Supporting Information  
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**One Collision – Two Substituents:**

**Barrierless Gas-Phase Preparation of Xylenes under Single-Collision Conditions**

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**Abstract:** The fundamental reaction pathways to the simplest dialkylsubstituted aromatics – xylenes (C6H4(CH3)2) – in high temperature combustion flames and in low temperature extraterrestrial environments are still unknown, but critical to understand the chemistry and molecular mass growth processes in these extreme environments. Exploiting crossed molecular beam experiments augmented by state-of-the-art electronic structure and statistical calculations, this study uncovers a previously elusive, facile gas-phase synthesis of xylenes through an isomer-selective reaction of 1-propynyl radical (methylethynyl, CH3CC) with 2-methyl-1,3-butadiene (isoprene, C5H8). The reaction dynamics are driven by a barrierless addition of radical to the diene moiety of 2-methyl-1,3-butadiene followed by extensive isomerization (hydrogen shifts, cyclization) prior to unimolecular decomposition accompanied by aromatization via atomic hydrogen loss. This overall exoergic reaction affords a preparation of xylenes not only in high-temperature environments such as in combustion flames and around circumstellar enveloped of carbon-rich Asymptotic Giant Branch (AGB) stars, but also in low-temperature cold molecular clouds (10 K) and in hydrocarbon-rich atmospheres of planets and their moons such as Triton and Titan. Our study established a hitherto unknown gas-phase route to xylenes and potentially more complex, disubstituted benzenes via a single collision event highlighting the significance of an alkyl-substituted ethynyl-mediated preparation of aromatic molecules in our Universe.

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Experimental Procedures

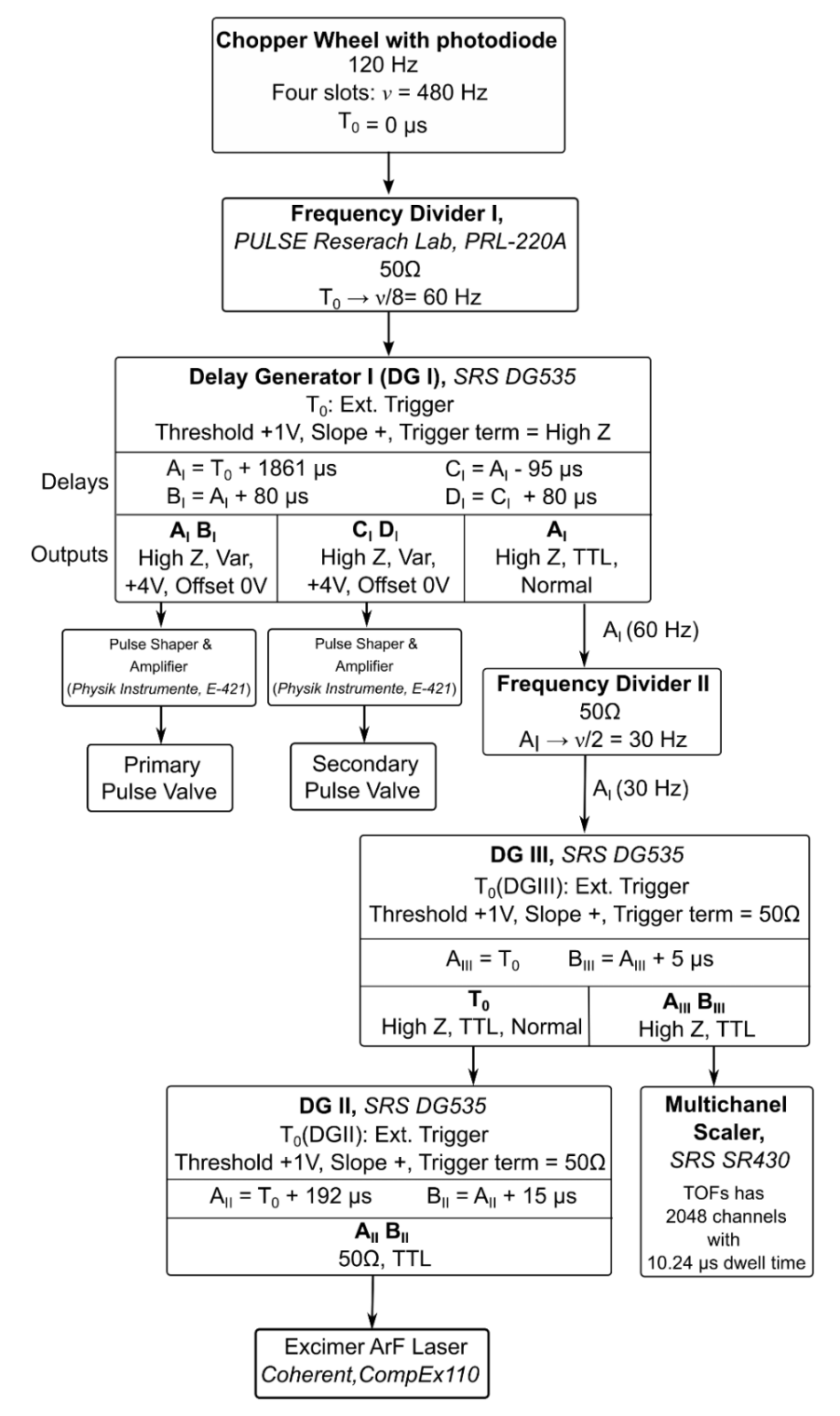
Crossed molecular beams

The gas-phase reactions of the 1-propynyl radical (CH3CC; X2A1) with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') and 1,3-pentadiene (CH3CHCHCHCH2, X1A') were carried out under single-collision conditions using the crossed molecular beams machine.[1,2]. The crossed beams apparatus consists of two fixed orthogonal source chambers (primary and secondary), the main scattering chamber, and an ultrahigh-vacuum (UHV; 10–12 Torr), rotatable, differentially pumped detector. In the primary source chamber, the pulsed supersonic beam of 1-propynyl radical was generated by photodissociation of 1-iodopropyne (CH3CCI; TCI, 99%+) seeded at a level of 0.5% in helium (99.9999 %, Matheson), using the focused 193 nm output of the excimer laser (Coherent, CompEx110; 20 mJ pulse–1; 30 Hz).[3–5] The secondary molecular beam was produced using 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; Sigma, 99%) or 1,3-pentadiene (*cis-* and *trans-* mixture of CH3CHCHCHCH2; TCI, >96.0%) released by Proch-Trickl pulsed valve[6] at backing pressures of 430 Torr and 350 Torr, respectively. A four-slot chopper wheel located after the skimmer selected a part of the 1-propynyl radical beam with a well-defined peak velocity (*v*p) and speed ratio (S) that intersected in the interaction region of the scattering chamber with the secondary beams. The peak velocities (*v*p), speed ratios (S), center-of-mass angles (ΘCM), and collision energies (EC) of the hydrocarbons beams are summarized in Table S1. We should note that it is possible that the propargyl radical (2-propynyl, CH2CCH) may be produced during generation of 1-propynyl by photodissociation of CH3CCI via isomerization through hydrogen shift in the 1-propynyl radical in the photolysis zone, too. However, the entrance barrier for the addition of the propargyl radical to the diene moiety was shown to be about 80 kJ mol−1,[7] which is well above the collision energy in our experiments (43 ± 2 kJ mol–1). Therefore, even if propargyl is present in the molecular beam, it will not contribute to the reactive scattering signal.

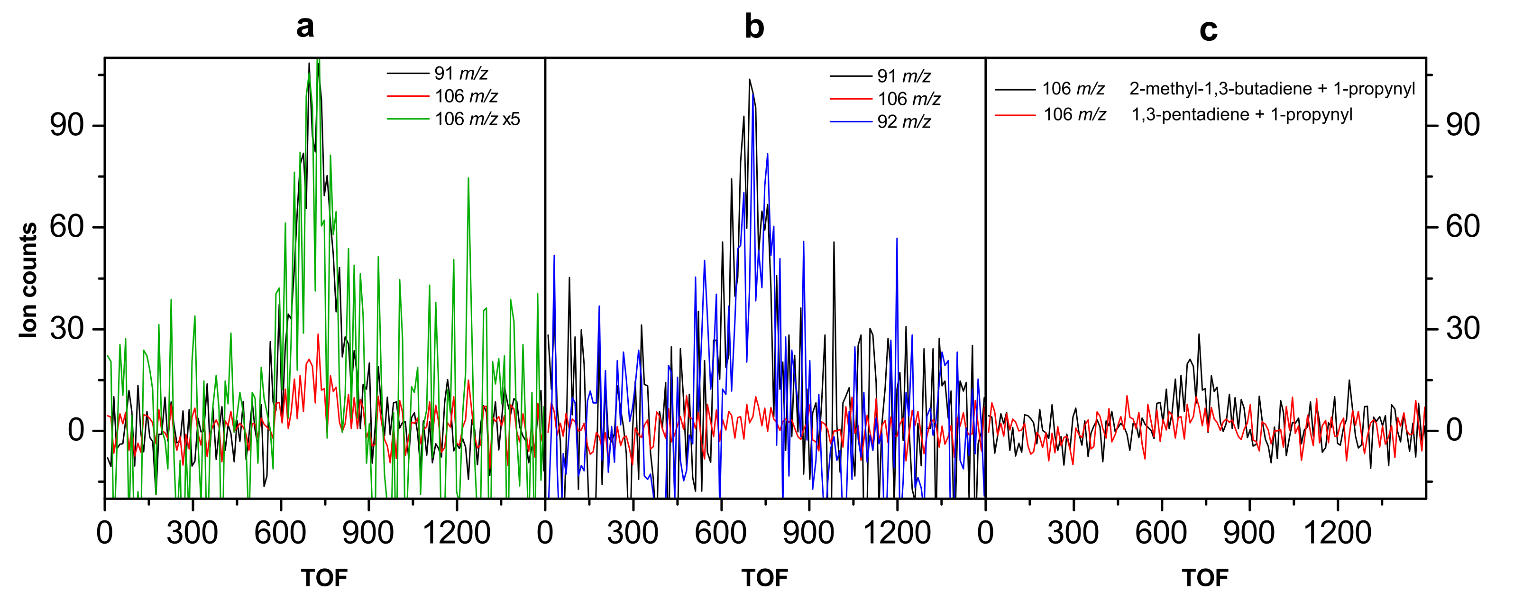
The scattering products of collision events are ionized by electron impact at 80 eV (2 mA) at the entrance of the rotatable detector, filtered according to mass-to-charge (*m/z*) ratios using the QMS (Extrel, QC 150; 1.2 MHz) and then detected using a Daly-type particle ion counter.[8] The pulse scheme of the experiment is represented in Figure S1. Angular resolved time-of-flight (TOF) spectra were recorded in the plane of the reactant beams at discrete laboratory angles, which were integrated and normalized with respect to TOF at ΘCM to extract the laboratory angular distribution (LAD). TOF and LAD were fit using a forward-convolution routine that is constrained by the reactant beam divergences, velocity spreads, and various machine parameters. This is an iterative method where user-defined center-of-mass (CM) translational energy (P(ET)) and angular (T(θ)) flux distributions simulate the measured signal under our experimental conditions.[9,10] CM functions are varied until a suitable fit of the TOF spectra and LAD is achieved. Together, the CM functions represent the reactive differential cross section I(θ, u), which can be divided into components of the CM scattering angle θ and the CM velocity u, I(u, θ) ∼ P(u) × T(θ), which is represented as a flux contour maps (Fig. 2) and reveals an overall image of the reaction outcome.

**Table S1**. Peak velocities (*v*p) and speed ratios (S) of the 1-propynyl radical (C3H3), 2‑methyl‑1,3‑butadiene (CH2C(CH3)CHCH2), and 1,3-pentadiene (CH3CHCHCHCH2) beams along with the corresponding collision energies (EC) and center-of-mass angles (ΘCM)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Beam | *v*p (m s–1) | S | EC (kJ mol–1) | ΘCM (degree) |
| 1-propynyl radical (CH3CC, X2A1) | 1722 ± 50 | 10.3 ± 1.5 | – | – |
| 2‑methyl‑1,3‑butadiene (CH2C(CH3)CHCH2, X1A') | 701 ± 19 | 5.1 ± 0.5 | 43 ± 2 | 35.4 ± 1.2 |
| 1,3-pentadiene (CH3CHCHCHCH2, X1A') | 708 ± 17 | 5.7 ± 0.5 | 43 ± 2 | 35.9 ± 0.9 |



**Figure S1.** Pulse sequence for the crossed molecular beam experiment for the reaction of the 1-propynyl radical (CH3CC; X2A1) with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2, X1A') and 1,3-pentadiene (CH3CHCHCHCH2, X1A').



**Figure S2.** Time-of-flight (TOF) spectra for the reactions of 1-propynyl radical (CH3CC; X2A1) with (a) 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2, X1A') and (b) 1,3‑pentadiene (CH3CHCHCHCH2, X1A') taken at different m/z. On the (c) depicted the direct comparison of the reactive scattering signal recorded at *m*/*z* = 106 for the 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2, X1A') and 1,3‑pentadiene (CH3CHCHCHCH2, X1A') systems.

Sample preparation

Samples of 1-iodopropyne (CH3CCI; TCI, 99%+), 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; Sigma, 99%), and 1,3-pentadiene (cis- and trans- mixture of CH3CHCHCHCH2; TCI, >96.0%) were purified by several cycles of freeze-pump-thaw method. 1-iodopropyne (CH3CCI; TCI, 99%+) was then diluted at a level of 0.5% in helium (99.9999%; Matheson) in a Teflon-coated sample cylinder (Swagelok); teflon coating is recommended to prevent sample degradation over time. This mixture was used at backing pressure of 760 Torr in the primary chamber pulsed valve. Neat 2-methyl-1,3-butadiene and 1,3-pentadiene were fed into the secondary chamber pulsed valve at backing pressures of 450 Torr and 400 Torr, respectively.

Electronic structure calculations

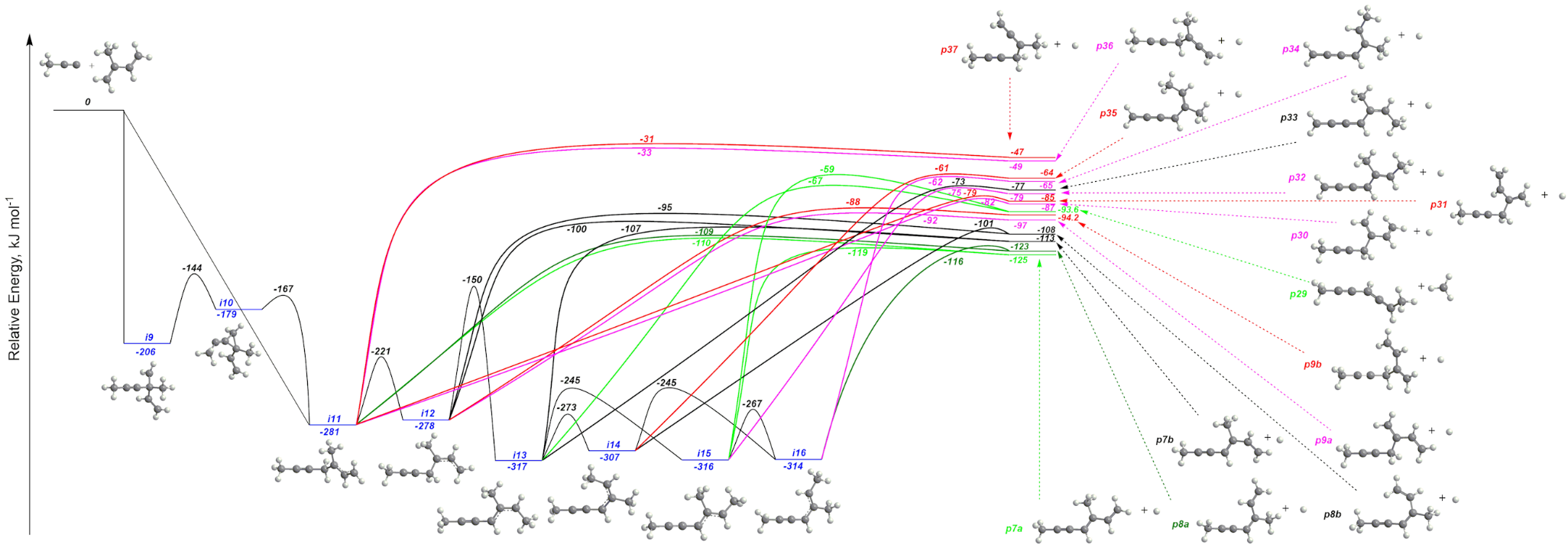
Geometry optimization of different structures on the C8H11 potential energy surface (PES) accessed by the reactions of the propynyl radical with two C5H8 isomers, 2-methyl-1,3-butadiene (isoprene) and 1,3-pentadiene, was carried out at the density functional ωB97X-D level of theory [11] with the 6-311G(d,p) basis set. Vibrational frequencies for all optimized stationary points were computed at the same ωB97X-D/6-311G(d,p) level. The calculations of frequencies allowed us to characterize all structures as either local minima or transition states and to evaluate zero-point vibrational energy corrections (ZPE). The frequencies were also used for calculations of energy-dependent rate constants. Single-point energies for each stationary point on the PES were rectified using the G3(MP2,CC) model chemistry scheme in which the coupled cluster CCSD(T)/6-311G(d,p) energy is upgraded by a basis set correction to the G3Large basis set evaluated at the Moller-Plesset second-order perturbation theory (MP2) level.[12–14] The resulting G3(MP2,CC)//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) relative energies are known to be typically accurate within 10 kJ mol–1 or better.[14] The GAUSSIAN 09[15] and MOLPRO 2015[16] program packages were employed for the electronic calculations.



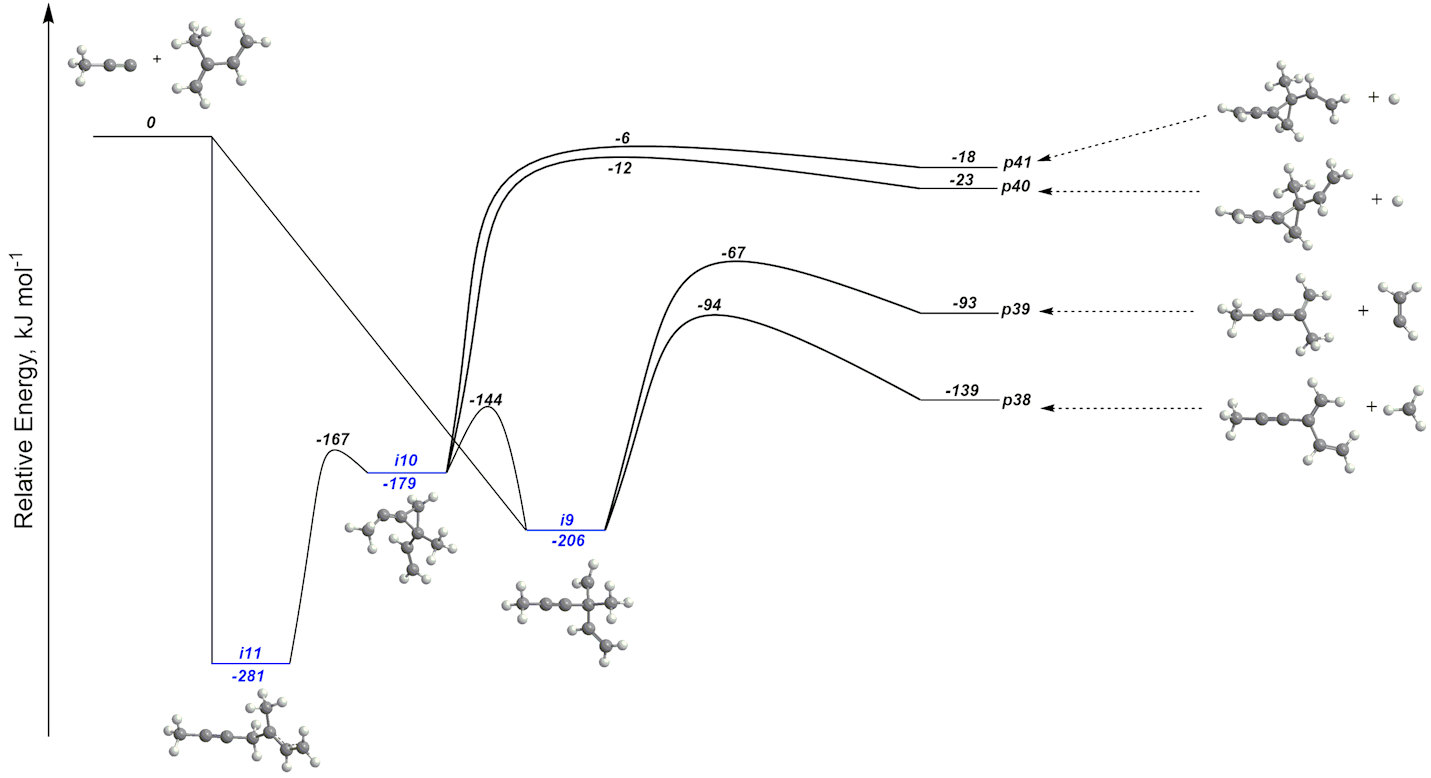
**Figure S3.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part I.

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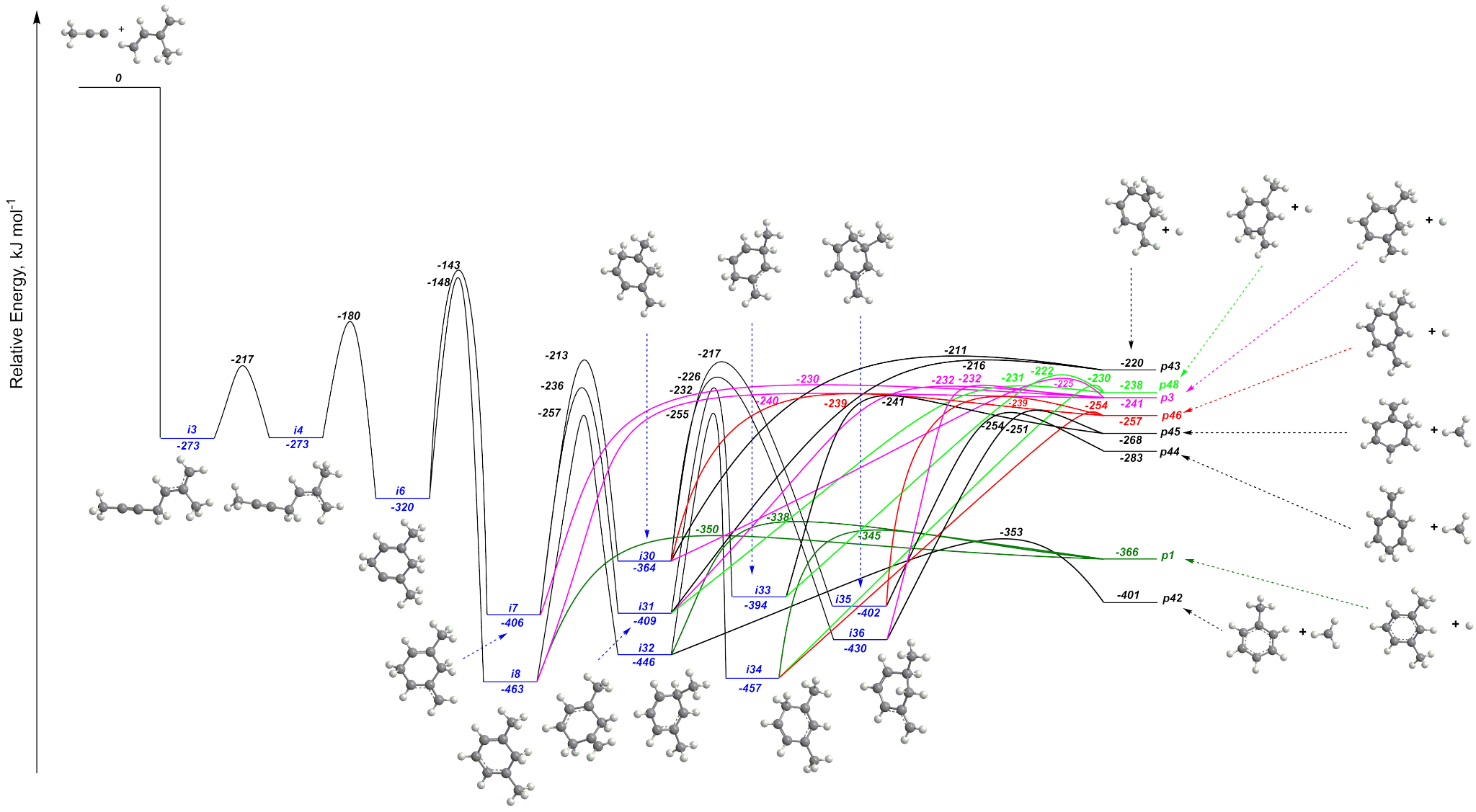
**Figure S4.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part II.



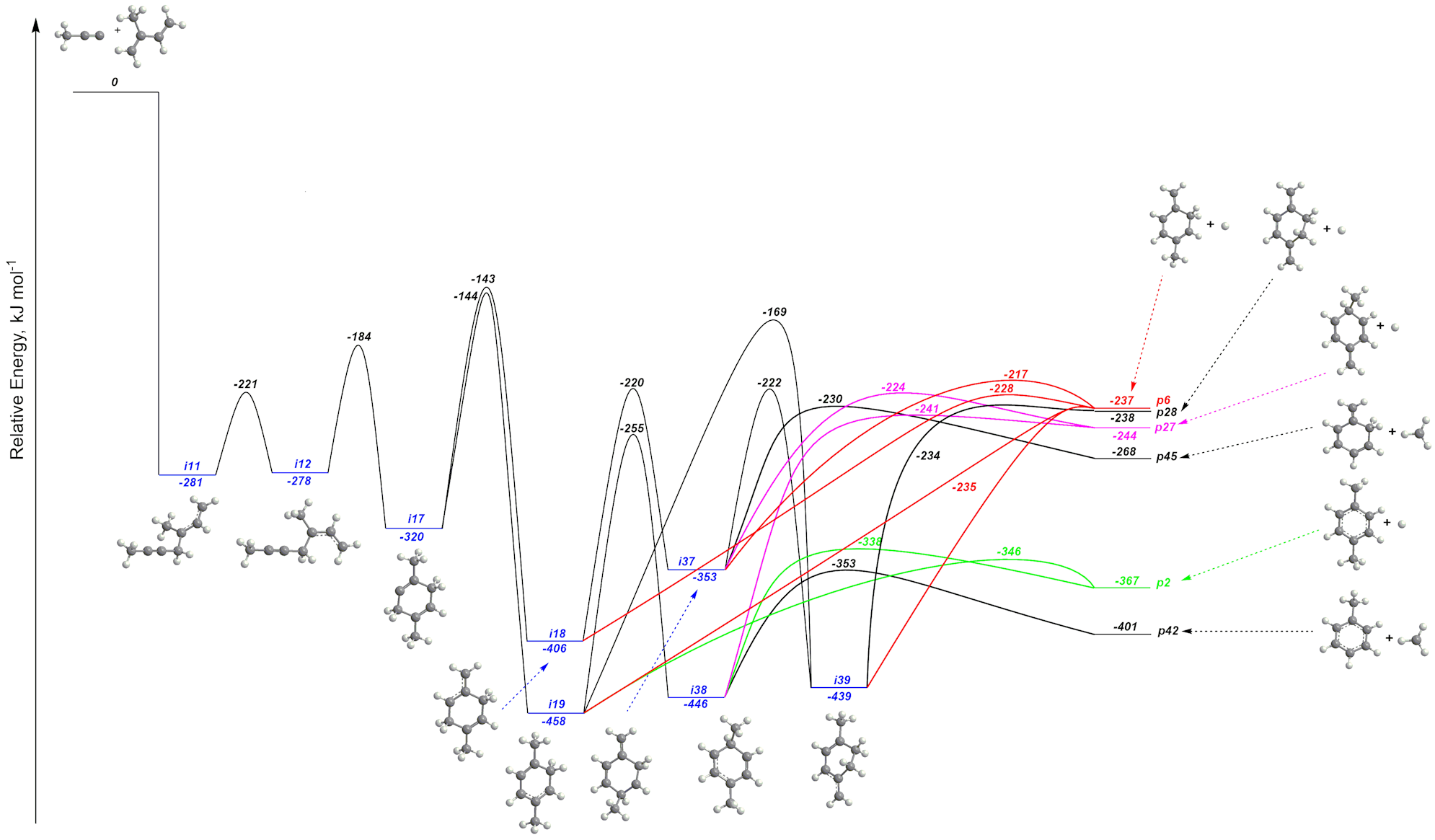
**Figure S5.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part III.



**Figure S6.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part IV.



**Figure S7.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part V.



**Figure S8**. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with 2-methyl-1,3-butadiene (CH2C(CH3)CHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part VI.

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**Figure S9.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part I.

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**Figure S10.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part II.

**g:\My Drive\C3H3 + C5H8\QuantumChem\pentadiene+propynyl\pentadiene+propynyl PES 3_renamed.tiffFigure S11.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part III.

**g:\My Drive\C3H3 + C5H8\QuantumChem\pentadiene+propynyl\pentadiene+propynyl PES 4_renamed.tiff**

**Figure S12**. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part IV.

**g:\My Drive\C3H3 + C5H8\QuantumChem\pentadiene+propynyl\pentadiene+propynyl PES 5_renamed.tiffFigure S13.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part V.

**g:\My Drive\C3H3 + C5H8\QuantumChem\pentadiene+propynyl\pentadiene+propynyl PES 6_renamed.tiffFigure S14.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part VI.

**g:\My Drive\C3H3 + C5H8\QuantumChem\pentadiene+propynyl\pentadiene+propynyl PES 7_renamed.tiffFigure S15.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part VII.

**g:\My Drive\C3H3 + C5H8\QuantumChem\pentadiene+propynyl\pentadiene+propynyl PES 8_renamed.tiffFigure S16.** Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) with 1,3-pentadiene (CH3CHCHCHCH2; X1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol–1. Part VIII.

Calculations of energy-dependent rate constants

Rice-Ramsperger-Kassel-Marcus (RRKM) theory[17–19]  was employed to compute microcanonical, internal energy-dependent rate constants of all unimolecular reaction steps on the C8H11 PES following the initial association of the H3CCC radical with the C5H8 isomers. We utilized our in-house code Unimol [20] to evaluate the rate constants as functions of the available internal energy of each intermediate or transition state within the harmonic approximation. Unimol is an updated version of our previous software code on energy dependent RRKM calculations of rate constants for multiwell and multichannel unimolecular reactions under single-collision conditions and for solving a system of first-order kinetic equations. [21] The internal energy in these calculations is assumed to be equal to the sum of the collision energy and the chemical activation energy, that is, negative of the relative energy of a species with respect to the reactants. Since the calculations simulate the experimental crossed molecular beams conditions at a zero-pressure limit, only one energy level is considered throughout. With all RRKM rate constants in hand, product branching ratios are then computed by solving first-order kinetic equations within steady-state approximation. The calculated rate constants and product branching ratios depending on the initial reaction intermediate formed by recombination of the reactants are presented in Supporting Information (Tables S9-S10 and S2-S8, respectively).

**Table S2**. Statistical branching ratios (%) for the reaction of 2-methyl-1,3-butadiene + propynyl with ***i1***, ***i3***, ***i9***,and ***i11*** as initial intermediates at different collision energies (*EC,* kJ·mol-1)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | ***i1*** | | ***i3*** | | ***i9*** | | ***i11*** | |
| *EC* | **0** | **43** | **0** | **43** | **0** | **43** | **0** | **43** |
| ***p1*** | 3.7 | 1.5 | 3.7 | 1.5 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p2*** | 0.0 | 0.0 | 0.0 | 0.0 | 3.7 | 1.6 | 3.8 | 1.7 |
| ***p3*** | 3.2 | 1.4 | 3.2 | 1.4 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p4a*** | 38.7 | 33.4 | 39.0 | 34.3 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p4b*** | 27.8 | 31.5 | 28.0 | 32.4 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p5a*** | 10.0 | 10.1 | 10.1 | 10.4 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p5b*** | 15.0 | 18.6 | 15.1 | 19.1 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p6*** | 0.0 | 0.0 | 0.0 | 0.0 | 3.6 | 1.5 | 3.6 | 1.6 |
| ***p7a*** | 0.0 | 0.0 | 0.0 | 0.0 | 28.3 | 22.7 | 28.7 | 24.0 |
| ***p7b*** | 0.0 | 0.0 | 0.0 | 0.0 | 46.1 | 47.5 | 46.7 | 50.3 |
| ***p8a*** | 0.0 | 0.0 | 0.0 | 0.0 | 13.2 | 13.1 | 13.4 | 13.9 |
| ***p8b*** | 0.0 | 0.0 | 0.0 | 0.0 | 1.6 | 2.5 | 1.6 | 2.6 |
| ***p9a*** | 0.0 | 0.0 | 0.0 | 0.0 | 1.1 | 2.8 | 1.2 | 2.9 |
| ***p9b*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.4 | 0.1 | 0.4 |
| ***p14*** | 0.6 | 1.6 | 0.2 | 0.3 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p15*** | 0.3 | 1.0 | 0.1 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p16*** | 0.1 | 0.6 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p17*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p18*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p19*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p20*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p21*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p22*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p23/p23‘*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p24*** | 0.0 | 0.1 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p25*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p26*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p27*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p28*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p29*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.0 | 0.3 |
| ***p30*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.7 | 0.2 | 0.7 |
| ***p31*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.2 | 0.1 | 0.3 |
| ***p32*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.1 |
| ***p33*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p34*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p35*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p36*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p37*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p38*** | 0.0 | 0.0 | 0.0 | 0.0 | 1.8 | 6.5 | 0.5 | 1.2 |
| ***p39*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.0 | 0.0 |
| ***p40*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p41*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p42*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p43*** | 0.1 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p44*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p45*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.1 | 0.0 |
| ***p46*** | 0.1 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p48*** | 0.4 | 0.2 | 0.4 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 |

**Table S3**. Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene + propynyl with ***i1***, ***i3*** as initial intermediates at different collision energies (*EC,* kJ·mol-1) having the energies of *ts*[***i4-i5***] and *ts*[***i6-i7***] increased by 5 kJ·mol-1 and the energy of *ts*[***i6-i8***] decreased by 5 kJ·mol-1:

*ts*[***i4-i5***] := (-148 + 5) kJ·mol-1 = -143 kJ·mol-1 (reducing the contribution of p4-p5);

*ts*[***i6-i7***] := (-143 + 5) kJ·mol-1 = -138 kJ·mol-1 (reducing the contribution of p3);

*ts*[***i6-i8***] := (-148 - 5) kJ·mol-1 = -153 kJ·mol-1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***i1*** | | ***i3*** | |
| *EC* | **0** | **43** | **0** | **43** |
| ***p1*** | 8.4 | 3.6 | 8.5 | 3.7 |
| ***p3*** | 1.9 | 1.0 | 1.9 | 1.0 |
| ***p4a*** | 37.5 | 33.1 | 37.8 | 34.0 |
| ***p4b*** | 26.7 | 30.7 | 26.9 | 31.5 |
| ***p5a*** | 9.6 | 9.9 | 9.7 | 10.1 |
| ***p5b*** | 14.4 | 18.1 | 14.5 | 18.6 |

**Table S4**. Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene + propynyl with ***i1***, ***i3*** as initial intermediates at different collision energies (*EC,* kJ·mol-1) having the energies of *ts*[***i4-i5***], *ts*[***i6-i7***], *ts*[***i5-p4a/p4b***], and *ts*[***i5-p5a/p5b***] increased by 5 kJ·mol-1 and the energy of *ts*[***i6-i8***] decreased by 5 kJ·mol-1:

*ts*[***i4-i5***] := (-148 + 5) kJ·mol-1 = -143 kJ·mol-1 (reducing the contribution of p1-p4);

*ts*[***i6-i7***] := (-143 + 5) kJ·mol-1 = -138 kJ·mol-1 (reducing the contribution of p3);

*ts*[***i6-i8***] := (-148 - 5) kJ·mol-1 = -153 kJ·mol-1;

*ts*[***i5-p4a/p4b***] := (-117 + 5) kJ·mol-1 = -112 kJ·mol-1;

*ts*[***i5-p5a/p5b***] := (-110 + 5) kJ·mol-1 = -105 kJ·mol-1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***i1*** | | ***i3*** | |
| *EC* | **0** | **43** | **0** | **43** |
| ***p1*** | 14.1 | 4.8 | 14.2 | 4.9 |
| ***p3*** | 3.1 | 1.3 | 3.1 | 1.4 |
| ***p4a*** | 35.8 | 33.4 | 36.0 | 34.3 |
| ***p4b*** | 23.6 | 29.4 | 23.8 | 30.2 |
| ***p5a*** | 8.7 | 9.6 | 8.8 | 9.8 |
| ***p5b*** | 12.6 | 17.3 | 12.7 | 17.7 |

**Table S5**. Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene + propynyl with ***i9***, ***i11*** as initial intermediates at different collision energies (*EC,* kJ·mol-1) having the energies of *ts*[***i12-i13***] and *ts*[***i17-i18***] increased by 5 kJ·mol-1 and the energy of *ts*[***i17-i19***] decreased by 5 kJ·mol-1:

*ts*[***i12-i13***] := (-150 + 5) kJ·mol-1 = -145 kJ·mol-1 (reducing the contribution of p7-p8);

*ts*[***i17-i18***] := (-143 + 5) kJ·mol-1 = -138 kJ·mol-1 (reducing the contribution of p6);

*ts*[***i17-i19***] := (-144 - 5) kJ·mol-1 = -149 kJ·mol-1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***i9*** | | ***i11*** | |
| *EC* | **0** | **43** | **0** | **43** |
| ***p2*** | 8.6 | 3.7 | 8.7 | 3.9 |
| ***p6*** | 2.1 | 1.0 | 2.1 | 1.1 |
| ***p7a*** | 27.2 | 22.2 | 27.5 | 23.4 |
| ***p7b*** | 43.2 | 43.5 | 43.8 | 46.0 |
| ***p8a*** | 13.5 | 14.3 | 13.6 | 15.1 |
| ***p8b*** | 1.7 | 2.7 | 1.7 | 2.8 |
| ***p9a*** | 1.3 | 3.5 | 1.4 | 3.7 |
| ***p9b*** | 0.2 | 0.5 | 0.2 | 0.5 |

**Table S6**.

Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene +propynyl with ***i9***, ***i11*** as initial intermediates at different collision energies (*EC,* kJ·mol-1) having the value of *ts*[***i12-i13***], *ts*[***i17-i18***], *ts*[***i15-p7a/p7b***], and *ts*[***i16-p8a/p8b***] increased by 5 kJ·mol-1 and the value of *ts*[***i17-i19***] decreased by 5 kJ·mol-1:

*ts*[***i12-i13***] := (-150 + 5) kJ·mol-1 = -145 kJ·mol-1 (reducing the contribution of p7-p8);

*ts*[***i17-i18***] := (-143 + 5) kJ·mol-1 = -138 kJ·mol-1 (reducing the contribution of p6);

*ts*[***i17-i19***] := (-144 - 5) kJ·mol-1 = -149 kJ·mol-1;

*ts*[***i15-p7a/p7b***] := (-119 + 5) kJ·mol-1 = -114 kJ·mol-1;

*ts*[***i16-p8a/p8b***] := (-116 + 5) kJ·mol-1 = -111 kJ·mol-1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***I9*** | | ***i11*** | |
| *EC* | **0** | **43** | **0** | **43** |
| ***p2*** | 9.7 | 3.9 | 9.9 | 4.1 |
| ***p6*** | 2.4 | 1.1 | 2.4 | 1.2 |
| ***p7a*** | 17.0 | 15.7 | 17.2 | 16.6 |
| ***p7b*** | 54.1 | 51.1 | 54.8 | 54.1 |
| ***p8a*** | 10.6 | 12.3 | 10.7 | 13.0 |
| ***p8b*** | 2.0 | 3.0 | 2.0 | 3.1 |
| ***p9a*** | 1.5 | 3.7 | 1.5 | 3.9 |
| ***p9b*** | 0.2 | 0.5 | 0.2 | 0.6 |

**Table S7**.

Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene+propynyl with ***i9***, ***i11*** as initial intermediates at different collision energies (*EC,* kJ·mol-1) having the value of *ts*[***i12-i13***], *ts*[***i17-i18***], *ts*[***i15-p7a/p7b***], *ts*[***i16-p8a/p8b***], *ts*[***i11-p7a/p7b***], *ts*[***i10-p8a/p8b***], and *ts*[***i13-p7a/p7b***] increased by 5 kJ·mol-1 and the value of *ts*[***i17-i19***] decreased by 5 kJ·mol-1:

*ts*[***i12-i13***] := (-150 + 5) kJ·mol-1 = -145 kJ·mol-1 (reducing the contribution of p7-p8);

*ts*[***i17-i18***] := (-143 + 5) kJ·mol-1 = -138 kJ·mol-1 (reducing the contribution of p6);

*ts*[***i17-i19***] := (-144 - 5) kJ·mol-1 = -149 kJ·mol-1;

*ts*[***i15-p7a/7b***] := (-119 + 5) kJ·mol-1 = -114 kJ·mol-1;

*ts*[***i16-p8a/8b***] := (-116 + 5) kJ·mol-1 = -111 kJ·mol-1;

*ts*[***i11-p7a/p7b***] := (-110 + 5) kJ·mol-1 = -105 kJ·mol-1;

*ts*[***i11-p8a/p8b***] := (-109 + 5) kJ·mol-1 = -104 kJ·mol-1;

*ts*[***i13-p7a/p7b***] := (-107 + 5) kJ·mol-1 = -102 kJ·mol-1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***i9*** | | ***i11*** | |
| *EC* | **0** | **43** | **0** | **43** |
| ***p2*** | 14.4 | 5.1 | 14.5 | 5.4 |
| ***p6*** | 3.5 | 1.4 | 3.6 | 1.5 |
| ***p7a*** | 24.8 | 20.5 | 25.1 | 21.7 |
| ***p7b*** | 37.2 | 41.7 | 37.7 | 44.1 |
| ***p8a*** | 11.2 | 11.5 | 11.4 | 12.2 |
| ***p8b*** | 3.3 | 4.5 | 3.3 | 4.7 |
| ***p9a*** | 2.2 | 4.8 | 2.3 | 5.0 |
| ***p9b*** | 0.3 | 0.7 | 0.3 | 0.7 |

**Table S8**. Statistical branching ratios (%) for the reaction of 1,3-pentadiene + propynyl with ***i1***, ***i3***, ***i18***,and ***i20*** as initial intermediates at different collision energies (*EC,* kJ·mol-1)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | ***i20*** | | ***i22*** | | ***i24*** | | ***i26*** | |
| *EC* | **0** | **43** | **0** | **43** | **0** | **43** | **0** | **43** |
| ***p10a*** | 19.0 | 18.2 | 19.0 | 18.4 | 17.5 | 13.2 | 17.9 | 14.1 |
| ***p11a*** | 66.7 | 63.4 | 66.8 | 64.4 | 49.6 | 36.7 | 50.6 | 39.1 |
| ***p10b*** | 6.0 | 7.2 | 6.1 | 7.3 | 10.6 | 10.1 | 10.9 | 10.7 |
| ***p11b*** | 6.0 | 7.7 | 6.0 | 7.8 | 8.6 | 7.8 | 8.7 | 8.3 |
| ***p12a*** | 0.4 | 0.6 | 0.4 | 0.6 | 0.1 | 0.2 | 0.0 | 0.1 |
| ***p13a*** | 0.1 | 0.3 | 0.1 | 0.3 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p12b*** | 0.0 | 0.1 | 0.0 | 0.1 | 0.0 | 0.1 | 0.0 | 0.0 |
| ***p13b*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p39*** | 0.0 | 0.1 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p49*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p50*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p51*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p52*** | 0.0 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p53*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p54*** | 0.0 | 0.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p55*** | 0.1 | 1.2 | 0.0 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p56*** | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p57*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p42*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.8 | 0.6 | 0.8 | 0.6 |
| ***p1*** | 0.8 | 0.3 | 0.8 | 0.3 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p44*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p45*** | 0.3 | 0.1 | 0.3 | 0.2 | 0.2 | 0.1 | 0.2 | 0.1 |
| ***p46*** | 0.4 | 0.2 | 0.4 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p3*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p48*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p43*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p58*** | 0.0 | 0.0 | 0.0 | 0.0 | 4.1 | 9.1 | 3.0 | 6.9 |
| ***p59*** | 0.0 | 0.0 | 0.0 | 0.0 | 3.7 | 8.2 | 3.7 | 8.7 |
| ***p60*** | 0.0 | 0.0 | 0.0 | 0.0 | 1.3 | 3.0 | 1.3 | 3.2 |
| ***p61*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.6 | 1.5 | 0.6 | 1.6 |
| ***p62*** | 0.0 | 0.0 | 0.0 | 0.0 | 1.8 | 5.7 | 1.0 | 3.1 |
| ***p63*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 1.1 | 0.3 | 1.2 |
| ***p64*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.1 |
| ***p65*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.3 | 0.1 | 0.3 |
| ***p66*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.6 | 0.2 | 0.6 |
| ***p67*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.4 | 0.1 | 0.4 |
| ***p68*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.1 |
| ***p69*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p70*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p71*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p72*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p73*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p74*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p75*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p76*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p76'*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.7 | 0.0 | 0.3 |
| ***p77*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p78*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p79*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p80*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p81*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p82*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.1 | 0.0 | 0.1 |
| ***p83*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p84*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 |
| ***p85*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p86*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p87*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p88*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p89*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p90*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p91*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p92*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 0.2 | 0.3 | 0.2 |
| ***p93*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p94*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

**Table S9**. RRKM calculated rate constants (*k(E)*, s-1) of the reaction of 2-methyl-1,3-butadiene + propynyl as functions of the internal energy (*E,* kJ mol-1) of the intermediate states for unimolecular reaction steps at different collision energies (*EC,* kJ mol-1)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ***EC*** | **0** | | **43** | | ***EC*** | **0** | | **43** | |
| **Reaction step** | *k(E)* | *E* | *k(E)* | *E* | **Reaction step** | *k(E)* | *E* | *k(E)* | *E* |
| ***i4 – p23‘*** | 3.89E-01 | 273 | 1.62E+02 | 316 | ***i8 – p3*** | 6.02E+07 | 463 | 2.44E+08 | 506 |
| ***i4 – p4b*** | 3.26E+03 | 273 | 6.22E+04 | 316 | ***i33 – p45*** | 2.44E+09 | 394 | 7.19E+09 | 437 |
| ***i11 – p36*** | 1.38E-02 | 281 | 1.05E+01 | 324 | ***i33 – p48*** | 3.26E+07 | 394 | 1.16E+08 | 437 |
| ***i11 – p7a*** | 8.99E+04 | 281 | 1.18E+06 | 324 | ***i35 – p44*** | 2.19E+09 | 402 | 5.85E+09 | 445 |
| ***i3 – p23‘*** | 7.10E-01 | 273 | 2.20E+02 | 316 | ***i35 – p46*** | 1.10E+08 | 402 | 3.38E+08 | 445 |
| ***i3 – p1*** | 2.24E+04 | 273 | 3.03E+05 | 316 | ***i36 – p45*** | 3.41E+08 | 430 | 1.07E+09 | 473 |
| ***i2 – i1*** | 5.89E+11 | 177 | 1.10E+12 | 220 | ***i36 – p3*** | 1.68E+07 | 430 | 6.28E+07 | 473 |
| ***i1 – i2*** | 7.02E+08 | 217 | 1.99E+09 | 260 | ***i30 – p46*** | 2.22E+09 | 364 | 5.75E+09 | 407 |
| ***i12 – p7b*** | 3.88E+04 | 278 | 6.83E+05 | 321 | ***i31 – p48*** | 1.35E+08 | 409 | 4.74E+08 | 452 |
| ***i2 – p21*** | 5.72E-01 | 177 | 3.24E+03 | 220 | ***i1 – i69*** | 3.93E+06 | 217 | 3.33E+07 | 260 |
| ***i3 – i2*** | 7.03E+06 | 273 | 2.31E+07 | 316 | ***i69 – i1*** | 7.71E+02 | 320 | 1.58E+04 | 363 |
| ***i2 – i3*** | 6.74E+12 | 177 | 8.58E+12 | 220 | ***i12 – i13*** | 1.15E+07 | 278 | 4.96E+07 | 321 |
| ***i9 – p39*** | 1.84E+05 | 206 | 5.92E+06 | 249 | ***i13 – i12*** | 3.15E+05 | 317 | 1.76E+06 | 360 |
| ***i9 – p38*** | 2.47E+07 | 206 | 2.62E+08 | 249 | ***i12 – p9a*** | 4.17E+04 | 278 | 9.60E+05 | 321 |
| ***i2 – p22*** | 3.40E-01 | 177 | 2.62E+03 | 220 | ***i19 – i39*** | 5.26E+02 | 458 | 3.92E+03 | 501 |
| ***i10 – p41*** | 3.94E-02 | 179 | 8.87E+02 | 222 | ***i39 – i19*** | 6.52E+03 | 439 | 4.58E+04 | 482 |
| ***i1 – p14*** | 2.80E+05 | 217 | 4.05E+06 | 260 | ***i37 – i39*** | 1.28E+08 | 353 | 3.33E+08 | 396 |
| ***i1 – p16*** | 4.83E+05 | 217 | 8.22E+06 | 260 | ***i39 – i37*** | 8.05E+05 | 439 | 3.12E+06 | 482 |
| ***i1 – p15*** | 1.15E+05 | 217 | 2.38E+06 | 260 | ***i11 – p30*** | 5.31E+03 | 281 | 1.80E+05 | 324 |
| ***i10 – p40*** | 4.67E-01 | 179 | 2.06E+03 | 222 | ***i1 – i68*** | 6.03E+09 | 217 | 1.18E+10 | 260 |
| ***i11 – i10*** | 1.63E+07 | 281 | 5.62E+07 | 324 | ***i68 – i1*** | 8.05E+10 | 210 | 1.49E+11 | 253 |
| ***i10 – i11*** | 5.15E+12 | 179 | 6.42E+12 | 222 | ***i13 – p7b*** | 6.08E+04 | 317 | 1.16E+06 | 360 |
| ***i11 – i12*** | 3.16E+10 | 281 | 5.45E+10 | 324 | ***i13 – p29*** | 5.58E+01 | 317 | 5.71E+03 | 360 |
| ***i12 – i11*** | 4.29E+10 | 278 | 7.27E+10 | 321 | ***i69 – p15*** | 1.20E+04 | 320 | 2.65E+05 | 363 |
| ***i4 – i3*** | 1.68E+09 | 273 | 2.79E+09 | 316 | ***i68 – p20*** | 1.05E+01 | 210 | 1.12E+04 | 253 |
| ***i3 – i4*** | 3.23E+09 | 273 | 5.40E+09 | 316 | ***i39 – p6*** | 6.66E+07 | 439 | 2.58E+08 | 482 |
| ***i4 – i6*** | 2.12E+06 | 273 | 5.36E+06 | 316 | ***i39 – p28*** | 3.55E+07 | 439 | 1.36E+08 | 482 |
| ***i6 – i4*** | 9.44E+07 | 320 | 3.61E+08 | 363 | ***i13 – i14*** | 5.45E+10 | 317 | 7.46E+10 | 360 |
| ***i6 – i8*** | 1.02E+06 | 320 | 5.66E+06 | 363 | ***i14 – i13*** | 6.44E+10 | 307 | 8.28E+10 | 350 |
| ***i8 – i6*** | 5.48E+01 | 463 | 5.89E+02 | 506 | ***i14 – i16*** | 1.57E+10 | 307 | 2.60E+10 | 350 |
| ***i6 – i7*** | 1.05E+06 | 320 | 6.03E+06 | 363 | ***i16 – i14*** | 8.89E+09 | 314 | 1.54E+10 | 357 |
| ***i7 – i6*** | 4.50E+02 | 406 | 3.99E+03 | 449 | ***i69 – p18*** | 3.08E+01 | 320 | 1.59E+03 | 363 |
| ***i10 – i9*** | 3.74E+11 | 179 | 7.03E+11 | 222 | ***i69 – p19*** | 1.60E+00 | 320 | 1.58E+02 | 363 |
| ***i9 – i10*** | 2.09E+09 | 206 | 5.13E+09 | 249 | ***i13 – p33*** | 1.57E+01 | 317 | 1.09E+03 | 360 |
| ***i12 – i17*** | 3.17E+07 | 278 | 8.06E+07 | 321 | ***i4 – p5b*** | 2.08E+03 | 273 | 4.41E+04 | 316 |
| ***i17 – i12*** | 1.87E+08 | 320 | 6.79E+08 | 363 | ***i3 – p23*** | 2.13E-01 | 273 | 7.29E+01 | 316 |
| ***i17 – i18*** | 8.07E+05 | 320 | 4.61E+06 | 363 | ***i3 – p5a*** | 2.03E+03 | 273 | 3.55E+04 | 316 |
| ***i18 – i17*** | 4.01E+02 | 406 | 3.52E+03 | 449 | ***i11 – p37*** | 9.99E-03 | 281 | 9.11E+00 | 324 |
| ***i17 – i19*** | 8.09E+05 | 320 | 4.81E+06 | 363 | ***i12 – p8b*** | 2.07E+04 | 278 | 4.25E+05 | 321 |
| ***i19 – i17*** | 1.77E+01 | 458 | 2.00E+02 | 501 | ***i12 – p9b*** | 5.32E+03 | 278 | 1.37E+05 | 321 |
| ***i7 – p3*** | 3.10E+07 | 406 | 1.07E+08 | 449 | ***i14 – p8b*** | 1.70E+03 | 307 | 3.57E+04 | 350 |
| ***i8 – p1*** | 7.85E+10 | 463 | 1.39E+11 | 506 | ***i14 – p35*** | 7.80E-01 | 307 | 9.07E+01 | 350 |
| ***i18 – p6*** | 3.47E+07 | 406 | 1.23E+08 | 449 | ***i15 – p29*** | 8.25E-01 | 316 | 1.15E+02 | 359 |
| ***i19 – p2*** | 8.58E+10 | 458 | 1.52E+11 | 501 | ***i15 – p32*** | 4.11E+01 | 316 | 2.62E+03 | 359 |
| ***i8 – i32*** | 3.79E+06 | 463 | 1.15E+07 | 506 | ***i15 – p7a*** | 3.34E+04 | 316 | 4.59E+05 | 359 |
| ***i32 – i8*** | 1.48E+07 | 446 | 4.23E+07 | 489 | ***i11 – p31*** | 1.60E+03 | 281 | 5.97E+04 | 324 |
| ***i18 – i37*** | 1.30E+06 | 406 | 4.49E+06 | 449 | ***i11 – p8a*** | 1.29E+05 | 281 | 1.73E+06 | 324 |
| ***i37 – i18*** | 1.13E+08 | 353 | 3.05E+08 | 396 | ***i13 – i15*** | 1.06E+10 | 317 | 1.87E+10 | 360 |
| ***i19 – i38*** | 2.13E+06 | 458 | 6.43E+06 | 501 | ***i15 – i13*** | 1.05E+10 | 316 | 1.86E+10 | 359 |
| ***i38 – i19*** | 5.32E+06 | 446 | 1.54E+07 | 489 | ***i15 – i16*** | 4.35E+10 | 316 | 6.26E+10 | 359 |
| ***i7 – i30*** | 1.18E+06 | 406 | 4.35E+06 | 449 | ***i16 – i15*** | 2.92E+10 | 314 | 4.13E+10 | 357 |
| ***i30 – i7*** | 4.09E+07 | 364 | 1.25E+08 | 407 | ***i69 – p17*** | 1.59E+02 | 320 | 1.28E+04 | 363 |
| ***i7 – i31*** | 1.03E+07 | 406 | 3.03E+07 | 449 | ***i69 – p14*** | 2.44E+04 | 320 | 4.09E+05 | 363 |
| ***i31 – i7*** | 3.67E+07 | 409 | 1.10E+08 | 452 | ***i16 – p8a*** | 7.57E+03 | 314 | 1.08E+05 | 357 |
| ***i38 – p42*** | 6.22E+10 | 446 | 9.92E+10 | 489 | ***i16 – p34*** | 4.12E+00 | 314 | 4.95E+02 | 357 |
| ***i38 – p2*** | 6.87E+09 | 446 | 1.21E+10 | 489 | ***i4 – i5*** | 2.52E+06 | 273 | 1.06E+07 | 316 |
| ***i37 – p45*** | 4.66E+09 | 353 | 1.23E+10 | 396 | ***i5 – i4*** | 3.80E+05 | 321 | 2.28E+06 | 364 |
| ***i37 – p6*** | 1.78E+08 | 353 | 5.39E+08 | 396 | ***i5 – p24*** | 1.76E+01 | 321 | 1.13E+03 | 364 |
| ***i32 – p42*** | 3.02E+11 | 446 | 4.82E+11 | 489 | ***i5 – p4b*** | 3.22E+04 | 321 | 6.46E+05 | 364 |
| ***i32 – p1*** | 3.05E+10 | 446 | 5.37E+10 | 489 | ***i5 – p4a*** | 4.35E+04 | 321 | 6.48E+05 | 364 |
| ***i30 – i36*** | 6.10E+07 | 364 | 1.61E+08 | 407 | ***i5 – p25*** | 2.23E+00 | 321 | 2.17E+02 | 364 |
| ***i36 – i30*** | 3.26E+06 | 430 | 1.16E+07 | 473 | ***i5 – p5a*** | 1.16E+04 | 321 | 2.08E+05 | 364 |
| ***i30 – p3*** | 1.27E+09 | 364 | 3.82E+09 | 407 | ***i5 – p5b*** | 1.73E+04 | 321 | 3.77E+05 | 364 |
| ***i30 – i35*** | 2.62E+07 | 364 | 7.61E+07 | 407 | ***i5 – p26*** | 9.14E-02 | 321 | 3.00E+01 | 364 |
| ***i35 – i30*** | 7.52E+06 | 402 | 2.61E+07 | 445 | ***i38 – p27*** | 1.02E+07 | 446 | 3.76E+07 | 489 |
| ***i31 – i33*** | 1.14E+07 | 409 | 3.55E+07 | 452 | ***i37 – p27*** | 6.15E+08 | 353 | 1.73E+09 | 396 |
| ***i33 – i31*** | 3.12E+07 | 394 | 9.08E+07 | 437 | ***i34 – p1*** | 1.59E+10 | 457 | 2.80E+10 | 500 |
| ***i31 – p3*** | 1.02E+08 | 409 | 3.52E+08 | 452 | ***i34 – i32*** | 3.32E+06 | 457 | 1.00E+07 | 500 |
| ***i19 – p6*** | 1.18E+07 | 458 | 4.91E+07 | 501 | ***i32 – i34*** | 2.40E+07 | 446 | 6.95E+07 | 489 |
| ***i30 – p43*** | 1.59E+08 | 364 | 5.47E+08 | 407 | ***i34 – p48*** | 2.32E+07 | 457 | 9.49E+07 | 500 |
| ***i31 – p43*** | 3.53E+07 | 409 | 1.44E+08 | 452 | ***i34 – p46*** | 6.91E+07 | 457 | 2.39E+08 | 500 |

**Table S10**. RRKM calculated rate constants (*k(E)*, s-1) of the reaction of 1,3-pentadiene+propynyl as functions of the internal energy (*E,* kJ mol-1) of the intermediate states for unimolecular reaction steps at different collision energies (*EC,* kJ mol-1)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ***EC*** | 0 | | 43 | | ***EC*** | 0 | | 43 | |
| **Reaction step** | *k(E)* | *E* | *k(E)* | *E* | **Reaction step** | *k(E)* | *E* | *k(E)* | *E* |
| ***i55 – i27*** | 8.48E+08 | 308 | 2.98E+09 | 351 | ***i40 – p39*** | 1.38E+05 | 268 | 3.05E+06 | 311 |
| ***i27 – i55*** | 7.09E+06 | 276 | 1.82E+07 | 319 | ***i33 – i43*** | 6.87E+05 | 395 | 3.32E+06 | 438 |
| ***i55 – i56*** | 1.13E+06 | 308 | 6.84E+06 | 351 | ***i43 – i33*** | 2.15E+07 | 328 | 7.27E+07 | 371 |
| ***i56 – i55*** | 7.70E+02 | 395 | 7.32E+03 | 438 | ***i43 – i31*** | 6.05E+07 | 328 | 1.81E+08 | 371 |
| ***i55 – i57*** | 1.93E+06 | 308 | 1.15E+07 | 351 | ***i31 – i43*** | 7.09E+05 | 410 | 3.23E+06 | 453 |
| ***i57 – i55*** | 4.53E+01 | 449 | 5.32E+02 | 492 | ***i64 – p93*** | 3.48E+07 | 345 | 1.17E+08 | 388 |
| ***i57 – p42*** | 1.96E+11 | 449 | 3.10E+11 | 492 | ***i64 – i66*** | 2.46E+07 | 345 | 8.23E+07 | 388 |
| ***i57 – p89*** | 1.07E+10 | 449 | 1.87E+10 | 492 | ***i66 – i64*** | 4.63E+05 | 407 | 2.10E+06 | 450 |
| ***i56 – p92*** | 4.13E+07 | 395 | 1.53E+08 | 438 | ***i62 – i65*** | 4.04E+07 | 329 | 1.27E+08 | 372 |
| ***i56 – i60*** | 3.05E+07 | 395 | 9.68E+07 | 438 | ***i65 – i62*** | 3.19E+05 | 402 | 1.46E+06 | 445 |
| ***i60 – i56*** | 3.30E+07 | 399 | 1.07E+08 | 442 | ***i61 – i59*** | 1.20E+07 | 453 | 3.65E+07 | 496 |
| ***i56 – i63*** | 2.69E+06 | 395 | 1.06E+07 | 438 | ***i59 – i61*** | 1.46E+07 | 452 | 4.46E+07 | 495 |
| ***i63 – i56*** | 2.86E+07 | 354 | 9.22E+07 | 397 | ***i23 – p13b*** | 1.16E+03 | 265 | 3.17E+04 | 308 |
| ***i60 – i62*** | 5.91E+05 | 399 | 2.68E+06 | 442 | ***i23 – p10b*** | 1.91E+06 | 265 | 1.92E+07 | 308 |
| ***i62 – i60*** | 1.61E+07 | 329 | 5.01E+07 | 372 | ***i22 – p10a*** | 7.09E+06 | 274 | 6.17E+07 | 317 |
| ***i56 – i59*** | 3.76E+04 | 395 | 2.08E+05 | 438 | ***i22 – p13a*** | 5.14E+04 | 274 | 8.93E+05 | 317 |
| ***i59 – i56*** | 6.71E+02 | 452 | 4.69E+03 | 495 | ***i22 – i40*** | 4.70E+04 | 274 | 5.04E+05 | 317 |
| ***i57 – i58*** | 6.08E+05 | 449 | 2.47E+06 | 492 | ***i40 – i22*** | 1.63E+04 | 268 | 1.68E+05 | 311 |
| ***i58 – i57*** | 7.16E+07 | 347 | 1.80E+08 | 390 | ***i50 – i54*** | 4.04E+05 | 205 | 4.52E+06 | 248 |
| ***i41 – i33*** | 9.35E+05 | 310 | 5.72E+06 | 353 | ***i54 – i50*** | 8.06E+01 | 311 | 2.32E+03 | 354 |
| ***i33 – i41*** | 7.01E+02 | 395 | 6.69E+03 | 438 | ***i50 – p85*** | 7.34E+03 | 205 | 1.77E+05 | 248 |
| ***i41 – i23*** | 2.39E+08 | 310 | 9.29E+08 | 353 | ***i26 – p59*** | 3.81E+04 | 280 | 5.62E+05 | 323 |
| ***i23 – i41*** | 2.65E+07 | 265 | 6.82E+07 | 308 | ***i26 – i47*** | 1.15E+10 | 280 | 2.04E+10 | 323 |
| ***i41 – i44*** | 1.49E+06 | 310 | 8.38E+06 | 353 | ***i47 – i26*** | 7.24E+10 | 276 | 1.25E+11 | 319 |
| ***i44 – i41*** | 1.57E+01 | 458 | 1.77E+02 | 501 | ***i27 – p63*** | 6.37E+03 | 276 | 1.35E+05 | 319 |
| ***i41 – i42*** | 1.99E+06 | 310 | 1.08E+07 | 353 | ***i51 – i49*** | 1.13E+10 | 263 | 2.34E+10 | 306 |
| ***i42 – i41*** | 8.75E+03 | 344 | 5.62E+04 | 387 | ***i49 – i51*** | 1.15E+12 | 210 | 1.43E+12 | 253 |
| ***i26 – i27*** | 5.31E+09 | 280 | 9.72E+09 | 323 | ***i28 – i29*** | 4.48E+10 | 303 | 8.69E+10 | 346 |
| ***i27 – i26*** | 9.48E+09 | 276 | 1.69E+10 | 319 | ***i29 – i28*** | 1.06E+11 | 305 | 2.09E+11 | 348 |
| ***i23 – i22*** | 3.40E+10 | 265 | 5.95E+10 | 308 | ***i46 – p3*** | 6.65E+08 | 348 | 2.09E+09 | 391 |
| ***i22 – i23*** | 4.02E+10 | 274 | 7.58E+10 | 317 | ***i46 – i8*** | 1.15E+08 | 348 | 2.80E+08 | 391 |
| ***i27 – p67*** | 1.29E+03 | 276 | 4.27E+04 | 319 | ***i8 – i46*** | 3.29E+05 | 465 | 1.37E+06 | 508 |
| ***i27 – p62*** | 5.03E+03 | 276 | 9.98E+04 | 319 | ***i43 – p43*** | 5.34E+07 | 328 | 1.76E+08 | 371 |
| ***i27 – i28*** | 1.70E+06 | 276 | 8.41E+06 | 319 | ***i20 – p54*** | 2.77E+05 | 212 | 6.46E+06 | 255 |
| ***i28 – i27*** | 6.42E+05 | 303 | 3.90E+06 | 346 | ***i20 – p53*** | 3.14E+04 | 212 | 7.28E+05 | 255 |
| ***i27 – p70*** | 8.01E-04 | 276 | 1.47E+00 | 319 | ***i40 – p49*** | 5.80E+04 | 268 | 1.48E+06 | 311 |
| ***i23 – p11b*** | 1.88E+06 | 265 | 2.06E+07 | 308 | ***i40 – p50*** | 6.66E+00 | 268 | 1.30E+03 | 311 |
| ***i23 – p12b*** | 8.05E+03 | 265 | 1.70E+05 | 308 | ***i53 – p82*** | 9.31E+03 | 320 | 1.51E+05 | 363 |
| ***i23 – p51*** | 6.29E-04 | 265 | 2.03E+00 | 308 | ***i53 – p86*** | 1.63E+01 | 320 | 1.30E+03 | 363 |
| ***i60 – p92*** | 5.28E+07 | 399 | 1.93E+08 | 442 | ***i53 – p88*** | 1.51E-02 | 320 | 4.56E+00 | 363 |
| ***i60 – p45*** | 1.54E+09 | 399 | 4.50E+09 | 442 | ***i53 – p12a*** | 1.42E+04 | 320 | 2.07E+05 | 363 |
| ***i60 – p91*** | 2.36E+07 | 399 | 8.32E+07 | 442 | ***i53 – i54*** | 1.06E+10 | 320 | 1.93E+10 | 363 |
| ***i63 – p92*** | 2.68E+08 | 354 | 8.29E+08 | 397 | ***i54 – i53*** | 2.57E+10 | 311 | 4.42E+10 | 354 |
| ***i63 – p44*** | 7.35E+09 | 354 | 1.68E+10 | 397 | ***i54 – p87*** | 7.49E+00 | 311 | 7.32E+02 | 354 |
| ***i63 – p90*** | 2.65E+08 | 354 | 7.07E+08 | 397 | ***i54 – p84*** | 5.35E+03 | 311 | 1.28E+05 | 354 |
| ***i59 – p89*** | 1.41E+10 | 452 | 2.47E+10 | 495 | ***i54 – p88*** | 6.33E-02 | 311 | 1.51E+01 | 354 |
| ***i59 – p90*** | 4.21E+07 | 452 | 1.46E+08 | 495 | ***i54 – p12b*** | 7.28E+03 | 311 | 1.48E+05 | 354 |
| ***i58 – p91*** | 5.93E+07 | 347 | 1.71E+08 | 390 | ***i40 – p12a*** | 1.98E+05 | 268 | 2.36E+06 | 311 |
| ***i44 – p1*** | 1.57E+10 | 458 | 2.76E+10 | 501 | ***i47 – p60*** | 6.94E+04 | 276 | 1.15E+06 | 319 |
| ***i44 – i32*** | 3.44E+06 | 458 | 1.03E+07 | 501 | ***i51 – p76'*** | 1.21E+04 | 263 | 3.57E+05 | 306 |
| ***i32 – i44*** | 1.27E+07 | 447 | 3.67E+07 | 490 | ***i51 – p78*** | 1.56E+00 | 263 | 4.72E+02 | 306 |
| ***i44 – p48*** | 2.43E+07 | 458 | 9.85E+07 | 501 | ***i51 – p58*** | 2.20E+05 | 263 | 2.85E+06 | 306 |
| ***i44 – p46*** | 7.19E+07 | 458 | 2.47E+08 | 501 | ***i47 – p68*** | 1.01E+03 | 276 | 4.05E+04 | 319 |
| ***i42 – p46*** | 2.69E+08 | 344 | 6.99E+08 | 387 | ***i47 – p71*** | 6.29E-03 | 276 | 1.10E+01 | 319 |
| ***i26 – p58*** | 2.30E+04 | 280 | 3.28E+05 | 323 | ***i47 – p61*** | 3.91E+04 | 276 | 6.45E+05 | 319 |
| ***i26 – p66*** | 1.58E+03 | 280 | 3.96E+04 | 323 | ***i29 – p10a*** | 5.75E+06 | 305 | 5.26E+07 | 348 |
| ***i26 – p71*** | 7.43E-05 | 280 | 2.39E-01 | 323 | ***i29 – p72*** | 7.39E+00 | 305 | 7.86E+02 | 348 |
| ***i57 – p92*** | 1.37E+07 | 449 | 5.80E+07 | 492 | ***i29 – p74*** | 9.01E-03 | 305 | 8.60E+00 | 348 |
| ***i57 – i61*** | 9.73E+06 | 449 | 2.85E+07 | 492 | ***i49 – p77*** | 6.88E+02 | 210 | 4.71E+04 | 253 |
| ***i61 – i57*** | 2.07E+06 | 453 | 6.09E+06 | 496 | ***i49 – p79*** | 1.73E-04 | 210 | 3.68E+00 | 253 |
| ***i60 – i65*** | 3.07E+07 | 399 | 8.86E+07 | 442 | ***i49 – i50*** | 1.72E+10 | 210 | 3.30E+10 | 253 |
| ***i65 – i60*** | 6.59E+06 | 402 | 1.91E+07 | 445 | ***i50 – i49*** | 1.83E+10 | 205 | 3.21E+10 | 248 |
| ***i63 – i66*** | 8.10E+07 | 354 | 2.26E+08 | 397 | ***i29 – p60*** | 6.56E+04 | 305 | 1.14E+06 | 348 |
| ***i66 – i63*** | 1.91E+06 | 407 | 6.91E+06 | 450 | ***i47 – i48*** | 2.88E+10 | 276 | 5.04E+10 | 319 |
| ***i22 – p12a*** | 1.23E+05 | 274 | 1.80E+06 | 317 | ***i48 – i47*** | 2.21E+10 | 265 | 3.54E+10 | 308 |
| ***i22 – p51*** | 1.45E-03 | 274 | 3.43E+00 | 317 | ***i50 – i52*** | 7.26E+08 | 205 | 2.17E+09 | 248 |
| ***i22 – p11a*** | 2.49E+07 | 274 | 2.15E+08 | 317 | ***i52 – i50*** | 3.00E+11 | 170 | 6.09E+11 | 213 |
| ***i25 – i24*** | 7.76E+11 | 174 | 1.48E+12 | 217 | ***i27 – i48*** | 2.23E+10 | 276 | 3.89E+10 | 319 |
| ***i24 – i25*** | 3.79E+09 | 208 | 1.04E+10 | 251 | ***i48 – i27*** | 6.05E+10 | 265 | 9.65E+10 | 308 |
| ***i25 – i26*** | 4.64E+12 | 174 | 5.88E+12 | 217 | ***i50 – p76*** | 2.21E+04 | 205 | 7.67E+05 | 248 |
| ***i26 – i25*** | 3.31E+06 | 280 | 1.22E+07 | 323 | ***i47 – i52*** | 2.01E+07 | 276 | 7.59E+07 | 319 |
| ***i21 – i1*** | 8.99E+11 | 175 | 1.71E+12 | 218 | ***i52 – i47*** | 3.84E+12 | 170 | 4.87E+12 | 213 |
| ***i20 – i21*** | 1.16E+09 | 212 | 3.32E+09 | 255 | ***i52 – p81*** | 5.82E-03 | 170 | 5.57E+02 | 213 |
| ***i22 – i21*** | 1.03E+08 | 274 | 3.47E+08 | 317 | ***i48 – p69*** | 2.10E+02 | 265 | 1.03E+04 | 308 |
| ***i21 – i22*** | 5.72E+12 | 175 | 7.05E+12 | 218 | ***i48 – p65*** | 3.06E+03 | 265 | 7.62E+04 | 308 |
| ***i25 – p80*** | 1.15E-01 | 174 | 1.66E+03 | 217 | ***i48 – p64*** | 1.43E+03 | 265 | 3.36E+04 | 308 |
| ***i21 – p57*** | 1.73E-01 | 175 | 1.77E+03 | 218 | ***i42 – i30*** | 7.15E+06 | 344 | 2.44E+07 | 387 |
| ***i63 – i64*** | 4.64E+06 | 354 | 1.95E+07 | 397 | ***i30 – i42*** | 1.30E+07 | 366 | 5.07E+07 | 409 |
| ***i64 – i63*** | 5.84E+06 | 345 | 2.33E+07 | 388 | ***i42 – i45*** | 6.33E+06 | 344 | 2.13E+07 | 387 |
| ***i44 – i42*** | 3.92E+05 | 458 | 1.60E+06 | 501 | ***i45 – i42*** | 3.15E+06 | 366 | 1.20E+07 | 409 |
| ***i42 – i44*** | 1.64E+08 | 344 | 3.94E+08 | 387 | ***i45 – p48*** | 3.17E+08 | 366 | 9.47E+08 | 409 |
| ***i61 – p89*** | 1.00E+10 | 453 | 1.74E+10 | 496 | ***i45 – p46*** | 1.03E+09 | 366 | 2.73E+09 | 409 |
| ***i61 – p91*** | 1.25E+07 | 453 | 4.99E+07 | 496 | ***i45 – i33*** | 7.23E+06 | 366 | 2.30E+07 | 409 |
| ***i58 – i61*** | 1.16E+08 | 347 | 2.86E+08 | 390 | ***i33 – i45*** | 2.48E+06 | 395 | 9.15E+06 | 438 |
| ***i61 – i58*** | 2.09E+05 | 453 | 8.41E+05 | 496 | ***i51 – p62*** | 1.57E+05 | 263 | 2.98E+06 | 306 |
| ***i65 – p94*** | 3.88E+06 | 402 | 1.85E+07 | 445 | ***i28 –p11b*** | 1.18E+06 | 303 | 1.29E+07 | 346 |
| ***i65 – p91*** | 4.42E+07 | 402 | 1.53E+08 | 445 | ***i29 – p11a*** | 1.62E+07 | 305 | 1.46E+08 | 348 |
| ***i66 – p93*** | 2.53E+07 | 407 | 9.59E+07 | 450 | ***i8 – p1*** | 7.95E+10 | 465 | 1.40E+11 | 508 |
| ***i66 – p90*** | 1.56E+08 | 407 | 4.76E+08 | 450 | ***i8 – i32*** | 4.03E+06 | 465 | 1.22E+07 | 508 |
| ***i62 – p94*** | 8.68E+06 | 329 | 3.63E+07 | 372 | ***i32 – i8*** | 1.57E+07 | 447 | 4.47E+07 | 490 |
| ***i24 – p83*** | 1.47E+05 | 208 | 3.21E+06 | 251 | ***i32 – p42*** | 3.14E+11 | 447 | 5.00E+11 | 490 |
| ***i24 – i53*** | 3.81E+06 | 208 | 3.16E+07 | 251 | ***i32 – p1*** | 3.19E+10 | 447 | 5.60E+10 | 490 |
| ***i53 – i24*** | 1.33E+02 | 320 | 2.93E+03 | 363 | ***i30 – p3*** | 1.32E+09 | 366 | 3.93E+09 | 409 |
| ***i24 – p76'*** | 4.80E+05 | 208 | 1.48E+07 | 251 | ***i30 – i35*** | 2.71E+07 | 366 | 7.83E+07 | 409 |
| ***i24 – i49*** | 1.43E+11 | 208 | 2.48E+11 | 251 | ***i35 – i30*** | 8.06E+06 | 403 | 2.78E+07 | 446 |
| ***i49 – i24*** | 5.75E+10 | 210 | 1.05E+11 | 253 | ***i31 – i33*** | 1.18E+07 | 410 | 3.66E+07 | 453 |
| ***i26 – i51*** | 3.69E+04 | 280 | 4.29E+05 | 323 | ***i33 – i31*** | 3.23E+07 | 395 | 9.34E+07 | 438 |
| ***i51 – i26*** | 9.92E+05 | 263 | 1.02E+07 | 306 | ***i31 – p3*** | 1.01E+08 | 410 | 3.51E+08 | 453 |
| ***i20 – p56*** | 5.87E+04 | 212 | 3.00E+06 | 255 | ***i30 – p43*** | 1.65E+08 | 366 | 5.65E+08 | 409 |
| ***i20 – p52*** | 2.87E+05 | 212 | 5.15E+06 | 255 | ***i31 – p43*** | 3.69E+07 | 410 | 1.49E+08 | 453 |
| ***i20 – p55*** | 1.07E+06 | 212 | 2.71E+07 | 255 | ***i8 – p3*** | 6.20E+07 | 465 | 2.50E+08 | 508 |
| ***i28 – p62*** | 2.79E+04 | 303 | 6.28E+05 | 346 | ***i33 – p45*** | 2.52E+09 | 395 | 7.40E+09 | 438 |
| ***i28 – p10b*** | 1.47E+06 | 303 | 1.66E+07 | 346 | ***i33 – p48*** | 3.40E+07 | 395 | 1.20E+08 | 438 |
| ***i28 – p75*** | 1.73E-02 | 303 | 1.36E+01 | 346 | ***i35 – p44*** | 2.33E+09 | 403 | 6.17E+09 | 446 |
| ***i28 – p73*** | 3.91E+00 | 303 | 5.28E+02 | 346 | ***i35 – p46*** | 1.18E+08 | 403 | 3.58E+08 | 446 |
| ***i32 – i46*** | 2.90E+05 | 447 | 1.20E+06 | 490 | ***i30 – p46*** | 2.29E+09 | 366 | 5.90E+09 | 409 |
| ***i46 – i32*** | 2.59E+07 | 348 | 6.71E+07 | 391 | ***i31 – p48*** | 1.35E+08 | 410 | 4.72E+08 | 453 |
|  |  |  |  |  |  |  |  |  |  |

**Table S11**. Natural charge analysis of 1,3-pentadiene

|  |  |
| --- | --- |
| **Atom** | ***Natural charges*** |
| ***1,3-pentadiene***  D:\My scientific research in chemistry\Chemical reactions\C5H8+C3H3(doing)\1,3-pentadiene\заряды\1,3-pentadiene.tiff |
| C1 | -0.14496 |
| C2 | -0.23605 |
| C3 | -0.20426 |
| C4 | -0.36267 |
| C5 | -0.60189 |
| H6 | 0.18865 |
| H7 | 0.18054 |
| H8 | 0.19192 |
| H9 | 0.19093 |
| H10 | 0.18309 |
| H11 | 0.20723 |
| H12 | 0.20023 |
| H13 | 0.20724 |
| **Total** | 0 |

**Table S12**. Calculated lifetimes for the different initial complecxes in the reaction of the 1-propynyl radical with 2-methyl-1,3-butadiene and 1,3-pentadiene

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 1-propynyl + 2-methyl-1,3-butadiene | | | | |
| Initial complex | i1 | i3 | i9 | i11 |
| Lifetime, ns | 0.72 | 98.94 | 0.253 | 41.08 |
| 1-propynyl + 1,3-pentadiene | | | | |
| Initial complex | i20 | i22 | i24 | i26 |
| Lifetime, ns | 0.46 | 3.05 | 0.11 | 160.59 |

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# Author Contributions

R.I.K designed experiments. I.A.M, C.H. and Z.H.Y. performed experiments. A.M.M. and A.A.N. carried out the theoretical calculations. I.A.M, A.M.M. and R.I.K. wrote the manuscript, which was read, revised, and approved by all co-authors.

Appendix

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm−1) for all intermediates, transition states, reactants, and products involved in the 2-methyl-1,3-butadiene + 1-propynyl reactions at the ωB97P-D/6-311G(d,p) level.

***Reactants***

***(trans-)2-methyl-1,3-butadiene***

C 1.973854 0.006578 0.000167

C 0.833035 -0.680452 -0.000194

H 2.931617 -0.500421 0.000144

H 1.996166 1.091273 0.000490

H 0.874839 -1.767502 -0.000613

C -0.517629 -0.100332 -0.000109

C -1.583514 -0.904863 0.000160

C -0.653664 1.397459 -0.000078

H -2.593738 -0.510187 0.000344

H -1.474113 -1.984540 0.000162

H -1.702903 1.695636 -0.000034

H -0.172206 1.832714 -0.881248

H -0.172155 1.832679 0.881081

**Frequencies**

137.3939 225.5480 297.6232

401.6022 437.5583 541.3986

639.7032 785.0651 801.3264

928.0969 943.5573 972.6251

1015.7076 1028.9680 1076.1723

1094.4048 1327.0370 1340.6146

1418.9358 1443.5148 1464.2737

1488.5355 1511.4583 1691.9826

1743.8405 3047.6580 3110.6408

3139.9049 3154.9701 3160.7078

3172.2382 3243.8763 3253.1487

***(trans-)1,3-pentadiene***

C -2.517576 -0.260302 0.000007

C -1.358229 0.395795 -0.000002

C -0.049303 -0.246709 -0.000014

C 1.107341 0.417464 0.000001

C 2.462545 -0.214923 0.000005

H -3.466470 0.262808 0.000021

H -2.552191 -1.345860 0.000002

H -1.361331 1.484318 -0.000015

H -0.039804 -1.336165 -0.000017

H 1.080386 1.506611 0.000000

H 3.038178 0.092906 -0.879154

H 2.394546 -1.305140 -0.000204

H 3.038016 0.092576 0.879387

**Frequencies**

116.2996 190.2383 201.0248

244.1542 461.6287 488.6761

642.4576 849.5210 915.9246

936.5777 984.1635 995.3123

1043.7708 1067.1296 1108.0483

1212.0422 1294.8272 1324.2103

1340.3223 1416.0599 1455.8048

1478.9669 1493.9892 1700.8253

1765.1114 3034.3836 3092.1631

3126.5166 3148.6404 3151.9411

3155.3764 3164.9185 3248.3316

***1-propynyl***

C -1.123766 0.000034 0.000188

C 0.336608 -0.000571 -0.000814

C 1.540300 0.000283 0.000377

H -1.504993 0.615339 0.817821

H -1.506845 -1.015014 0.124083

H -1.507018 0.401203 -0.940410

***Frequencies***

200.1523 203.0213 952.8370

1014.5159 1022.1101 1413.0112

1478.5078 1483.7864 2276.0322

3059.2654 3134.4920 3139.5728

***i1***

C -0.758962 1.919431 0.528457

C -0.470348 0.764220 -0.383565

C 3.443950 -0.506816 -0.076342

C 2.061473 -0.054842 -0.186553

C 0.923441 0.315894 -0.280545

H -0.050724 2.229783 1.284912

H -1.726791 2.402361 0.466747

H -0.642545 1.090388 -1.418866

H 3.712467 -0.683052 0.968230

H 4.131770 0.239729 -0.480999

H 3.593420 -1.439289 -0.626079

C -1.450322 -0.386128 -0.121123

C -2.368113 -0.710128 -1.025169

C -1.323283 -1.075225 1.206641

H -3.085634 -1.502851 -0.840598

H -2.433938 -0.197735 -1.979561

H -2.081776 -1.850640 1.324358

H -1.428916 -0.354837 2.024213

H -0.334347 -1.532287 1.306845

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 62.3355 | 88.5296 | 92.1546 |
| 137.8212 | 142.456 | 205.6978 |
| 236.3967 | 270.7907 | 304.73 |
| 394.8174 | 415.386 | 472.4497 |
| 509.0041 | 553.334 | 595.6581 |
| 730.2493 | 772.9026 | 830.3167 |
| 945.1615 | 973.9402 | 999.4444 |
| 1036.496 | 1059.139 | 1063.052 |
| 1082.99 | 1103.893 | 1179.987 |
| 1225.601 | 1296.75 | 1338.724 |
| 1415.638 | 1422.269 | 1450.894 |
| 1454.301 | 1485.637 | 1487.446 |
| 1491.202 | 1502.671 | 1744.314 |
| 2395.098 | 3013.603 | 3043.021 |
| 3051.577 | 3106.876 | 3122.456 |
| 3126.419 | 3137.852 | 3149.524 |
| 3163.2 | 3234.671 | 3285.266 |

***i2***

C 0.088957 1.885199 -0.037697

C -0.406246 0.606225 -0.711628

C -1.424872 -0.285063 -0.097534

C -2.191137 -1.056100 -0.868731

C -1.541801 -0.291742 1.402058

C 2.699793 -1.212955 0.013574

C 2.069129 0.105319 0.178716

C 0.973101 0.716611 -0.101416

H 0.304150 2.728003 -0.686831

H -0.328346 2.150729 0.928573

H -0.427765 0.637895 -1.797523

H -2.928126 -1.727845 -0.442200

H -2.104781 -1.039016 -1.950252

H -2.210677 -1.085077 1.737670

H -1.940025 0.660563 1.766914

H -0.563784 -0.436448 1.870716

H 3.645139 -1.133564 -0.530214

H 2.038569 -1.889785 -0.544397

H 2.914100 -1.670415 0.983494

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 58.4259 | 79.1364 | 124.3839 |
| 170.9379 | 201.1269 | 228.5389 |
| 287.535 | 374.9556 | 410.005 |
| 463.8513 | 504.2346 | 552.2834 |
| 661.928 | 743.7214 | 767.5677 |
| 839.4418 | 904.5862 | 921.5697 |
| 950.4005 | 1007.409 | 1031.067 |
| 1050.219 | 1053.467 | 1061.528 |
| 1073.628 | 1079.342 | 1099.312 |
| 1197.437 | 1312.846 | 1353.614 |
| 1405.234 | 1421.246 | 1451.091 |
| 1465.563 | 1467.507 | 1482.908 |
| 1489.013 | 1508.134 | 1726.935 |
| 1886.968 | 3009.831 | 3042.865 |
| 3091.378 | 3103.092 | 3115.52 |
| 3129.884 | 3145.227 | 3150.71 |
| 3159.909 | 3217.702 | 3237.922 |

***i3***

C -0.219178 -0.762535 -0.036247

C 0.731217 0.402709 -0.025376

C 2.117916 0.263898 0.002133

C 2.938576 1.372302 0.005577

C 2.723617 -1.120735 0.029126

C -4.179704 0.372905 0.024794

C -2.778365 -0.031910 0.003118

C -1.626492 -0.368365 -0.014276

H -0.019313 -1.420339 0.821313

H -0.038195 -1.387851 -0.922535

H 0.301456 1.398346 -0.045293

H 4.017653 1.277140 0.026709

H 2.522138 2.373181 -0.012599

H 3.813317 -1.075450 0.035535

H 2.414825 -1.704340 -0.843616

H 2.403630 -1.674061 0.917542

H -4.789725 -0.304072 -0.578413

H -4.298710 1.382469 -0.376245

H -4.572598 0.365363 1.044509

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 12.139 | 41.6526 | 79.8575 |
| 139.3793 | 185.2888 | 198.3576 |
| 212.7249 | 290.6685 | 385.4865 |
| 411.5126 | 481.5263 | 502.1147 |
| 526.9928 | 573.2427 | 683.2899 |
| 787.9445 | 794.249 | 868.9236 |
| 913.437 | 985.5128 | 1020.547 |
| 1058.107 | 1058.839 | 1059.573 |
| 1127.11 | 1178.138 | 1225.088 |
| 1260.597 | 1333.477 | 1387.695 |
| 1420.329 | 1429.583 | 1448.205 |
| 1467.36 | 1486.253 | 1486.785 |
| 1493.111 | 1502.873 | 1531.551 |
| 2399.148 | 2999.624 | 3022.179 |
| 3042.057 | 3047.231 | 3103.054 |
| 3119.929 | 3120.512 | 3138.996 |
| 3153.643 | 3191.85 | 3251.341 |

***i4***

C -0.265501 -0.850225 0.000735

C 0.733365 0.273520 0.000466

C -4.171476 0.462940 -0.000520

C -2.789305 -0.003780 0.000062

C -1.653809 -0.392444 0.000367

C 2.118721 0.084124 -0.000158

C 2.693760 -1.164429 -0.000707

C 2.994662 1.318918 -0.000025

H -0.101461 -1.495439 0.874883

H -0.101243 -1.496067 -0.872897

H 0.339603 1.284581 0.000941

H -4.721509 0.051577 -0.850547

H -4.213403 1.552948 -0.066749

H -4.686020 0.160047 0.914785

H 3.770639 -1.284059 -0.001217

H 2.099378 -2.070523 -0.000651

H 4.053672 1.055588 -0.002354

H 2.800558 1.933510 0.883204

H 2.797293 1.936090 -0.880716

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 24.205 | 32.646 | 42.3382 |
| 78.7787 | 175.5922 | 206.176 |
| 220.5036 | 293.1935 | 387.4386 |
| 389.6971 | 481.7588 | 510.4465 |
| 522.4042 | 577.8029 | 660.653 |
| 780.5432 | 807.899 | 900.8756 |
| 919.9465 | 992.1853 | 1038.82 |
| 1059.231 | 1059.351 | 1063.149 |
| 1112.119 | 1177.749 | 1228.634 |
| 1253.806 | 1326.265 | 1363.637 |
| 1416.235 | 1420.52 | 1456.891 |
| 1483.927 | 1486.116 | 1486.893 |
| 1491.881 | 1501.836 | 1556.408 |
| 2399.125 | 3006.371 | 3030.671 |
| 3047.133 | 3047.542 | 3114.581 |
| 3119.534 | 3120.358 | 3136.001 |
| 3159.799 | 3187.785 | 3251.928 |

***i5***

C 0.329285 0.627281 0.000849

C -0.687063 -0.343321 -0.004445

C 4.286488 -0.306164 0.000848

C 2.868733 0.026023 -0.000469

C 1.688503 0.299665 0.000001

C -2.040505 -0.123961 -0.005738

C -2.671484 1.235909 -0.000406

C -2.999832 -1.276395 0.003105

H -1.956333 2.045428 -0.143530

H 0.079879 1.683208 0.009222

H -0.353169 -1.378565 -0.004941

H 4.894092 0.582361 -0.188027

H 4.515625 -1.044883 -0.772123

H 4.589683 -0.725096 0.964807

H -3.426405 1.308884 -0.790994

H -3.192478 1.410523 0.948764

H -3.676001 -1.215360 0.864571

H -2.485205 -2.238082 0.041366

H -3.634434 -1.262640 -0.891588

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 57.3121 | 71.9314 | 80.3252 |
| 111.3967 | 123.5204 | 216.7447 |
| 229.7661 | 234.1674 | 299.5739 |
| 382.6394 | 398.1878 | 462.5146 |
| 492.2241 | 534.585 | 735.5088 |
| 807.3223 | 865.337 | 909.3535 |
| 974.8465 | 1003.23 | 1041.486 |
| 1051.397 | 1064.58 | 1080.627 |
| 1169.666 | 1217.376 | 1235.474 |
| 1340.088 | 1409.761 | 1420.206 |
| 1422.703 | 1447.866 | 1471.824 |
| 1478.947 | 1484.302 | 1486.372 |
| 1491.745 | 1494.175 | 1558.185 |
| 2264.95 | 3019.955 | 3031.926 |
| 3044.45 | 3070.462 | 3083.061 |
| 3111.184 | 3121.671 | 3134.908 |
| 3150.784 | 3161.347 | 3186.731 |

***i6***

C 2.446259 -1.143968 -0.000021

C 1.213355 -0.284680 0.000003

C -0.093187 -1.039504 0.000041

C -1.331142 -0.158987 -0.000018

C -1.164459 1.141704 -0.000034

C 0.067557 1.954922 0.000019

C 1.276773 1.044551 -0.000004

C -2.661569 -0.858317 -0.000016

H 2.464266 -1.796721 -0.879841

H 2.464263 -1.796759 0.879772

H 3.358361 -0.544343 -0.000004

H -0.124628 -1.708413 0.872935

H -0.124621 -1.708540 -0.872750

H 0.098039 2.615576 -0.875648

H 0.098012 2.615506 0.875739

H 2.247438 1.534984 -0.000025

H -3.484581 -0.143201 -0.000309

H -2.759159 -1.500949 0.881802

H -2.758918 -1.501466 -0.881486

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 83.4124 | 121.4427 | 151.0743 |
| 230.2841 | 260.2654 | 262.2348 |
| 387.2731 | 421.2414 | 465.8643 |
| 466.4409 | 501.5996 | 698.321 |
| 790.8007 | 848.0587 | 904.7779 |
| 919.3005 | 931.2447 | 976.4261 |
| 995.1383 | 1044.843 | 1070.286 |
| 1082.697 | 1114.454 | 1173.947 |
| 1210.389 | 1215.058 | 1235.592 |
| 1314.164 | 1352.909 | 1403.657 |
| 1410.734 | 1422.706 | 1466.929 |
| 1472.437 | 1482.859 | 1485.687 |
| 1487.987 | 1490.797 | 1767.075 |
| 1801.882 | 3000.338 | 3023.106 |
| 3026.017 | 3030.247 | 3036.317 |
| 3050.544 | 3087.34 | 3093.454 |
| 3129.47 | 3149.598 | 3167.889 |

***i7***

C 2.556578 -0.907326 0.000016

C 1.232313 -0.198815 -0.000017

C 0.023567 -1.096718 0.000008

C -1.316890 -0.388964 0.000016

C -1.368109 0.991825 0.000012

C -0.166352 1.875960 -0.000002

C 1.132364 1.126771 -0.000030

C -2.470638 -1.157830 -0.000003

H 2.651763 -1.553530 -0.879759

H 2.651976 -1.552999 0.880158

H 3.390350 -0.202788 -0.000282

H 0.077003 -1.762202 0.871862

H 0.076981 -1.762237 -0.871818

H -0.203366 2.549306 -0.869400

H -0.203330 2.549312 0.869391

H 2.039082 1.726910 -0.000051

H -2.342062 1.473165 0.000002

H -3.449940 -0.693278 0.000205

H -2.425451 -2.241071 -0.000302

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 35.6033 | 131.2169 | 194.9589 |
| 251.4234 | 290.3053 | 413.7416 |
| 417.4993 | 482.0156 | 482.4788 |
| 505.1915 | 520.2974 | 706.5145 |
| 712.9466 | 753.4632 | 815.7129 |
| 876.7537 | 917.6087 | 924.2151 |
| 959.1972 | 966.0118 | 1003.715 |
| 1062.272 | 1072.615 | 1111.714 |
| 1167.855 | 1217.41 | 1253.425 |
| 1256.529 | 1318.008 | 1387.098 |
| 1391.695 | 1418.267 | 1438.983 |
| 1460.286 | 1467.118 | 1484.861 |
| 1489.493 | 1490.692 | 1527.866 |
| 1787.558 | 2998.586 | 3011.166 |
| 3020.967 | 3034.069 | 3046.575 |
| 3090.07 | 3136.515 | 3158.248 |
| 3158.712 | 3180.361 | 3256.985 |

***i8***

C 2.549259 -0.989396 -0.000009

C 1.268948 -0.215171 -0.000002

C 0.000001 -1.018373 0.000024

C -1.268949 -0.215172 0.000009

C -1.223843 1.145347 0.000009

C 0.000001 1.852482 0.000000

C 1.223844 1.145348 -0.000008

C -2.549260 -0.989395 -0.000017

H 2.613056 -1.641975 -0.879422

H 2.612986 -1.642107 0.879309

H 3.420073 -0.330862 0.000074

H 0.000006 -1.703959 0.867206

H 0.000002 -1.704027 -0.867101

H 0.000000 2.935517 0.000000

H -2.155453 1.704163 0.000010

H 2.155454 1.704164 -0.000018

H -3.420069 -0.330855 0.000160

H -2.612956 -1.642197 0.879237

H -2.613099 -1.641882 -0.879495

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 105.322 | 121.3122 | 146.1784 |
| 233.321 | 271.5806 | 308.6448 |
| 395.1505 | 463.7989 | 492.2639 |
| 514.9125 | 529.5915 | 699.5178 |
| 730.1448 | 864.4786 | 876.2869 |
| 910.5745 | 921.8337 | 943.6904 |
| 997.9289 | 1011.912 | 1041.236 |
| 1065.802 | 1078.291 | 1128.882 |
| 1170.816 | 1221.361 | 1244.254 |
| 1315.34 | 1337.058 | 1398.717 |
| 1414.088 | 1417.337 | 1444.038 |
| 1463.725 | 1481.334 | 1481.776 |
| 1482.105 | 1489.225 | 1570.73 |
| 1652.126 | 2940.093 | 2940.697 |
| 3018.134 | 3019.617 | 3069.454 |
| 3069.581 | 3127.566 | 3127.888 |
| 3175.596 | 3177.772 | 3220.278 |

***i9***

C -2.349466 1.456940 0.074456

C -1.357128 0.838970 -0.548699

C -0.618890 -0.403860 -0.072285

C -0.780118 -1.488487 -1.106961

C -1.100878 -0.901576 1.299025

C 3.421952 0.480963 0.086931

C 1.997423 0.173089 0.035835

C 0.822355 -0.076900 -0.000199

H -2.812883 2.335208 -0.360467

H -2.738129 1.121898 1.029701

H -1.002759 1.223293 -1.503043

H -0.617658 -2.522130 -0.823742

H -0.798254 -1.232874 -2.159815

H -0.528783 -1.783741 1.592995

H -2.158534 -1.172564 1.252376

H -0.961138 -0.133140 2.062103

H 3.629661 1.239744 0.845492

H 3.773096 0.860627 -0.875848

H 4.003880 -0.411151 0.331632

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 74.2628 | 94.877 | 98.6481 |
| 119.2503 | 137.3561 | 275.4394 |
| 289.1235 | 303.7181 | 316.7995 |
| 330.2069 | 375.8219 | 464.9857 |
| 504.6145 | 540.4581 | 574.2549 |
| 648.942 | 731.1389 | 857.2406 |
| 936.5041 | 962.3061 | 977.0588 |
| 1044.306 | 1045.609 | 1054.235 |
| 1058.279 | 1076.676 | 1208.038 |
| 1222.232 | 1260.374 | 1342.169 |
| 1408.368 | 1415.409 | 1446.77 |
| 1458.054 | 1485.35 | 1489.202 |
| 1503.581 | 1507.71 | 1734.159 |
| 2377.707 | 3047.892 | 3051.646 |
| 3120.136 | 3120.838 | 3135.755 |
| 3138.576 | 3150.791 | 3153.144 |
| 3168.111 | 3248.123 | 3268.115 |

***i10***

C 2.282923 -1.420854 -0.184144

C 1.342939 -0.631353 -0.694942

C 0.617320 0.435050 0.031652

C 0.109839 1.615377 -0.802451

C 0.993434 0.698066 1.471071

C -2.718066 -1.072077 0.295561

C -2.023597 0.094197 -0.270159

C -0.844923 0.600461 -0.347397

H 2.759623 -2.182486 -0.789947

H 2.611720 -1.336273 0.846166

H 1.049195 -0.762508 -1.734721

H 0.093548 2.585883 -0.315397

H 0.367205 1.639876 -1.857504

H 0.366313 1.485390 1.893569

H 2.040223 1.008973 1.548364

H 0.858444 -0.201351 2.078164

H -3.458154 -0.766998 1.040430

H -2.003258 -1.752067 0.778697

H -3.244078 -1.631634 -0.482965

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 68.073 | 101.1221 | 130.958 |
| 146.5619 | 220.0881 | 238.1919 |
| 287.1907 | 330.6533 | 379.4441 |
| 449.4175 | 462.3179 | 513.3329 |
| 618.424 | 706.5186 | 754.8261 |
| 829.937 | 927.6966 | 931.3841 |
| 961.2905 | 983.5208 | 1035.68 |
| 1045.225 | 1049.868 | 1051.457 |
| 1061.184 | 1096.538 | 1127.883 |
| 1266.275 | 1314.308 | 1348.687 |
| 1400.821 | 1413.518 | 1452.189 |
| 1464.328 | 1468.334 | 1483.523 |
| 1486.451 | 1507.938 | 1719.94 |
| 1888.322 | 3008.385 | 3045.228 |
| 3090.178 | 3114.856 | 3115.69 |
| 3119.324 | 3139.556 | 3157.515 |
| 3169.661 | 3207.498 | 3250.216 |

***i11***

C 3.235973 -0.010889 0.892106

C 2.143759 -0.628164 0.324311

C 1.091953 -0.019262 -0.351814

C -0.042366 -0.858219 -0.890797

C 0.980850 1.458211 -0.558268

C -3.693774 0.241264 0.684779

C -2.404724 -0.149402 0.124650

C -1.345917 -0.478813 -0.335636

H 3.996660 -0.593588 1.396114

H 3.376659 1.062978 0.863189

H 2.089286 -1.711396 0.419214

H -0.088046 -0.748843 -1.983630

H 0.142357 -1.917558 -0.689885

H 0.575893 1.679112 -1.551084

H 1.940311 1.967175 -0.460191

H 0.286444 1.896556 0.168299

H -3.857953 -0.235445 1.654308

H -4.510838 -0.050907 0.020401

H -3.745288 1.323562 0.827282

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 34.819 | 68.747 | 96.7725 |
| 111.3163 | 183.563 | 209.75 |
| 264.0643 | 298.345 | 363.769 |
| 387.0372 | 401.9712 | 459.1644 |
| 556.307 | 607.2626 | 765.8929 |
| 778.5052 | 790.6495 | 922.224 |
| 978.6712 | 999.7615 | 1033.143 |
| 1054.432 | 1057.976 | 1064.623 |
| 1167.162 | 1214.502 | 1233.966 |
| 1246.147 | 1334.613 | 1387.951 |
| 1420.624 | 1425.472 | 1460.904 |
| 1471.791 | 1488.162 | 1493.054 |
| 1495.185 | 1510.345 | 1527.466 |
| 2396.173 | 3012.865 | 3033.23 |
| 3050.697 | 3088.125 | 3090.098 |
| 3121.825 | 3124.658 | 3144.968 |
| 3147.829 | 3169.833 | 3262.73 |

***i12***

C 3.184133 -0.943703 0.091464

C 2.498508 0.247635 0.089097

H 4.262330 -0.960729 0.188519

H 2.685908 -1.901506 -0.004627

H 3.085235 1.159585 0.179121

C 1.118457 0.413154 -0.023666

C 0.228123 -0.803759 -0.158300

C 0.500722 1.772907 -0.054925

C -3.822871 -0.094110 0.105443

C -2.387892 -0.339132 0.009522

C -1.207815 -0.545575 -0.066230

H 0.436493 -1.295181 -1.119349

H 0.501531 -1.538494 0.608908

H -0.232929 1.893421 0.749683

H -0.047495 1.934387 -0.990879

H 1.257943 2.553150 0.041022

H -4.083126 0.320076 1.082641

H -4.383456 -1.022438 -0.029097

H -4.150624 0.613221 -0.660364

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 26.2614 | 70.2711 | 89.8777 |
| 177.9595 | 198.6185 | 230.355 |
| 231.3176 | 285.8393 | 337.838 |
| 396.3709 | 397.9303 | 516.3181 |
| 536.9574 | 585.2154 | 770.4785 |
| 797.2951 | 808.9205 | 891.0093 |
| 974.2147 | 988.9393 | 1038.766 |
| 1057.198 | 1061.583 | 1063.775 |
| 1177.003 | 1231.054 | 1240.729 |
| 1253.808 | 1309.532 | 1386.801 |
| 1420.152 | 1423.988 | 1461.751 |
| 1467.615 | 1477.546 | 1486.431 |
| 1489.702 | 1508.882 | 1538.321 |
| 2399.24 | 3012.781 | 3028.913 |
| 3050.574 | 3053.527 | 3081.334 |
| 3125.02 | 3127.631 | 3131.575 |
| 3157.56 | 3167.872 | 3259.18 |

***i13***

C 3.172976 -1.027368 -0.003493

C 2.413346 0.259738 -0.002308

C 1.053749 0.430415 -0.000257

C 0.147090 -0.656708 0.003969

C 0.480235 1.827035 0.000113

C -3.892013 -0.207821 -0.002473

C -2.444890 -0.367340 -0.000104

C -1.239764 -0.500860 0.002175

H 3.963177 -1.002803 -0.760345

H 3.666485 -1.187558 0.962424

H 3.023445 1.159681 0.011208

H 0.524726 -1.672680 0.013577

H 2.548882 -1.898459 -0.205396

H -0.153293 1.986339 0.877132

H -0.148287 1.987779 -0.880296

H 1.270650 2.579232 0.002406

H -4.276809 -0.105497 1.016575

H -4.378515 -1.072790 -0.460526

H -4.184833 0.684206 -0.562494

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 64.5341 | 69.7866 | 86.0206 |
| 87.7087 | 112.8042 | 208.5106 |
| 242.034 | 248.4229 | 279.7677 |
| 404.3287 | 439.2814 | 472.2754 |
| 514.5803 | 549.3286 | 725.9904 |
| 773.4526 | 806.1686 | 851.1141 |
| 977.34 | 1042.557 | 1043.12 |
| 1058.236 | 1060.636 | 1065.297 |
| 1116.821 | 1219.266 | 1270.875 |
| 1324.015 | 1407.676 | 1417.135 |
| 1419.842 | 1426.383 | 1480.892 |
| 1484.602 | 1485.129 | 1486.299 |
| 1492.927 | 1498.07 | 1575.66 |
| 2255.682 | 3034.155 | 3043.212 |
| 3054.467 | 3090.281 | 3110.299 |
| 3118.54 | 3120.511 | 3138.713 |
| 3144.408 | 3161.255 | 3202.247 |

***i14***

C 0.290475 2.020952 -0.000012

C 1.495583 1.133209 0.000011

C 1.519855 -0.237544 0.000003

C 0.387100 -1.086043 -0.000011

C 2.859440 -0.945050 0.000001

C -3.563928 -0.137882 0.000001

C -2.147871 -0.473942 0.000013

C -0.961543 -0.721896 0.000004

H -0.341621 1.844215 0.876036

H 0.588231 3.070900 -0.000174

H -0.341775 1.843974 -0.875896

H 2.460490 1.632651 0.000034

H 0.577928 -2.156442 -0.000031

H 2.963558 -1.583989 -0.881904

H 2.963512 -1.584089 0.881839

H 3.686792 -0.233814 0.000062

H -4.063368 -0.546429 0.883052

H -4.062760 -0.543949 -0.884540

H -3.705663 0.946152 0.001465

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 38.7034 | 58.0788 | 85.7587 |
| 90.0574 | 120.4387 | 205.2971 |
| 247.2714 | 249.166 | 313.3354 |
| 355.116 | 440.7697 | 470.3567 |
| 492.08 | 571.1115 | 727.2087 |
| 756.1042 | 827.0024 | 869.5643 |
| 999.3428 | 1031.419 | 1044.242 |
| 1055.671 | 1064.386 | 1089.228 |
| 1107.07 | 1211.894 | 1238.24 |
| 1348.307 | 1394.642 | 1416.109 |
| 1418.753 | 1420.557 | 1480.333 |
| 1482.139 | 1484.034 | 1487.919 |
| 1490.743 | 1503.025 | 1581.369 |
| 2259.049 | 3035.691 | 3039.048 |
| 3043.356 | 3091.527 | 3107.074 |
| 3108.341 | 3114.092 | 3127.191 |
| 3135.611 | 3155.905 | 3167.057 |

***i15***

C -3.555834 0.100486 -0.012159

C -2.262985 -0.646031 0.003057

C -1.007704 -0.090441 0.007534

C 0.120561 -0.941286 0.008728

C -0.816172 1.407873 0.008976

C 4.006380 0.251784 -0.009528

C 2.611779 -0.166754 -0.001300

C 1.450843 -0.515407 0.005262

H -4.080689 -0.047513 -0.964094

H -4.227146 -0.263875 0.772740

H -3.422218 1.173890 0.129655

H -2.334075 -1.731338 -0.005372

H -0.051951 -2.014001 0.009759

H 0.242729 1.665641 -0.004413

H -1.262779 1.859064 0.899444

H -1.287914 1.864503 -0.865295

H 4.622987 -0.459202 -0.565677

H 4.403589 0.318117 1.007702

H 4.116259 1.233371 -0.477875

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.5974 | 64.5798 | 85.6599 |
| 89.2758 | 122.8289 | 192.8774 |
| 247.0468 | 268.7597 | 294.1518 |
| 386.5907 | 443.7115 | 448.1226 |
| 478.1843 | 608.9243 | 719.4954 |
| 792.9951 | 816.0392 | 837.0154 |
| 961.9144 | 1035.093 | 1045.125 |
| 1054.221 | 1057.417 | 1062.054 |
| 1125.472 | 1213.93 | 1240.324 |
| 1384.898 | 1414.034 | 1420.235 |
| 1426.165 | 1439.295 | 1477.153 |
| 1481.874 | 1485.725 | 1487.232 |
| 1503.867 | 1505.785 | 1551.549 |
| 2259.316 | 3028.604 | 3043.216 |
| 3054.317 | 3080.685 | 3110.245 |
| 3118.154 | 3120.007 | 3136.119 |
| 3149.584 | 3163.423 | 3174.757 |

***i16***

C -2.389506 1.739908 0.000062

C -1.159671 0.894326 -0.000008

C -1.121454 -0.478612 -0.000048

C 0.103572 -1.181178 0.000055

C -2.395714 -1.294445 -0.000199

C 3.792330 0.532294 -0.000264

C 2.468716 -0.074962 0.000562

C 1.369518 -0.581627 0.000270

H -2.409126 2.396806 -0.877408

H -3.309492 1.153517 0.000019

H -2.409122 2.396635 0.877666

H -0.209475 1.421364 -0.000085

H 0.078303 -2.266506 -0.000008

H -2.177641 -2.363537 -0.000425

H -3.005522 -1.079093 -0.882097

H -3.005499 -1.079460 0.881804

H 3.975468 1.070030 -0.934892

H 4.569092 -0.228481 0.109861

H 3.896268 1.244499 0.822989

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 31.9769 | 66.4275 | 82.3036 |
| 88.1229 | 128.8519 | 199.0461 |
| 238.9491 | 255.6298 | 309.5971 |
| 381.1779 | 446.9458 | 459.3498 |
| 484.3871 | 608.7245 | 715.539 |
| 797.4352 | 801.7105 | 847.9121 |
| 980.1294 | 1029.141 | 1038.007 |
| 1046.808 | 1056.918 | 1057.763 |
| 1146.674 | 1220.435 | 1256.575 |
| 1298.164 | 1408.959 | 1417.403 |
| 1421.294 | 1443.639 | 1480.114 |
| 1482.274 | 1483.444 | 1489.69 |
| 1500.68 | 1507.308 | 1562.146 |
| 2280.847 | 3023.874 | 3040.662 |
| 3046.518 | 3071.659 | 3109.044 |
| 3110.384 | 3117.515 | 3133.174 |
| 3136.228 | 3173.633 | 3176.081 |

***i17***

C 2.920394 0.065469 -0.000007

C 1.418933 0.061483 0.000005

C 0.690330 1.174779 -0.000003

C -0.811080 1.231544 0.000007

C -1.474332 -0.135643 0.000018

C -0.698980 -1.193118 0.000026

C 0.771528 -1.314573 -0.000006

C -2.977029 -0.165713 -0.000013

H 3.310992 -0.456830 0.880267

H 3.320348 1.081293 0.000034

H 3.310984 -0.456769 -0.880321

H 1.203612 2.133689 -0.000006

H -1.160773 1.800001 0.873504

H -1.160787 1.800000 -0.873486

H 1.118514 -1.878814 -0.875846

H 1.118549 -1.878853 0.875794

H -3.373117 0.350327 0.881339

H -3.353853 -1.188928 0.000432

H -3.373057 0.349517 -0.881872

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 63.7905 | 157.0146 | 163.0922 |
| 228.496 | 257.1797 | 270.3686 |
| 365.8184 | 417.3741 | 428.7065 |
| 447.5565 | 590.7947 | 704.3292 |
| 767.7063 | 801.4587 | 909.4865 |
| 935.8212 | 936.3204 | 960.0613 |
| 994.4407 | 1062.101 | 1072.815 |
| 1077.506 | 1123.276 | 1174.23 |
| 1199.091 | 1215.555 | 1216.587 |
| 1323.068 | 1363.285 | 1372.302 |
| 1410.612 | 1419.182 | 1473.308 |
| 1474.913 | 1479.788 | 1484.587 |
| 1492.874 | 1498.667 | 1769.293 |
| 1802.097 | 3007.385 | 3018.71 |
| 3030.135 | 3037.093 | 3038.79 |
| 3043.752 | 3094.272 | 3096.199 |
| 3135.078 | 3147.27 | 3166.344 |

***i18***

C -2.877528 0.043857 -0.000247

C -1.376171 0.071144 -0.000036

C -0.679012 1.202860 -0.000038

C 0.818323 1.291055 0.000287

C 1.529762 -0.047280 -0.000052

C 0.792456 -1.215705 -0.000046

C -0.698894 -1.273242 0.000313

C 2.916268 -0.064978 -0.000258

H -3.257642 -0.486902 -0.880318

H -3.299685 1.050560 -0.000384

H -3.257865 -0.486744 0.879824

H -1.212285 2.150832 -0.000233

H 1.147591 1.869995 -0.871717

H 1.147222 1.869309 0.872896

H -1.047754 -1.851087 0.870151

H -1.048169 -1.851809 -0.868860

H 3.461815 -1.001717 -0.000437

H 1.324639 -2.163014 -0.000233

H 3.490912 0.854309 -0.000224

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 32.6252 | 153.5709 | 189.199 |
| 245.8089 | 301.2721 | 395.0139 |
| 431.3302 | 433.3352 | 463.8853 |
| 536.5198 | 589.9348 | 721.328 |
| 732.991 | 766.1395 | 777.7106 |
| 815.7619 | 911.7521 | 947.6633 |
| 950.4064 | 984.1298 | 1004.267 |
| 1069.124 | 1084.533 | 1106.792 |
| 1177.612 | 1221.373 | 1239.392 |
| 1246.751 | 1339.659 | 1345.158 |
| 1414.246 | 1423.053 | 1432.475 |
| 1460.198 | 1474.305 | 1480.037 |
| 1487.803 | 1499.26 | 1527.05 |
| 1788.242 | 2990.066 | 3003.447 |
| 3026.46 | 3035.137 | 3051.372 |
| 3090.763 | 3135.365 | 3154.065 |
| 3164.311 | 3176.584 | 3253.121 |

***i19***

C -2.950150 -0.029540 0.000006

C -1.444129 0.008453 -0.000008

C -0.760122 1.181736 -0.000011

C 0.734660 1.252464 0.000006

C 1.421390 -0.081870 -0.000002

C 0.686374 -1.229521 -0.000002

C -0.724412 -1.220233 -0.000001

C 2.917452 -0.072511 0.000001

H -3.326172 -0.557698 -0.881343

H -3.375761 0.975720 -0.000199

H -3.326162 -0.557335 0.881578

H -1.301246 2.123479 -0.000021

H 1.083023 1.840363 -0.867336

H 1.083002 1.840336 0.867377

H 1.202403 -2.185722 -0.000005

H -1.268546 -2.158323 -0.000001

H 3.307051 0.454554 -0.879445

H 3.328985 -1.083778 -0.000011

H 3.307046 0.454531 0.879463

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 82.9468 | 93.9118 | 146.7413 |
| 223.5167 | 285.8258 | 293.3116 |
| 380.6338 | 439.5918 | 442.8224 |
| 556.0239 | 609.5425 | 722.5785 |
| 725.2389 | 771.15 | 795.8223 |
| 893.2767 | 940.3589 | 947.0813 |
| 988.6598 | 1018.376 | 1051.262 |
| 1064.275 | 1083.699 | 1132.562 |
| 1192.214 | 1201.929 | 1226.009 |
| 1324.471 | 1338.469 | 1378.562 |
| 1417.283 | 1419.706 | 1439.303 |
| 1449.111 | 1476.679 | 1483.867 |
| 1493.813 | 1502.522 | 1594.581 |
| 1655.192 | 2949.82 | 2951.659 |
| 3024.435 | 3048.341 | 3074.636 |
| 3111.26 | 3132.17 | 3137.908 |
| 3176.217 | 3180.537 | 3203.048 |

***i30***

C -2.487474 -0.952693 -0.209095

C -1.171384 -0.267632 -0.083352

C 0.015237 -1.041040 0.394640

C 1.336845 -0.401551 0.027613

C 1.352425 1.062609 -0.025456

C 0.242914 1.802209 0.002934

C -1.140074 1.220078 0.041835

C 2.436455 -1.120902 -0.201901

H -2.966310 -1.100032 0.773829

H -2.382910 -1.944017 -0.661054

H -3.186371 -0.370877 -0.817844

H -0.021905 -2.069967 0.023384

H -0.021213 -1.117714 1.498446

H 2.322653 1.545499 -0.098866

H -1.635960 1.539484 0.978273

H 0.319877 2.885117 -0.027567

H -1.744746 1.674330 -0.755471

H 3.383979 -0.643094 -0.428319

H 2.423254 -2.205201 -0.168118

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 79.4057 | 93.8658 | 176.1463 |
| 248.8528 | 300.3684 | 311.4142 |
| 412.4887 | 447.0551 | 479.0285 |
| 550.7268 | 665.3452 | 706.5412 |
| 792.0506 | 847.4082 | 871.1036 |
| 894.454 | 922.8413 | 936.2658 |
| 960.6553 | 1002.119 | 1009.902 |
| 1021.254 | 1028.195 | 1168.008 |
| 1187.315 | 1198.469 | 1241.474 |
| 1302.457 | 1334.236 | 1342.396 |
| 1401.6 | 1416.749 | 1430.599 |
| 1450.221 | 1459.394 | 1469.511 |
| 1487.737 | 1495.112 | 1700.63 |
| 1750.893 | 2919.809 | 2927.767 |
| 2962.281 | 3025.068 | 3060.466 |
| 3078.118 | 3108.928 | 3153.85 |
| 3168.558 | 3191.707 | 3240.987 |

***i31***

C -2.593336 -0.710666 -0.117123

C -1.230166 -0.114940 0.014043

C -0.118872 -1.014692 0.489701

C 1.242375 -0.509800 0.081965

C 1.468574 0.959801 0.335176

C 0.291513 1.781073 -0.107108

C -0.962258 1.218993 -0.251005

C 2.156511 -1.292155 -0.479182

H -2.920368 -1.162970 0.827817

H -2.601559 -1.513057 -0.865526

H -3.335267 0.034680 -0.410917

H -0.270732 -2.033292 0.118019

H -0.167766 -1.080958 1.589352

H 2.383658 1.294374 -0.161595

H 1.632160 1.115801 1.414054

H 0.441271 2.837581 -0.297092

H -1.781954 1.853862 -0.577921

H 3.126360 -0.905903 -0.776126

H 1.968149 -2.345803 -0.658865

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 96.4348 | 131.4849 | 180.1724 |
| 278.7265 | 316.9265 | 384.5447 |
| 435.6697 | 457.2317 | 477.6432 |
| 565.6806 | 655.0619 | 688.2445 |
| 740.3267 | 848.5894 | 888.4527 |
| 916.7675 | 938.4153 | 941.423 |
| 946.8391 | 991.9668 | 1010.85 |
| 1021.234 | 1041.957 | 1159.928 |
| 1176.765 | 1209.453 | 1239.146 |
| 1305.14 | 1314.646 | 1352.852 |
| 1358.19 | 1421.729 | 1453.239 |
| 1463.859 | 1477.486 | 1481.182 |
| 1483.851 | 1490.352 | 1527.517 |
| 1755.176 | 2976.726 | 2981.521 |
| 3016.765 | 3064.256 | 3076.174 |
| 3088.244 | 3129.688 | 3148.2 |
| 3167.114 | 3205.381 | 3233.558 |

***i32***

C 2.228030 -1.105781 0.519544

C 1.259958 -0.388108 -0.447879

C -0.123747 -0.958546 -0.342887

C -1.223181 -0.223433 -0.029867

C -1.092062 1.177006 0.193013

C 0.168234 1.803104 0.080226

C 1.285889 1.094575 -0.231066

C -2.586964 -0.853125 0.086298

H 2.242174 -2.181775 0.324855

H 1.914401 -0.945959 1.554034

H 3.246137 -0.723800 0.403391

H -0.223366 -2.027762 -0.513165

H 1.639685 -0.593221 -1.464061

H -1.968973 1.763433 0.444135

H 0.240769 2.873479 0.244518

H 2.246792 1.593424 -0.312977

H -2.998449 -0.706450 1.089433

H -2.549813 -1.925873 -0.111986

H -3.286300 -0.399656 -0.622476

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 85.9816 | 114.2778 | 174.0151 |
| 248.4061 | 288.2139 | 358.7597 |
| 417.4039 | 469.5766 | 503.6676 |
| 560.7307 | 615.7196 | 701.1058 |
| 749.3744 | 787.3221 | 818.1258 |
| 874.4487 | 955.449 | 970.7935 |
| 982.4908 | 1004.982 | 1056.894 |
| 1065.063 | 1077.435 | 1095.725 |
| 1144.149 | 1189.234 | 1212.73 |
| 1289.56 | 1329.652 | 1337.855 |
| 1378.729 | 1401.469 | 1420.146 |
| 1449.491 | 1488.381 | 1496.472 |
| 1501.277 | 1503.436 | 1583.228 |
| 1641.794 | 2944.394 | 3038.905 |
| 3041.423 | 3105.163 | 3118.466 |
| 3127.024 | 3132.417 | 3161.83 |
| 3170.182 | 3186.214 | 3201.231 |

***i33***

C 2.275786 -0.980177 0.528621

C 1.260316 -0.356644 -0.447559

C -0.076138 -1.020382 -0.328735

C -1.262313 -0.378756 -0.025038

C -1.277052 1.119996 0.205295

C 0.059596 1.779910 0.047536

C 1.177996 1.131260 -0.249470

C -2.456834 -1.075926 0.074912

H 2.375645 -2.055297 0.355842

H 1.952535 -0.825460 1.561240

H 3.262342 -0.524128 0.405019

H -0.100772 -2.096304 -0.486164

H 1.644521 -0.542038 -1.462809

H -1.667607 1.324655 1.209804

H -1.993849 1.582090 -0.484671

H 0.087597 2.856960 0.188124

H 2.110366 1.681783 -0.346613

H -3.386556 -0.570153 0.309672

H -2.492370 -2.147788 -0.082815

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 70.0778 | 132.5585 | 261.2191 |
| 274.4211 | 343.7674 | 408.6712 |
| 469.8981 | 481.3361 | 507.3989 |
| 545.5132 | 575.3951 | 717.878 |
| 752.0301 | 761.0988 | 809.9405 |
| 861.4819 | 921.8451 | 932.5121 |
| 974.5356 | 1014.088 | 1019.47 |
| 1030.787 | 1057.279 | 1086.44 |
| 1158.529 | 1203.358 | 1236.833 |
| 1244.765 | 1311.143 | 1334.889 |
| 1376.46 | 1408.355 | 1426.379 |
| 1431.08 | 1471.692 | 1479.916 |
| 1502.55 | 1508.33 | 1525.162 |
| 1765.876 | 2988.375 | 3032.529 |
| 3041.537 | 3058.611 | 3117.334 |
| 3129.72 | 3156.438 | 3161.912 |
| 3165.402 | 3186.702 | 3254.86 |

***i34***

C 2.570450 -1.014346 0.010424

C 1.259348 -0.286741 -0.011609

C 0.026741 -0.985166 -0.008752

C -1.183887 -0.361273 -0.000416

C -1.273442 1.138380 0.010120

C 0.055862 1.825036 -0.000581

C 1.221995 1.135573 -0.009302

C -2.479494 -1.109809 -0.000479

H 2.436884 -2.082559 -0.173900

H 3.070146 -0.905901 0.980812

H 3.257644 -0.624536 -0.747730

H 0.052278 -2.072770 -0.015069

H -1.860856 1.464059 0.886788

H -1.880307 1.475017 -0.848612

H 0.062994 2.910037 -0.001648

H 2.163158 1.678907 -0.016144

H -2.323402 -2.190336 -0.010600

H -3.077502 -0.858476 0.884247

H -3.086482 -0.843372 -0.874578

**Frequencies**

|  |  |  |
| --- | --- | --- |
| 102.931 | 116.0062 | 130.0723 |
| 194.7818 | 276.2467 | 301.8438 |
| 399.9382 | 430.1645 | 486.0878 |
| 532.3924 | 548.824 | 693.2966 |
| 715.9051 | 871.9445 | 880.193 |
| 929.3859 | 940.6525 | 971.4278 |
| 994.484 | 1006.453 | 1033.661 |
| 1045.747 | 1051.247 | 1162.291 |
| 1191.543 | 1205.092 | 1260.657 |
| 1282.746 | 1335.71 | 1420.465 |
| 1425.24 | 1435.637 | 1447.421 |
| 1455.954 | 1476.691 | 1491.096 |
| 1493.807 | 1500.359 | 1557.749 |
| 1650.739 | 2946.638 | 2951.201 |
| 3015.827 | 3023.499 | 3065.289 |
| 3079.909 | 3126.291 | 3130.617 |
| 3164.143 | 3172.125 | 3199.686 |

***i35***

C -2.457205 -0.960788 0.105921

C -1.193820 -0.238687 -0.359256

C 0.049324 -1.030566 -0.079215

C 1.307678 -0.424675 -0.014947

C 1.356465 1.047522 -0.122276

C 0.257709 1.791720 -0.003278

C -1.088735 1.168588 0.244280

C 2.472462 -1.145733 0.145095

H -2.437213 -1.113060 1.189467

H -2.549012 -1.940527 -0.370883

H -3.352344 -0.382517 -0.139219

H -1.258949 -0.114521 -1.453852

H -0.023900 -2.112803 -0.015885

H 2.326857 1.511647 -0.267978

H 0.326468 2.874336 -0.042919

H -1.258229 1.109818 1.329809

H -1.885397 1.802037 -0.156898

H 3.436644 -0.653350 0.191299

H 2.451802 -2.225341 0.239112

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 127.6151 | 147.4309 | 270.0247 |
| 276.5751 | 323.4568 | 396.2373 |
| 447.3198 | 454.8029 | 532.2385 |
| 556.053 | 596.9184 | 691.1269 |
| 712.68 | 765.9744 | 801.267 |
| 877.1029 | 892.9122 | 934.0126 |
| 957.6913 | 1007.516 | 1019.353 |
| 1028.981 | 1077.428 | 1109.683 |
| 1182.438 | 1193.827 | 1238.738 |
| 1274.452 | 1314.286 | 1337.99 |
| 1361.483 | 1374.36 | 1413.272 |
| 1450.093 | 1452.656 | 1484.685 |
| 1503.243 | 1512.218 | 1526.815 |
| 1726.102 | 2959.792 | 3010.96 |
| 3040.424 | 3090.278 | 3117.557 |
| 3118.17 | 3159.723 | 3172.25 |
| 3173.394 | 3196.149 | 3258.09 |

***i36***

C 2.513751 -0.845407 0.070056

C 1.168409 -0.266756 -0.365270

C 0.000821 -1.016121 0.288685

C -1.341075 -0.361894 0.035953

C -1.351472 1.066167 0.054098

C -0.151308 1.803890 0.095949

C 1.063436 1.205792 -0.078087

C -2.468372 -1.090032 -0.134566

H 2.580614 -1.909749 -0.171391

H 2.649131 -0.733807 1.150399

H 3.342929 -0.334847 -0.427643

H 0.169344 -1.025312 1.374545

H -0.013436 -2.058013 -0.042450

H -2.304744 1.583617 0.035868

H -0.204232 2.880202 0.226282

H 1.079905 -0.391843 -1.456527

H 1.972674 1.799354 -0.079264

H -3.431080 -0.609278 -0.271519

H -2.446246 -2.174157 -0.139219

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 123.6878 | 140.5176 | 262.392 |
| 281.3956 | 344.6476 | 413.5174 |
| 437.7204 | 496.6413 | 525.7228 |
| 552.8468 | 642.6765 | 701.9464 |
| 743.8607 | 796.0961 | 865.1197 |
| 874.0613 | 890.187 | 949.4998 |
| 967.8399 | 979.8493 | 993.9248 |
| 1071.376 | 1099.735 | 1118.821 |
| 1149.161 | 1188.727 | 1219.487 |
| 1301.937 | 1315.957 | 1332.218 |
| 1358.393 | 1382.296 | 1419.134 |
| 1443.94 | 1447.65 | 1469.76 |
| 1506.01 | 1509.943 | 1556.341 |
| 1607.761 | 2979.765 | 3027.321 |
| 3039.289 | 3096.958 | 3113.457 |
| 3120.573 | 3151.993 | 3171.924 |
| 3189.054 | 3205.065 | 3245.125 |

***i37***

C 2.663558 -0.064848 0.570994

C 1.444436 0.063263 -0.355279

C 0.611202 1.252516 -0.011429

C -0.849291 1.258680 -0.306130

C -1.513095 -0.059751 0.034632

C -0.684377 -1.255250 -0.142435

C 0.633115 -1.206786 -0.346785

C -2.782226 -0.138205 0.436407

H 2.341715 -0.221966 1.603667

H 3.271934 0.842901 0.535081

H 3.294924 -0.907224 0.274737

H 1.110961 2.181417 0.242179

H -1.351110 2.082442 0.207454

H -1.005349 1.431649 -1.387151

H -1.188213 -2.216811 -0.099821

H 1.838149 0.188200 -1.382247

H 1.187059 -2.131519 -0.487822

H -3.248701 -1.096015 0.642388

H -3.391305 0.749215 0.571686

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 61.9599 | 131.7195 | 233.4363 |
| 259.4158 | 311.59 | 353.5711 |
| 403.8179 | 426.1038 | 510.4969 |
| 525.0636 | 614.1826 | 706.6455 |
| 761.5595 | 791.0572 | 824.2863 |
| 879.2005 | 922.2864 | 929.4553 |
| 966.1975 | 988.8026 | 1013.412 |
| 1030.047 | 1083.365 | 1099.876 |
| 1147.115 | 1196.878 | 1211.716 |
| 1295.182 | 1314.052 | 1328.387 |
| 1352.698 | 1398.606 | 1408.774 |
| 1420.952 | 1456.891 | 1468.878 |
| 1501.252 | 1503.6 | 1698.089 |
| 1748.808 | 2917.162 | 2930.569 |
| 3040.645 | 3091.397 | 3118.545 |
| 3124.713 | 3147.072 | 3157.448 |
| 3181.18 | 3186.243 | 3234.597 |

***i38***

C 2.866730 -0.000494 0.300109

C 1.394975 0.001182 0.015549

C 0.670739 -1.215045 -0.107905

C -0.669020 -1.242660 -0.319999

C -1.505664 -0.000168 -0.407735

C -0.669998 1.242916 -0.319723

C 0.670304 1.216204 -0.107456

C -2.614640 -0.000836 0.668238

H 3.359340 -0.866511 -0.150258

H 3.063841 -0.040511 1.378963

H 3.348700 0.902211 -0.084055

H 1.216349 -2.152130 -0.035509

H -2.026025 -0.000365 -1.380887

H -1.184231 -2.193966 -0.414884

H -1.185813 2.193897 -0.414342

H 1.215021 2.153742 -0.034685

H -3.247969 -0.887137 0.570981

H -3.248671 0.884985 0.571277

H -2.171095 -0.000811 1.666928

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 31.3531 | 67.0681 | 218.4332 |
| 238.7979 | 269.1787 | 350.0759 |
| 389.2727 | 439.6859 | 492.4607 |
| 613.7858 | 633.2436 | 745.8777 |
| 751.856 | 759.4227 | 807.2247 |
| 942.67 | 968.0922 | 976.7075 |
| 980.931 | 995.0394 | 1036.044 |
| 1041.721 | 1073.794 | 1110.352 |
| 1184.519 | 1200.422 | 1255.272 |
| 1276.983 | 1297.552 | 1348.657 |
| 1401.23 | 1418.161 | 1418.94 |
| 1480.531 | 1487.227 | 1489.014 |
| 1498.052 | 1503.548 | 1546.347 |
| 1637.582 | 2950.033 | 3019.086 |
| 3038.366 | 3085.106 | 3118.126 |
| 3120.922 | 3126.315 | 3160.648 |
| 3161.73 | 3181.766 | 3185.399 |

***i39***

C -2.872757 0.056986 -0.158564

C -1.533116 0.064643 0.032183

C -0.765388 -1.201169 0.349787

C 0.631466 -1.204519 -0.274855

C 1.366386 0.084741 -0.023737

C 0.645012 1.241818 0.088285

C -0.762061 1.265952 0.015104

C 2.860452 0.049941 -0.006437

H -3.442563 -0.865196 -0.132753

H -1.330222 -2.081757 0.035029

H -3.417254 0.977304 -0.340933

H -0.656833 -1.259986 1.440250

H 1.209213 -2.052604 0.106266

H 0.552068 -1.351188 -1.362630

H 1.174592 2.185341 0.189313

H -1.278642 2.217502 -0.053186

H 3.228059 -0.580079 0.812337

H 3.290818 1.046687 0.109957

H 3.250796 -0.386382 -0.934247

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 98.766 | 174.162 | 178.868 |
| 297.0049 | 316.6259 | 378.5171 |
| 420.9092 | 442.2269 | 523.253 |
| 570.3798 | 656.4859 | 729.1508 |
| 772.2143 | 776.4198 | 792.3128 |
| 865.6486 | 918.1024 | 943.8353 |
| 971.1904 | 1007.506 | 1021.067 |
| 1051.36 | 1067.015 | 1123.081 |
| 1191.83 | 1204.74 | 1243.794 |
| 1315.76 | 1343.087 | 1363.326 |
| 1371.346 | 1419.269 | 1432.643 |
| 1451.421 | 1475.03 | 1482.619 |
| 1487.38 | 1492.814 | 1566.819 |
| 1613.2 | 3002.288 | 3021.155 |
| 3034.697 | 3072.772 | 3081.711 |
| 3103.836 | 3125.281 | 3152.584 |
| 3172.046 | 3197.634 | 3245.294 |

***i68***

C 1.116717 -0.943323 1.016349

C 0.318192 -0.823835 -0.254107

C -3.630429 0.263894 -0.123121

C -2.225788 -0.125761 -0.169021

C -1.068844 -0.448162 -0.209455

C 1.432770 0.201341 0.066420

C 1.049313 1.553611 0.451373

C 2.697461 0.082740 -0.759303

H 0.608593 -0.698774 1.940938

H 1.839101 -1.749158 1.084182

H 0.573965 -1.520908 -1.046058

H -3.796250 1.020962 0.647682

H -4.268357 -0.593860 0.104912

H -3.952390 0.682472 -1.080018

H 1.676839 2.394274 0.184330

H 0.111397 1.739350 0.958651

H 3.552171 0.488306 -0.210229

H 2.599881 0.634349 -1.698349

H 2.918703 -0.960042 -1.000848

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 89.6418 | 93.1368 | 102.7952 |
| 182.4453 | 210.8472 | 250.0674 |
| 264.3337 | 336.8315 | 374.0059 |
| 381.7653 | 408.7911 | 486.927 |
| 529.5634 | 564.0217 | 716.468 |
| 736.2403 | 799.0308 | 932.2291 |
| 939.7564 | 949.3797 | 985.1335 |
| 1051.539 | 1053.718 | 1056.241 |
| 1072.874 | 1104.281 | 1122.04 |
| 1218.955 | 1286.946 | 1334.092 |
| 1404.008 | 1416.104 | 1430.14 |
| 1465.472 | 1485.011 | 1487.546 |
| 1489.592 | 1500.212 | 1509.636 |
| 2392.8 | 3044.392 | 3046.888 |
| 3117.404 | 3120.045 | 3120.302 |
| 3123.219 | 3144.059 | 3165.754 |
| 3167.782 | 3242.562 | 3276.098 |

***i69***

C -0.882805 2.029523 -0.000115

C -0.464773 0.584063 -0.000523

C 3.518836 -0.236136 0.000639

C 2.092010 0.053184 -0.000357

C 0.902437 0.290796 -0.000714

C -1.428552 -0.474914 -0.000060

C -2.763793 -0.222226 0.000858

C -0.924841 -1.897568 -0.000456

H -0.011628 2.683912 -0.001109

H -1.487034 2.264250 0.883001

H -1.489099 2.264266 -0.881792

H 3.697796 -1.311762 0.072059

H 4.014059 0.247322 0.847462

H 3.991761 0.127229 -0.916176

H -3.482647 -1.033182 0.001277

H -3.163613 0.784327 0.001288

H -1.754233 -2.606344 -0.000254

H -0.302939 -2.090296 0.878050

H -0.303539 -2.090049 -0.879434

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 40.129 | 71.4481 | 93.8393 |
| 125.8713 | 152.882 | 174.9158 |
| 273.1527 | 286.7731 | 328.1529 |
| 424.1345 | 436.1929 | 437.669 |
| 550.3512 | 593.4978 | 643.0224 |
| 653.7907 | 854.1958 | 872.9141 |
| 967.1359 | 1018.856 | 1022.352 |
| 1045.887 | 1052.045 | 1062.93 |
| 1064.522 | 1166.984 | 1345.335 |
| 1356.536 | 1395.999 | 1409.469 |
| 1426.39 | 1437.057 | 1479.94 |
| 1485.906 | 1486.712 | 1489.38 |
| 1495.139 | 1502.627 | 1585.819 |
| 2245.934 | 3030.376 | 3044.376 |
| 3053.966 | 3086.672 | 3111.085 |
| 3118.196 | 3123.302 | 3145.611 |
| 3148.55 | 3172.812 | 3261.649 |

***Transition states***

***i4 – p23***

C 0.383556 -0.988528 0.741919

C -0.763990 -0.012557 0.568116

C 3.959812 0.635537 -0.510913

C 2.697998 0.056069 -0.064135

C 1.659956 -0.425439 0.298903

C -1.836473 -0.314415 -0.121603

C -2.624221 -1.082719 -0.874622

H 0.167780 -1.906997 0.190192

H 0.465294 -1.262307 1.800630

H -0.647752 0.954865 1.042841

H 4.625920 0.823033 0.334949

H 3.790218 1.584733 -1.025338

H 4.472588 -0.036564 -1.203487

H -3.409340 -1.682979 -0.426440

H -2.603528 -1.004977 -1.956824

C -3.050661 1.647716 0.104725

H -3.968566 1.472518 -0.442052

H -2.327814 2.311113 -0.354675

H -3.120665 1.653584 1.185865

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -524.882 | 23.1781 | 36.0978 |
| 45.907 | 83.8396 | 125.6289 |
| 174.7322 | 199.2855 | 238.273 |
| 300.4985 | 321.2879 | 398.3154 |
| 440.5207 | 466.5085 | 482.4191 |
| 524.2345 | 562.1733 | 773.0305 |
| 797.912 | 845.1525 | 869.192 |
| 932.4045 | 1025.18 | 1032.627 |
| 1058.86 | 1059.967 | 1116.962 |
| 1173.314 | 1226.303 | 1312.902 |
| 1377.229 | 1419.662 | 1420.275 |
| 1429.381 | 1465.667 | 1472.211 |
| 1486.013 | 1486.377 | 1947.524 |
| 2394.213 | 3038.418 | 3046.586 |
| 3099.203 | 3099.804 | 3119.011 |
| 3119.932 | 3138.218 | 3194.978 |
| 3225.866 | 3268.168 | 3268.881 |

***i4 – p4b***

C 0.255849 -0.562427 -0.218396

C -0.730317 0.281849 0.169483

C 4.232132 0.341533 0.038179

C 2.813321 0.022433 -0.047805

C 1.641548 -0.241606 -0.111509

C -2.165739 0.029673 0.027581

C -2.678960 -1.204660 0.000637

C -3.035330 1.258633 -0.048725

H 0.006093 -1.444855 -0.800665

H 0.170641 -1.911305 1.323888

H -0.442404 1.226227 0.624959

H 4.684843 -0.137785 0.910089

H 4.383287 1.419948 0.128420

H 4.762492 -0.003964 -0.852575

H -3.744752 -1.365565 -0.117612

H -2.056568 -2.084473 0.121351

H -4.088927 0.997119 -0.156784

H -2.746618 1.889214 -0.895198

H -2.923117 1.862874 0.857458

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -729.82 | 51.4711 | 79.3246 |
| 84.1694 | 104.7347 | 160.2956 |
| 219.2751 | 239.0138 | 308.8992 |
| 333.2526 | 348.7458 | 395.8244 |
| 446.6108 | 515.839 | 530.3522 |
| 538.9378 | 705.695 | 808.8473 |
| 891.2799 | 914.1334 | 934.5635 |
| 986.2355 | 1005.404 | 1033.058 |
| 1057.037 | 1062.953 | 1072.805 |
| 1199.636 | 1251.136 | 1309.968 |
| 1352.959 | 1415.205 | 1424.917 |
| 1446.935 | 1483.764 | 1487.596 |
| 1487.903 | 1498.591 | 1626.718 |
| 1709.567 | 2378.019 | 3043.752 |
| 3051.578 | 3104.819 | 3123.344 |
| 3126.731 | 3145.434 | 3161.124 |
| 3169.223 | 3177.74 | 3249.524 |

***i11 – p36***

C -3.125400 -1.065683 -0.648438

C -2.186149 -0.312991 -0.142757

C -1.078688 0.352103 0.128646

C -0.056765 -0.237973 1.083702

C -0.852488 1.756592 -0.352102

C 3.727780 -0.302762 -0.550159

C 2.390825 -0.277021 0.032516

C 1.291435 -0.262801 0.514598

H -4.101648 -1.156921 -0.188518

H -2.935989 -1.624501 -1.560303

H -3.118558 0.349994 1.495891

H -0.049151 0.361610 2.003563

H -0.359060 -1.248922 1.366692

H -0.847092 2.451395 0.495608

H -1.627552 2.067807 -1.051910

H 0.123057 1.830008 -0.841244

H 3.808142 -1.087895 -1.305869

H 4.482471 -0.491426 0.217252

H 3.962075 0.652065 -1.027197

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -704.657 | 34.575 | 89.2646 |
| 101.4763 | 102.5042 | 179.4779 |
| 185.1878 | 204.6773 | 250.9511 |
| 301.4917 | 352.1747 | 397.5136 |
| 458.751 | 480.6688 | 549.3136 |
| 595.8821 | 668.4907 | 782.3708 |
| 788.7337 | 913.2074 | 920.776 |
| 1010.46 | 1028.73 | 1056.378 |
| 1060.335 | 1065.26 | 1170.315 |
| 1193.616 | 1235.217 | 1303.704 |
| 1359.561 | 1412.43 | 1424.204 |
| 1464.721 | 1476.392 | 1484.701 |
| 1490.011 | 1494.878 | 1510.306 |
| 2021.935 | 2397.095 | 3029.333 |
| 3040.248 | 3051.225 | 3105.759 |
| 3107.857 | 3122.95 | 3125.746 |
| 3147.32 | 3158.398 | 3236.924 |

***i11 – p7a***

C -3.525503 0.089437 -0.109800

C -2.384911 -0.604743 -0.115319

C -1.047280 -0.035666 -0.009493

C 0.019174 -0.885014 0.001307

C -0.889322 1.447064 0.128773

C 3.944819 0.241465 -0.090402

C 2.542199 -0.150205 -0.052897

C 1.383654 -0.473319 -0.016106

H -4.482834 -0.410481 -0.195608

H -3.544088 1.170203 -0.020477

H -2.432477 -1.687849 -0.203545

H -0.160021 -1.943449 -0.166102

H 0.162070 1.727897 0.180142

H -1.389090 1.801833 1.036121

H -1.348118 1.964074 -0.719670

H 4.117228 0.998875 -0.859373

H 4.581158 -0.618671 -0.311936

H 4.257889 0.657331 0.870785

H -0.018694 -1.433884 1.973290

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -704.823 | 71.4255 | 85.0857 |
| 94.0716 | 151.5305 | 165.9834 |
| 231.1752 | 252.4304 | 297.769 |
| 302.7745 | 336.3613 | 395.6933 |
| 437.6017 | 452.9303 | 536.9052 |
| 597.3534 | 699.8729 | 821.9496 |
| 836.7278 | 936.7372 | 950.4037 |
| 991.1049 | 1032.49 | 1050.887 |
| 1052.84 | 1059.991 | 1086.407 |
| 1210.51 | 1243.718 | 1333.426 |
| 1383.279 | 1411.676 | 1432.443 |
| 1454.098 | 1481.384 | 1487.669 |
| 1487.812 | 1493.842 | 1613.317 |
| 1689.621 | 2374.533 | 3046.128 |
| 3048.384 | 3105.383 | 3118.933 |
| 3124.808 | 3157.984 | 3158.423 |
| 3170.009 | 3173.4 | 3253.396 |

***i3 – p23***

C -0.063821 -1.307824 0.477250

C 0.973988 -0.908148 -0.544928

C 2.054940 -0.190597 -0.241030

C 3.331343 0.024102 -0.032306

C -3.676713 0.561079 -0.208278

C -2.402848 -0.104615 0.040381

C -1.355369 -0.653183 0.249871

H 0.298888 -1.069267 1.480708

H -0.206240 -2.394349 0.440982

H 0.731314 -1.077113 -1.590571

H 3.743832 1.013769 0.117684

H 4.015834 -0.818666 0.000200

H -4.425901 -0.149906 -0.565211

H -3.565027 1.343030 -0.963513

H -4.057632 1.025128 0.704825

C 1.164106 1.898037 0.203464

H 1.581039 2.054651 1.191279

H 0.093666 1.744086 0.140236

H 1.636467 2.415531 -0.623169

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -561.957 | 31.5615 | 34.2126 |
| 56.4336 | 91.9255 | 126.9622 |
| 181.2839 | 216.5675 | 249.7489 |
| 286.4341 | 333.6092 | 399.6932 |
| 449.3654 | 479.7481 | 545.1901 |
| 572.4651 | 584.6761 | 775.9255 |
| 817.9212 | 844.4237 | 893.0862 |
| 908.7114 | 1018.107 | 1028.217 |
| 1059.345 | 1060.1 | 1129.648 |
| 1169.973 | 1225.143 | 1307.288 |
| 1383.471 | 1417.606 | 1420.587 |
| 1431.37 | 1469.089 | 1479.809 |
| 1486.016 | 1486.577 | 1937.852 |
| 2391.046 | 3039.56 | 3047.416 |
| 3094.835 | 3096.081 | 3119.937 |
| 3121.113 | 3143.605 | 3167.084 |
| 3235.989 | 3263.999 | 3265.711 |

***i3 – p4a***

C 0.214521 -0.511480 0.012550

C -0.732948 0.460508 0.034019

C -2.167077 0.224855 -0.029929

C -3.010035 1.265912 0.016496

C -2.663044 -1.191645 -0.134634

C 4.227201 0.252158 -0.067516

C 2.795252 -0.013807 -0.036465

C 1.612641 -0.231298 -0.004032

H -0.068826 -1.541694 -0.180376

H 0.078819 -1.178902 1.934926

H -0.409596 1.491897 0.140832

H -4.084568 1.128382 -0.029084

H -2.643222 2.283492 0.100245

H -3.752882 -1.225063 -0.155146

H -2.315667 -1.785617 0.716934

H -2.289073 -1.672645 -1.043741

H 4.781478 -0.556853 0.414622

H 4.459751 1.183487 0.454489

H 4.584719 0.342302 -1.096629

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -738.138 | 51.6053 | 80.6083 |
| 81.8326 | 140.2837 | 213.9521 |
| 222.6907 | 227.9622 | 303.9014 |
| 332.506 | 377.3573 | 412.9783 |
| 455.7929 | 499.4519 | 534.9834 |
| 537.6267 | 704.048 | 819.7433 |
| 872.7091 | 894.5095 | 931.913 |
| 997.7217 | 1000.326 | 1045.426 |
| 1050.351 | 1056.558 | 1070.973 |
| 1207.071 | 1288.507 | 1310.328 |
| 1349.285 | 1413.788 | 1418.245 |
| 1449.626 | 1481.304 | 1486.164 |
| 1486.721 | 1504.927 | 1617.662 |
| 1687.233 | 2376.425 | 3045.211 |
| 3050.834 | 3107.324 | 3121.899 |
| 3126.866 | 3146.821 | 3157.571 |
| 3183.381 | 3191.311 | 3248.071 |

***i2 – i1***

C 0.082894 1.429322 0.998591

C -0.508883 0.832143 -0.245360

C -1.626572 -0.171246 -0.138480

C -2.680834 -0.075577 -0.942579

C -1.486640 -1.256672 0.890133

C 3.350273 -0.588351 -0.239281

C 1.958078 -0.200671 -0.434606

C 0.859149 0.335176 -0.261449

H 0.463309 2.440283 0.972925

H -0.026163 0.928113 1.949576

H -0.702768 1.567820 -1.026079

H -3.496223 -0.789272 -0.890836

H -2.762759 0.714832 -1.681426

H -2.294000 -1.984942 0.803332

H -1.512668 -0.841662 1.902762

H -0.530416 -1.775154 0.775172

H 3.772771 -0.122450 0.659363

H 3.962106 -0.289797 -1.094810

H 3.442015 -1.672517 -0.131787

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -701.408 | 47.6671 | 89.1969 |
| 109.3249 | 133.4152 | 183.1116 |
| 239.9172 | 281.4139 | 349.7103 |
| 381.0386 | 425.6427 | 470.0384 |
| 537.1517 | 618.3779 | 674.9309 |
| 719.9661 | 783.1061 | 817.6419 |
| 945.4904 | 948.451 | 1006.605 |
| 1034.251 | 1056.018 | 1064.238 |
| 1075.613 | 1093.52 | 1180.812 |
| 1224.869 | 1311.519 | 1347.088 |
| 1414.1 | 1418.4 | 1445.464 |
| 1463.448 | 1480.92 | 1482.66 |
| 1488.43 | 1504.547 | 1746.288 |
| 2093.87 | 3021.843 | 3048.979 |
| 3090.699 | 3111.609 | 3112.647 |
| 3113.413 | 3144.625 | 3152.517 |
| 3180.085 | 3238.78 | 3300.162 |

***i12 – p7b***

C -3.131748 -1.024745 0.106434

C -2.515525 0.109439 -0.227262

C -1.081638 0.381964 -0.086813

C -0.166314 -0.620042 -0.166164

C -0.698814 1.807345 0.178028

C 3.886402 -0.131602 0.008157

C 2.439651 -0.293378 -0.050784

C 1.244717 -0.429224 -0.091428

H -4.199521 -1.143277 -0.035672

H -2.596308 -1.857882 0.550283

H -3.113407 0.937617 -0.603697

H -0.426355 -1.402648 1.732656

H -0.497871 -1.605020 -0.479756

H 0.382733 1.938323 0.203861

H -1.114765 2.141036 1.134812

H -1.113000 2.461449 -0.596473

H 4.307936 -0.011609 -0.993351

H 4.354001 -1.005099 0.469311

H 4.156168 0.748563 0.597019

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -633.268 | 72.3244 | 82.1737 |
| 94.3808 | 107.3674 | 136.4271 |
| 236.8147 | 244.0919 | 285.369 |
| 287.8809 | 355.9344 | 398.1012 |
| 426.3269 | 512.0417 | 535.8708 |
| 557.8188 | 697.2862 | 818.3842 |
| 846.7278 | 918.6349 | 968.386 |
| 1008.021 | 1034.344 | 1045.698 |
| 1058.158 | 1061.707 | 1082.442 |
| 1199.381 | 1247.272 | 1320.376 |
| 1359.071 | 1414.667 | 1423.422 |
| 1464.587 | 1483.286 | 1484.842 |
| 1485.042 | 1489.867 | 1624.565 |
| 1706.79 | 2374.317 | 3039.961 |
| 3047.227 | 3097.878 | 3117.138 |
| 3123.702 | 3153.044 | 3157.3 |
| 3163.865 | 3185.248 | 3249.64 |

***i2 – p21***

C 0.121380 1.777412 0.278875

C -0.486360 0.683930 -0.600192

C -1.533344 -0.252255 -0.102165

C -2.453691 -0.722285 -0.941226

C -1.499556 -0.640558 1.349907

C 3.080314 -0.827660 -0.011088

C 1.997383 -0.080885 -0.038231

C 0.914774 0.599808 -0.103210

H 0.351540 2.724854 -0.196666

H -0.202851 1.849309 1.311752

H -0.580121 0.943931 -1.650889

H -3.220441 -1.413135 -0.608250

H -2.468230 -0.434883 -1.987254

H -2.243764 -1.408319 1.563721

H -1.709611 0.220101 1.993095

H -0.513722 -1.023749 1.629088

H 3.887179 -0.661910 -0.716567

H 3.262056 -1.513278 0.809395

H 2.592573 -2.507953 -1.143443

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -546.244 | 41.9363 | 81.1754 |
| 159.3043 | 187.4334 | 195.6447 |
| 271.6711 | 289.4926 | 319.1018 |
| 394.2563 | 411.7304 | 477.5827 |
| 522.1399 | 594.8356 | 652.0954 |
| 683.1569 | 749.1173 | 790.8776 |
| 901.2393 | 927.8465 | 931.7804 |
| 940.6602 | 978.393 | 1012.33 |
| 1029.487 | 1059.362 | 1067.247 |
| 1076.282 | 1077.876 | 1120.855 |
| 1310.209 | 1330.788 | 1384.991 |
| 1420.999 | 1455.298 | 1465.145 |
| 1491.181 | 1506.385 | 1531.509 |
| 1737.921 | 2103.776 | 3043.327 |
| 3105.628 | 3130.94 | 3143.472 |
| 3146.638 | 3149.816 | 3155.291 |
| 3220.386 | 3232.531 | 3236.912 |

***i3 – i2***

C 0.060829 1.838201 -0.192079

C -0.523554 0.588627 -0.791292

C -1.445108 -0.300621 -0.107956

C -2.050335 -1.298731 -0.775137

C -1.688746 -0.083279 1.362792

C 2.773192 -1.181677 0.145242

C 2.062898 0.096957 0.170955

C 1.059019 0.799435 -0.064749

H 0.282736 2.642113 -0.890417

H -0.382099 2.196937 0.734673

H -0.420297 0.476114 -1.864073

H -2.734347 -1.976607 -0.277622

H -1.879294 -1.454505 -1.835055

H -2.322336 -0.870322 1.773068

H -2.183551 0.876837 1.540755

H -0.745095 -0.075211 1.917102

H 3.629863 -1.136608 -0.532531

H 2.112500 -1.991381 -0.189802

H 3.152749 -1.440843 1.137251

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -698.816 | 55.4511 | 64.1783 |
| 77.7788 | 164.8181 | 206.8121 |
| 217.9118 | 297.4839 | 378.7437 |
| 407.6049 | 436.4949 | 513.5577 |
| 538.9123 | 694.8245 | 711.4371 |
| 789.3757 | 840.8337 | 889.6471 |
| 947.6647 | 1002.365 | 1026.831 |
| 1035.616 | 1059.455 | 1072.511 |
| 1090.161 | 1114.119 | 1170.54 |
| 1218.925 | 1319.106 | 1384.55 |
| 1405.878 | 1424.201 | 1451.984 |
| 1472.206 | 1475.737 | 1477.96 |
| 1491.151 | 1511.092 | 1651.665 |
| 2027.739 | 3017.872 | 3045.469 |
| 3094.891 | 3105.567 | 3107.386 |
| 3119.006 | 3147.705 | 3156.254 |
| 3178.566 | 3201.336 | 3246.602 |

***i9 – p39***

C -2.437111 -1.625896 -0.134381

C -1.358364 -1.212798 0.483000

H -2.909663 -2.576848 0.115590

H -2.907856 -1.048847 -0.927283

H -0.772317 -1.640275 1.286347

C -0.427006 0.828981 0.073193

C -0.862439 1.475816 1.195298

C -1.083324 1.075966 -1.269074

C 3.402170 -0.625409 -0.108357

C 2.039823 -0.112678 -0.034458

C 0.916770 0.311987 0.029738

H -1.826393 1.971014 1.202969

H -0.297924 1.438462 2.118255

H -0.604880 1.932443 -1.752752

H -2.144427 1.300864 -1.142504

H -0.977197 0.213624 -1.927777

H 3.490174 -1.384941 -0.889081

H 3.698496 -1.078548 0.840921

H 4.108874 0.177245 -0.334434

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -490.664 | 32.8687 | 51.3055 |
| 90.2675 | 116.777 | 179.3437 |
| 189.4539 | 229.5812 | 252.0917 |
| 306.1207 | 334.1075 | 367.858 |
| 371.7024 | 484.6617 | 575.6637 |
| 642.7123 | 657.6315 | 819.4134 |
| 834.5975 | 906.1744 | 924.1898 |
| 940.9788 | 1017.517 | 1048.858 |
| 1056.116 | 1058.533 | 1088.056 |
| 1103.363 | 1318.329 | 1390.407 |
| 1405.042 | 1418.452 | 1421.474 |
| 1484.209 | 1485.501 | 1488.332 |
| 1504.027 | 1554.945 | 1664.396 |
| 2377.519 | 3046.202 | 3051.117 |
| 3088.629 | 3118.3 | 3120.918 |
| 3123.951 | 3151.52 | 3159.536 |
| 3173.201 | 3229.279 | 3261.889 |

***i9 – p38***

C -2.555277 -1.322067 -0.330689

C -1.421518 -0.694292 -0.620669

C -0.582243 0.065418 0.350544

C -1.070792 0.475644 1.568516

C 3.456548 -0.479555 -0.123393

C 2.023065 -0.275532 0.044508

C 0.841632 -0.109440 0.191456

H -3.109097 -1.848543 -1.099172

H -2.961304 -1.344607 0.674843

H -1.029850 -0.738845 -1.632515

H -0.403105 0.849701 2.333144

H -2.137655 0.527134 1.748235

H 3.652618 -1.247222 -0.875958

H 3.915936 -0.800420 0.814843

H 3.948362 0.442538 -0.443870

C -0.668151 1.964630 -0.852784

H -0.069475 2.616527 -0.228143

H -1.735152 2.154361 -0.875212

H -0.210861 1.640547 -1.781133

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -578.442 | 27.7135 | 70.0477 |
| 104.0049 | 108.9103 | 150.1505 |
| 216.4567 | 226.1364 | 285.4122 |
| 329.6382 | 335.1033 | 437.3237 |
| 486.3285 | 558.7386 | 565.4085 |
| 589.9311 | 617.5747 | 674.9921 |
| 725.5607 | 805.232 | 890.9343 |
| 937.4983 | 955.9603 | 1040.325 |
| 1056.23 | 1057.93 | 1065.076 |
| 1092.039 | 1285.62 | 1333.654 |
| 1391.572 | 1419.563 | 1420.349 |
| 1424.999 | 1452.415 | 1484.49 |
| 1485.207 | 1524.569 | 1719.87 |
| 2379.337 | 3046.671 | 3091.536 |
| 3117.903 | 3122.043 | 3155.679 |
| 3165.992 | 3180.444 | 3246.046 |
| 3257.476 | 3263.275 | 3268.956 |

***i2 – p22***

C -0.002227 1.874781 -0.100156

C -0.505348 0.579924 -0.711152

C -1.501836 -0.302430 -0.029745

C -2.448013 0.180413 0.768635

C -1.337084 -1.766759 -0.323804

C 3.055258 -0.596463 0.402574

C 1.960175 0.083052 0.136573

C 0.866473 0.682216 -0.151154

H 0.224815 2.697410 -0.769955

H -0.384547 2.163026 0.873387

H -0.546709 0.555165 -1.799117

H -3.157839 -0.476843 1.259416

H -2.548031 1.243983 0.955339

H -2.089682 -2.368024 0.188770

H -0.342856 -2.105346 -0.014610

H -1.416997 -1.956199 -1.399601

H 3.902756 -0.574708 -0.273914

H 3.194782 -1.067822 1.369425

H 2.639918 -2.519050 -0.339763

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -504.716 | 56.1049 | 71.7882 |
| 163.6965 | 181.8591 | 190.5104 |
| 245.8664 | 281.1267 | 302.1874 |
| 377.3821 | 405.8086 | 475.2053 |
| 526.0618 | 591.4257 | 667.0045 |
| 694.1811 | 727.0016 | 807.9008 |
| 900.3068 | 935.6801 | 940.9816 |
| 946.3284 | 977.3398 | 1026.392 |
| 1030.256 | 1045.197 | 1069.774 |
| 1083.222 | 1094.497 | 1118.19 |
| 1260.837 | 1338.209 | 1398.028 |
| 1421.86 | 1447.176 | 1462.575 |
| 1483.716 | 1498.171 | 1533.111 |
| 1746.883 | 2107.314 | 3035.341 |
| 3096.625 | 3126.141 | 3131.101 |
| 3136.733 | 3145.735 | 3152.08 |
| 3221.204 | 3231.57 | 3238.204 |

***i10 – p41***

C -2.392388 -1.386438 -0.083740

C -1.457333 -0.655675 -0.674902

H -2.931033 -2.154925 -0.626083

H -2.653878 -1.244194 0.960144

H -1.232023 -0.818031 -1.727388

C -0.662910 0.430563 -0.029224

C -0.358359 0.355432 1.459153

C -0.833160 1.799197 -0.661886

C 3.124137 -0.559635 -0.197418

C 1.903531 -0.235531 0.172894

C 0.697372 0.078338 0.463239

H -0.300733 1.289988 2.008513

H -0.736267 -0.488746 2.026134

H -0.179546 2.533390 -0.185739

H -1.869700 2.134585 -0.566584

H -0.580247 1.762037 -1.724977

H 3.896169 0.196130 -0.292806

H 3.425967 -1.599166 -0.265817

H 3.035957 -0.568579 -2.294102

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -512.377 | 65.897 | 108.9247 |
| 118.0951 | 192.0844 | 221.2204 |
| 259.3807 | 282.945 | 306.9342 |
| 335.9343 | 369.292 | 446.017 |
| 481.804 | 580.2507 | 652.4302 |
| 692.2567 | 711.1649 | 750.7347 |
| 900.0926 | 914.039 | 939.1267 |
| 966.7496 | 980.2972 | 1011.524 |
| 1030.641 | 1038.604 | 1065.53 |
| 1068.421 | 1118.27 | 1215.996 |
| 1277.74 | 1332.256 | 1382.202 |
| 1416.825 | 1452.793 | 1462.626 |
| 1491.752 | 1500.773 | 1534.096 |
| 1734.368 | 2103.139 | 3042.287 |
| 3118.704 | 3126.202 | 3131.139 |
| 3145.904 | 3146.016 | 3158.403 |
| 3215.98 | 3231.835 | 3240.44 |

***i1 – p14***

C 0.786956 1.897250 -0.225479

C 0.416326 0.612204 0.042005

C -3.583525 -0.286303 0.004081

C -2.160911 0.028356 0.020231

C -0.988942 0.291672 0.040395

C 1.392677 -0.520407 -0.013442

C 0.976979 -1.777799 -0.153350

C 2.851896 -0.173140 0.085248

H 0.042212 2.679241 -0.290401

H 1.827567 2.178509 -0.318058

H 0.563296 0.685479 1.900327

H -4.085094 0.223184 -0.822378

H -4.059338 0.027155 0.936618

H -3.741744 -1.361004 -0.113239

H 1.688806 -2.594144 -0.202079

H -0.075914 -2.023186 -0.222933

H 3.457747 -1.078364 0.135631

H 3.049286 0.425670 0.979986

H 3.184439 0.406458 -0.781605

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1026.14 | 40.8961 | 60.8315 |
| 94.4746 | 162.0119 | 222.8125 |
| 285.6213 | 335.244 | 344.2247 |
| 376.131 | 409.6603 | 449.6786 |
| 460.4892 | 485.2043 | 574.3125 |
| 612.2435 | 661.248 | 698.1449 |
| 773.7923 | 845.0577 | 893.6337 |
| 948.1353 | 966.8492 | 1027.363 |
| 1058.704 | 1064.607 | 1071.006 |
| 1079.439 | 1223.324 | 1370.076 |
| 1411.435 | 1414.955 | 1427.987 |
| 1442.791 | 1483.565 | 1487.721 |
| 1489.586 | 1500.692 | 1575.447 |
| 1729.228 | 2386.575 | 3042.368 |
| 3050.97 | 3104.761 | 3122.761 |
| 3127.155 | 3142.381 | 3166.478 |
| 3184.176 | 3258.24 | 3284.555 |

***i1 – p16***

C -0.672406 2.079782 0.652297

C -0.261542 1.228584 -0.328568

C 3.336406 -0.717108 -0.155941

C 2.054850 -0.025219 -0.214433

C 0.999457 0.549094 -0.264928

C -1.598445 -0.603589 -0.098899

C -2.548913 -0.690548 -0.997624

C -1.205293 -1.364430 1.098470

H -0.152557 2.135812 1.601073

H -1.571998 2.669125 0.525988

H -0.707970 1.306528 -1.315041

H 3.808715 -0.579818 0.819838

H 4.019544 -0.334906 -0.918753

H 3.208735 -1.789520 -0.324579

H -3.286194 -1.495024 -0.964580

H -2.647740 0.023959 -1.810446

H -1.894636 -2.198586 1.278389

H -1.207856 -0.715370 1.979297

H -0.192729 -1.761598 0.986571

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -435.94 | 33.3574 | 76.5873 |
| 129.9863 | 133.3908 | 142.8912 |
| 172.3298 | 201.462 | 260.5091 |
| 325.9889 | 333.8185 | 349.8603 |
| 426.1379 | 543.4631 | 565.9799 |
| 608.6234 | 724.3133 | 843.4183 |
| 902.7271 | 913.1049 | 942.6011 |
| 980.0084 | 1039.446 | 1062.204 |
| 1062.739 | 1066.895 | 1119.624 |
| 1190.602 | 1275.514 | 1392.56 |
| 1423.51 | 1431.189 | 1433.801 |
| 1462.606 | 1481.757 | 1491.38 |
| 1492.669 | 1562.888 | 1758.578 |
| 2379.853 | 3022.32 | 3048.013 |
| 3092.147 | 3096.769 | 3115.826 |
| 3120.14 | 3120.835 | 3167.623 |
| 3173.658 | 3182.911 | 3270.067 |

***i1 – p15***

C 0.827107 1.900876 -0.578200

C 0.467676 0.707034 -0.032556

C -3.488431 -0.349414 0.181035

C -2.083807 0.030079 0.105914

C -0.927215 0.352307 0.054348

C 1.471065 -0.408123 0.077390

C 2.638602 -0.225595 0.686895

C 1.084958 -1.706243 -0.575790

H 0.089258 2.671470 -0.763446

H 1.867541 2.114147 -0.789075

H 0.502022 1.177645 1.762192

H -4.041586 0.026880 -0.682951

H -3.950232 0.057166 1.084368

H -3.594862 -1.436593 0.206510

H 3.385279 -1.011589 0.714313

H 2.873984 0.706355 1.188949

H 1.900035 -2.428843 -0.516067

H 0.827113 -1.550099 -1.627862

H 0.201716 -2.132072 -0.091146

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1075.8 | 31.2903 | 48.0291 |
| 89.8311 | 150.6231 | 192.2274 |
| 260.3004 | 301.9252 | 317.8944 |
| 387.3962 | 408.8642 | 457.7713 |
| 484.1152 | 513.8881 | 578.3638 |
| 621.3782 | 671.917 | 704.0058 |
| 764.946 | 847.9078 | 903.1758 |
| 941.742 | 968.2118 | 1032.421 |
| 1055.118 | 1058.521 | 1070.817 |
| 1083.883 | 1231.687 | 1332.062 |
| 1408.704 | 1419.63 | 1425.257 |
| 1447.504 | 1481.204 | 1483.222 |
| 1484.424 | 1498.317 | 1577.423 |
| 1735.763 | 2380.994 | 3044 |
| 3047.706 | 3108.8 | 3120.683 |
| 3122.983 | 3141.248 | 3152.908 |
| 3164.758 | 3242.021 | 3269.844 |

***i10 – p40***

C 2.465802 -1.333571 -0.055197

C 1.424900 -0.723456 -0.609474

C 0.658636 0.398136 -0.008794

C 0.044822 1.402548 -0.990434

C 1.096085 0.909903 1.344798

C -3.090220 -0.708872 0.187542

C -1.948049 -0.117212 -0.089551

C -0.805020 0.415152 -0.310394

H 2.968221 -2.147635 -0.564083

H 2.852128 -1.050656 0.917974

H 1.071313 -1.053136 -1.584331

H -0.019844 2.436156 -0.665256

H 0.238154 1.264006 -2.049710

H 0.447716 1.723313 1.675719

H 2.124276 1.281104 1.301837

H 1.045591 0.113766 2.091801

H -3.747758 -0.315702 0.955157

H -3.472763 -1.501710 -0.445896

H -2.588770 -2.205272 1.555806

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -532.445 | 73.7158 | 101.622 |
| 151.8368 | 192.1581 | 255.0327 |
| 270.7402 | 287.5533 | 312.1471 |
| 365.9901 | 373.9401 | 449.39 |
| 464.7378 | 582.1255 | 619.951 |
| 689.51 | 725.4503 | 764.6853 |
| 901.5466 | 909.4986 | 938.9119 |
| 948.4242 | 975.8576 | 1011.078 |
| 1029.236 | 1037.473 | 1057.685 |
| 1058.389 | 1107.68 | 1204.369 |
| 1313.763 | 1337.834 | 1380.578 |
| 1420.377 | 1451.503 | 1462.366 |
| 1494.28 | 1508.789 | 1533.246 |
| 1728.288 | 2102.522 | 3045.513 |
| 3120.406 | 3121.736 | 3135.992 |
| 3146.857 | 3151.281 | 3164.369 |
| 3212.332 | 3233.025 | 3245.973 |

***i11 – i10***

C 2.185829 -1.527073 -0.201004

C 1.383935 -0.586928 -0.719228

C 0.750686 0.488743 0.017678

C 0.118101 1.624422 -0.748878

C 1.036178 0.674364 1.480466

C -2.739349 -1.083292 0.283758

C -2.004587 0.078609 -0.217943

C -0.934260 0.697020 -0.397211

H 2.613152 -2.299747 -0.828428

H 2.442649 -1.549895 0.852460

H 1.166946 -0.618833 -1.785452

H 0.104882 2.590421 -0.247976

H 0.366594 1.700273 -1.806087

H 0.398876 1.450845 1.907656

H 2.082735 0.963198 1.635842

H 0.858983 -0.248842 2.038802

H -3.449130 -0.791232 1.062211

H -2.055180 -1.831975 0.703561

H -3.309709 -1.559399 -0.518417

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -674.989 | 65.392 | 94.8079 |
| 106.3635 | 156.0476 | 189.7353 |
| 232.0662 | 279.8304 | 306.5326 |
| 400.0833 | 419.4551 | 448.8706 |
| 521.7674 | 670.7621 | 722.0728 |
| 749.3807 | 892.2257 | 942.3724 |
| 985.8026 | 1018.351 | 1032.043 |
| 1034.469 | 1055.251 | 1061.569 |
| 1077.232 | 1132.752 | 1192.534 |
| 1270.217 | 1340.168 | 1346.38 |
| 1409.933 | 1422.522 | 1450.634 |
| 1475.495 | 1477.554 | 1480.704 |
| 1486.555 | 1512.463 | 1654.901 |
| 2022.33 | 3012.874 | 3032.961 |
| 3091.548 | 3100.058 | 3102.421 |
| 3117.976 | 3138.049 | 3153.356 |
| 3165.485 | 3176.094 | 3252.337 |

***i11 – i12***

C -1.152164 1.729304 -0.655755

C -1.150738 0.469226 0.146498

C 2.276661 -0.201656 0.103161

C 1.221811 0.022887 0.632336

C -0.098332 0.302376 1.215881

C 3.564203 -0.476930 -0.525128

H -0.959444 2.602681 -0.025221

H -2.105617 1.870131 -1.170710

H -0.363399 1.709460 -1.424428

H -0.034126 1.215182 1.819643

H -0.375463 -0.514227 1.889783

H 4.261486 0.349621 -0.367110

H 3.448510 -0.620688 -1.602310

H 4.013901 -1.382468 -0.110219

C -1.733712 -0.750275 -0.443603

C -2.914176 -1.263450 -0.115388

H -1.133651 -1.257568 -1.205571

H -3.544894 -0.794731 0.633930

H -3.288628 -2.166278 -0.585807

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -147.058 | 34.3044 | 81.6436 |
| 95.9098 | 157.5185 | 189.9641 |
| 203.4845 | 263.6702 | 309.9992 |
| 356.8782 | 398.925 | 439.0489 |
| 575.1925 | 708.1482 | 739.5433 |
| 770.1566 | 919.7596 | 970.0317 |
| 977.3853 | 994.7873 | 1018.245 |
| 1059.745 | 1063.33 | 1075.173 |
| 1159.047 | 1177.745 | 1247.552 |
| 1308.255 | 1320.203 | 1333.595 |
| 1405.848 | 1423.166 | 1451.167 |
| 1465.36 | 1483.828 | 1488.602 |
| 1491.423 | 1493.001 | 1719.525 |
| 2387.067 | 2984.956 | 3039.476 |
| 3051.407 | 3073.881 | 3082.41 |
| 3091.709 | 3122.554 | 3124.537 |
| 3124.85 | 3151.953 | 3240.859 |

***i4 – i3***

C 0.040129 -1.462743 -0.208030

C -1.015420 -0.818195 0.649291

C 3.577539 0.658017 -0.006556

C 2.332781 -0.097903 -0.090050

C 1.311666 -0.726756 -0.160344

H -0.308210 -1.517357 -1.244730

H 0.216727 -2.491203 0.125823

H -0.913761 -0.916466 1.727002

H 4.313675 0.128606 0.603530

H 3.407787 1.638858 0.444792

H 4.008813 0.812069 -0.998776

C -1.880504 0.251152 0.109233

C -3.118329 -0.000150 -0.311868

C -1.269839 1.631967 0.050264

H -3.747927 0.787618 -0.714311

H -3.540895 -0.997802 -0.261479

H -1.973223 2.361723 -0.356785

H -0.366105 1.624265 -0.566801

H -0.965018 1.957360 1.050098

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -93.2091 | 47.5529 | 101.7009 |
| 108.1742 | 180.9254 | 212.6218 |
| 234.5857 | 288.5656 | 303.2885 |
| 396.2759 | 415.1969 | 459.2143 |
| 557.2799 | 603.078 | 727.8384 |
| 755.8939 | 793.9416 | 927.5875 |
| 939.4851 | 998.8341 | 1028.31 |
| 1058.64 | 1064.915 | 1077.889 |
| 1091.329 | 1163.033 | 1218.329 |
| 1262.674 | 1311.145 | 1387.473 |
| 1413.66 | 1422.621 | 1443.562 |
| 1466.724 | 1487.12 | 1489.143 |
| 1491.08 | 1500.609 | 1725.713 |
| 2387.273 | 3038.665 | 3043.785 |
| 3048.725 | 3088.091 | 3105.533 |
| 3118.477 | 3124.09 | 3128.121 |
| 3150.048 | 3167.927 | 3238.953 |

***i4 – i6***

C -2.438533 -1.163158 -0.330708

C -1.277325 -0.303569 0.109813

C -0.141046 -0.997146 0.701947

C 1.645328 0.028528 -0.111499

C 1.152478 1.158086 -0.118441

C -0.082676 1.925301 0.104008

C -1.290621 1.026981 -0.083231

C 2.688657 -0.992667 -0.263233

H -2.880607 -1.700231 0.513793

H -2.098957 -1.915388 -1.051013

H -3.219840 -0.567075 -0.806722

H -0.036490 -2.059430 0.489793

H 0.197024 -0.701812 1.688950

H -0.060383 2.364497 1.110556

H -0.150670 2.767289 -0.590898

H -2.177746 1.496416 -0.497986

H 3.628027 -0.527674 -0.570979

H 2.404210 -1.730956 -1.016732

H 2.857863 -1.519779 0.679304

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -642.031 | 77.5611 | 164.9747 |
| 169.1398 | 189.8538 | 213.0475 |
| 230.2698 | 345.8609 | 387.0732 |
| 416.3187 | 455.4259 | 490.6052 |
| 606.7755 | 681.1735 | 744.8598 |
| 790.1591 | 841.1022 | 870.6072 |
| 950.3452 | 981.1273 | 996.0668 |
| 1041.763 | 1069.888 | 1071.621 |
| 1103.035 | 1150.079 | 1210.874 |
| 1220.292 | 1322.806 | 1366.226 |
| 1415.855 | 1419.413 | 1472.542 |
| 1479.366 | 1483.936 | 1487.394 |
| 1495.445 | 1500.138 | 1672.385 |
| 2124.887 | 3026.299 | 3037.423 |
| 3052.587 | 3085.653 | 3099.628 |
| 3123.747 | 3127.278 | 3132.195 |
| 3133.526 | 3181.937 | 3220.423 |

***i6 – i8***

C 2.439616 -1.043501 0.194732

C 1.214445 -0.208181 -0.018955

C -0.010605 -0.931116 -0.555399

C -1.282118 -0.218805 -0.136517

C -1.259102 1.132178 -0.202589

C -0.046132 1.861784 -0.072356

C 1.183621 1.114008 0.208406

C -2.435181 -1.030568 0.361705

H 2.715440 -1.561872 -0.730505

H 2.250457 -1.818081 0.946202

H 3.291172 -0.444197 0.521681

H -0.022784 -1.961175 -0.177024

H 0.080672 -1.026405 -1.648754

H 0.013147 2.884462 -0.435542

H -1.020719 1.991013 0.802389

H 2.063396 1.636212 0.570901

H -3.267058 -0.388401 0.653910

H -2.138135 -1.636428 1.226939

H -2.792854 -1.729929 -0.404346

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1818.04 | 93.0292 | 162.7188 |
| 196.0278 | 224.9553 | 282.9233 |
| 319.5589 | 379.4166 | 453.1106 |
| 465.6395 | 511.8668 | 554.1508 |
| 691.4772 | 746.7065 | 832.0497 |
| 876.5234 | 885.9863 | 911.8095 |
| 960.5316 | 1004.201 | 1034.332 |
| 1065.364 | 1075.386 | 1154.665 |
| 1163.953 | 1207.255 | 1224.227 |
| 1239.391 | 1319.03 | 1368.545 |
| 1397.779 | 1409.911 | 1416.95 |
| 1463.762 | 1478.208 | 1483.054 |
| 1488.934 | 1494.367 | 1578.704 |
| 1698.105 | 2099.084 | 2983.686 |
| 3015.395 | 3032.202 | 3048.145 |
| 3065.04 | 3089.997 | 3133.631 |
| 3139.302 | 3166.261 | 3191.352 |

***i6 – i7***

C 2.638230 -0.788217 -0.000004

C 1.262503 -0.183493 -0.000004

C 0.122481 -1.184604 0.000011

C -1.188455 -0.478037 0.000006

C -1.337973 0.830560 0.000004

C -0.257193 1.857130 0.000004

C 1.076904 1.138219 -0.000006

C -2.628855 -0.887377 -0.000009

H 2.782251 -1.425001 -0.879946

H 2.782288 -1.424908 0.879999

H 3.417451 -0.023916 -0.000058

H 0.212777 -1.845742 0.873306

H 0.212771 -1.845766 -0.873266

H -0.331394 2.513031 -0.875605

H -0.331384 2.513023 0.875620

H 1.954219 1.782012 -0.000014

H -2.717059 0.521359 -0.000010

H -3.053897 -1.294591 0.918202

H -3.053876 -1.294589 -0.918232

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2256.92 | 77.4138 | 119.8993 |
| 190.2783 | 252.8833 | 306.1788 |
| 388.3743 | 419.8058 | 443.4742 |
| 472.3626 | 487.2263 | 552.0982 |
| 723.8559 | 800.6449 | 839.8882 |
| 903.7115 | 936.4053 | 956.0645 |
| 964.9409 | 986.5816 | 1043.791 |
| 1067.153 | 1079.631 | 1086.132 |
| 1086.972 | 1164.007 | 1200.931 |
| 1225.344 | 1242.03 | 1319.626 |
| 1356.551 | 1407.712 | 1422.292 |
| 1446.162 | 1466.731 | 1468.538 |
| 1484.013 | 1491.022 | 1751.232 |
| 1804.249 | 1876.04 | 3014.227 |
| 3036.196 | 3036.351 | 3036.391 |
| 3062.096 | 3077.25 | 3092.675 |
| 3136.965 | 3149.186 | 3169.979 |

***i10 – i9***

C -2.649925 -1.159308 -0.243222

C -1.490056 -0.892383 0.340822

C -0.651654 0.332769 0.112192

C -0.067102 0.920182 1.367987

C -1.203115 1.337178 -0.887092

C 3.365920 -0.496866 -0.277800

C 1.922572 -0.295794 -0.315213

C 0.773368 0.042202 -0.020204

H -3.189514 -2.070979 -0.013758

H -3.103186 -0.490567 -0.966825

H -1.073034 -1.599538 1.054568

H 0.184018 1.971712 1.392829

H -0.068939 0.348945 2.286222

H -0.512351 2.174979 -0.996269

H -2.166321 1.722077 -0.541218

H -1.334550 0.873845 -1.867545

H 3.846599 -0.028951 -1.141164

H 3.610459 -1.562236 -0.301540

H 3.806764 -0.067167 0.629873

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -684.988 | 78.4559 | 82.7192 |
| 106.872 | 138.441 | 262.7133 |
| 277.2584 | 289.3994 | 308.6293 |
| 371.5363 | 399.4933 | 436.7246 |
| 481.7435 | 628.3544 | 644.3966 |
| 676.6092 | 736.7171 | 825.6045 |
| 940.144 | 957.4773 | 982.9087 |
| 1035.64 | 1044.768 | 1047.736 |
| 1061.689 | 1082.037 | 1171.186 |
| 1279.821 | 1294.187 | 1353.157 |
| 1412.539 | 1418.761 | 1441.643 |
| 1458.2 | 1477.746 | 1483.157 |
| 1497.033 | 1509.516 | 1736.235 |
| 2098.894 | 3022.514 | 3051.045 |
| 3092.328 | 3115.922 | 3130.002 |
| 3144.216 | 3152.199 | 3166.286 |
| 3167.446 | 3247.57 | 3288.69 |

***i12 – i17***

C -2.852099 -0.046859 0.437088

C -1.431240 0.068580 -0.027616

C -0.746561 1.228825 0.001601

C 0.600343 1.412822 -0.487507

C 1.632374 -0.439932 0.092854

C 0.677635 -1.200152 -0.093577

C -0.753780 -1.234963 -0.431514

C 3.020713 -0.083811 0.412744

H -3.490562 -0.457395 -0.354097

H -3.260501 0.923175 0.727169

H -2.932294 -0.727207 1.292883

H -1.220597 2.084054 0.481714

H 0.831167 1.147158 -1.513373

H 1.161333 2.263881 -0.109553

H -1.256848 -2.068055 0.069979

H -0.871421 -1.416486 -1.508684

H 3.597870 -0.985089 0.632251

H 3.063030 0.575595 1.283020

H 3.494525 0.433311 -0.425753

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -677.016 | 74.5539 | 138.5372 |
| 151.4244 | 193.0927 | 214.6667 |
| 251.8043 | 347.0251 | 375.2344 |
| 405.7434 | 434.3718 | 505.5519 |
| 629.0838 | 636.2828 | 761.1252 |
| 797.0334 | 815.8054 | 886.8709 |
| 935.9816 | 981.0006 | 1036.397 |
| 1052.057 | 1064.275 | 1071.393 |
| 1151.095 | 1159.711 | 1202.215 |
| 1227.792 | 1327.41 | 1362.259 |
| 1414.712 | 1416.409 | 1472.162 |
| 1480.254 | 1481.486 | 1485.947 |
| 1489.15 | 1497.196 | 1659.452 |
| 2108.778 | 3023.868 | 3028.917 |
| 3047.567 | 3072.203 | 3081.691 |
| 3118.732 | 3128.414 | 3128.891 |
| 3133.089 | 3139.015 | 3217.51 |

***i17 – i18***

C 2.861398 -0.129874 -0.000151

C 1.364426 0.007268 -0.000001

C 0.764614 1.199567 0.000000

C -0.725961 1.445448 0.000129

C -1.446159 0.141932 0.000111

C -0.856938 -1.035978 0.000167

C 0.607222 -1.313806 0.000123

C -2.876541 -0.301790 -0.000220

H 3.200693 -0.687309 0.879917

H 3.356288 0.843214 -0.000022

H 3.200540 -0.687013 -0.880466

H 1.391880 2.088122 -0.000115

H -1.007827 2.048218 0.873929

H -1.007981 2.048256 -0.873594

H 0.901344 -1.906452 -0.875405

H 0.901418 -1.906327 0.875713

H -3.454077 -0.193482 0.918520

H -2.180927 -1.530647 -0.000269

H -3.453721 -0.193180 -0.919151

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2281.91 | 74.5615 | 149.72 |
| 198.2813 | 257.0886 | 315.1591 |
| 385.0558 | 406.8803 | 447.626 |
| 458.9099 | 482.6761 | 595.1089 |
| 735.2443 | 783.8861 | 809.0648 |
| 915.0014 | 946.9913 | 956.343 |
| 958.4254 | 982.9209 | 1057.642 |
| 1063.82 | 1071.947 | 1088.774 |
| 1093.711 | 1168.514 | 1214.887 |
| 1220.723 | 1238.595 | 1318.702 |
| 1372.769 | 1400.446 | 1423.243 |
| 1435.657 | 1469.102 | 1472.558 |
| 1479.922 | 1497.113 | 1752.891 |
| 1805.641 | 1874.582 | 3015.856 |
| 3024.125 | 3033.321 | 3037.748 |
| 3050.332 | 3081.938 | 3089.316 |
| 3135.014 | 3154.362 | 3176.26 |

***i17 – i19***

C 2.850728 0.013891 -0.407270

C 1.401333 0.057919 -0.017249

C 0.674629 1.182100 0.047363

C -0.786070 1.200918 0.446275

C -1.440210 -0.123477 0.096524

C -0.702049 -1.228609 0.342502

C 0.717936 -1.198657 0.345230

C -2.800408 -0.122809 -0.524238

H 3.447329 -0.483995 0.364201

H 3.256828 1.016276 -0.556040

H 2.987966 -0.551059 -1.334865

H 1.143917 2.137153 -0.176047

H -0.876528 1.435028 1.518091

H -1.303639 2.016697 -0.071820

H 0.044190 -1.937943 -0.514284

H 1.276378 -1.979998 0.856981

H -3.536752 0.357805 0.131802

H -3.136662 -1.140118 -0.728514

H -2.798358 0.442496 -1.464335

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1851.11 | 100.1097 | 151.5409 |
| 155.8352 | 241.1512 | 256.3712 |
| 295.6796 | 365.2282 | 438.2125 |
| 456.1039 | 525.4716 | 575.9572 |
| 691.1847 | 752.6188 | 789.7945 |
| 839.9615 | 910.353 | 938.0847 |
| 963.5191 | 998.4452 | 1044.566 |
| 1066.574 | 1075.759 | 1155.928 |
| 1183.533 | 1204.881 | 1213.668 |
| 1235.104 | 1337.243 | 1347.774 |
| 1401.23 | 1411.854 | 1423.287 |
| 1471.821 | 1479.967 | 1485.257 |
| 1488.814 | 1496.573 | 1583.756 |
| 1709.882 | 2103.192 | 2991.666 |
| 3021.059 | 3040.922 | 3051.088 |
| 3071.793 | 3101.535 | 3132.166 |
| 3142.481 | 3150.177 | 3170.061 |

***i7 – p3***

C 2.565629 -0.856711 -0.104207

C 1.234985 -0.175611 -0.023961

C 0.052565 -1.043720 0.328766

C -1.302945 -0.446338 0.014257

C -1.375029 1.003905 -0.044421

C -0.251233 1.758944 -0.088486

C 1.071091 1.141621 -0.178188

C -2.386265 -1.210065 -0.178147

H 2.573013 -1.600578 -0.908470

H 2.781663 -1.393824 0.826530

H 3.372979 -0.145031 -0.285282

H 0.103087 -1.224079 1.414201

H 0.150324 -2.028226 -0.139381

H -2.353701 1.469675 -0.089147

H -0.329575 2.830820 -0.229222

H -0.185680 2.336998 1.950558

H 1.924519 1.781694 -0.376033

H -3.361987 -0.766445 -0.344192

H -2.327432 -2.293153 -0.173239

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -594.292 | 77.2221 | 161.6409 |
| 195.7223 | 220.253 | 289.1179 |
| 297.5619 | 374.4621 | 418.1956 |
| 481.6659 | 487.3599 | 512.1192 |
| 576.8434 | 686.1358 | 736.8592 |
| 821.2468 | 868.8919 | 878.9565 |
| 904.2307 | 929.561 | 953.2568 |
| 980.2637 | 999.304 | 1010.317 |
| 1068.629 | 1077.473 | 1180.038 |
| 1200.744 | 1239.379 | 1321.12 |
| 1338.839 | 1382.23 | 1419.034 |
| 1431.98 | 1453.843 | 1470.117 |
| 1483.541 | 1494.48 | 1590.217 |
| 1680.191 | 1741.303 | 2992.682 |
| 3028.819 | 3076.374 | 3085.751 |
| 3132.87 | 3150.194 | 3182.394 |
| 3189.087 | 3208.5 | 3239.366 |

***i8 – p1***

C 2.514641 -1.009682 -0.068819

C 1.227413 -0.234940 -0.047447

C 0.000000 -0.922647 -0.023528

C -1.227413 -0.234940 -0.047447

C -1.207883 1.152327 0.002142

C 0.000000 1.841750 0.034607

C 1.207883 1.152327 0.002142

C -2.514641 -1.009682 -0.068819

H 2.532029 -1.725835 -0.895077

H 2.631402 -1.577964 0.859921

H 3.377226 -0.349139 -0.172769

H 0.000000 -1.432869 1.820580

H 0.000000 -1.997229 -0.186404

H -2.143603 1.701704 0.007195

H 0.000000 2.925495 0.070311

H 2.143603 1.701704 0.007195

H -3.377226 -0.349139 -0.172770

H -2.631403 -1.577963 0.859922

H -2.532028 -1.725835 -0.895076

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -723.097 | 71.8511 | 78.1466 |
| 181.7583 | 224.6108 | 275.5878 |
| 300.1297 | 358.9788 | 416.8444 |
| 489.8595 | 527.2639 | 543.0044 |
| 548.3253 | 726.9405 | 744.2945 |
| 792.0956 | 920.5589 | 927.324 |
| 969.7551 | 996.8228 | 1003.57 |
| 1026.68 | 1042.196 | 1063.988 |
| 1068.398 | 1130.236 | 1186.081 |
| 1200.327 | 1288.249 | 1324.52 |
| 1345.546 | 1417.023 | 1419.373 |
| 1448.115 | 1488.994 | 1489.519 |
| 1495.05 | 1509.196 | 1545.477 |
| 1657.922 | 1658.373 | 3038.807 |
| 3039.447 | 3103.54 | 3103.714 |
| 3134.663 | 3134.888 | 3165.047 |
| 3180.126 | 3188.257 | 3206.962 |

***i18 – p6***

C 2.838128 -0.013347 -0.239588

C 1.349323 -0.081400 -0.061106

C 0.666955 -1.226541 0.010432

C -0.813904 -1.270202 0.264482

C -1.536295 0.031071 -0.016068

C -0.730882 1.241851 0.018942

C 0.619752 1.192096 0.040956

C -2.850844 0.079069 -0.265562

H 3.099944 0.544477 -1.144574

H 3.277712 -1.009595 -0.312225

H 3.301090 0.505799 0.606455

H 1.188555 -2.176714 -0.057135

H -1.277142 -2.086207 -0.297377

H -0.962330 -1.518431 1.326602

H -1.243200 2.198062 -0.010225

H 0.981592 1.511031 2.140230

H 1.191340 2.112245 -0.026550

H -3.360228 1.025997 -0.408396

H -3.450732 -0.822242 -0.331725

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -539.124 | 62.588 | 171.3562 |
| 199.9894 | 230.9786 | 267.1546 |
| 308.3102 | 317.9989 | 408.4914 |
| 429.7671 | 490.1952 | 573.6736 |
| 625.2268 | 702.3437 | 744.9249 |
| 783.6702 | 815.6526 | 834.0671 |
| 910.5515 | 941.724 | 960.447 |
| 983.8524 | 999.7156 | 1012.906 |
| 1073.695 | 1088.889 | 1196.108 |
| 1200.508 | 1232.769 | 1313.081 |
| 1345.462 | 1371.674 | 1420.177 |
| 1431.168 | 1457.352 | 1474.305 |
| 1485.571 | 1499.735 | 1600.724 |
| 1684.304 | 1753.137 | 2996.696 |
| 3034.343 | 3082.663 | 3094.564 |
| 3134.171 | 3149.613 | 3175.837 |
| 3177.032 | 3196.638 | 3238.769 |

***i19 – p2***

C -2.939346 0.001395 -0.008035

C -1.433060 -0.005902 -0.023357

C -0.705809 1.172894 -0.099944

C 0.696810 1.162647 -0.054613

C 1.402249 -0.057093 -0.048138

C 0.665164 -1.230819 0.025643

C -0.725489 -1.208685 0.048650

C 2.904123 -0.057203 -0.059476

H -3.346329 -0.780330 -0.654236

H -3.335035 0.961148 -0.346131

H -3.317710 -0.176878 1.003283

H -1.224935 2.123313 -0.168257

H 1.237794 2.083519 -0.248538

H 0.997783 1.606483 1.742231

H 1.183524 -2.184062 0.056456

H -1.272239 -2.145062 0.103714

H 3.294599 0.518924 -0.903086

H 3.303211 -1.070883 -0.126906

H 3.291489 0.400421 0.857088

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -830.99 | 33.7783 | 83.1182 |
| 137.9549 | 277.255 | 294.5886 |
| 312.7605 | 379.5933 | 413.1963 |
| 454.7494 | 467.7179 | 534.7883 |
| 659.3395 | 723.7633 | 742.8255 |
| 828.2979 | 844.8143 | 883.0991 |
| 973.3059 | 993.431 | 1016.652 |
| 1030.38 | 1046.082 | 1066.514 |
| 1070.623 | 1140.76 | 1211.509 |
| 1234.738 | 1248.486 | 1324.612 |
| 1342.391 | 1418.979 | 1421.094 |
| 1437.138 | 1489.286 | 1492.428 |
| 1495.407 | 1506.755 | 1562.488 |
| 1628.713 | 1675.072 | 3037.874 |
| 3044.138 | 3101.913 | 3110.262 |
| 3132.555 | 3133.234 | 3173.953 |
| 3175.546 | 3190.939 | 3194.15 |

***i8 – i32***

C -2.522478 -1.034962 -0.165265

C -1.278559 -0.256939 0.143038

C 0.052978 -0.987059 0.139285

C 1.274185 -0.232739 0.009871

C 1.236743 1.123392 -0.029999

C -0.032500 1.840949 -0.023103

C -1.210023 1.173461 0.023298

C 2.561043 -1.001382 -0.080927

H -2.532218 -1.997274 0.355777

H -2.597786 -1.248742 -1.240042

H -3.417760 -0.484971 0.135033

H 0.038673 -2.061508 0.002906

H -0.636474 -0.654347 1.188052

H 2.159822 1.686989 -0.105479

H -0.024076 2.922645 -0.085349

H -2.147977 1.718444 -0.030897

H 3.421778 -0.333352 -0.139627

H 2.562833 -1.643736 -0.967633

H 2.684855 -1.652480 0.790076

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2570.45 | 126.8398 | 140.8083 |
| 180.8906 | 211.5815 | 265.3566 |
| 321.62 | 385.5976 | 485.5923 |
| 496.7639 | 516.1098 | 610.93 |
| 685.2722 | 716.9955 | 745.1167 |
| 830.8386 | 869.0689 | 940.5473 |
| 967.6035 | 981.0734 | 1021.812 |
| 1044.363 | 1061.603 | 1069.76 |
| 1152.375 | 1185.48 | 1221.558 |
| 1248.968 | 1298.453 | 1314.907 |
| 1390.063 | 1415.013 | 1425.467 |
| 1457.38 | 1482.751 | 1486.394 |
| 1497.16 | 1503.02 | 1601.065 |
| 1628.462 | 2206.181 | 3004.853 |
| 3036.822 | 3075.355 | 3098.188 |
| 3116.738 | 3136.318 | 3173.36 |
| 3190.34 | 3203.391 | 3210.394 |

***i18 – i37***

C -2.834240 -0.012514 -0.302781

C -1.371614 0.056952 0.055761

C -0.640292 1.230299 -0.031870

C 0.823704 1.250115 0.296084

C 1.532590 -0.059201 -0.023023

C 0.752831 -1.260253 0.104281

C -0.629146 -1.223136 0.188199

C 2.841870 -0.076515 -0.341912

H -2.947104 -0.212877 -1.372134

H -3.339805 0.926818 -0.072012

H -3.342146 -0.813651 0.240587

H -1.153993 2.166779 -0.214616

H 1.319524 2.080010 -0.214840

H 0.954601 1.443590 1.375217

H 1.257931 -2.219142 0.112352

H -1.164630 -0.501851 1.239606

H -1.218103 -2.133196 0.187974

H 3.366486 -1.010895 -0.510604

H 3.413016 0.839928 -0.439968

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1929.63 | 84.2207 | 171.8189 |
| 198.8154 | 283.7729 | 318.0246 |
| 405.5229 | 427.5348 | 493.4521 |
| 562.6892 | 606.0233 | 641.3738 |
| 674.3518 | 746.8996 | 760.7051 |
| 788.6859 | 860.1443 | 884.4449 |
| 926.3654 | 944.1152 | 987.6594 |
| 1004.994 | 1067.663 | 1085.863 |
| 1140.911 | 1168.949 | 1205.078 |
| 1234.68 | 1296.735 | 1333.391 |
| 1350.372 | 1399.933 | 1425.096 |
| 1446.688 | 1472.502 | 1488.793 |
| 1496.93 | 1522.588 | 1562.422 |
| 1625.02 | 1797.361 | 2946.923 |
| 3045.339 | 3080.837 | 3114.068 |
| 3134.469 | 3148.613 | 3191.513 |
| 3198.642 | 3208.894 | 3238.649 |

***i19 – i38***

C -2.940202 0.025189 -0.096683

C -1.445123 -0.039173 -0.011569

C -0.755600 -1.205100 -0.014665

C 0.676191 -1.257342 0.097828

C 1.448763 0.046470 0.134189

C 0.655798 1.241606 0.073415

C -0.698249 1.224338 0.044498

C 2.910865 0.030441 -0.199335

H -3.362037 0.527889 0.781534

H -3.382845 -0.970765 -0.162598

H -3.258113 0.599580 -0.974368

H -1.290336 -2.146394 -0.101911

H 1.127379 -0.652023 1.163392

H 1.229413 -2.170307 -0.077804

H 1.184306 2.190741 0.049821

H -1.253204 2.156028 0.026239

H 3.421508 -0.807779 0.284630

H 3.401495 0.951219 0.125858

H 3.067777 -0.076760 -1.280862

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2664.31 | 103.3298 | 172.0547 |
| 189.2124 | 252.8315 | 275.3707 |
| 348.9925 | 371.4981 | 405.3156 |
| 434.7162 | 612.1496 | 633.5801 |
| 675.5163 | 707.8419 | 752.2534 |
| 787.2885 | 890.6399 | 928.6603 |
| 966.7737 | 977.6013 | 1019.871 |
| 1048.345 | 1063.236 | 1092.644 |
| 1170.053 | 1186.114 | 1222.133 |
| 1255.104 | 1295.989 | 1336.587 |
| 1388.784 | 1418.844 | 1424.499 |
| 1463.189 | 1480.978 | 1486.626 |
| 1498.419 | 1503.813 | 1591.179 |
| 1638.505 | 2199.493 | 3007.423 |
| 3021.793 | 3074.994 | 3076.1 |
| 3116.689 | 3125.939 | 3168.317 |
| 3175.017 | 3195.82 | 3218.859 |

***i7 – i30***

C 2.537880 -0.902618 0.148159

C 1.218226 -0.212070 0.039308

C 0.018558 -1.046436 -0.318930

C -1.326299 -0.400699 -0.013170

C -1.384735 1.034815 -0.002279

C -0.236869 1.808916 0.009983

C 1.097400 1.165898 0.071530

C -2.418057 -1.166936 0.185009

H 2.788583 -1.431736 -0.782036

H 2.521859 -1.659289 0.941525

H 3.347267 -0.202050 0.365820

H 0.082595 -2.021298 0.177010

H 0.054456 -1.267067 -1.400658

H -2.352900 1.520461 0.031012

H 0.609709 1.668446 -1.060779

H -0.280572 2.881997 0.149007

H 1.943000 1.796340 0.324503

H -3.392876 -0.721393 0.351330

H -2.357738 -2.249635 0.185610

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1946.12 | 82.9745 | 163.2867 |
| 200.4973 | 277.9997 | 308.2269 |
| 414.0912 | 462.9222 | 481.9342 |
| 508.5414 | 573.0457 | 650.1073 |
| 721.4634 | 732.8031 | 808.2979 |
| 857.9705 | 866.3154 | 908.7672 |
| 949.0721 | 963.6323 | 986.6479 |
| 1007.535 | 1044.859 | 1060.574 |
| 1127.737 | 1190.356 | 1202.797 |
| 1237.039 | 1303.96 | 1324.737 |
| 1361.959 | 1399.151 | 1419.907 |
| 1447.249 | 1473.845 | 1478.098 |
| 1494.617 | 1531.46 | 1574.456 |
| 1623.086 | 1796.102 | 2948.933 |
| 3006.92 | 3059.264 | 3062.056 |
| 3123.962 | 3150.931 | 3192.179 |
| 3204.273 | 3223.985 | 3241.312 |

***i7 – i31***

C -2.549159 -0.871955 -0.131672

C -1.231548 -0.170797 -0.011536

C -0.046915 -1.036584 0.342680

C 1.307220 -0.425541 0.025327

C 1.393138 1.009319 0.038893

C 0.162417 1.830206 -0.001657

C -1.106228 1.170688 -0.111908

C 2.373339 -1.206990 -0.239457

H -2.788357 -1.418468 0.789287

H -2.524555 -1.613286 -0.938851

H -3.362927 -0.172643 -0.333941

H -0.131036 -2.007541 -0.157215

H -0.091069 -1.257507 1.422002

H 2.339560 1.501657 -0.148873

H 0.825722 1.571816 1.092455

H 0.268386 2.887272 -0.205728

H -1.985130 1.785664 -0.276652

H 3.348640 -0.779737 -0.445665

H 2.287181 -2.287304 -0.260840

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1886.66 | 81.306 | 174.8912 |
| 210.5956 | 291.2886 | 327.5392 |
| 415.9977 | 461.7037 | 479.2132 |
| 501.8966 | 548.0304 | 639.8229 |
| 697.0269 | 726.8551 | 834.6501 |
| 844.6633 | 863.9994 | 894.7973 |
| 927.0543 | 948.1691 | 964.056 |
| 1013.85 | 1049.451 | 1064.195 |
| 1142.533 | 1188.524 | 1234.563 |
| 1245.739 | 1301.923 | 1334.844 |
| 1370.014 | 1398.735 | 1419.484 |
| 1436.326 | 1466.454 | 1479.415 |
| 1483.986 | 1498.35 | 1635.395 |
| 1651.666 | 2123.277 | 2974.906 |
| 3022.246 | 3063.613 | 3074.986 |
| 3130.181 | 3154.96 | 3190.393 |
| 3207.2 | 3229.911 | 3245.126 |

***i38 – p42***

C 2.754923 -0.000057 0.515048

C 1.327583 0.000080 0.038736

C 0.646204 -1.201282 -0.196554

C -0.674774 -1.211378 -0.595674

C -1.402760 0.000035 -0.692223

C -0.674846 1.211450 -0.595589

C 0.646162 1.201385 -0.196424

C -2.494203 -0.000127 1.194593

H 3.292425 -0.882921 0.160710

H 2.803176 -0.003941 1.609393

H 3.290521 0.886431 0.166999

H 1.177397 -2.141440 -0.081221

H -1.177248 -2.152574 -0.789067

H -2.355161 0.000024 -1.209794

H -1.177350 2.152642 -0.788917

H 1.177284 2.141567 -0.080981

H -3.070009 -0.919127 1.146816

H -3.070150 0.918786 1.146876

H -1.660622 -0.000085 1.887710

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -581.638 | 52.0435 | 87.8642 |
| 140.0722 | 169.1611 | 226.7923 |
| 349.7375 | 422.9284 | 436.0288 |
| 520.2384 | 566.0435 | 604.4288 |
| 634.9271 | 689.868 | 782.3013 |
| 797.8959 | 837.4894 | 880.9895 |
| 957.8567 | 985.2093 | 994.9585 |
| 1003.975 | 1026.941 | 1033.243 |
| 1061.953 | 1108.619 | 1178.939 |
| 1207.456 | 1248.286 | 1311.955 |
| 1358.011 | 1420.055 | 1426.193 |
| 1428.706 | 1479.247 | 1493.394 |
| 1508.13 | 1514.225 | 1597.059 |
| 1646.535 | 3036.63 | 3081.617 |
| 3101.49 | 3127.591 | 3172.531 |
| 3173.385 | 3184.654 | 3198.658 |
| 3206.323 | 3237.479 | 3249.598 |

***i38 – p2***

C 2.943502 -0.000104 0.008803

C 1.438791 0.000246 0.026316

C 0.718807 -1.197543 0.032387

C -0.662634 -1.203575 0.008137

C -1.394807 0.000008 -0.078407

C -0.662880 1.203612 0.008195

C 0.718691 1.197803 0.032343

C -2.890463 -0.000186 0.145075

H 3.319229 -0.012015 -1.019587

H 3.346840 -0.879392 0.516274

H 3.347136 0.890297 0.496112

H 1.256220 -2.140300 0.065557

H -1.200216 -2.146111 0.018619

H -1.560755 -0.000068 -1.887480

H -1.200573 2.146081 0.018743

H 1.255909 2.140660 0.065441

H -3.355968 -0.883877 -0.294868

H -3.356088 0.883776 -0.294193

H -3.105775 -0.000615 1.218280

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -966.938 | 51.8738 | 127.0476 |
| 183.6667 | 286.7652 | 305.9737 |
| 375.9995 | 410.9792 | 442.9888 |
| 456.9941 | 514.1546 | 552.3559 |
| 657.4287 | 719.3778 | 740.802 |
| 821.7594 | 844.5084 | 849.4608 |
| 973.4791 | 989.9427 | 995.684 |
| 1030.876 | 1036.27 | 1064.517 |
| 1068.093 | 1153.236 | 1210.38 |
| 1238.815 | 1250.025 | 1311.156 |
| 1343.156 | 1419.988 | 1421.179 |
| 1454.085 | 1491.483 | 1493.977 |
| 1495.402 | 1508.103 | 1547.183 |
| 1615.623 | 1673.088 | 3041.327 |
| 3046.454 | 3107.587 | 3118.628 |
| 3131.459 | 3142.044 | 3175.738 |
| 3175.846 | 3193.621 | 3196.784 |

***i37 – p45***

C -2.346637 0.321810 1.303982

C -1.364434 -0.219122 -0.670525

C -0.641041 -1.351856 -0.430714

C 0.824651 -1.310408 -0.118942

C 1.396854 0.082788 0.066915

C 0.628371 1.196189 -0.493429

C -0.658423 1.059338 -0.835431

C 2.555954 0.288102 0.698703

H -1.453654 0.455619 1.902705

H -2.946355 -0.556744 1.513006

H -2.887696 1.224176 1.038820

H -2.362559 -0.305466 -1.083045

H -1.123047 -2.323235 -0.455146

H 1.045963 -1.922247 0.762786

H 1.360647 -1.796226 -0.948616

H 1.121852 2.159300 -0.576144

H -1.219824 1.909288 -1.208176

H 2.976518 1.283827 0.790218

H 3.116382 -0.529331 1.140226

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -532.672 | 39.6114 | 111.596 |
| 127.2961 | 164.0879 | 271.1685 |
| 383.9728 | 408.186 | 487.6466 |
| 526.7756 | 546.6807 | 560.9126 |
| 599.3956 | 693.9896 | 709.6288 |
| 770.7632 | 815.4854 | 851.2677 |
| 905.686 | 929.555 | 948.1655 |
| 954.3233 | 964.7147 | 989.2527 |
| 1005.327 | 1033.708 | 1180.658 |
| 1196.417 | 1219.845 | 1319.888 |
| 1344.583 | 1397.552 | 1421.271 |
| 1423.256 | 1434.652 | 1452.516 |
| 1469.845 | 1543.691 | 1679.577 |
| 1724.005 | 2994.374 | 3055.048 |
| 3088.789 | 3147.859 | 3176.148 |
| 3183.033 | 3196.447 | 3207.203 |
| 3235.435 | 3249.411 | 3260.619 |

***i37 – p6***

C -2.801517 -0.062501 -0.349783

C -1.346568 0.038535 0.031997

C -0.654549 1.200503 -0.046836

C 0.815072 1.260446 0.241022

C 1.543061 -0.042414 -0.012831

C 0.743800 -1.259500 0.131804

C -0.593366 -1.221963 0.174307

C 2.841850 -0.089929 -0.318551

H -2.891084 -0.453897 -1.368579

H -3.289942 0.912525 -0.311786

H -3.339450 -0.742018 0.315046

H -1.692636 0.198477 1.940717

H -1.180472 2.133385 -0.223112

H 1.286489 2.076755 -0.312092

H 0.933227 1.510168 1.308287

H 1.267625 -2.209517 0.166397

H -1.164340 -2.139911 0.270104

H 3.356455 -1.037740 -0.435344

H 3.427432 0.812722 -0.456408

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -782.405 | 74.4434 | 185.1682 |
| 225.5014 | 275.677 | 309.5929 |
| 382.2872 | 402.7057 | 412.4924 |
| 479.9787 | 502.4816 | 564.9302 |
| 623.8035 | 712.7702 | 746.6687 |
| 780.8415 | 795.2823 | 824.903 |
| 915.6642 | 944.3268 | 952.2038 |
| 984.5319 | 1006.618 | 1011.612 |
| 1061.6 | 1090.428 | 1193.619 |
| 1200.52 | 1228.163 | 1312.453 |
| 1345.913 | 1366.621 | 1420.262 |
| 1430.182 | 1452.823 | 1471.965 |
| 1488.529 | 1498.981 | 1619.853 |
| 1689.797 | 1732.447 | 2979.136 |
| 3042.808 | 3091.986 | 3112.353 |
| 3140.719 | 3149.106 | 3176.074 |
| 3184.14 | 3197.681 | 3237.213 |

***i32 – p42***

C 2.133354 -1.279218 0.889838

C 1.125594 -0.298720 -0.773935

C -0.175710 -0.852309 -0.671862

C -1.201506 -0.160924 -0.053226

C -0.957753 1.144936 0.397984

C 0.277336 1.754343 0.181980

C 1.302310 1.064332 -0.436078

C -2.562980 -0.780420 0.129223

H 2.022397 -2.333153 0.655094

H 1.529020 -0.910755 1.710877

H 3.144072 -0.887649 0.832446

H 1.838160 -0.769031 -1.442218

H -0.350043 -1.858689 -1.039371

H -1.754932 1.698774 0.883661

H 0.426728 2.784464 0.487183

H 2.258451 1.542389 -0.615656

H -2.777945 -0.941320 1.189968

H -2.632033 -1.745547 -0.376379

H -3.347750 -0.131607 -0.269142

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -577.333 | 37.9523 | 108.1316 |
| 138.741 | 145.4494 | 240.6212 |
| 349.5952 | 402.3133 | 477.2827 |
| 525.0235 | 571.6423 | 584.3113 |
| 644.5639 | 676.7589 | 766.104 |
| 807.6077 | 863.4974 | 885.9665 |
| 901.564 | 991.589 | 1000.768 |
| 1004.862 | 1008.644 | 1052.843 |
| 1066.2 | 1105.994 | 1180.941 |
| 1195.595 | 1234.774 | 1324.146 |
| 1352.261 | 1419.54 | 1425.971 |
| 1428.692 | 1463.105 | 1491.288 |
| 1504.086 | 1527.272 | 1612.018 |
| 1641.887 | 3043.443 | 3082.269 |
| 3108.559 | 3131.186 | 3174.399 |
| 3177.206 | 3188.245 | 3193.905 |
| 3208.863 | 3238.727 | 3251.007 |

***i32 – p1***

C -2.497876 -1.017345 -0.145293

C -1.205184 -0.264028 0.075813

C 0.028434 -0.947898 0.002204

C 1.239171 -0.274261 -0.017012

C 1.226243 1.124519 -0.022216

C 0.023460 1.822341 -0.036597

C -1.181358 1.143190 -0.015163

C 2.545908 -1.023742 -0.019648

H -2.460407 -2.010218 0.306243

H -2.675777 -1.137928 -1.218526

H -3.346707 -0.480275 0.281380

H -1.353055 -0.327253 1.882242

H 0.020095 -2.034128 0.001246

H 2.165840 1.667551 -0.038071

H 0.030607 2.906120 -0.072702

H -2.118959 1.688469 -0.029206

H 3.244405 -0.598490 -0.744626

H 2.399898 -2.077378 -0.265241

H 3.021274 -0.973120 0.964722

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -981.233 | 42.6135 | 171.0109 |
| 192.9587 | 215.6632 | 275.6231 |
| 388.4217 | 439.4285 | 461.4139 |
| 481.6591 | 529.8271 | 554.4428 |
| 580.9013 | 701.1786 | 741.8312 |
| 793.4969 | 892.1052 | 915.0551 |
| 931.4845 | 1002.029 | 1006.167 |
| 1014.591 | 1038.645 | 1067.446 |
| 1067.701 | 1133.134 | 1187.259 |
| 1199.125 | 1279.678 | 1316.693 |
| 1347.448 | 1419.041 | 1421.877 |
| 1453.325 | 1491.972 | 1493.895 |
| 1496.158 | 1512.236 | 1530.313 |
| 1635.469 | 1663.594 | 3045.144 |
| 3047.235 | 3111.76 | 3119.727 |
| 3133.633 | 3143.384 | 3174.271 |
| 3179.438 | 3189.453 | 3206.769 |

***i30 – i36***

C -2.560075 -0.846191 0.020922

C -1.195104 -0.247470 0.122298

C -0.007394 -1.065304 -0.288521

C 1.333960 -0.399453 -0.033274

C 1.376492 1.050640 -0.124522

C 0.251212 1.809651 -0.081961

C -1.044894 1.224254 0.118446

C 2.425013 -1.135869 0.214491

H -2.606547 -1.829771 0.496853

H -2.842844 -0.976808 -1.034468

H -3.317386 -0.207596 0.483935

H -0.092742 -1.241903 -1.376358

H -0.035864 -2.053008 0.182166

H 2.350072 1.525306 -0.184088

H 0.321018 2.890751 -0.120069

H -1.079622 0.616605 1.209367

H -1.943257 1.824008 0.018864

H 3.394811 -0.671532 0.358109

H 2.377101 -2.217601 0.278416

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1882.36 | 99.984 | 159.3703 |
| 202.992 | 284.0164 | 307.4447 |
| 411.3166 | 424.8013 | 464.0123 |
| 497.4767 | 581.5944 | 672.9759 |
| 717.8158 | 765.5764 | 837.6516 |
| 855.817 | 887.7154 | 912.1342 |
| 946.1538 | 959.7825 | 970.1662 |
| 1006.652 | 1047.653 | 1084.807 |
| 1167.288 | 1177.516 | 1221.329 |
| 1253.17 | 1300.301 | 1325.777 |
| 1354.561 | 1401.788 | 1418.124 |
| 1456.095 | 1473.765 | 1480.883 |
| 1489.981 | 1506.037 | 1586.053 |
| 1686.995 | 2194.752 | 2938.827 |
| 2995.749 | 3074.168 | 3078.997 |
| 3121.32 | 3149.224 | 3186.144 |
| 3193.354 | 3211.697 | 3237.566 |

***i30 – p3***

C -2.536419 -0.883847 -0.015014

C -1.209866 -0.199816 0.051250

C -0.000543 -1.082243 0.199649

C 1.342630 -0.400258 0.025403

C 1.366333 1.057073 0.142046

C 0.239618 1.779048 0.110548

C -1.072836 1.144098 -0.029004

C 2.457537 -1.097723 -0.209664

H -2.666303 -1.569292 0.829979

H -2.609788 -1.487142 -0.927711

H -3.360318 -0.168455 -0.012799

H -0.079825 -1.931842 -0.488128

H -0.044952 -1.521829 1.207891

H 2.333777 1.544105 0.206116

H 0.280867 2.861368 0.157597

H -1.955217 1.774534 -0.006900

H -1.277784 1.381439 -1.995773

H 3.420006 -0.604854 -0.292812

H 2.440807 -2.176026 -0.328745

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -680.825 | 39.581 | 121.2738 |
| 182.0176 | 271.9952 | 296.7835 |
| 312.1466 | 362.6369 | 419.0748 |
| 491.4592 | 495.9954 | 526.1404 |
| 573.7447 | 702.6141 | 733.448 |
| 814.7247 | 872.8831 | 887.7767 |
| 921.7883 | 929.0248 | 966.0124 |
| 979.4523 | 1002.27 | 1010.437 |
| 1059.993 | 1076.073 | 1183.681 |
| 1205.979 | 1235.157 | 1317.734 |
| 1341.669 | 1378.287 | 1417.203 |
| 1431.024 | 1448.795 | 1469.069 |
| 1482.025 | 1486.861 | 1638.111 |
| 1686.336 | 1730.457 | 3001.464 |
| 3030.626 | 3064.271 | 3086.852 |
| 3142.143 | 3153.317 | 3183.119 |
| 3190.026 | 3213.307 | 3241.02 |

***i30 – i35***

C -2.511773 -0.957007 0.084021

C -1.214750 -0.251029 -0.144964

C 0.044434 -1.050954 -0.130621

C 1.344735 -0.424316 -0.004616

C 1.360585 1.045409 -0.070154

C 0.254846 1.788734 -0.027867

C -1.130116 1.222436 0.129640

C 2.490119 -1.121799 0.142911

H -2.696717 -1.092790 1.160727

H -2.515247 -1.951079 -0.372237

H -3.354166 -0.394361 -0.328326

H -0.516043 -0.708774 -1.212614

H -0.049049 -2.122287 0.012641

H 2.331574 1.524918 -0.146254

H 0.338180 2.870728 -0.065458

H -1.467195 1.412840 1.165379

H -1.836563 1.772346 -0.504521

H 3.445684 -0.616037 0.216972

H 2.491061 -2.204338 0.203600

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1935.45 | 106.6649 | 154.842 |
| 218.8728 | 276.5805 | 318.9613 |
| 350.4168 | 404.3864 | 456.9397 |
| 508.6659 | 576.3534 | 643.6226 |
| 696.8945 | 776.5033 | 804.2774 |
| 852.4817 | 870.1872 | 911.9176 |
| 926.8199 | 961.1164 | 1006.937 |
| 1016.835 | 1036.21 | 1056.128 |
| 1159.8 | 1211.576 | 1213.716 |
| 1268.118 | 1299.019 | 1329.235 |
| 1366.257 | 1397.78 | 1422.063 |
| 1455.169 | 1469.305 | 1480.464 |
| 1487.602 | 1502.444 | 1633.412 |
| 1740.305 | 2197.671 | 2933.594 |
| 2988.236 | 3040.45 | 3077.388 |
| 3119.543 | 3159.629 | 3173.264 |
| 3188.57 | 3196.122 | 3250.381 |

***i31 – i33***

C -2.578962 -0.849335 -0.101843

C -1.250206 -0.187746 0.124968

C -0.033901 -1.035692 0.170917

C 1.282745 -0.471896 0.025864

C 1.412609 1.031637 0.206917

C 0.160132 1.789246 -0.136548

C -1.060063 1.218560 -0.119053

C 2.362859 -1.233463 -0.234722

H -2.651147 -1.799606 0.434133

H -2.722966 -1.062634 -1.168047

H -3.400639 -0.210907 0.230479

H -0.174853 -2.108620 0.102530

H -0.691510 -0.585841 1.232890

H 2.258015 1.397853 -0.382783

H 1.673774 1.233674 1.257916

H 0.256692 2.851744 -0.332278

H -1.947067 1.818508 -0.297246

H 3.346050 -0.792489 -0.352503

H 2.282377 -2.309547 -0.344082

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1888.36 | 83.5136 | 159.9186 |
| 219.6904 | 287.0987 | 309.8815 |
| 414.1763 | 442.3332 | 501.0148 |
| 528.33 | 554.5279 | 660.0897 |
| 696.5138 | 720.9859 | 796.5233 |
| 855.2651 | 863.2358 | 933.6855 |
| 945.3566 | 965.3899 | 974.0469 |
| 1022.986 | 1039.011 | 1057.474 |
| 1165.9 | 1188.178 | 1228.345 |
| 1257.135 | 1307.392 | 1339.048 |
| 1344.116 | 1404.071 | 1425.495 |
| 1450.463 | 1467.199 | 1477.624 |
| 1494.602 | 1508.317 | 1635.003 |
| 1641.316 | 2115.737 | 2980.217 |
| 3027.954 | 3081.237 | 3097.034 |
| 3129.837 | 3150.907 | 3181.181 |
| 3199.696 | 3203.572 | 3240.564 |

***i31 – p3***

C -2.604639 -0.770752 -0.072005

C -1.254328 -0.129032 -0.009456

C -0.093002 -1.024238 0.345774

C 1.265701 -0.464470 -0.003421

C 1.378195 0.996315 0.038383

C 0.274187 1.767138 -0.092390

C -1.052352 1.184631 -0.186455

C 2.302080 -1.241762 -0.322995

H -2.830111 -1.285694 0.869029

H -2.637939 -1.528060 -0.862824

H -3.391623 -0.038547 -0.260794

H -0.223511 -2.014841 -0.100785

H -0.130108 -1.177909 1.436408

H 2.367632 1.438188 -0.004454

H 1.584318 1.151415 2.197972

H 0.373624 2.845449 -0.148700

H -1.891123 1.840413 -0.397148

H 3.283035 -0.818596 -0.510862

H 2.200764 -2.318791 -0.402451

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -537.547 | 100.4084 | 147.3914 |
| 206.8674 | 236.4631 | 276.496 |
| 300.6162 | 353.6639 | 418.338 |
| 477.8869 | 488.332 | 518.4463 |
| 587.6054 | 701.6079 | 741.7143 |
| 801.3142 | 876.14 | 879.781 |
| 914.0303 | 934.4336 | 957.3403 |
| 985.2648 | 989.1289 | 1015.58 |
| 1067.159 | 1084.166 | 1181.979 |
| 1202.708 | 1231.679 | 1319.957 |
| 1343.9 | 1381.935 | 1421.702 |
| 1434.834 | 1457.083 | 1473.385 |
| 1482.526 | 1500.615 | 1596.324 |
| 1707.948 | 1738.296 | 2992.513 |
| 3033.553 | 3076.407 | 3090.623 |
| 3135.246 | 3152.184 | 3184.478 |
| 3195.6 | 3212.697 | 3240.611 |

***i19 – p6***

C -2.926548 0.049064 -0.083383

C -1.429492 -0.037928 0.008019

C -0.760844 -1.194323 -0.009681

C 0.734041 -1.269162 0.127217

C 1.454571 0.044910 -0.086279

C 0.659838 1.259185 0.068062

C -0.679268 1.219249 0.115857

C 2.762897 0.100348 -0.373414

H -3.342816 0.534000 0.805806

H -3.379966 -0.939371 -0.176469

H -3.229926 0.647349 -0.948770

H -1.298628 -2.135410 -0.079984

H 0.961871 -1.621559 1.144826

H 1.139416 -2.032616 -0.543616

H 1.184728 2.208793 0.097775

H -1.244141 2.142868 0.201669

H 3.699309 -0.084883 1.925712

H 3.273017 1.051096 -0.482516

H 3.345981 -0.798323 -0.542815

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -309.493 | 55.2738 | 107.0304 |
| 137.6063 | 172.3746 | 237.659 |
| 277.4278 | 308.8099 | 407.5865 |
| 428.4462 | 480.3408 | 575.2893 |
| 621.6159 | 725.6004 | 746.8121 |
| 782.5177 | 811.6791 | 829.2351 |
| 909.6298 | 945.1701 | 959.8392 |
| 983.6876 | 1004.458 | 1015.302 |
| 1076.161 | 1090.947 | 1203.184 |
| 1206.505 | 1231.259 | 1317.291 |
| 1346.226 | 1376.076 | 1425.151 |
| 1435.083 | 1452.819 | 1476.534 |
| 1488.222 | 1502.31 | 1662.66 |
| 1684.444 | 1762.981 | 3002.328 |
| 3037.747 | 3079.951 | 3097.976 |
| 3133.096 | 3156.555 | 3178.324 |
| 3180.957 | 3201.341 | 3246.438 |

***i30 – p43***

C -2.118465 -1.167348 -0.375152

C -1.182121 -0.394194 0.185291

C 0.111916 -0.941053 0.722093

C 1.300914 -0.277745 0.057996

C 1.150418 1.154087 -0.218832

C -0.016209 1.791394 -0.107275

C -1.304067 1.103385 0.263038

C 2.421211 -0.940599 -0.229237

H -2.019451 -2.247337 -0.392417

H -1.498928 -1.188958 -2.424298

H -3.053489 -0.750846 -0.734455

H 0.160227 -2.025416 0.606414

H 0.163733 -0.719202 1.797674

H 2.038289 1.697477 -0.528251

H -0.068948 2.857717 -0.304595

H -1.584556 1.397452 1.285466

H -2.111995 1.451837 -0.386965

H 3.272494 -0.438330 -0.676606

H 2.521042 -2.001962 -0.029510

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -460.676 | 92.3907 | 100.2039 |
| 189.6793 | 250.1643 | 305.3323 |
| 358.6606 | 411.7283 | 438.3215 |
| 470.5255 | 546.2872 | 571.1321 |
| 688.7834 | 726.1104 | 770.6119 |
| 813.825 | 860.5979 | 920.1302 |
| 933.3263 | 939.2083 | 947.2796 |
| 951.204 | 998.1782 | 1009.954 |
| 1015.483 | 1027.211 | 1173.992 |
| 1199.482 | 1231.239 | 1298.956 |
| 1316.861 | 1338.696 | 1353.294 |
| 1412.159 | 1450.352 | 1460.935 |
| 1470.329 | 1482.558 | 1697.29 |
| 1706.679 | 1751.249 | 3009.254 |
| 3019.245 | 3089.269 | 3117.068 |
| 3150.843 | 3155.354 | 3173.397 |
| 3196.94 | 3240.639 | 3242.786 |

***i31 – p43***

C -2.400567 -0.764634 -0.377843

C -1.228209 -0.201428 -0.057566

C -0.102112 -0.985289 0.578525

C 1.239204 -0.494452 0.099394

C 1.451918 0.984501 0.293890

C 0.225826 1.777580 -0.073682

C -0.977651 1.226617 -0.251151

C 2.139337 -1.287285 -0.468409

H -3.517508 -0.593509 1.684854

H -2.568198 -1.829345 -0.260604

H -3.202828 -0.181524 -0.817112

H -0.221898 -2.054440 0.393564

H -0.164991 -0.829532 1.665275

H 2.309105 1.327355 -0.292666

H 1.700647 1.185345 1.346547

H 0.352483 2.847449 -0.208291

H -1.819039 1.845326 -0.548846

H 3.092072 -0.902963 -0.818339

H 1.953689 -2.347816 -0.603322

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -284.447 | 98.2215 | 119.4481 |
| 140.3261 | 181.5556 | 314.5786 |
| 358.1265 | 406.5297 | 439.0338 |
| 470.2843 | 546.8477 | 574.4974 |
| 697.7707 | 724.8166 | 744.0813 |
| 819.3186 | 864.1913 | 917.3324 |
| 932.5242 | 939.2216 | 945.4289 |
| 953.0611 | 998.9313 | 1012.758 |
| 1019.493 | 1029.798 | 1176.561 |
| 1206.739 | 1237.139 | 1301.485 |
| 1320.897 | 1340.468 | 1357.384 |
| 1414.14 | 1456.852 | 1463.935 |
| 1472.835 | 1486.096 | 1678.2 |
| 1725.006 | 1760.007 | 3008.467 |
| 3017.725 | 3087.142 | 3117.252 |
| 3147.291 | 3157.924 | 3170.925 |
| 3194.139 | 3233.703 | 3248.26 |

***i8 – p3***

C 2.572074 -0.934663 -0.064833

C 1.276412 -0.187397 0.000944

C 0.029602 -1.019943 0.165348

C -1.277948 -0.297102 -0.079407

C -1.252989 1.157511 0.029543

C -0.093058 1.831130 0.057445

C 1.193070 1.147263 -0.020205

C -2.409792 -0.962176 -0.350838

H 2.601104 -1.585465 -0.945805

H 2.690277 -1.582654 0.811276

H 3.426188 -0.256628 -0.108632

H 0.026610 -1.392612 1.201832

H 0.089625 -1.914691 -0.463212

H -2.201878 1.683690 0.037232

H -0.097014 2.914727 0.107132

H 2.094394 1.747189 -0.096508

H -3.350978 -0.439144 -0.479615

H -3.083170 -1.543657 1.993049

H -2.419386 -2.038498 -0.484729

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -264.732 | 53.19 | 110.6568 |
| 132.4853 | 148.2568 | 203.7069 |
| 292.893 | 336.5894 | 416.73 |
| 465.7359 | 491.6159 | 513.2424 |
| 578.8419 | 706.5367 | 737.1182 |
| 814.2171 | 874.1593 | 876.3841 |
| 909.5433 | 927.9238 | 950.801 |
| 979.7606 | 1001.924 | 1009.057 |
| 1066.721 | 1081.442 | 1181.454 |
| 1204.687 | 1234.233 | 1320.16 |
| 1341.339 | 1379.188 | 1416.321 |
| 1433.361 | 1445.442 | 1469.216 |
| 1483.31 | 1487.837 | 1662.682 |
| 1682.121 | 1751.466 | 2997.047 |
| 3031.529 | 3070.577 | 3087.373 |
| 3136.632 | 3156.305 | 3182.459 |
| 3191.888 | 3211.494 | 3245.15 |

***i33 – p45***

C 2.371065 -1.041157 0.986328

C 1.002388 -0.381641 -0.848989

C -0.195207 -1.001998 -0.623196

C -1.302885 -0.320356 0.008675

C -1.034585 1.061124 0.579055

C 0.173222 1.745183 0.001214

C 1.126226 1.063928 -0.633843

C -2.515566 -0.892065 0.104653

H 2.371136 -2.118361 0.873941

H 1.756211 -0.621564 1.772186

H 3.281678 -0.511373 0.731826

H 1.746391 -0.874072 -1.462920

H -0.340955 -2.032327 -0.931378

H -0.876388 0.959013 1.663104

H -1.921940 1.691191 0.469882

H 0.270884 2.814184 0.158901

H 2.012898 1.565163 -1.006300

H -3.358302 -0.370627 0.545570

H -2.689554 -1.899328 -0.258195

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -438.287 | 63.7536 | 73.0236 |
| 91.5879 | 149.4269 | 280.8033 |
| 386.4981 | 447.441 | 456.2346 |
| 475.0298 | 490.9479 | 533.9588 |
| 600.5418 | 660.7498 | 729.5824 |
| 775.4801 | 781.4026 | 822.7327 |
| 880.266 | 927.5389 | 945.6481 |
| 950.8801 | 965.7803 | 993.026 |
| 1010.962 | 1033.763 | 1174.535 |
| 1201.548 | 1230.119 | 1321.105 |
| 1338.208 | 1401.366 | 1412.256 |
| 1415.566 | 1435.119 | 1461.71 |
| 1470.592 | 1521.912 | 1648.287 |
| 1722.518 | 3003.962 | 3087.41 |
| 3103.125 | 3154.639 | 3185.269 |
| 3190.535 | 3207.254 | 3221.035 |
| 3243.798 | 3269.235 | 3280 |

***i33 – p47***

C -2.549406 -0.847759 -0.080177

C -1.172402 -0.253376 0.046070

C -0.053626 -1.029039 0.070443

C 1.282595 -0.464829 0.011834

C 1.396964 1.028946 0.226940

C 0.158291 1.790642 -0.146409

C -1.031063 1.193252 -0.190636

C 2.359043 -1.236272 -0.193109

H -2.562255 -1.895649 0.223152

H -2.882581 -0.785930 -1.122194

H -3.272978 -0.302568 0.529956

H -1.262732 -0.113673 2.069325

H -0.149970 -2.110198 0.108175

H 2.273928 1.425081 -0.291340

H 1.574998 1.202155 1.300039

H 0.249270 2.857642 -0.319694

H -1.931397 1.759362 -0.406918

H 3.353873 -0.812396 -0.276303

H 2.267468 -2.313217 -0.283933

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -721.294 | 97.2153 | 150.2086 |
| 183.8703 | 288.6364 | 336.9192 |
| 362.1559 | 406.1769 | 437.9556 |
| 455.9379 | 532.319 | 545.4822 |
| 567.1099 | 686.7606 | 708.9024 |
| 753.3822 | 863.8459 | 873.4212 |
| 904.7625 | 939.9723 | 957.2309 |
| 984.1315 | 1011.704 | 1026.167 |
| 1047.886 | 1054.148 | 1190.19 |
| 1205.023 | 1235.502 | 1317.897 |
| 1350.387 | 1375.649 | 1409.741 |
| 1439.477 | 1454.071 | 1463.455 |
| 1482.114 | 1495.225 | 1594.297 |
| 1678.832 | 1730.976 | 2996.817 |
| 3043.092 | 3099.536 | 3114.053 |
| 3144.256 | 3152.41 | 3180.752 |
| 3181.525 | 3205.7 | 3242.025 |

***i35 – p44***

C -2.065222 -1.270090 1.045752

C -0.998447 -0.378634 -0.853794

C 0.244971 -0.917714 -0.736273

C 1.320035 -0.234570 -0.038468

C 1.006146 1.100337 0.488752

C -0.161183 1.701659 0.259649

C -1.249493 1.077953 -0.562187

C 2.533540 -0.790625 0.131759

H -1.533178 -0.677183 1.779821

H -1.813461 -2.321506 0.985968

H -3.092832 -0.997350 0.831754

H -1.738905 -0.889797 -1.459108

H 0.431972 -1.926498 -1.090801

H 1.771287 1.597890 1.076988

H -0.344819 2.695286 0.656864

H -2.219076 1.217438 -0.074013

H -1.327735 1.617147 -1.518350

H 3.324671 -0.268817 0.658561

H 2.759988 -1.776502 -0.258828

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -465.924 | 86.8318 | 94.7276 |
| 130.3904 | 207.3587 | 328.6946 |
| 367.3433 | 378.2031 | 477.9442 |
| 482.9017 | 520.2108 | 572.7417 |
| 609.2664 | 670.541 | 778.9565 |
| 794.2252 | 803.52 | 822.2718 |
| 891.2311 | 893.1538 | 940.0698 |
| 954.2695 | 969.0171 | 989.6774 |
| 1013.081 | 1032.204 | 1172.604 |
| 1209.375 | 1225.717 | 1334.155 |
| 1387.317 | 1388.379 | 1416.746 |
| 1422.435 | 1441.917 | 1468.847 |
| 1476.803 | 1566.192 | 1646.73 |
| 1741.845 | 3006.464 | 3071.132 |
| 3098.11 | 3155.658 | 3174.641 |
| 3183.154 | 3197.113 | 3205.009 |
| 3246.773 | 3262.001 | 3275.004 |

***i35 – p46***

C 2.488348 -0.940231 -0.075435

C 1.132176 -0.299943 0.032944

C -0.009287 -1.024512 -0.018333

C -1.334778 -0.419998 -0.019008

C -1.380844 1.045222 0.032916

C -0.276462 1.789091 -0.000439

C 1.096631 1.201249 -0.109029

C -2.451642 -1.164266 -0.051922

H 2.889644 -0.793305 -1.084706

H 2.441312 -2.012283 0.122341

H 3.195426 -0.490323 0.626051

H 1.095259 -0.269303 2.044490

H 0.047734 -2.109418 -0.001464

H -2.357234 1.514437 0.100982

H -0.350516 2.871531 0.034871

H 1.529206 1.462300 -1.087309

H 1.764712 1.659557 0.629123

H -3.434056 -0.705727 -0.048530

H -2.406334 -2.247138 -0.086016

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -718.547 | 112.7264 | 164.8934 |
| 219.5348 | 289.1501 | 337.3275 |
| 378.3345 | 410.987 | 470.0226 |
| 484.2458 | 497.817 | 546.7634 |
| 588.9342 | 684.1999 | 710.4336 |
| 793.4263 | 875.3562 | 882.9482 |
| 903.0589 | 928.5809 | 950.8266 |
| 977.9556 | 1010.293 | 1020.868 |
| 1045.345 | 1065.641 | 1177.748 |
| 1206.979 | 1228.821 | 1321.027 |
| 1366.818 | 1400.196 | 1418.526 |
| 1436.752 | 1464.999 | 1468.692 |
| 1489.868 | 1496.874 | 1650.384 |
| 1669.702 | 1751.146 | 3003.295 |
| 3039.244 | 3059.043 | 3105.321 |
| 3143.92 | 3162.234 | 3177.279 |
| 3178.308 | 3199.821 | 3253.284 |

***i36 – p45***

C 1.669963 -1.593195 1.080392

C 1.196039 -0.110116 -0.826281

C -0.184437 -0.653080 -1.091357

C -1.224693 -0.157046 -0.110816

C -0.997222 1.176915 0.436706

C 0.208024 1.778398 0.344070

C 1.340539 1.113379 -0.257388

C -2.303931 -0.879373 0.211090

H 1.772757 -2.526370 0.539272

H 0.733111 -1.399337 1.586996

H 2.567188 -1.139825 1.480590

H 2.027817 -0.574604 -1.342956

H -0.185154 -1.743852 -1.136078

H -0.477184 -0.301831 -2.093493

H -1.814187 1.657124 0.965654

H 0.353548 2.761258 0.779501

H 2.318755 1.575678 -0.190439

H -3.070243 -0.481574 0.868020

H -2.452098 -1.881964 -0.175561

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -364.153 | 88.2349 | 99.2975 |
| 129.4772 | 185.1686 | 288.4849 |
| 391.6509 | 426.8055 | 438.6112 |
| 473.9216 | 499.7098 | 564.8519 |
| 605.1714 | 672.7329 | 747.1323 |
| 775.9265 | 782.7131 | 830.687 |
| 898.2904 | 929.8846 | 947.3824 |
| 962.6319 | 975.8157 | 997.7267 |
| 1005.875 | 1038.844 | 1182.012 |
| 1197.956 | 1218.144 | 1318.767 |
| 1333.575 | 1401.173 | 1415.189 |
| 1421.873 | 1442.221 | 1455.923 |
| 1480.409 | 1514.64 | 1659.3 |
| 1704.287 | 2997.779 | 3105.817 |
| 3112.141 | 3152.291 | 3176.025 |
| 3190.305 | 3198.847 | 3213.143 |
| 3240.467 | 3275.959 | 3285.555 |

***i36 – p3***

C -2.555396 -0.800843 0.029782

C -1.208273 -0.142496 0.009681

C -0.032592 -1.011926 -0.365289

C 1.318207 -0.406846 -0.059919

C 1.388596 1.051120 -0.104281

C 0.273089 1.800114 -0.053617

C -1.040164 1.195586 0.073355

C 2.391461 -1.157145 0.209004

H -2.578913 -1.629615 0.742434

H -2.782899 -1.216913 -0.958870

H -3.343273 -0.093807 0.294751

H -0.790456 -0.349684 2.122959

H -0.100023 -1.170563 -1.454007

H -0.123218 -2.000688 0.091679

H 2.368369 1.517075 -0.119832

H 0.345799 2.882162 -0.049961

H -1.895669 1.839756 0.248997

H 3.364790 -0.705730 0.368439

H 2.325919 -2.237380 0.281108

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -537.939 | 103.6555 | 164.4699 |
| 202.0768 | 281.8299 | 308.3085 |
| 342.6708 | 377.206 | 419.483 |
| 482.3875 | 488.3819 | 516.0567 |
| 589.0871 | 684.2102 | 740.1304 |
| 799.5513 | 874.3244 | 878.3524 |
| 911.3496 | 931.9555 | 961.7282 |
| 986.7704 | 994.7005 | 1014.918 |
| 1059.161 | 1085.223 | 1183.584 |
| 1201.872 | 1234.075 | 1320.498 |
| 1341.268 | 1380.009 | 1420.904 |
| 1435.018 | 1461.063 | 1475.345 |
| 1484.244 | 1496.725 | 1611.644 |
| 1685.007 | 1724.552 | 2988.838 |
| 3037.633 | 3093.126 | 3103.943 |
| 3144.4 | 3150.868 | 3186.551 |
| 3195.82 | 3213.035 | 3239.865 |

***i30 – p46***

C -2.501241 -0.924960 -0.096575

C -1.150374 -0.284159 -0.056902

C -0.012006 -1.010635 0.024946

C 1.325769 -0.398132 -0.026469

C 1.364714 1.065831 0.007515

C 0.256878 1.804954 0.025268

C -1.119810 1.215038 -0.000286

C 2.438261 -1.136804 -0.108374

H -3.063433 -0.687481 0.814608

H -2.430761 -2.010652 -0.179829

H -3.088146 -0.548861 -0.941306

H -0.063715 -2.090161 -0.084095

H -0.087481 -1.354697 1.955300

H 2.340699 1.540805 0.015696

H 0.328390 2.887856 0.053936

H -1.681855 1.549240 0.885353

H -1.681298 1.621718 -0.853781

H 3.417764 -0.674311 -0.154553

H 2.396690 -2.220253 -0.126072

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -724.75 | 93.6802 | 114.2323 |
| 184.5505 | 267.2623 | 295.0597 |
| 321.6667 | 374.8245 | 420.039 |
| 485.7444 | 508.6162 | 542.6435 |
| 593.6542 | 708.4731 | 711.7194 |
| 795.3319 | 883.7707 | 904.4821 |
| 912.5915 | 931.3785 | 969.2915 |
| 973.2737 | 1008.826 | 1018.01 |
| 1045.246 | 1062.26 | 1182.593 |
| 1207.129 | 1228.726 | 1317.218 |
| 1361.647 | 1403.197 | 1417.292 |
| 1435.661 | 1455.99 | 1468.484 |
| 1481.718 | 1490.546 | 1653.113 |
| 1694.186 | 1762.391 | 2998.869 |
| 3023.621 | 3030.523 | 3089.687 |
| 3137.215 | 3161.13 | 3176.401 |
| 3179.363 | 3203.158 | 3250.894 |

***i31 – p47***

C -2.573575 -0.802882 -0.041143

C -1.185877 -0.237529 -0.047643

C -0.084635 -1.014556 0.086133

C 1.266608 -0.454138 -0.006176

C 1.388092 1.024584 0.279217

C 0.155029 1.804401 -0.076026

C -1.032529 1.207986 -0.207032

C 2.321233 -1.213946 -0.308445

H -3.154151 -0.382889 0.787168

H -2.564989 -1.888803 0.064255

H -3.100602 -0.547680 -0.966419

H -0.184408 -2.095765 0.099164

H -0.209297 -1.161031 2.272777

H 2.269460 1.440089 -0.216379

H 1.559395 1.152621 1.359655

H 0.246461 2.880758 -0.177676

H -1.920478 1.792958 -0.426597

H 3.313620 -0.789641 -0.416425

H 2.218918 -2.284152 -0.452827

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -456.252 | 109.9989 | 137.4999 |
| 173.01 | 209.2957 | 250.6275 |
| 297.0099 | 337.3102 | 427.1846 |
| 453.0704 | 527.2979 | 552.0258 |
| 577.5938 | 701.6832 | 719.8991 |
| 760.7194 | 875.5035 | 885.4012 |
| 921.9987 | 944.4212 | 957.4426 |
| 984.5153 | 1008.891 | 1023.536 |
| 1047.393 | 1064.51 | 1197.475 |
| 1208.276 | 1229.032 | 1317.303 |
| 1352.807 | 1371.219 | 1413.681 |
| 1446.281 | 1454.073 | 1464.417 |
| 1484.621 | 1493.437 | 1619.398 |
| 1707.908 | 1737.704 | 2996.51 |
| 3040.409 | 3097.703 | 3100.359 |
| 3141.709 | 3151.307 | 3175.315 |
| 3184.019 | 3200.057 | 3239.761 |

***i1 – i69***

C -0.842894 2.064530 -0.150296

C -0.466359 0.624694 -0.179765

C 3.503308 -0.293696 0.197417

C 2.090127 0.036357 0.062940

C 0.920480 0.303277 -0.043864

C -1.465077 -0.444844 0.034281

C -2.695582 -0.189128 0.494661

C -1.029045 -1.843237 -0.317211

H -0.064246 2.806795 -0.058672

H -1.883847 2.348790 -0.155620

H -0.629719 1.238658 -1.247730

H 3.653519 -1.374505 0.136275

H 3.899056 0.049274 1.156999

H 4.090533 0.172933 -0.597871

H -3.421041 -0.986814 0.606362

H -3.008752 0.802930 0.795716

H -1.849241 -2.550331 -0.185531

H -0.193685 -2.157656 0.314664

H -0.682329 -1.897789 -1.353572

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1855.51 | 24.1153 | 60.1399 |
| 88.8029 | 155.3513 | 174.137 |
| 269.8574 | 295.846 | 320.2414 |
| 387.5745 | 418.8729 | 434.5443 |
| 486.1933 | 560.737 | 573.5971 |
| 640.7592 | 653.8766 | 763.5284 |
| 839.0956 | 900.7009 | 961.0981 |
| 1015.638 | 1049.032 | 1054.55 |
| 1057.122 | 1072.534 | 1170.739 |
| 1204.341 | 1330.69 | 1357.617 |
| 1418.217 | 1421.042 | 1425.32 |
| 1451.652 | 1482.445 | 1483.279 |
| 1486.321 | 1500.56 | 1685.529 |
| 2234.779 | 2353.066 | 3043.867 |
| 3045.822 | 3109.902 | 3114.222 |
| 3118.859 | 3140.668 | 3162.205 |
| 3190.876 | 3248.726 | 3317.477 |

***i12 – i13***

C -1.986153 -1.717427 -0.197528

C -2.197640 -0.275094 -0.494017

C -1.284360 0.537925 0.037546

C -0.272140 -0.222371 0.861672

C -1.192489 2.021725 -0.107959

C 3.618684 -0.143330 -0.404965

C 2.236955 -0.163806 0.058345

C 1.093773 -0.176952 0.441513

H -2.727121 -2.226691 0.419064

H -1.598547 -2.341545 -1.003267

H -3.029675 0.080323 -1.096702

H -0.395756 -0.107796 1.942270

H -0.837549 -1.380468 0.586317

H -0.230495 2.300660 -0.549268

H -1.252679 2.514122 0.868296

H -1.992249 2.409435 -0.742560

H 3.791503 -0.924372 -1.150330

H 4.312491 -0.306209 0.423509

H 3.860293 0.818515 -0.864970

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1883.97 | 64.5446 | 84.5566 |
| 93.167 | 167.8091 | 214.2727 |
| 228.4182 | 246.9739 | 345.1512 |
| 373.1434 | 419.1873 | 457.3327 |
| 549.4892 | 601.7041 | 634.3038 |
| 771.1781 | 833.6231 | 897.1603 |
| 923.2052 | 941.498 | 1034.678 |
| 1051.96 | 1052.826 | 1055.213 |
| 1074.592 | 1104.512 | 1197.929 |
| 1210.805 | 1290.976 | 1343.373 |
| 1391.35 | 1416.72 | 1419.876 |
| 1449.213 | 1479.688 | 1481.967 |
| 1490.24 | 1494.226 | 1655.268 |
| 1754.222 | 2339.628 | 3041.059 |
| 3047.731 | 3084.961 | 3096.445 |
| 3103.368 | 3115.701 | 3124.27 |
| 3135.23 | 3172.355 | 3175.784 |

***i12 – p9a***

C 3.162310 -0.954492 0.039197

C 2.540692 0.219774 -0.069191

C 1.090913 0.434429 -0.084389

C 0.205152 -0.787694 0.047109

C 0.597357 1.676859 -0.187577

C -3.850239 -0.076754 -0.025836

C -2.412687 -0.322890 -0.003656

C -1.230459 -0.528885 0.017612

H 4.244230 -1.012058 0.041160

H 2.627121 -1.893651 0.129239

H 3.140978 1.122448 -0.154479

H 0.458942 -1.492078 -0.754145

H 0.457023 -1.298854 0.984437

H -0.469385 1.857771 -0.236235

H 1.260071 2.527675 -0.300747

H 0.363596 2.262891 1.984016

H -4.122489 0.701650 0.691137

H -4.402275 -0.983353 0.233864

H -4.176044 0.245470 -1.017855

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -412.304 | 30.2132 | 55.9375 |
| 89.3692 | 136.2742 | 159.769 |
| 213.3686 | 216.0612 | 238.803 |
| 294.1526 | 388.0361 | 417.6251 |
| 421.772 | 517.0392 | 535.6675 |
| 659.4085 | 802.5731 | 814.4994 |
| 840.2729 | 944.2629 | 951.5168 |
| 959.6592 | 974.9938 | 1037.73 |
| 1058.48 | 1059.218 | 1066.043 |
| 1181.067 | 1253.677 | 1280.341 |
| 1334.395 | 1393.888 | 1420.436 |
| 1425.892 | 1463.544 | 1477.184 |
| 1485.983 | 1486.518 | 1664.174 |
| 1714.497 | 2398.687 | 3033.448 |
| 3047.82 | 3065.244 | 3121.043 |
| 3121.377 | 3155.98 | 3160.93 |
| 3167.428 | 3246.949 | 3256.491 |

***i19 – i39***

C -2.819952 -0.156096 -0.156676

C -1.437048 0.296227 0.145614

C -0.829368 -1.046197 0.350270

C 0.529646 -1.209283 -0.283511

C 1.363850 0.045554 -0.030102

C 0.765208 1.239138 0.081614

C -0.694868 1.386070 -0.029373

C 2.850262 -0.135719 0.016219

H -3.507388 -0.275067 0.680546

H -2.079229 -1.383192 -0.229532

H -3.280358 0.137202 -1.097493

H -0.956871 -1.449875 1.358387

H 1.042966 -2.093647 0.102841

H 0.446315 -1.346836 -1.371714

H 1.369297 2.131857 0.214582

H -1.120743 2.346948 -0.297917

H 3.141449 -0.783996 0.850171

H 3.369617 0.818470 0.125741

H 3.208567 -0.620026 -0.899945

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2292.89 | 114.0621 | 183.3099 |
| 206.9802 | 272.9619 | 312.3189 |
| 338.9974 | 399.548 | 452.4148 |
| 493.9042 | 540.2548 | 579.9488 |
| 730.1812 | 803.2946 | 819.9181 |
| 841.4707 | 891.6372 | 924.6973 |
| 932.7382 | 970.1663 | 981.782 |
| 1039.577 | 1067.29 | 1081.75 |
| 1100.194 | 1167.013 | 1206.557 |
| 1209.743 | 1303.025 | 1315.921 |
| 1333.814 | 1366.402 | 1385.276 |
| 1422.526 | 1427.373 | 1474.693 |
| 1485.156 | 1496.496 | 1692.168 |
| 1729.831 | 1835.051 | 3005.257 |
| 3029.484 | 3084.256 | 3085.865 |
| 3103.556 | 3105.073 | 3130.917 |
| 3182.925 | 3202.603 | 3204.423 |

***i37 – i39***

C 2.861856 -0.026835 0.023243

C 1.366836 -0.049608 -0.155640

C 0.622907 1.228203 -0.142450

C -0.808839 1.255937 0.294830

C -1.536141 -0.054546 0.041180

C -0.742184 -1.269977 0.123792

C 0.614027 -1.258322 0.065156

C -2.853026 -0.073237 -0.200950

H 3.114523 0.095003 1.082427

H 3.315500 0.806546 -0.520120

H 3.317691 -0.952796 -0.334307

H 1.000805 0.444350 -1.239582

H 1.201292 2.142696 -0.191263

H -0.832992 1.442925 1.382042

H -1.348860 2.083867 -0.171708

H -1.271901 -2.214555 0.190292

H 1.167103 -2.191036 0.111202

H -3.383065 -1.008495 -0.346794

H -3.432717 0.841804 -0.257148

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1892.11 | 86.1115 | 174.3918 |
| 215.0498 | 274.7716 | 304.6332 |
| 399.5378 | 431.9519 | 456.1435 |
| 542.8648 | 615.6037 | 638.1216 |
| 695.5422 | 730.6423 | 773.2558 |
| 796.3898 | 896.0891 | 926.949 |
| 943.6204 | 950.5378 | 985.1167 |
| 1009.789 | 1051.12 | 1077.787 |
| 1162.46 | 1178.88 | 1202.891 |
| 1255.023 | 1304.848 | 1330.088 |
| 1352.513 | 1418.025 | 1424.215 |
| 1433.94 | 1473.853 | 1482.557 |
| 1494.978 | 1509.992 | 1588.056 |
| 1689.102 | 2207.561 | 2959.363 |
| 3036.019 | 3085.126 | 3103.079 |
| 3129.417 | 3152.59 | 3180.853 |
| 3200.443 | 3209.545 | 3241.247 |

***i11 – p30***

C -3.499070 0.147592 0.282879

C -2.437754 -0.505891 -0.182995

C -1.058993 0.012945 -0.190678

C 0.004881 -1.036146 0.072822

C -0.776270 1.302688 -0.405594

C 3.900254 0.298198 0.049709

C 2.518551 -0.169140 0.053005

C 1.383453 -0.559309 0.058764

H -4.488740 -0.292940 0.248134

H -3.406653 1.134173 0.725565

H -2.568807 -1.517374 -0.565460

H -0.204164 -1.505524 1.042246

H -0.108731 -1.834985 -0.671225

H 0.248072 1.656069 -0.407855

H -0.929487 2.138075 1.716517

H -1.557455 2.007115 -0.665383

H 4.382042 0.086593 -0.907939

H 4.477277 -0.193287 0.836865

H 3.946329 1.376468 0.221057

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -372.387 | 44.7061 | 54.9081 |
| 84.8536 | 119.2166 | 148.384 |
| 184.053 | 213.2251 | 255.1998 |
| 302.423 | 356.2786 | 393.4151 |
| 417.5714 | 468.6694 | 593.8976 |
| 672.9857 | 787.1198 | 802.7225 |
| 858.5141 | 943.5478 | 961.2884 |
| 967.5075 | 973.9108 | 1028.104 |
| 1055.595 | 1062.518 | 1100.615 |
| 1177.835 | 1217.113 | 1254.021 |
| 1341.928 | 1380.663 | 1421.011 |
| 1430.459 | 1466.527 | 1473.684 |
| 1484.488 | 1490.424 | 1686.249 |
| 1721.903 | 2400.38 | 3030.821 |
| 3052.92 | 3060.415 | 3124.862 |
| 3126.353 | 3144.692 | 3158.783 |
| 3169.659 | 3249.241 | 3263.745 |

***i1 – i68***

C 0.973676 -1.293755 0.936921

C 0.361497 -0.736916 -0.300122

C -3.616127 0.285762 -0.119635

C -2.204297 -0.073643 -0.183002

C -1.043052 -0.372830 -0.241323

C 1.388884 0.338153 -0.039966

C 1.084909 1.496180 0.631899

C 2.718373 0.176654 -0.738100

H 0.513843 -1.078644 1.890089

H 1.777250 -2.014259 0.881120

H 0.585901 -1.309452 -1.201057

H -3.738000 1.363831 0.010835

H -4.108617 -0.214982 0.717623

H -4.131289 -0.003665 -1.038876

H 1.854176 2.232179 0.832145

H 0.086984 1.679660 1.011118

H 3.520839 0.659091 -0.176449

H 2.669742 0.641322 -1.728298

H 2.985993 -0.872715 -0.878286

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -630.056 | 69.8109 | 91.2281 |
| 96.1745 | 170.635 | 224.8719 |
| 278.6758 | 328.0906 | 351.092 |
| 385.837 | 418.7125 | 507.3958 |
| 546.1565 | 573.1642 | 579.3729 |
| 686.3105 | 754.601 | 759.155 |
| 835.39 | 968.1967 | 987.4461 |
| 1020.995 | 1059.122 | 1061.696 |
| 1063.861 | 1115.419 | 1175.269 |
| 1213.881 | 1273.088 | 1385.425 |
| 1403.562 | 1426.333 | 1431.568 |
| 1455.584 | 1485.974 | 1490.655 |
| 1497.796 | 1500.711 | 1543.452 |
| 2399.699 | 3047.07 | 3050.376 |
| 3103.446 | 3116.168 | 3121.376 |
| 3125.283 | 3138.764 | 3161.571 |
| 3182.253 | 3260.089 | 3306.054 |

***i13 – p7b***

C 3.087804 -0.926614 -0.370014

C 2.471244 0.151585 0.129231

C 1.028536 0.418236 0.070102

C 0.138411 -0.589674 0.132592

C 0.625732 1.861928 -0.033336

C -3.921498 -0.208207 -0.072792

C -2.471681 -0.333055 -0.001037

C -1.273117 -0.433735 0.058506

H 4.162161 -1.042992 -0.291279

H 2.920430 -2.431376 1.323020

H 2.550165 -1.674036 -0.943572

H 3.073760 0.919585 0.611087

H 0.502195 -1.603891 0.271226

H 1.046493 2.432904 0.801128

H -0.457928 1.977790 -0.022436

H 1.016173 2.304422 -0.955275

H -4.391345 -1.190878 -0.160083

H -4.219709 0.389358 -0.938076

H -4.314978 0.276323 0.824753

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -411.67 | 9.0604 | 81.1692 |
| 87.8341 | 108.7597 | 131.4124 |
| 160.2154 | 231.6205 | 242.9554 |
| 276.4982 | 302.6136 | 398.6258 |
| 414.3231 | 507.3333 | 517.7363 |
| 556.1239 | 714.8019 | 820.3912 |
| 846.6871 | 899.5283 | 960.4289 |
| 1008.635 | 1028.325 | 1052.354 |
| 1054.305 | 1057.808 | 1086.189 |
| 1206.436 | 1247.613 | 1321.695 |
| 1367.578 | 1418.415 | 1420.841 |
| 1458.248 | 1483.657 | 1484.108 |
| 1486.075 | 1491.924 | 1663.078 |
| 1705.452 | 2367.763 | 3038.618 |
| 3045.537 | 3097.918 | 3116.409 |
| 3121.362 | 3147.521 | 3151.255 |
| 3159.52 | 3171.308 | 3249.213 |

***i13 – p29***

C 2.776705 -1.581164 -0.338718

C 2.244313 -0.173787 -0.271151

C 1.117265 0.134762 0.316295

C 0.013738 -0.042852 1.051734

C 0.898363 2.445731 -0.312125

C -3.727993 -0.463593 -0.518020

C -2.391458 -0.311527 0.041284

C -1.281088 -0.193921 0.494323

H 2.896004 -1.895964 -1.379875

H 3.761398 -1.640977 0.135104

H 2.105721 -2.280807 0.160761

H 2.838598 0.600003 -0.747145

H 0.088379 0.048373 2.133126

H 1.790557 2.810630 0.181675

H -0.059187 2.706914 0.118553

H 0.935518 2.280777 -1.381401

H -4.074404 0.474295 -0.960575

H -4.441965 -0.755759 0.256001

H -3.739682 -1.229371 -1.297952

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -468.032 | 20.3377 | 32.9219 |
| 57.3725 | 78.4441 | 135.9341 |
| 160.6939 | 166.3631 | 185.5148 |
| 249.4081 | 304.8555 | 385.5872 |
| 425.5624 | 453.3682 | 462.9273 |
| 486.9854 | 565.0637 | 735.3659 |
| 786.9093 | 807.14 | 873.68 |
| 907.6135 | 1052.353 | 1057.158 |
| 1063.965 | 1089.688 | 1111.528 |
| 1209.872 | 1320.691 | 1408.787 |
| 1411.546 | 1415.718 | 1423.003 |
| 1430.576 | 1482.676 | 1484.361 |
| 1488.138 | 1498.652 | 1961.121 |
| 2348.26 | 3040.016 | 3044.206 |
| 3102.936 | 3103.709 | 3114.635 |
| 3119.832 | 3142.616 | 3147.439 |
| 3175.567 | 3276.104 | 3279.768 |

***i69 – p15***

C 0.841569 1.948307 0.200403

C 0.463265 0.671901 0.008714

C -3.490357 -0.358763 -0.209046

C -2.083489 0.010405 -0.130517

C -0.924214 0.326286 -0.066756

C 1.449671 -0.441015 -0.089033

C 2.557092 -0.306401 -0.816983

C 1.119888 -1.701009 0.663682

H 0.869995 2.088195 2.506621

H 0.112749 2.748664 0.230309

H 1.890685 2.207689 0.275503

H -3.612051 -1.442794 -0.146981

H -3.925916 -0.021858 -1.153237

H -4.057300 0.095891 0.607108

H 3.291370 -1.102936 -0.871748

H 2.753246 0.592440 -1.390447

H 1.917302 -2.438528 0.562014

H 0.188710 -2.137659 0.291561

H 0.970659 -1.487374 1.726512

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -374.851 | 22.8963 | 55.2585 |
| 90.1183 | 134.8737 | 149.041 |
| 186.3497 | 211.0292 | 262.9175 |
| 300.1701 | 328.933 | 405.4131 |
| 410.7096 | 484.0822 | 582.2276 |
| 639.454 | 676.4525 | 764.4912 |
| 796.5174 | 850.1542 | 944.3777 |
| 947.6688 | 971.0036 | 1033.715 |
| 1053.767 | 1058.185 | 1073.779 |
| 1085.311 | 1239.632 | 1348.388 |
| 1412.719 | 1419.935 | 1433.615 |
| 1448.773 | 1482.479 | 1483.13 |
| 1483.67 | 1499.971 | 1645.583 |
| 1727.315 | 2370.671 | 3044.684 |
| 3047.65 | 3110.15 | 3120.308 |
| 3123.441 | 3140.562 | 3153.353 |
| 3166.046 | 3242.641 | 3265.198 |

***i68 – p20***

C 0.997575 -0.728890 1.210967

C 0.226211 -0.689454 -0.129437

C -3.780689 0.175984 -0.207647

C -2.356439 -0.135215 -0.178390

C -1.182519 -0.389444 -0.152113

C 1.200275 0.366754 0.252578

C 1.310936 1.702943 0.205337

H 0.433501 -0.504790 2.109822

H 1.740100 -1.511021 1.312986

H 0.548181 -1.425255 -0.858363

H -3.946018 1.252423 -0.115438

H -4.307604 -0.319574 0.611771

H -4.230138 -0.155118 -1.147263

H 1.877914 2.242867 0.955822

H 0.913351 2.262339 -0.634292

C 3.112830 -0.386636 -0.885563

H 3.879368 0.044131 -0.253849

H 2.950284 0.078040 -1.849816

H 2.971984 -1.460294 -0.825772

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -484.796 | 16.8826 | 63.8288 |
| 82.8719 | 103.2781 | 174.0393 |
| 204.1792 | 234.2749 | 303.7351 |
| 320.6629 | 373.8987 | 482.2717 |
| 491.2881 | 505.3156 | 541.6033 |
| 584.0371 | 717.9512 | 766.5874 |
| 837.3558 | 857.7246 | 914.7833 |
| 937.215 | 1007.792 | 1032.358 |
| 1057.022 | 1058.745 | 1071.836 |
| 1107.58 | 1132.953 | 1217.71 |
| 1361.078 | 1417.724 | 1420.127 |
| 1423.659 | 1443.008 | 1477.034 |
| 1484.833 | 1486.679 | 1699.966 |
| 2391.571 | 3045.615 | 3096.553 |
| 3117.288 | 3119.013 | 3139.1 |
| 3144.94 | 3168.686 | 3230.808 |
| 3239.544 | 3260.212 | 3273.055 |

***i39 – p6***

C 2.821556 0.079135 0.293292

C 1.526798 0.055819 -0.034436

C 0.794483 -1.224943 -0.367262

C -0.684340 -1.168102 -0.101277

C -1.352218 -0.005495 -0.040671

C -0.604280 1.250618 -0.134553

C 0.736455 1.283205 -0.119086

C -2.838679 0.074839 0.151200

H 3.399126 -0.833446 0.394228

H 3.338781 1.016195 0.470114

H 1.250347 -2.069852 0.154619

H 0.929169 -1.424283 -1.441909

H -1.223765 -2.109469 -0.061593

H -0.510215 -1.373998 2.275945

H -1.168881 2.177734 -0.164358

H 1.265045 2.231255 -0.115309

H -3.308070 0.616762 -0.676458

H -3.081760 0.616348 1.071246

H -3.288427 -0.917696 0.210229

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -328.445 | 72.9869 | 132.1287 |
| 160.6375 | 195.8294 | 253.4712 |
| 282.3075 | 311.6722 | 408.664 |
| 426.3041 | 485.409 | 568.9321 |
| 626.2178 | 711.6813 | 746.7967 |
| 785.9445 | 819.0008 | 832.6634 |
| 915.9025 | 944.7797 | 960.3596 |
| 986.4887 | 1005.835 | 1012.978 |
| 1070.212 | 1087.264 | 1200.851 |
| 1202.977 | 1231.043 | 1313.851 |
| 1346.521 | 1371.219 | 1420.219 |
| 1435.021 | 1457.202 | 1475.802 |
| 1485.115 | 1498.695 | 1642.947 |
| 1702.748 | 1744.336 | 2992.442 |
| 3035.935 | 3093.512 | 3096.384 |
| 3135.064 | 3149.295 | 3172.373 |
| 3180.52 | 3194.678 | 3237.747 |

***i39 – p28***

C -2.836178 0.035877 -0.039732

C -1.506935 0.037768 0.081373

C -0.701670 -1.213120 0.336042

C 0.618208 -1.192110 -0.441974

C 1.398945 0.067262 -0.160241

C 0.608324 1.290240 -0.048066

C -0.732414 1.278450 0.017178

C 2.734833 0.080737 -0.043886

H -3.408315 -0.884314 0.008999

H -3.389652 0.957175 -0.188985

H -1.285023 -2.101166 0.082764

H -0.476263 -1.263981 1.408339

H 1.219689 -2.072941 -0.206356

H 0.395906 -1.225228 -1.515860

H 1.143729 2.234844 -0.036094

H -1.281963 2.214708 0.042642

H 2.984152 -0.353443 2.249828

H 3.277435 1.007544 0.108960

H 3.321629 -0.823827 -0.158406

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -324.854 | 79.5821 | 132.0041 |
| 165.3741 | 201.8081 | 296.2891 |
| 359.4363 | 384.9303 | 439.391 |
| 445.8972 | 558.8872 | 621.038 |
| 714.5381 | 749.76 | 765.6932 |
| 779.3586 | 805.0995 | 855.6551 |
| 929.2756 | 935.058 | 938.0897 |
| 984.9299 | 996.2147 | 1012.943 |
| 1035.636 | 1062.737 | 1181.396 |
| 1202.332 | 1247.503 | 1310.236 |
| 1346.084 | 1360.446 | 1362.437 |
| 1428.477 | 1445.687 | 1472.275 |
| 1486.134 | 1487.357 | 1655.66 |
| 1693.979 | 1730.588 | 3033.973 |
| 3042.145 | 3106.207 | 3108.148 |
| 3148.967 | 3151.412 | 3170.92 |
| 3192.066 | 3237.574 | 3242.15 |

***i13 – i14***

C 1.884259 1.934709 -0.077382

C 2.048396 0.479374 -0.390342

C 1.276357 -0.512205 0.053050

C 1.508278 -1.952575 -0.328416

H 2.789702 2.339222 0.386860

H 1.711929 2.509123 -0.993500

H 1.043040 2.111320 0.595605

H 2.875134 0.221645 -1.050538

H 0.623285 -2.362152 -0.825740

H 1.688863 -2.566839 0.560042

H 2.364111 -2.053874 -0.999730

C 0.125387 -0.277005 0.965552

C -3.632796 0.250905 -0.447548

C -2.287792 0.048069 0.068726

C -1.156679 -0.107928 0.497665

H 0.290851 -0.304231 2.039624

H -3.830222 1.315141 -0.610636

H -4.382762 -0.125808 0.252928

H -3.766383 -0.263607 -1.402755

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -95.4265 | 86.0189 | 131.82 |
| 133.4484 | 154.9263 | 178.0093 |
| 202.963 | 247.834 | 257.6437 |
| 323.39 | 386.5347 | 429.9505 |
| 495.7372 | 572.4856 | 624.9553 |
| 785.3952 | 839.3972 | 864.8171 |
| 973.9304 | 1044.478 | 1054.141 |
| 1061.894 | 1066.783 | 1072.198 |
| 1106.144 | 1210.621 | 1223.175 |
| 1349.218 | 1406.096 | 1411.394 |
| 1419.92 | 1436.05 | 1476.351 |
| 1484.368 | 1485.391 | 1488.963 |
| 1490.081 | 1500.167 | 1761.501 |
| 2175.69 | 3038.249 | 3039.872 |
| 3040.877 | 3097.709 | 3101.506 |
| 3105.853 | 3119.475 | 3130.618 |
| 3133.477 | 3153.104 | 3163.56 |

***i14 – i16***

C 1.089847 2.061862 -0.367348

C 1.197520 0.936312 0.602247

H 1.206766 3.032181 0.119671

H 1.841932 1.980612 -1.161212

H 0.109161 2.050919 -0.866252

H 1.026171 1.110414 1.659841

C 1.327821 -0.453161 0.122874

C 0.254069 -1.189361 -0.200162

C 2.725515 -0.998454 -0.005779

C -3.603517 0.132795 0.073170

C -2.226011 -0.333047 -0.023410

C -1.087576 -0.716773 -0.099446

H 0.387362 -2.206024 -0.561815

H 2.730635 -2.013599 -0.408899

H 3.222963 -1.006410 0.969507

H 3.326456 -0.359886 -0.661759

H -3.998206 -0.020201 1.081232

H -4.246451 -0.407987 -0.625867

H -3.672796 1.198950 -0.157331

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -168.751 | 62.1589 | 76.2303 |
| 103.3731 | 155.2806 | 185.1444 |
| 205.8686 | 232.6339 | 278.6325 |
| 299.8659 | 369.654 | 434.596 |
| 479.0948 | 547.5119 | 598.3171 |
| 806.4729 | 835.4686 | 855.7607 |
| 983.5014 | 1013.55 | 1040.034 |
| 1052.301 | 1058.47 | 1077.344 |
| 1122.153 | 1199.432 | 1211.731 |
| 1327.021 | 1408.792 | 1414.749 |
| 1416.022 | 1419.903 | 1476.591 |
| 1482.377 | 1482.864 | 1490.13 |
| 1494.321 | 1494.885 | 1705.868 |
| 2375.387 | 2994.689 | 3037.566 |
| 3049.483 | 3054.376 | 3098.845 |
| 3118.176 | 3120.273 | 3124.685 |
| 3133.102 | 3165.587 | 3182.858 |

***i69 – p18***

C 0.869749 2.036451 -0.009362

C 0.424055 0.596424 0.021388

C -3.390066 -0.228827 0.160120

C -2.102153 0.049923 0.124614

C -0.869552 0.310501 0.075800

C 1.424232 -0.488907 -0.012225

C 2.733101 -0.223256 -0.078733

C 0.912107 -1.903402 0.033001

H 0.010689 2.705045 0.026703

H 1.434794 2.245314 -0.922723

H 1.520323 2.258133 0.841877

H -4.001614 -0.371922 -2.170034

H -4.133371 0.559536 0.205229

H -3.738978 -1.254752 0.207361

H 3.461896 -1.025522 -0.103467

H 3.123089 0.786795 -0.110986

H 1.734850 -2.617968 -0.013583

H 0.231842 -2.097424 -0.800799

H 0.347646 -2.080674 0.952803

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -393.204 | 57.2647 | 90.3309 |
| 125.1276 | 136.9201 | 165.9269 |
| 187.2305 | 214.0356 | 275.4042 |
| 319.9633 | 345.6483 | 411.3223 |
| 427.6859 | 514.4664 | 562.5947 |
| 589.7419 | 599.1527 | 659.8905 |
| 740.8948 | 875.4713 | 896.0877 |
| 936.3125 | 976.1891 | 1020.721 |
| 1034.027 | 1046.811 | 1073.18 |
| 1150.749 | 1161.358 | 1350.245 |
| 1405.573 | 1417.722 | 1438.898 |
| 1445.949 | 1481.659 | 1489.003 |
| 1493.828 | 1503.015 | 1683.799 |
| 1713.985 | 2163.426 | 3048.325 |
| 3055.642 | 3112.187 | 3120.149 |
| 3148.449 | 3152.493 | 3158.656 |
| 3171.224 | 3239.516 | 3256.143 |

***i69 – p19***

C 0.807807 1.934368 -0.293077

C 0.341838 0.516038 -0.075403

C -3.464825 -0.236904 0.338925

C -2.178454 0.018700 0.205334

C -0.948748 0.256800 0.062109

H -0.039202 2.617606 -0.339099

H 1.372617 2.013721 -1.227611

H 1.469854 2.257595 0.516021

H -4.181287 -0.703072 -1.926482

H -4.201611 0.558044 0.302014

H -3.816297 -1.241207 0.549065

C 1.354466 -0.569082 -0.023208

C 1.041553 -1.826387 -0.343868

C 2.751261 -0.184809 0.392718

H 1.781834 -2.617066 -0.294064

H 0.041614 -2.093345 -0.666703

H 3.399207 -1.061466 0.426357

H 2.752811 0.281405 1.383030

H 3.191073 0.535442 -0.303702

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -377.428 | 38.7858 | 89.4124 |
| 122.5935 | 132.9334 | 187.3475 |
| 226.7857 | 247.1079 | 285.1837 |
| 323.0576 | 326.1671 | 407.1581 |
| 452.4615 | 512.8955 | 571.2748 |
| 583.6145 | 622.5085 | 662.4084 |
| 737.1735 | 878.3858 | 902.085 |
| 941.5695 | 976.6564 | 1024.615 |
| 1032.826 | 1051.379 | 1074.52 |
| 1140.923 | 1172.125 | 1324.415 |
| 1407.821 | 1418.056 | 1443.513 |
| 1446.292 | 1482.995 | 1492.022 |
| 1500.125 | 1512.841 | 1690.204 |
| 1717.887 | 2169.603 | 3044.009 |
| 3047.704 | 3106.288 | 3108.36 |
| 3141.464 | 3154.334 | 3160.229 |
| 3162.427 | 3240.916 | 3254.22 |

***i13 – p33***

C 3.144918 -1.035684 -0.056386

C 2.386041 0.253951 -0.041259

C 1.058045 0.448153 0.007049

C 0.108091 -0.662260 0.052762

C 0.476894 1.836959 0.014700

C -3.766873 -0.211935 0.142317

C -2.457828 -0.364556 0.123043

C -1.205845 -0.510867 0.090559

H 3.707888 -1.133399 -0.990664

H 3.877701 -1.052937 0.756459

H 2.514147 -1.918727 0.045401

H 3.009309 1.145406 -0.078975

H 0.495747 -1.676405 0.051986

H -0.107549 2.006257 0.924041

H -0.202576 1.978214 -0.830952

H 1.261539 2.593011 -0.038897

H -4.215062 0.775389 0.168026

H -4.430072 -1.068655 0.194013

H -4.371741 -0.170720 -2.197156

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -401.606 | 51.537 | 85.2664 |
| 91.0652 | 128.7273 | 153.5568 |
| 162.004 | 241.1535 | 251.4597 |
| 268.6275 | 288.7985 | 387.8779 |
| 409.322 | 517.7112 | 542.606 |
| 557.7938 | 640.4488 | 801.275 |
| 843.5016 | 875.4688 | 882.7209 |
| 930.0815 | 1001.767 | 1033.678 |
| 1064.699 | 1072.324 | 1073.767 |
| 1119.161 | 1264.187 | 1304.596 |
| 1393.726 | 1422.131 | 1428.998 |
| 1450.584 | 1481.973 | 1483.849 |
| 1493.179 | 1502.87 | 1680.726 |
| 1728.989 | 2158.844 | 3046.937 |
| 3051.222 | 3100.437 | 3114.03 |
| 3141.16 | 3144.926 | 3152.197 |
| 3158.273 | 3188.24 | 3239.368 |

***i4 – p5b***

C 0.114433 1.480716 0.037097

C -1.172680 1.046226 0.013162

C 3.517310 -0.761394 -0.235599

C 2.300434 0.032116 -0.134763

C 1.284757 0.670169 -0.042415

C -1.686875 -0.320733 0.076986

C -1.013679 -1.337864 0.626779

C -3.072268 -0.506179 -0.491563

H 0.275511 1.909551 2.020581

H 0.283192 2.546398 -0.084813

H -1.930831 1.822864 -0.054856

H 4.398933 -0.151133 -0.025417

H 3.625112 -1.180163 -1.239454

H 3.499356 -1.590637 0.476323

H -1.448110 -2.331271 0.662451

H -0.033577 -1.206249 1.066173

H -3.409692 -1.538484 -0.387808

H -3.097816 -0.240730 -1.553010

H -3.790675 0.141519 0.021725

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -756.175 | 39.5674 | 49.7655 |
| 81.4298 | 157.5055 | 164.4846 |
| 212.3795 | 239.1073 | 318.5285 |
| 332.9594 | 366.581 | 412.9996 |
| 446.1801 | 470.4122 | 591.3496 |
| 669.3507 | 708.3376 | 755.6425 |
| 823.5233 | 908.0939 | 949.3104 |
| 988.1412 | 1004.669 | 1033.184 |
| 1054.859 | 1057.396 | 1070.421 |
| 1164.028 | 1272.948 | 1284.732 |
| 1409.779 | 1418.398 | 1454.141 |
| 1464.218 | 1482.565 | 1485.384 |
| 1486.623 | 1500.789 | 1605.485 |
| 1707.425 | 2374.766 | 3042.473 |
| 3049.958 | 3103.203 | 3121.532 |
| 3125.356 | 3143.629 | 3161.231 |
| 3165.299 | 3183.965 | 3260.459 |

***i3 – p23’***

C -0.046929 1.717913 -0.072977

C -1.336820 1.122737 0.437827

C -1.569527 -0.185292 0.537194

C -1.763535 -1.323858 1.155220

C -1.553521 -0.823587 -1.689026

C 3.159944 -0.862595 0.068184

C 2.030176 0.057908 0.012209

C 1.098661 0.813243 -0.027742

H 0.178136 2.620743 0.506011

H -0.194852 2.058675 -1.107527

H -2.170807 1.809684 0.556523

H -2.069428 -2.227823 0.644827

H -1.598654 -1.381151 2.227113

H -2.298291 -1.609500 -1.648914

H -0.511241 -1.116373 -1.721516

H -1.827067 0.073044 -2.232489

H 3.890936 -0.631927 -0.710677

H 2.826145 -1.893373 -0.074261

H 3.664431 -0.800812 1.035579

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -564.302 | 39.4364 | 62.0575 |
| 79.4002 | 94.9008 | 106.118 |
| 174.4178 | 202.4188 | 247.654 |
| 312.1528 | 335.6772 | 393.2596 |
| 438.2237 | 498.5712 | 517.4568 |
| 525.6553 | 657.3135 | 768.026 |
| 801.4616 | 832.4908 | 906.8059 |
| 918.4048 | 942.7155 | 1016.89 |
| 1050.72 | 1064.555 | 1115.345 |
| 1186.288 | 1240.111 | 1325.488 |
| 1379.7 | 1414.76 | 1417.64 |
| 1426.096 | 1458.879 | 1480.827 |
| 1486.943 | 1491.444 | 1943.917 |
| 2402.432 | 3016.9 | 3052.622 |
| 3063.364 | 3099.529 | 3124.362 |
| 3126.617 | 3152.981 | 3171.007 |
| 3244.962 | 3262.984 | 3273.786 |

***i3 – p5a***

C 0.029224 1.483310 -0.032363

C -1.259216 1.053858 -0.104919

C -1.801114 -0.296347 -0.024419

C -3.128899 -0.453133 -0.136345

C -0.896302 -1.478669 0.195093

C 3.504247 -0.663654 -0.083884

C 2.260515 0.093887 -0.060944

C 1.218363 0.693994 -0.033693

H 0.097061 1.994083 1.935320

H 0.197507 2.547092 -0.173021

H -2.007271 1.836530 -0.196728

H -3.590016 -1.432823 -0.080109

H -3.789009 0.394592 -0.287450

H -1.480915 -2.396688 0.274513

H -0.311264 -1.355642 1.110027

H -0.182926 -1.587277 -0.624643

H 4.358462 -0.016306 0.128379

H 3.661372 -1.123896 -1.062896

H 3.486088 -1.459147 0.665447

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -745.574 | 44.6253 | 82.0669 |
| 100.9767 | 174.3934 | 221.3587 |
| 250.9043 | 305.3135 | 309.5852 |
| 339.0506 | 384.7454 | 435.0099 |
| 453.4153 | 456.4103 | 589.3276 |
| 685.1452 | 706.0071 | 761.4641 |
| 839.7231 | 868.5364 | 927.8735 |
| 991.4238 | 1009.04 | 1048.834 |
| 1056.901 | 1060.954 | 1071.436 |
| 1156.126 | 1269.244 | 1351.386 |
| 1411.647 | 1419.543 | 1438.74 |
| 1469.648 | 1485.999 | 1488.635 |
| 1494.927 | 1509.288 | 1604.124 |
| 1678.977 | 2373.607 | 3049.086 |
| 3061.276 | 3119.442 | 3126.265 |
| 3133.467 | 3145.244 | 3158.656 |
| 3165.57 | 3183.259 | 3248.359 |

***i11 – p37***

C 0.892748 2.281323 0.107387

C 1.151601 1.015536 -0.071210

C 1.391385 -0.276650 0.049194

C 0.298744 -1.316567 -0.102398

C 2.790993 -0.811579 0.176036

C -3.538364 0.162149 0.069534

C -2.183484 -0.373218 0.008390

C -1.065352 -0.804595 -0.042343

H 0.846021 2.981950 -0.717123

H 0.709101 2.658777 1.108894

H 1.376060 0.977340 -2.057536

H 0.454230 -1.836488 -1.057487

H 0.440830 -2.075740 0.676727

H 3.044769 -1.429234 -0.693167

H 2.875632 -1.446138 1.064443

H 3.520743 -0.006027 0.250697

H -3.725524 0.635056 1.036721

H -4.278394 -0.629867 -0.069541

H -3.693100 0.911977 -0.710168

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -697.083 | 55.4768 | 72.2706 |
| 103.4942 | 109.1337 | 115.2179 |
| 182.5388 | 210.1651 | 260.5431 |
| 286.5209 | 333.0107 | 398.7954 |
| 457.3839 | 478.0704 | 531.3598 |
| 616.0399 | 659.7414 | 772.1178 |
| 796.4537 | 912.8962 | 927.1544 |
| 992.5518 | 1018.785 | 1056.055 |
| 1061.426 | 1065.949 | 1178.452 |
| 1189.777 | 1249.962 | 1302.553 |
| 1373.676 | 1412.237 | 1424.711 |
| 1466.298 | 1473.206 | 1485.958 |
| 1486.285 | 1495.213 | 1503.459 |
| 2027.579 | 2405.175 | 3023.304 |
| 3032.735 | 3048.655 | 3055.844 |
| 3092.759 | 3120.998 | 3121.974 |
| 3150.999 | 3155.627 | 3241.397 |

***i12 – p8b***

C 0.495283 2.037051 0.253925

C 1.427212 1.199998 -0.205830

C 1.452386 -0.257879 -0.083388

C 0.362026 -1.054829 0.084537

C 2.820562 -0.880348 -0.123144

C -3.583660 -0.028329 -0.141643

C -2.173298 -0.382412 -0.058093

C -1.003882 -0.656278 0.015171

H 0.605620 3.106718 0.116244

H -0.382634 1.689337 0.783468

H 2.303667 1.626358 -0.691146

H 0.524290 -2.128968 0.100052

H 0.503395 -1.260262 2.137343

H 3.329554 -0.628701 -1.059613

H 2.775256 -1.966820 -0.037171

H 3.441325 -0.496530 0.693295

H -3.708035 1.053078 -0.239103

H -4.118384 -0.353667 0.754451

H -4.053819 -0.502387 -1.007032

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -635.517 | 64.3515 | 78.7894 |
| 88.1144 | 114.1054 | 152.0892 |
| 218.9314 | 253.3678 | 278.1416 |
| 311.5427 | 337.3315 | 368.6109 |
| 428.3721 | 478.0219 | 514.7441 |
| 574.0147 | 721.8244 | 814.1211 |
| 848.2001 | 883.1104 | 976.3075 |
| 1019.854 | 1041.406 | 1055.247 |
| 1058.309 | 1063.037 | 1105.988 |
| 1189.64 | 1223.544 | 1354.222 |
| 1377.495 | 1415.387 | 1423.768 |
| 1467.627 | 1482.951 | 1483.317 |
| 1487.966 | 1494.999 | 1618.512 |
| 1707.297 | 2373.891 | 3041.568 |
| 3048.798 | 3101.755 | 3121.577 |
| 3122.082 | 3142.542 | 3151.074 |
| 3172.846 | 3174.388 | 3269.076 |

***i12 – p9b***

C 0.962088 2.088339 -0.224032

C 1.625548 1.076118 0.333183

C 1.385479 -0.346915 0.083741

C 0.310168 -0.755287 -0.904051

C 2.134638 -1.277093 0.695160

C -3.502422 0.013843 0.463634

C -2.158583 -0.255862 -0.034702

C -1.047927 -0.477666 -0.431720

H 1.212993 3.115487 0.013265

H 0.142347 1.931895 -0.916590

H 2.425721 1.294181 1.036679

H 0.476207 -0.235711 -1.855146

H 0.407011 -1.823969 -1.112672

H 1.955228 -2.336341 0.551053

H 2.896199 -0.998990 1.415626

H 3.810552 -1.596170 -0.814640

H -3.459773 0.541457 1.419699

H -4.054786 -0.916818 0.615132

H -4.065638 0.632125 -0.239686

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -428.088 | 57.7697 | 85.989 |
| 99.7673 | 143.5785 | 161.8 |
| 203.5726 | 214.2236 | 250.3895 |
| 320.5064 | 402.7124 | 419.3461 |
| 423.9033 | 492.658 | 575.9963 |
| 676.6878 | 811.0397 | 823.4281 |
| 826.2534 | 957.2223 | 961.6923 |
| 963.2576 | 982.2476 | 1037.679 |
| 1055.992 | 1061.57 | 1076.804 |
| 1174.537 | 1229.088 | 1332.018 |
| 1334.227 | 1363.924 | 1418.152 |
| 1439.9 | 1470.419 | 1488.725 |
| 1489.32 | 1500.262 | 1665.972 |
| 1717.565 | 2399.034 | 3049.772 |
| 3053.763 | 3101.645 | 3126.437 |
| 3126.79 | 3159.328 | 3162.132 |
| 3172.894 | 3251.989 | 3252.631 |

***i14 – p8b***

C -0.466502 1.982702 -0.291274

C -1.438178 1.156371 0.119842

C -1.478297 -0.304656 0.012327

C -0.403391 -1.115109 -0.063175

C -2.862576 -0.900299 0.029646

C 3.550463 -0.114408 0.038478

C 2.138962 -0.469517 -0.006026

C 0.964148 -0.734284 -0.034479

H -0.584342 3.055174 -0.188282

H 0.950119 2.093604 1.462703

H 0.413589 1.624020 -0.809226

H -2.325554 1.600051 0.568159

H -0.580358 -2.185486 -0.131278

H -3.378885 -0.642206 0.960459

H -2.836417 -1.987537 -0.056207

H -3.465979 -0.504012 -0.793056

H 4.059104 -0.421225 -0.879168

H 4.047738 -0.602753 0.880541

H 3.673210 0.965569 0.153318

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -406.59 | 67.0101 | 83.0797 |
| 89.2378 | 113.6344 | 168.6228 |
| 216.0342 | 248.8785 | 265.4978 |
| 282.1235 | 331.4095 | 366.453 |
| 419.5625 | 477.8241 | 507.3717 |
| 572.5355 | 743.8027 | 817.6996 |
| 848.9221 | 858.8719 | 980.8665 |
| 1021.459 | 1038.353 | 1056.934 |
| 1061.55 | 1065.503 | 1113.982 |
| 1185.839 | 1228.41 | 1352.709 |
| 1382.595 | 1415.749 | 1423.786 |
| 1469.886 | 1482.011 | 1484.827 |
| 1488.028 | 1497.676 | 1653.98 |
| 1709.449 | 2365.089 | 3043.014 |
| 3047.225 | 3103.941 | 3118.781 |
| 3122.063 | 3141.978 | 3151.038 |
| 3167.118 | 3174.118 | 3269.973 |

***i14 – p35***

C 0.320184 2.040224 -0.093107

C 1.487044 1.123475 0.099998

C 1.508131 -0.213416 -0.012897

C 0.338002 -1.037684 -0.334174

C 2.791129 -0.989254 0.157519

C -3.420788 -0.242304 0.340367

C -2.151647 -0.514864 0.113369

C -0.932837 -0.748391 -0.110274

H -0.242352 2.167519 0.838686

H 0.661003 3.029126 -0.407904

H -0.381866 1.657781 -0.837331

H 2.431167 1.604757 0.345940

H 0.549034 -2.011990 -0.774264

H 3.033924 -1.542987 -0.755908

H 2.703799 -1.722045 0.965830

H 3.628031 -0.327374 0.385404

H -4.200942 -0.950821 0.083931

H -4.102934 0.917748 -1.655225

H -3.714170 0.671572 0.846043

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -398.826 | 48.3701 | 76.5851 |
| 124.0974 | 152.7983 | 171.5098 |
| 186.0049 | 245.7614 | 256.9894 |
| 291.7921 | 329.0109 | 350.6944 |
| 427.2224 | 463.9307 | 553.4497 |
| 586.5323 | 652.5722 | 819.3566 |
| 847.6733 | 887.1529 | 902.4193 |
| 922.6952 | 1018.492 | 1035.264 |
| 1055.632 | 1075.748 | 1087.16 |
| 1106.535 | 1214.262 | 1336.761 |
| 1389.82 | 1417.831 | 1424.468 |
| 1457.647 | 1484.864 | 1486.802 |
| 1503.751 | 1506.056 | 1688.09 |
| 1726.685 | 2168.159 | 3038.864 |
| 3043.009 | 3098.584 | 3105.507 |
| 3133.536 | 3136.722 | 3140.089 |
| 3152.244 | 3165.114 | 3239.897 |

***i15 – p29***

C 3.443759 0.221582 -0.175161

C 2.335157 -0.562080 0.460809

C 1.068789 -0.561599 0.077175

C -0.068481 -1.144469 -0.281582

C 0.542736 1.736248 -0.048447

C -3.864791 0.300757 0.122385

C -2.508193 -0.212210 -0.016050

C -1.380996 -0.620300 -0.123024

H 3.805053 1.008222 0.496804

H 4.293656 -0.432716 -0.390878

H 3.119625 0.685475 -1.107282

H 2.577852 -1.126419 1.360233

H 0.009004 -2.111320 -0.775446

H -0.147643 1.733597 0.784987

H 0.113868 1.761488 -1.042489

H 1.502075 2.216505 0.099205

H -4.261807 0.093925 1.119767

H -4.533058 -0.159067 -0.609945

H -3.886507 1.382736 -0.031590

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -502.062 | 30.2114 | 64.1477 |
| 81.913 | 139.7837 | 156.4596 |
| 163.8765 | 221.8099 | 240.1055 |
| 285.7509 | 307.1884 | 345.2683 |
| 449.3541 | 461.6253 | 480.6333 |
| 537.7699 | 598.9215 | 704.7846 |
| 784.0257 | 844.6902 | 868.9398 |
| 905.3268 | 1046.35 | 1048.902 |
| 1055.987 | 1080.684 | 1130.125 |
| 1216.055 | 1304.734 | 1404.571 |
| 1412.082 | 1419.882 | 1430.114 |
| 1450.293 | 1482.636 | 1488.145 |
| 1491.676 | 1503.065 | 1923.814 |
| 2371.859 | 3038.047 | 3049.456 |
| 3099.042 | 3108.873 | 3119.839 |
| 3123.465 | 3134.293 | 3144.56 |
| 3151.558 | 3277.004 | 3284.645 |

***i15 – p32***

C 3.564792 0.085116 -0.064216

C 2.239175 -0.605083 -0.040673

C 1.015823 -0.053846 0.012091

C -0.142616 -0.948453 0.023619

C 0.729896 1.421003 0.060006

C -3.863759 0.218251 0.143424

C -2.605555 -0.172960 0.112808

C -1.403370 -0.551923 0.070107

H 4.194024 -0.270391 0.758238

H 4.099125 -0.147095 -0.991704

H 3.487175 1.169147 0.016942

H 2.289796 -1.692222 -0.074743

H 0.058739 -2.017415 -0.010182

H 0.183934 1.671177 0.974399

H 0.090163 1.708730 -0.779268

H 1.634610 2.025762 0.024164

H -4.672554 -0.503731 0.171776

H -4.450252 0.433245 -2.195273

H -4.121076 1.270168 0.202650

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -375.118 | 51.7943 | 78.5457 |
| 82.7276 | 94.9954 | 127.0598 |
| 151.5534 | 227.3574 | 262.1139 |
| 295.8058 | 311.4377 | 383.6992 |
| 438.6469 | 445.0633 | 533.9484 |
| 608.5839 | 620.7687 | 812.6267 |
| 838.3165 | 876.3026 | 902.3287 |
| 923.1837 | 1002.295 | 1034.874 |
| 1054.378 | 1059.675 | 1067.104 |
| 1128.372 | 1252.785 | 1326.614 |
| 1384.376 | 1425.102 | 1435.834 |
| 1453.118 | 1481.931 | 1487.603 |
| 1488.807 | 1501.637 | 1686.662 |
| 1729.378 | 2163.703 | 3043.284 |
| 3054.801 | 3096.5 | 3112.451 |
| 3141.231 | 3152.426 | 3154.233 |
| 3157.694 | 3165.701 | 3240.568 |

***i15 – p7a***

C 3.460589 0.026670 -0.120983

C 2.310244 -0.659354 -0.071531

C 0.973869 -0.072863 -0.057390

C -0.090889 -0.900467 -0.012719

C 0.837303 1.420602 -0.085174

C -4.014696 0.221120 0.047411

C -2.611587 -0.169824 0.025096

C -1.450361 -0.488915 0.006769

H 3.911675 0.436437 2.094618

H 4.413971 -0.486576 -0.151785

H 3.485152 1.107334 -0.205027

H 2.352651 -1.744964 -0.022440

H 0.082170 -1.973433 0.011002

H -0.210203 1.719836 -0.066017

H 1.300793 1.834655 -0.985942

H 1.343441 1.866485 0.776889

H -4.655147 -0.641496 0.246270

H -4.313524 0.652746 -0.911474

H -4.197818 0.967166 0.825027

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -390.84 | 63.079 | 79.5525 |
| 84.0907 | 122.0673 | 159.5834 |
| 194.5073 | 236.6589 | 256.0114 |
| 299.1745 | 309.0101 | 397.6892 |
| 429.4008 | 453.1052 | 506.2951 |
| 597.6534 | 710.3573 | 823.5243 |
| 837.4068 | 884.9899 | 946.379 |
| 994.5094 | 1020.957 | 1049.521 |
| 1052.05 | 1067.343 | 1088.905 |
| 1215.363 | 1247.07 | 1328.525 |
| 1386.438 | 1410.839 | 1436.86 |
| 1453.076 | 1480.171 | 1487.235 |
| 1492.895 | 1497.814 | 1661.889 |
| 1688.625 | 2368.452 | 3048.313 |
| 3049.152 | 3109.068 | 3119.076 |
| 3125.781 | 3154.959 | 3162.87 |
| 3170.834 | 3173.719 | 3259.286 |

***i11 – p31***

C 1.920550 1.894204 0.065312

C 1.360315 0.895434 -0.612007

C 1.270997 -0.498138 -0.147833

C 0.059502 -1.280193 -0.617392

C 2.200996 -1.067241 0.630298

C -3.479662 0.578640 0.386588

C -2.234155 -0.087778 0.024639

C -1.207141 -0.635956 -0.267172

H 1.959512 2.896717 -0.344507

H 2.340492 1.744927 1.054911

H 0.891384 1.105464 -1.571366

H 0.112921 -1.387003 -1.708716

H 0.089369 -2.291026 -0.202235

H 2.106739 -2.096605 0.957744

H 1.468845 -0.486991 2.700444

H 3.116547 -0.547369 0.887257

H -4.205159 -0.139301 0.777180

H -3.925147 1.072273 -0.480642

H -3.303915 1.335079 1.155325

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -424.981 | 47.3842 | 64.9605 |
| 122.648 | 125.4452 | 154.193 |
| 187.0536 | 208.5398 | 248.8293 |
| 305.7778 | 386.5986 | 398.9868 |
| 413.2165 | 509.0314 | 549.6286 |
| 695.2318 | 784.6172 | 814.5219 |
| 822.7035 | 931.9068 | 949.9219 |
| 965.2055 | 976.848 | 1036.219 |
| 1058.955 | 1066.325 | 1102.529 |
| 1174.496 | 1209.477 | 1282.642 |
| 1332.252 | 1347.907 | 1422.99 |
| 1444.898 | 1464.556 | 1476.166 |
| 1489.036 | 1492.788 | 1681.079 |
| 1721.501 | 2398.516 | 3032.986 |
| 3048.581 | 3100.412 | 3120.041 |
| 3123.648 | 3152.114 | 3161.906 |
| 3164.5 | 3247.963 | 3253.826 |

***i11 – p8a***

C 2.260370 1.814603 0.049692

C 1.171140 1.041311 0.037994

C 1.178121 -0.411766 -0.055689

C 0.013797 -1.119770 -0.031357

C 2.490092 -1.135024 -0.130395

C -3.748742 0.472368 -0.041321

C -2.402333 -0.083864 -0.036015

C -1.290013 -0.542549 -0.025608

H 2.175988 2.892603 0.119861

H 3.263883 1.406951 -0.009864

H 0.191424 1.505883 0.101120

H 0.054224 -2.193679 -0.187119

H 0.096440 -1.732419 1.941195

H 2.343790 -2.213540 -0.200382

H 3.094673 -0.929958 0.759089

H 3.068463 -0.808360 -1.000044

H -3.744542 1.503738 0.319552

H -4.410881 -0.110718 0.603578

H -4.168053 0.467643 -1.050788

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -648.571 | 40.6092 | 84.2021 |
| 97.1791 | 140.7485 | 200.3645 |
| 232.9338 | 245.5581 | 299.9234 |
| 312.6088 | 322.9685 | 389.3695 |
| 432.6001 | 463.9336 | 513.408 |
| 600.7753 | 728.6628 | 797.5363 |
| 845.7104 | 903.9538 | 952.309 |
| 1005.517 | 1042.353 | 1054.609 |
| 1058.464 | 1063.278 | 1073.886 |
| 1211.319 | 1260.486 | 1329.862 |
| 1376.831 | 1418.702 | 1423.075 |
| 1456.809 | 1483.252 | 1484.217 |
| 1486.071 | 1502.752 | 1612.337 |
| 1685.801 | 2373.21 | 3040.251 |
| 3046.502 | 3101.721 | 3118.462 |
| 3122.626 | 3140.287 | 3158.553 |
| 3173.283 | 3182.255 | 3247.459 |

***i13 – i15***

C 3.305431 -0.465398 0.660494

C 2.394324 -0.258437 -0.501379

H 4.255370 -0.908564 0.354943

H 3.535927 0.483068 1.170940

H 2.842557 -1.115485 1.411388

H 2.817177 -0.159867 -1.497574

C 0.989044 0.145237 -0.293283

C 0.002755 -0.764022 -0.326705

C 0.747016 1.609224 -0.032437

C -3.968290 0.013464 0.251995

C -2.551483 -0.257430 0.042995

C -1.379660 -0.475680 -0.125813

H 0.254217 -1.803106 -0.520199

H 1.306848 1.935805 0.850243

H -0.311298 1.820007 0.126704

H 1.104174 2.207644 -0.877006

H -4.252347 -0.178712 1.290107

H -4.585662 -0.619454 -0.390421

H -4.201784 1.056912 0.025676

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -172.21 | 75.1523 | 94.2005 |
| 99.0473 | 132.7184 | 159.7283 |
| 208.4581 | 216.7049 | 283.4779 |
| 314.905 | 406.0382 | 443.8161 |
| 502.3959 | 518.4936 | 577.2569 |
| 817.4933 | 827.6698 | 900.3914 |
| 978.6211 | 987.4556 | 1036.667 |
| 1058.159 | 1067.015 | 1078.018 |
| 1114.491 | 1197.101 | 1229.704 |
| 1339.631 | 1375.716 | 1405.583 |
| 1411.318 | 1423.459 | 1474.419 |
| 1485.995 | 1488.266 | 1489.38 |
| 1491.681 | 1493.126 | 1713.485 |
| 2373.388 | 2984.796 | 3038.838 |
| 3045.375 | 3061.779 | 3098.019 |
| 3117.166 | 3118.67 | 3127.007 |
| 3147.512 | 3166.333 | 3170.789 |

***i15 – i16***

C -3.085505 -1.071947 -0.384500

C -1.797496 -0.759337 0.315847

C -1.065464 0.352296 0.232116

C -1.389625 1.560101 -0.609864

H -2.984063 -1.987459 -0.976064

H -3.883228 -1.252870 0.343511

H -3.415933 -0.277061 -1.053718

H -1.424332 -1.546859 0.967709

H -0.596282 1.724664 -1.346050

H -1.434729 2.458044 0.015039

H -2.337630 1.467354 -1.140419

C 0.192959 0.471359 1.019794

C 3.799421 -0.498262 -0.545896

C 2.505556 -0.152904 0.022557

C 1.421040 0.144995 0.495051

H 0.147799 0.901859 2.016931

H 4.479809 -0.869202 0.225394

H 4.266786 0.375315 -1.011356

H 3.696485 -1.271590 -1.311611

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -96.6971 | 75.2794 | 86.8434 |
| 128.697 | 152.717 | 177.513 |
| 210.7692 | 264.6599 | 285.134 |
| 338.5288 | 387.8739 | 429.3017 |
| 468.5411 | 599.0674 | 631.8916 |
| 771.4755 | 825.2176 | 890.8933 |
| 982.777 | 1026.686 | 1040.741 |
| 1057.428 | 1062.861 | 1069.739 |
| 1115.59 | 1212.976 | 1227.195 |
| 1364.284 | 1396.53 | 1413.799 |
| 1424.078 | 1427.231 | 1483.98 |
| 1484.945 | 1487.136 | 1488.101 |
| 1491.584 | 1504.254 | 1763.911 |
| 2175.991 | 3039.115 | 3040.235 |
| 3044.157 | 3096.866 | 3097.582 |
| 3105.106 | 3117.559 | 3139.869 |
| 3151.592 | 3162.287 | 3163.462 |

***i69 – p17***

C 0.644363 2.043756 -0.292689

C 0.340991 0.657828 0.222461

C -3.531575 -0.615359 -0.017440

C -2.148197 -0.166677 0.066349

C -1.000437 0.191101 0.148127

C 1.324633 -0.175700 0.582483

C 2.170085 -0.790408 1.365799

C 1.952800 -1.059665 -1.562068

H 0.455100 2.102418 -1.369782

H 1.686434 2.305891 -0.106561

H -0.001577 2.777356 0.196625

H -3.593675 -1.589562 -0.509302

H -4.136743 0.092467 -0.589180

H -3.971895 -0.711554 0.978634

H 2.885893 -1.517189 1.001683

H 2.163524 -0.578932 2.431951

H 2.984038 -0.729113 -1.564328

H 1.266176 -0.569480 -2.240288

H 1.746749 -2.091561 -1.307584

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -495.749 | 28.2622 | 33.5519 |
| 52.9681 | 87.9156 | 110.8667 |
| 132.6408 | 180.2129 | 199.6453 |
| 263.5331 | 306.1579 | 369.0908 |
| 409.0225 | 471.787 | 501.7121 |
| 532.974 | 572.8917 | 646.6407 |
| 698.2093 | 769.7813 | 911.6214 |
| 921.9857 | 1009.656 | 1048.509 |
| 1053.243 | 1057.926 | 1060.975 |
| 1239.757 | 1321.1 | 1406.912 |
| 1413.271 | 1419.247 | 1420.69 |
| 1466.206 | 1482.069 | 1483.083 |
| 1484.513 | 1498.885 | 1952.414 |
| 2348.299 | 3038.074 | 3044.697 |
| 3102.754 | 3106.523 | 3115.493 |
| 3120.463 | 3136.928 | 3146.877 |
| 3228.431 | 3273.892 | 3276.036 |

***i69 – p14***

C 0.644363 2.043756 -0.292689

C 0.340991 0.657828 0.222461

C -3.531575 -0.615359 -0.017440

C -2.148197 -0.166677 0.066349

C -1.000437 0.191101 0.148127

C 1.324633 -0.175700 0.582483

C 2.170085 -0.790408 1.365799

C 1.952800 -1.059665 -1.562068

H 0.455100 2.102418 -1.369782

H 1.686434 2.305891 -0.106561

H -0.001577 2.777356 0.196625

H -3.593675 -1.589562 -0.509302

H -4.136743 0.092467 -0.589180

H -3.971895 -0.711554 0.978634

H 2.885893 -1.517189 1.001683

H 2.163524 -0.578932 2.431951

H 2.984038 -0.729113 -1.564328

H 1.266176 -0.569480 -2.240288

H 1.746749 -2.091561 -1.307584

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -352.344 | 34.3911 | 58.4444 |
| 94.5091 | 126.3455 | 142.1766 |
| 196.1442 | 244.8158 | 290.8112 |
| 338.4445 | 350.5564 | 396.8789 |
| 429.7247 | 463.6666 | 578.1918 |
| 622.5813 | 686.9342 | 744.2897 |
| 800.2293 | 847.1382 | 938.592 |
| 955.2626 | 974.98 | 1032.402 |
| 1054.687 | 1058.733 | 1073.918 |
| 1080.729 | 1231.064 | 1385.41 |
| 1417.721 | 1422.717 | 1434.476 |
| 1450.821 | 1483.673 | 1483.817 |
| 1490.389 | 1509.711 | 1643.754 |
| 1720.048 | 2377.063 | 3042.271 |
| 3047.512 | 3104.363 | 3120.079 |
| 3123.105 | 3141.328 | 3160.683 |
| 3178.064 | 3252.299 | 3271.942 |

***i16 – p8a***

C 2.271334 1.682786 0.185735

C 1.153195 0.947116 0.108292

C 1.113274 -0.509084 0.026629

C -0.062895 -1.167568 -0.038572

C 2.410360 -1.267200 0.012278

C -3.790207 0.497685 -0.002251

C -2.455250 -0.085343 -0.017946

C -1.349646 -0.562669 -0.027798

H 2.220739 2.761905 0.267308

H 3.257148 1.235075 0.245678

H 2.825158 2.005239 -2.011607

H 0.190712 1.449657 0.087882

H -0.051818 -2.252311 -0.103198

H 2.239732 -2.340660 -0.077841

H 2.976898 -1.086558 0.931270

H 3.038415 -0.947342 -0.825194

H -3.987936 0.988425 0.954353

H -4.551573 -0.271432 -0.153046

H -3.898466 1.243670 -0.793810

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -393.891 | 81.6012 | 87.2631 |
| 114.3355 | 121.1197 | 157.342 |
| 198.2583 | 241.5556 | 260.9406 |
| 283.1101 | 326.1677 | 390.2982 |
| 426.9714 | 466.7278 | 489.7388 |
| 601.431 | 749.8818 | 798.6578 |
| 847.5634 | 868.6083 | 952.2244 |
| 1010.646 | 1032.345 | 1056.316 |
| 1065.568 | 1069.788 | 1080.949 |
| 1214.472 | 1258.518 | 1340.48 |
| 1378.087 | 1423.726 | 1426.836 |
| 1458.411 | 1483.919 | 1487.188 |
| 1492.729 | 1505.243 | 1657.656 |
| 1689.668 | 2369.041 | 3044.683 |
| 3047.021 | 3105.254 | 3119.024 |
| 3121.471 | 3144.131 | 3164.727 |
| 3172.653 | 3192.589 | 3254.868 |

***i16 – p34***

C 2.408559 1.763490 0.017501

C 1.196898 0.889149 -0.014034

C 1.139967 -0.450080 -0.024054

C -0.155816 -1.149580 -0.051268

C 2.336541 -1.366091 -0.013459

C -3.682362 0.496960 0.205660

C -2.489761 -0.059168 0.126618

C -1.351895 -0.594456 0.038490

H 2.412654 2.439506 -0.844018

H 2.395663 2.397316 0.910876

H 3.347112 1.209023 0.014600

H 0.246614 1.419477 -0.031185

H -0.115473 -2.232981 -0.153324

H 2.316114 -2.031025 -0.882963

H 2.323803 -2.001540 0.878061

H 3.283437 -0.828774 -0.026963

H -4.583505 -0.106582 0.192266

H -4.245407 0.987553 -2.114947

H -3.793792 1.566676 0.344875

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -362.131 | 33.1985 | 64.8757 |
| 80.972 | 91.5545 | 124.3256 |
| 152.2642 | 228.3815 | 253.798 |
| 263.251 | 329.2657 | 361.6108 |
| 430.6926 | 449.7084 | 541.8731 |
| 623.2233 | 631.1131 | 799.3933 |
| 855.2598 | 885.2276 | 907.0056 |
| 923.5147 | 1006.161 | 1033.594 |
| 1043.442 | 1062.325 | 1067.511 |
| 1137.688 | 1231.063 | 1315.956 |
| 1387.177 | 1422.256 | 1428.818 |
| 1457.793 | 1484.383 | 1485.557 |
| 1492.375 | 1502.041 | 1685.383 |
| 1734.839 | 2154.861 | 3038.433 |
| 3043.307 | 3090.073 | 3097.835 |
| 3144.21 | 3146.708 | 3148.548 |
| 3162.808 | 3168.89 | 3235.058 |

***i4 – i5***

C 0.168223 -0.449052 0.928543

C -0.914209 0.563628 0.686744

C 3.894204 0.326510 -0.579729

C 2.571037 0.049927 -0.034830

C 1.477163 -0.169775 0.421521

C -1.913690 0.101874 -0.065352

C -1.695218 -1.304681 -0.519192

C -3.149847 0.854256 -0.450159

H -0.450874 -1.350353 0.204327

H 0.180969 -0.877859 1.934124

H -0.864529 1.567962 1.095411

H 4.659664 -0.258559 -0.063802

H 4.145497 1.384780 -0.468933

H 3.938941 0.080361 -1.643990

H -2.389086 -2.062657 -0.153780

H -1.416277 -1.448013 -1.563672

H -3.234660 0.932961 -1.538796

H -3.149783 1.862104 -0.029197

H -4.045833 0.333146 -0.096962

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1901.24 | 44.8137 | 60.9985 |
| 86.1953 | 169.5854 | 201.7154 |
| 213.1315 | 293.55 | 349.9623 |
| 362.1435 | 423.5023 | 476.8498 |
| 502.4726 | 575.5678 | 653.6126 |
| 790.5876 | 841.3827 | 892.9856 |
| 946.1784 | 953.5497 | 996.3507 |
| 1033.588 | 1049.566 | 1054.13 |
| 1068.443 | 1109.119 | 1184.369 |
| 1220.671 | 1304.757 | 1334.775 |
| 1387.123 | 1414.837 | 1417.199 |
| 1452.94 | 1481.899 | 1483.084 |
| 1485.272 | 1490.503 | 1647.862 |
| 1744.227 | 2343.568 | 3038.521 |
| 3047.991 | 3091.912 | 3093.201 |
| 3098.787 | 3117.359 | 3122.498 |
| 3132.277 | 3172.664 | 3194.058 |

***i5 – p24***

C -0.368059 -0.625406 -0.035465

C 0.691907 0.366182 -0.033324

C -4.159787 0.290790 -0.152466

C -2.878641 -0.018052 -0.120563

C -1.654649 -0.316562 -0.079306

C 2.012547 0.125500 0.011120

C 2.636568 -1.239399 0.067269

C 2.995953 1.261564 0.007635

H -0.104964 -1.679092 0.000845

H 0.358435 1.399718 -0.071379

H -4.768850 0.491722 2.201154

H -4.921104 -0.481325 -0.175778

H -4.485090 1.323548 -0.213910

H 1.913751 -2.054050 0.069776

H 3.304216 -1.382534 -0.789229

H 3.254218 -1.332974 0.967029

H 3.621833 1.232405 0.906650

H 2.499420 2.232161 -0.034251

H 3.673100 1.182720 -0.850308

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -404.838 | 58.2303 | 80.9419 |
| 91.9362 | 116.3491 | 147.5156 |
| 171.9574 | 243.3039 | 245.6396 |
| 265.8322 | 309.0061 | 379.6578 |
| 453.4878 | 497.1219 | 530.0516 |
| 540.911 | 604.7678 | 846.9694 |
| 875.0406 | 885.7975 | 897.2015 |
| 940.6227 | 971.6067 | 1015.074 |
| 1034.477 | 1069.797 | 1103.84 |
| 1170.475 | 1232.623 | 1306.564 |
| 1387.769 | 1421.557 | 1428.568 |
| 1453.202 | 1472.797 | 1489.409 |
| 1494.53 | 1499.878 | 1680.136 |
| 1727.752 | 2157.318 | 3028.939 |
| 3038.289 | 3085.356 | 3091.601 |
| 3135.501 | 3147.286 | 3154.04 |
| 3166.756 | 3174.29 | 3234.629 |

***i5 – p4b***

C -0.284044 -0.516398 0.166881

C 0.676811 0.343759 -0.197888

C -4.288260 0.251882 -0.043843

C -2.858537 -0.017355 0.029071

C -1.675672 -0.232540 0.086199

C 2.118067 0.066327 -0.134454

C 2.621066 -1.156602 -0.351718

C 2.996114 1.244998 0.189213

H -0.007776 -1.488948 0.566932

H 0.385296 1.336791 -0.532886

H -4.557226 1.094565 0.598384

H -4.864691 -0.618423 0.278851

H -4.586071 0.497834 -1.066368

H 1.990567 -1.983325 -0.658052

H 3.687828 -1.342293 -0.295131

H 2.476144 -2.074253 1.829947

H 2.737032 1.662066 1.167483

H 2.854120 2.042398 -0.547768

H 4.051507 0.969162 0.197841

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -337.77 | 15.3051 | 74.2156 |
| 84.9323 | 119.7791 | 141.808 |
| 161.4519 | 180.2917 | 223.3525 |
| 264.3401 | 309.2458 | 379.9751 |
| 427.2901 | 518.6893 | 529.4336 |
| 552.7244 | 740.771 | 810.7205 |
| 892.7718 | 914.3055 | 936.2111 |
| 990.0729 | 1006.657 | 1031.387 |
| 1054.112 | 1058.038 | 1072.751 |
| 1204.916 | 1255.072 | 1331.17 |
| 1356.887 | 1416.291 | 1419.914 |
| 1443.737 | 1483.485 | 1483.727 |
| 1485.001 | 1499.104 | 1679.299 |
| 1714.007 | 2372.878 | 3038.129 |
| 3046.181 | 3099.802 | 3117.646 |
| 3122.149 | 3139.318 | 3156.271 |
| 3160.72 | 3166.069 | 3246.903 |

***i5 – p4a***

C 0.282465 -0.535653 0.011650

C -0.673795 0.401182 -0.089346

C 4.287142 0.256025 0.019150

C 2.857396 -0.022699 0.015753

C 1.674203 -0.244534 0.012338

C -2.109853 0.137768 -0.093928

C -2.592218 -1.280544 0.032436

C -2.970012 1.164644 -0.193669

H 0.012701 -1.584518 0.099291

H -0.373308 1.441952 -0.174243

H 4.606558 0.658955 -0.945532

H 4.860277 -0.653601 0.213994

H 4.538069 0.988336 0.790830

H -2.249627 -1.725189 0.972086

H -3.681527 -1.326289 0.010735

H -2.205991 -1.900275 -0.782624

H -4.041556 1.005078 -0.230637

H -2.618609 2.185169 -0.300961

H -3.378953 1.653244 2.060768

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -344.089 | 31.6694 | 80.4911 |
| 83.0481 | 134.4071 | 146.5207 |
| 200.7522 | 216.0021 | 225.6391 |
| 259.61 | 308.3182 | 414.0873 |
| 428.6891 | 500.6836 | 538.1523 |
| 549.8838 | 749.3082 | 818.9204 |
| 873.0556 | 889.0685 | 937.3679 |
| 998.4254 | 1000.663 | 1048.17 |
| 1053.392 | 1057.655 | 1070.484 |
| 1211.516 | 1295.634 | 1333.487 |
| 1351.412 | 1416.663 | 1420.838 |
| 1449.101 | 1483.139 | 1483.624 |
| 1489.021 | 1505.812 | 1669.326 |
| 1699.891 | 2371.134 | 3042.216 |
| 3046.041 | 3104.553 | 3117.341 |
| 3122.293 | 3141.988 | 3154.497 |
| 3171.327 | 3177.495 | 3245.58 |

***i5 – p25***

C 0.194566 1.491540 -0.070745

C -1.194364 1.081496 0.047863

C 3.464077 -0.641665 -0.088640

C 2.357741 0.075376 -0.095913

C 1.283854 0.735221 -0.090150

C -1.700429 -0.164181 0.003875

C -0.862455 -1.393953 -0.199034

C -3.175575 -0.392509 0.163494

H 0.358882 2.565587 -0.138733

H -1.893237 1.902742 0.179894

H 4.436373 -0.174720 -0.201772

H 3.428478 -1.724105 -0.024693

H 4.048381 -0.771173 2.285546

H -0.261553 -1.607845 0.691237

H -1.488592 -2.264887 -0.403867

H -0.157556 -1.264525 -1.024418

H -3.585172 -0.886105 -0.724931

H -3.722569 0.537638 0.326621

H -3.367917 -1.060556 1.010608

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -385.708 | 31.7799 | 81.615 |
| 115.0081 | 143.3804 | 171.0927 |
| 195.7875 | 236.6084 | 255.5113 |
| 274.181 | 313.0435 | 394.9125 |
| 436.1191 | 479.8644 | 533.6239 |
| 618.4825 | 718.8307 | 780.77 |
| 848.0722 | 871.5828 | 898.3468 |
| 925.7072 | 989.301 | 1003.761 |
| 1034.518 | 1051.176 | 1100.208 |
| 1157.842 | 1230.861 | 1340.347 |
| 1392.203 | 1419.082 | 1423.551 |
| 1456.217 | 1481.609 | 1487.283 |
| 1490.532 | 1502.329 | 1681.935 |
| 1704.288 | 2157.238 | 3028.288 |
| 3040.169 | 3085.698 | 3104.88 |
| 3129.915 | 3134.019 | 3140.937 |
| 3145.066 | 3171.323 | 3231.595 |

***i5 – p5a***

C 0.100960 1.516877 -0.002428

C -1.180873 1.114075 -0.047845

C 3.565733 -0.639724 0.044896

C 2.324311 0.121372 0.026961

C 1.281460 0.722668 0.011520

C -1.738527 -0.237373 -0.095632

C -0.839891 -1.442151 -0.085013

C -3.075331 -0.372570 -0.134007

H 0.280561 2.588292 0.027950

H -1.925537 1.905696 -0.048885

H 4.184268 -0.395326 -0.822553

H 3.363151 -1.713610 0.026668

H 4.144662 -0.417942 0.945117

H -0.221906 -1.458563 0.816299

H -1.429907 -2.359308 -0.122571

H -0.155002 -1.427894 -0.936314

H -3.543144 -1.348282 -0.199085

H -3.731488 0.490851 -0.158396

H -3.592711 -0.562951 2.161051

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -348.851 | 36.8007 | 48.2015 |
| 82.3623 | 137.5611 | 159.9541 |
| 192.5699 | 240.2311 | 247.6496 |
| 308.5583 | 328.4242 | 426.6652 |
| 434.4207 | 454.4391 | 599.7155 |
| 685.7578 | 741.4403 | 760.6418 |
| 822.2722 | 866.0554 | 935.8729 |
| 993.2518 | 1013.362 | 1047.604 |
| 1053.201 | 1057.956 | 1071.501 |
| 1164.063 | 1271.797 | 1350.714 |
| 1409.382 | 1418.21 | 1439.064 |
| 1464.91 | 1482.832 | 1483.409 |
| 1484.541 | 1503.626 | 1661.421 |
| 1695.882 | 2367.163 | 3045.148 |
| 3052.786 | 3118.001 | 3119.606 |
| 3122.552 | 3139.896 | 3153.178 |
| 3157.408 | 3178.206 | 3244.113 |

***i5 – p5b***

C 0.097827 1.544957 -0.077534

C -1.172146 1.108454 -0.127729

C 3.516860 -0.669603 0.154517

C 2.298824 0.122738 0.065356

C 1.274250 0.751584 -0.004331

C -1.679587 -0.267916 -0.129908

C -0.981905 -1.316373 -0.590909

C -3.072339 -0.431967 0.421567

H 0.262531 2.618833 -0.072580

H -1.940678 1.878321 -0.129969

H 4.213878 -0.402607 -0.643951

H 3.291029 -1.735598 0.071078

H 4.018541 -0.502503 1.111109

H 0.185583 -2.003031 1.324431

H -1.418620 -2.309112 -0.596142

H 0.000075 -1.201457 -1.030343

H -3.785794 0.182095 -0.138179

H -3.115392 -0.105416 1.465607

H -3.401851 -1.470775 0.372761

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -296.073 | 11.2643 | 42.0389 |
| 81.5018 | 159.8758 | 163.6243 |
| 184.0722 | 193.4651 | 245.8747 |
| 294.1937 | 347.4534 | 405.6785 |
| 428.0248 | 470.015 | 598.6124 |
| 672.6579 | 733.6652 | 757.7566 |
| 807.5473 | 908.6058 | 947.2095 |
| 987.0333 | 1007.978 | 1036.783 |
| 1052.953 | 1057.37 | 1072.729 |
| 1172.019 | 1276.573 | 1282.087 |
| 1415.378 | 1417.157 | 1449.645 |
| 1460.715 | 1481.029 | 1483.139 |
| 1486.581 | 1501.812 | 1665.202 |
| 1708.047 | 2367.114 | 3036.488 |
| 3045.72 | 3097.53 | 3118.95 |
| 3121.064 | 3138.429 | 3153.19 |
| 3162.418 | 3175.641 | 3260.84 |

***i5 – p26***

C 0.370066 0.011812 1.001146

C -0.764793 0.002131 0.336802

C 4.151876 -0.005579 -0.541749

C 2.802648 0.001055 0.007319

C 1.677873 0.005799 0.432666

C -2.036840 -0.000015 -0.010045

C -2.766838 1.282007 -0.306836

C -2.767505 -1.286273 -0.285944

H 0.311903 0.025313 2.088451

H -0.053742 -0.053016 -1.557679

H 4.759899 -0.783954 -0.073765

H 4.645057 0.955672 -0.375678

H 4.127371 -0.193184 -1.617976

H -2.176377 2.155974 -0.032281

H -3.000999 1.343547 -1.375672

H -3.716377 1.309880 0.237321

H -3.717691 -1.304525 0.257433

H -2.177797 -2.155875 0.003643

H -3.000167 -1.365454 -1.353955

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -705.004 | 14.6744 | 76.1111 |
| 80.5266 | 84.3299 | 154.7635 |
| 171.9587 | 174.0041 | 240.4973 |
| 298.0321 | 299.5321 | 357.1565 |
| 414.241 | 476.5283 | 502.215 |
| 522.0511 | 588.1559 | 794.3487 |
| 806.5334 | 833.5955 | 969.3938 |
| 988.5186 | 1023.819 | 1051.955 |
| 1059.664 | 1096.399 | 1190.854 |
| 1233.916 | 1248.514 | 1402.278 |
| 1413.899 | 1415.462 | 1445.859 |
| 1477.003 | 1482.939 | 1484.116 |
| 1488.09 | 1495.791 | 1517.2 |
| 2014.753 | 2383.573 | 3035.346 |
| 3038.1 | 3050.684 | 3098.517 |
| 3100.19 | 3120.912 | 3127.194 |
| 3142.982 | 3147.257 | 3148.835 |

***i38 – p27***

C 2.769055 0.000000 0.116240

C 1.436236 0.000000 -0.057615

C 0.666334 -1.241635 -0.154368

C -0.657122 -1.246071 -0.315565

C -1.491582 0.000000 -0.393551

C -0.657122 1.246071 -0.315565

C 0.666334 1.241635 -0.154368

C -2.580542 0.000000 0.695201

H 3.330904 -0.925810 0.166085

H 2.947030 0.000000 2.550399

H 3.330904 0.925810 0.166086

H 1.213741 -2.177104 -0.091176

H -1.189692 -2.191100 -0.381894

H -2.010405 0.000000 -1.364243

H -1.189692 2.191100 -0.381894

H 1.213741 2.177104 -0.091175

H -3.216744 -0.884967 0.608964

H -3.216743 0.884967 0.608964

H -2.122592 0.000000 1.687427

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -326.86 | 66.6779 | 123.7714 |
| 149.8823 | 236.4692 | 240.2884 |
| 274.3902 | 378.7948 | 423.4366 |
| 444.7331 | 501.2654 | 607.7049 |
| 677.662 | 712.6425 | 790.7084 |
| 802.2148 | 817.9588 | 834.5726 |
| 914.2111 | 939.9541 | 960.3912 |
| 992.1833 | 1015.846 | 1017.535 |
| 1048.165 | 1098.097 | 1130.461 |
| 1191.674 | 1225.828 | 1307.1 |
| 1335.459 | 1381.046 | 1391.815 |
| 1411.877 | 1446.811 | 1474.529 |
| 1500.388 | 1505.437 | 1661.061 |
| 1701.448 | 1760.725 | 2997.178 |
| 3041.899 | 3121.498 | 3127.861 |
| 3156.328 | 3162.907 | 3164.102 |
| 3187.212 | 3190.368 | 3247.666 |

***i37 – p27***

C -2.598396 -0.037380 -0.625134

C -1.441489 0.031468 0.388177

C -0.599045 1.249395 0.160074

C 0.744596 1.214978 0.030229

C 1.475808 -0.059665 -0.087825

C 0.681623 -1.270441 0.134470

C -0.630533 -1.233286 0.364141

C 2.777634 -0.103406 -0.390452

H -2.207662 -0.132803 -1.641292

H -3.213802 0.864899 -0.575124

H -3.241244 -0.897885 -0.421579

H -1.896608 0.122895 1.387198

H -1.113008 2.206327 0.150726

H 1.285930 2.124105 -0.211284

H 1.242218 1.587908 1.865790

H 1.204681 -2.221425 0.106890

H -1.175591 -2.159157 0.527229

H 3.301513 -1.047889 -0.485957

H 3.352386 0.803040 -0.544676

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -807.569 | 66.6585 | 203.6201 |
| 236.9221 | 262.917 | 313.0557 |
| 372.1346 | 387.8923 | 440.9654 |
| 469.9253 | 506.702 | 609.5075 |
| 682.5927 | 715.9644 | 785.5409 |
| 797.0691 | 813.6826 | 834.2148 |
| 922.3836 | 937.3999 | 957.6245 |
| 990.5626 | 1016.718 | 1023.603 |
| 1045.558 | 1097.308 | 1125.812 |
| 1190.098 | 1220.212 | 1305.829 |
| 1330.272 | 1377.513 | 1393.827 |
| 1412.621 | 1441.094 | 1473.459 |
| 1500.507 | 1505.756 | 1623.728 |
| 1692.634 | 1758.899 | 2986.427 |
| 3041.825 | 3121.201 | 3127.471 |
| 3154.813 | 3164.59 | 3169.549 |
| 3188.345 | 3191.374 | 3244.6 |

***i34 – p1***

C 2.571276 -0.988934 0.057746

C 1.251869 -0.267261 -0.006475

C 0.047639 -0.973064 -0.019363

C -1.182711 -0.331769 -0.054609

C -1.206299 1.076774 -0.031085

C -0.001768 1.794717 -0.090875

C 1.208427 1.129110 -0.056436

C -2.472451 -1.101413 -0.046174

H 2.450437 -2.057262 -0.131526

H 3.028190 -0.874488 1.045703

H 3.276482 -0.590467 -0.676473

H 0.074782 -2.059372 -0.010249

H -1.651154 1.278065 1.781992

H -2.146099 1.593434 -0.195778

H -0.027712 2.877331 -0.139435

H 2.136630 1.691430 -0.079720

H -2.303894 -2.168385 -0.202153

H -2.980732 -0.973949 0.915751

H -3.152826 -0.745295 -0.824489

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -813.404 | 130.2682 | 146.1397 |
| 192.1847 | 210.2601 | 281.8157 |
| 339.1612 | 375.3894 | 417.5071 |
| 459.0084 | 523.5133 | 544.3855 |
| 563.8394 | 723.1647 | 740.1261 |
| 810.679 | 896.5279 | 932.4744 |
| 961.7882 | 1005.676 | 1018.746 |
| 1027.746 | 1038.664 | 1071.678 |
| 1073.983 | 1122.841 | 1188.085 |
| 1199.543 | 1286.895 | 1313.801 |
| 1348.486 | 1425.873 | 1427.933 |
| 1463.881 | 1495.778 | 1498.296 |
| 1498.994 | 1520.146 | 1530.435 |
| 1631.7 | 1669.819 | 3042.011 |
| 3043.34 | 3106.603 | 3106.818 |
| 3135.89 | 3138.341 | 3178.488 |
| 3183.47 | 3189.62 | 3213.181 |

***i34 – i32***

C 2.554331 -1.023593 -0.022257

C 1.229715 -0.322594 0.012474

C 0.051566 -0.987909 0.076594

C -1.231111 -0.333792 0.144937

C -1.209876 1.180504 0.071905

C 0.056966 1.833636 -0.066084

C 1.222548 1.144571 -0.060067

C -2.510978 -1.053462 -0.154580

H 2.436936 -2.108498 0.013996

H 3.180873 -0.719836 0.824492

H 3.106856 -0.768442 -0.933763

H 0.051573 -2.075480 0.074332

H -1.292408 0.498095 1.153870

H -2.142588 1.695437 -0.117411

H 0.064742 2.913466 -0.174335

H 2.169241 1.665883 -0.147544

H -2.485000 -2.079817 0.220424

H -3.369053 -0.553240 0.304724

H -2.700135 -1.091736 -1.236315

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2649.02 | 135.388 | 139.0415 |
| 180.0321 | 193.1311 | 265.5705 |
| 373.0116 | 389.6796 | 418.454 |
| 472.5566 | 537.1573 | 609.9229 |
| 687.2009 | 703.8616 | 764.8061 |
| 839.5881 | 875.3774 | 961.7865 |
| 972.493 | 977.6797 | 1031.792 |
| 1052.018 | 1061.235 | 1072.368 |
| 1137.486 | 1183.212 | 1210.635 |
| 1268.646 | 1295.083 | 1333.81 |
| 1398.886 | 1420.017 | 1426.279 |
| 1456.139 | 1477.724 | 1484.802 |
| 1497.176 | 1501.538 | 1592.285 |
| 1642.022 | 2200.072 | 3005.927 |
| 3024.949 | 3078.188 | 3078.497 |
| 3119.904 | 3130.043 | 3169.692 |
| 3184.537 | 3205.102 | 3221.885 |

***i34 – p47***

C 2.580437 -0.932217 -0.000739

C 1.221315 -0.297129 -0.014546

C 0.089982 -1.008290 -0.160159

C -1.232480 -0.393495 -0.134161

C -1.294781 1.116003 -0.244546

C -0.009805 1.814178 0.092471

C 1.146343 1.156801 0.176980

C -2.345851 -1.134222 -0.030850

H 2.520739 -2.011307 -0.151367

H 3.084172 -0.744924 0.953545

H 3.214765 -0.509019 -0.786690

H 0.136937 -2.089741 -0.252854

H -2.112086 1.504569 0.370345

H -1.554660 1.379088 -1.280852

H -0.044235 2.890442 0.227168

H 2.067756 1.689765 0.391330

H -2.615419 -1.141448 2.437501

H -3.330146 -0.679699 -0.003505

H -2.298772 -2.217504 -0.011331

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -285.166 | 55.5996 | 95.5616 |
| 131.1956 | 171.9012 | 209.3735 |
| 294.0776 | 305.719 | 424.7324 |
| 458.3531 | 526.7927 | 547.3947 |
| 555.6475 | 700.6811 | 711.5805 |
| 763.4032 | 866.4372 | 884.6174 |
| 895.9389 | 941.2144 | 955.851 |
| 975.5056 | 1013.077 | 1026.281 |
| 1051.983 | 1072.072 | 1194.169 |
| 1206.672 | 1230.22 | 1318.415 |
| 1349.019 | 1373.51 | 1418.757 |
| 1446.219 | 1446.598 | 1457.528 |
| 1489.135 | 1498.158 | 1672.73 |
| 1679.165 | 1752.193 | 3002.854 |
| 3039.746 | 3086.233 | 3098.748 |
| 3140.4 | 3157.851 | 3176.172 |
| 3177.563 | 3201.572 | 3247.522 |

***i34 – p46***

C 2.439600 -1.011851 0.176390

C 1.284075 -0.328040 0.110320

C -0.014306 -1.001846 0.084340

C -1.177297 -0.347736 0.007889

C -1.226806 1.154310 -0.055406

C 0.115367 1.816683 -0.024655

C 1.257586 1.134851 0.049906

C -2.500402 -1.052466 -0.025136

H 2.923395 -1.366514 -2.224589

H 2.451525 -2.094119 0.240251

H 3.395397 -0.501584 0.211146

H -0.009283 -2.087858 0.127918

H -1.844026 1.530367 0.773726

H -1.768210 1.459685 -0.962901

H 0.132601 2.901429 -0.068542

H 2.209556 1.656192 0.067077

H -2.381730 -2.134921 0.046011

H -3.139056 -0.720881 0.800998

H -3.037066 -0.825225 -0.952987

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -289.866 | 94.8668 | 113.8081 |
| 129.308 | 149.949 | 208.9093 |
| 294.1842 | 341.5081 | 420.3231 |
| 443.5712 | 487.6937 | 538.146 |
| 589.8688 | 710.6859 | 716.0306 |
| 801.0208 | 882.3129 | 885.405 |
| 905.4548 | 931.1049 | 952.4072 |
| 974.445 | 1010.542 | 1017.781 |
| 1051.433 | 1070.194 | 1179.569 |
| 1203.263 | 1231.298 | 1319.134 |
| 1361.649 | 1402.113 | 1423.045 |
| 1441.017 | 1457.92 | 1465.898 |
| 1483.318 | 1495.794 | 1664.855 |
| 1716.76 | 1771.165 | 3007.258 |
| 3025.629 | 3034.867 | 3091.908 |
| 3136.477 | 3162.004 | 3175.011 |
| 3178.985 | 3202.096 | 3252.451 |

***Products***

***p1 + H***

C 2.514963 -1.033952 0.006534

C 1.218549 -0.265606 -0.006499

C 0.000002 -0.941214 -0.011637

C -1.218547 -0.265611 -0.006540

C -1.204417 1.127834 -0.000270

C -0.000003 1.818600 0.002619

C 1.204416 1.127837 -0.000223

C -2.514961 -1.033956 0.006561

H 2.510011 -1.829121 -0.743379

H 2.680066 -1.502609 0.981512

H 3.365844 -0.381223 -0.198287

H 0.000005 -2.028761 -0.022633

H -2.142370 1.673914 -0.001767

H -0.000004 2.903220 0.002943

H 2.142366 1.673921 -0.001681

H -3.365733 -0.381447 -0.199415

H -2.680609 -1.501586 0.981945

H -2.509586 -1.829902 -0.742511

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 101.1151 | 101.8826 | 197.0954 |
| 229.1919 | 276.9222 | 409.5253 |
| 442.0371 | 525.766 | 539.3609 |
| 549.2396 | 717.6343 | 744.0453 |
| 787.8462 | 902.4466 | 918.2242 |
| 927.3635 | 996.9835 | 1003.002 |
| 1027.264 | 1040.423 | 1072.154 |
| 1074.803 | 1136.274 | 1182.911 |
| 1203.896 | 1291.103 | 1321.434 |
| 1349.55 | 1420.062 | 1422.737 |
| 1467.381 | 1494.587 | 1495.267 |
| 1500.325 | 1519.841 | 1541.364 |
| 1666.199 | 1686.82 | 3047.079 |
| 3047.695 | 3113.249 | 3113.402 |
| 3136.376 | 3136.643 | 3169.041 |
| 3183.593 | 3191.635 | 3211.684 |

***p2 + H***

C 2.920815 -0.006989 0.006846

C 1.414238 0.005973 -0.002812

C 0.692766 -1.189501 -0.003647

C -0.692787 -1.189487 -0.003623

C -1.414238 0.006001 -0.002766

C -0.695777 1.196480 -0.003557

C 0.695799 1.196467 -0.003582

C -2.920815 -0.006977 0.006829

H 3.328831 0.996234 -0.131266

H 3.314313 -0.643560 -0.790400

H 3.303991 -0.396264 0.955075

H 1.227326 -2.134906 -0.007382

H -1.227366 -2.134882 -0.007339

H -1.228284 2.142624 -0.007012

H 1.228324 2.142600 -0.007058

H -3.314271 -0.642424 -0.791339

H -3.328844 0.996431 -0.129871

H -3.304026 -0.397654 0.954468

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 50.8421 | 53.1237 | 140.081 |
| 289.6258 | 314.3234 | 391.1122 |
| 419.1591 | 468.4956 | 500.9141 |
| 662.1979 | 729.5334 | 739.929 |
| 818.2806 | 848.6467 | 859.5028 |
| 966.3482 | 989.679 | 994.8395 |
| 1027.397 | 1047.969 | 1069.818 |
| 1073.135 | 1152.311 | 1222.46 |
| 1244.155 | 1251.368 | 1329.244 |
| 1350.768 | 1421.531 | 1421.855 |
| 1452.633 | 1493.772 | 1494.917 |
| 1495.476 | 1510.328 | 1570.401 |
| 1652.298 | 1698.392 | 3044.964 |
| 3045.256 | 3109.626 | 3109.793 |
| 3133.108 | 3133.153 | 3176.223 |
| 3180.226 | 3194.424 | 3199.459 |

***p3 + H***

C 2.564604 -0.812764 -0.108497

C 1.231008 -0.140155 -0.005522

C 0.048116 -1.028167 0.294126

C -1.307938 -0.407521 0.031775

C -1.371903 1.052817 0.084945

C -0.256682 1.794766 0.024932

C 1.063596 1.183393 -0.097202

C -2.390865 -1.149356 -0.216954

H 2.578131 -1.526363 -0.939572

H 2.780795 -1.383484 0.802267

H 3.369022 -0.090732 -0.259857

H 0.108286 -1.287484 1.363040

H 0.140318 -1.977270 -0.243421

H -2.350311 1.520954 0.115929

H -0.324608 2.877414 0.027976

H 1.918811 1.830187 -0.266337

H -3.365427 -0.691494 -0.348355

H -2.334628 -2.229809 -0.297297

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 82.2211 | 162.4214 | 205.9829 |
| 295.7255 | 340.1813 | 419.2479 |
| 466.0654 | 490.25 | 513.3584 |
| 581.8149 | 691.4093 | 737.8093 |
| 804.0696 | 873.9876 | 876.123 |
| 911.138 | 931.8734 | 955.9367 |
| 983.1314 | 997.4677 | 1013.343 |
| 1068.066 | 1082.527 | 1182.964 |
| 1205.094 | 1235.625 | 1319.217 |
| 1343.136 | 1380.113 | 1420.412 |
| 1434.82 | 1455.162 | 1472.642 |
| 1483.017 | 1496.219 | 1669.455 |
| 1710.937 | 1755.922 | 2993.247 |
| 3031.747 | 3079.574 | 3088.759 |
| 3134.631 | 3148.666 | 3183.174 |
| 3192.637 | 3210.643 | 3236.482 |

***p4a + H***

C -0.216585 -0.503344 0.000029

C 0.728450 0.448130 0.000503

C 2.171702 0.201094 0.000075

C 3.018269 1.235576 -0.000325

C 2.660932 -1.221921 0.000019

C -4.236277 0.213919 -0.000253

C -2.800384 -0.032611 -0.000104

C -1.613264 -0.231833 0.000083

H 0.065258 -1.552832 -0.000671

H 0.417377 1.489444 0.001164

H 4.092890 1.090074 -0.000784

H 2.657175 2.258796 -0.000230

H 3.750880 -1.261003 -0.000355

H 2.298293 -1.759366 -0.881628

H 2.298903 -1.759181 0.882034

H -4.788760 -0.716527 -0.151870

H -4.512280 0.908068 -0.798107

H -4.556798 0.648466 0.950280

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 65.9854 | 77.3066 | 81.2838 |
| 141.3035 | 175.3228 | 221.1408 |
| 251.5718 | 307.171 | 413.2139 |
| 420.7097 | 496.7486 | 537.3885 |
| 539.7464 | 707.3196 | 819.1777 |
| 872.6332 | 879.9678 | 927.1592 |
| 990.6811 | 999.1626 | 1040.813 |
| 1051.3 | 1059.804 | 1069.613 |
| 1211.086 | 1291.477 | 1333.861 |
| 1347.231 | 1413.458 | 1418.804 |
| 1452.218 | 1479.356 | 1483.298 |
| 1487.104 | 1501.337 | 1693.088 |
| 1732.885 | 2374.058 | 3047.791 |
| 3051.658 | 3109.621 | 3121.385 |
| 3128.303 | 3146.17 | 3156.42 |
| 3169.859 | 3175.743 | 3245.486 |

***p4b + H***

C 0.250828 0.512567 0.277268

C -0.725260 -0.270541 -0.199264

C 4.242830 -0.261261 -0.098650

C 2.817596 0.010496 0.032582

C 1.638471 0.228209 0.136373

C -2.165359 0.013461 -0.078925

C -2.655467 1.251331 -0.165757

C -3.048789 -1.189647 0.124319

H -0.008009 1.419039 0.818937

H -0.451293 -1.204258 -0.685964

H 4.536745 -0.298201 -1.150840

H 4.498325 -1.221311 0.357346

H 4.833641 0.515671 0.392506

H -3.717124 1.444518 -0.055821

H -2.014336 2.102275 -0.367200

H -4.100730 -0.907584 0.189491

H -2.773483 -1.723053 1.039405

H -2.932833 -1.894785 -0.705542

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 22.5545 | 74.5228 | 87.4451 |
| 118.5984 | 177.917 | 218.2704 |
| 258.1108 | 306.5348 | 378.9001 |
| 423.4704 | 518.9214 | 528.919 |
| 546.763 | 718.2159 | 809.42 |
| 893.3671 | 913.6025 | 938.6573 |
| 992.3557 | 1006.501 | 1032.24 |
| 1054.013 | 1057.934 | 1075.906 |
| 1204.178 | 1254.339 | 1332.261 |
| 1353.877 | 1416.89 | 1419.657 |
| 1447.086 | 1483.524 | 1483.937 |
| 1485.361 | 1499.914 | 1708.673 |
| 1728.108 | 2374.258 | 3037.782 |
| 3045.729 | 3099.512 | 3116.919 |
| 3121.764 | 3137.429 | 3152.411 |
| 3158.819 | 3165.23 | 3241.195 |

***p5a + H***

C -0.028044 1.505802 0.000160

C 1.250328 1.093384 0.000158

C 1.805266 -0.264290 0.000020

C 3.135871 -0.404380 -0.000522

C 0.897546 -1.464063 0.000488

C -3.515878 -0.616074 -0.000115

C -2.266160 0.132214 -0.000067

C -1.216813 0.722157 -0.000070

H -0.199636 2.579071 0.000471

H 2.000291 1.880080 0.000388

H 3.602522 -1.383233 -0.000583

H 3.796960 0.456133 -0.000969

H 1.482563 -2.385418 0.000904

H 0.245520 -1.462681 -0.876334

H 0.245537 -1.461918 0.877394

H -4.363779 0.039986 0.211082

H -3.497252 -1.402474 0.758875

H -3.685424 -1.088048 -0.971541

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 56.8869 | 84.3274 | 106.0189 |
| 177.8097 | 256.5123 | 309.5893 |
| 312.3303 | 321.342 | 424.2233 |
| 438.8249 | 455.3279 | 595.3162 |
| 685.7925 | 719.8847 | 760.1073 |
| 809.7163 | 866.3833 | 937.4719 |
| 992.3916 | 1013.248 | 1055.321 |
| 1057.842 | 1060.398 | 1074.219 |
| 1164.727 | 1276.95 | 1356.106 |
| 1415.38 | 1419.256 | 1439.364 |
| 1471.992 | 1485.751 | 1489.784 |
| 1498.06 | 1510.932 | 1684.203 |
| 1729.513 | 2372.504 | 3048.711 |
| 3055.167 | 3118.743 | 3125.025 |
| 3126.162 | 3139.967 | 3155.614 |
| 3163.434 | 3185.512 | 3244.967 |

***p5b + H***

C -0.103363 1.504008 -0.142918

C 1.166705 1.071987 -0.179625

C -3.518733 -0.699872 0.233266

C -2.296466 0.080755 0.100180

C -1.274396 0.706891 -0.011847

C 1.676354 -0.306088 -0.101348

C 1.010709 -1.363417 -0.570307

C 3.041426 -0.440183 0.525136

H -0.276651 2.574707 -0.205828

H 1.933416 1.841665 -0.238862

H -4.264967 -0.379547 -0.498215

H -3.950778 -0.579066 1.230112

H -3.320778 -1.763092 0.075814

H 1.432437 -2.360245 -0.494755

H 0.043840 -1.264073 -1.046671

H 3.367543 -1.481055 0.552554

H 3.039557 -0.050950 1.548159

H 3.782958 0.137173 -0.037527

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 43.1526 | 81.0124 | 132.825 |
| 154.5102 | 167.7401 | 226.2714 |
| 288.5302 | 341.9421 | 398.2488 |
| 419.9239 | 466.6237 | 592.5487 |
| 663.9805 | 719.832 | 756.2731 |
| 803.048 | 904.7755 | 954.0289 |
| 982.9897 | 1008.813 | 1031.18 |
| 1060.797 | 1065.498 | 1071.164 |
| 1171.418 | 1274.89 | 1286.972 |
| 1407.319 | 1426.201 | 1446.485 |
| 1464.269 | 1481.125 | 1489.457 |
| 1491.051 | 1498.797 | 1697.986 |
| 1730.214 | 2372.438 | 3041.208 |
| 3048.241 | 3102.853 | 3118.355 |
| 3124.218 | 3138.658 | 3155.998 |
| 3160.217 | 3180.974 | 3256.354 |

***p6 + H***

C -2.854163 -0.052880 -0.176806

C -1.363694 0.037518 -0.011545

C -0.697346 1.195062 0.001782

C 0.789030 1.270410 0.216973

C 1.520696 -0.039400 0.006619

C 0.721270 -1.257433 0.139250

C -0.617686 -1.219345 0.135692

C 2.827592 -0.091460 -0.265674

H -3.113490 -0.649778 -1.057417

H -3.305226 0.934668 -0.289325

H -3.311953 -0.541294 0.689898

H -1.232644 2.135045 -0.097026

H 1.226818 2.049739 -0.413579

H 0.961566 1.597219 1.253695

H 1.246182 -2.206099 0.192482

H -1.185375 -2.142709 0.204518

H 3.343202 -1.041144 -0.360454

H 3.416726 0.809511 -0.400541

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 57.5427 | 175.8774 | 240.0451 |
| 270.2503 | 308.9423 | 406.9 |
| 426.3477 | 477.8578 | 568.0475 |
| 621.2447 | 713.6911 | 746.0771 |
| 782.342 | 812.6579 | 826.612 |
| 911.9203 | 945.032 | 959.6387 |
| 983.7758 | 1004.455 | 1015.828 |
| 1076.497 | 1090.838 | 1202.884 |
| 1205.566 | 1232.444 | 1315.943 |
| 1346.159 | 1375.936 | 1425.196 |
| 1435.351 | 1452.172 | 1475.461 |
| 1490.45 | 1501.708 | 1670.828 |
| 1713.944 | 1766.61 | 3001.556 |
| 3035.741 | 3085.903 | 3095.917 |
| 3130.987 | 3154.874 | 3175.906 |
| 3180.969 | 3199.122 | 3243.01 |

***p7a + H***

C 3.528339 0.050147 0.000281

C 2.386690 -0.637703 0.000246

C 1.040957 -0.058491 -0.000044

C -0.017867 -0.891393 -0.000253

C 0.895894 1.434424 -0.000234

C -3.950551 0.205185 0.000429

C -2.544478 -0.176451 -0.000402

C -1.381255 -0.487948 -0.000422

H 4.485393 -0.457910 0.000491

H 3.550656 1.134627 0.000104

H 2.430653 -1.724742 0.000407

H 0.160566 -1.963783 -0.000248

H -0.153601 1.727371 0.000838

H 1.377661 1.867348 -0.882424

H 1.379546 1.867854 0.880661

H -4.235590 0.638276 0.962871

H -4.588598 -0.662512 -0.183754

H -4.153064 0.946854 -0.776554

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.0465 | 76.7708 | 84.8544 |
| 148.0809 | 191.3318 | 254.2638 |
| 280.9913 | 303.1753 | 396.7325 |
| 407.4392 | 451.9849 | 507.6309 |
| 597.0344 | 688.1567 | 823.5212 |
| 835.2667 | 885.1556 | 941.1339 |
| 995.2856 | 1026.165 | 1049.502 |
| 1052.068 | 1067.524 | 1090.256 |
| 1214.685 | 1247.414 | 1334.924 |
| 1386.284 | 1410.817 | 1436.577 |
| 1456.378 | 1480.214 | 1487.349 |
| 1492.852 | 1498.206 | 1687.807 |
| 1727.313 | 2371.848 | 3049.509 |
| 3050.07 | 3110.267 | 3119.812 |
| 3126.105 | 3154.207 | 3160.214 |
| 3169.766 | 3173.015 | 3255.41 |

***p7b + H***

C -3.121069 -1.047264 0.275050

C -2.523825 0.042204 -0.201755

C -1.086033 0.346702 -0.095201

C -0.164697 -0.624379 -0.219347

C -0.734511 1.788491 0.135315

C 3.879807 -0.151100 0.093737

C 2.435083 -0.307069 -0.014354

C 1.241122 -0.434553 -0.104169

H -4.185857 -1.205149 0.147977

H -2.567344 -1.807303 0.817139

H -3.131412 0.805593 -0.685627

H -0.495282 -1.635299 -0.440152

H 0.344178 1.937383 0.183260

H -1.180747 2.147080 1.068331

H -1.137121 2.409773 -0.671991

H 4.292967 0.293807 -0.815469

H 4.363525 -1.119203 0.245493

H 4.141835 0.495127 0.935387

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 72.8756 | 86.2873 | 93.0803 |
| 123.028 | 136.5801 | 224.0548 |
| 272.3293 | 288.9565 | 387.5662 |
| 409.4164 | 509.4569 | 517.6362 |
| 556.7462 | 698.448 | 821.484 |
| 846.86 | 903.2439 | 966.3233 |
| 1011.33 | 1034.317 | 1048.776 |
| 1058.618 | 1064.782 | 1087.79 |
| 1200.67 | 1245.107 | 1320.78 |
| 1361.5 | 1417.185 | 1426.412 |
| 1463.468 | 1485.091 | 1486.966 |
| 1489.737 | 1490.972 | 1704.893 |
| 1723.956 | 2374.031 | 3043.233 |
| 3047.871 | 3101.425 | 3118.742 |
| 3121.638 | 3148.153 | 3155.455 |
| 3160.278 | 3179.711 | 3247.005 |

***p8a + H***

C -2.274858 1.778068 -0.000114

C -1.180708 1.016477 -0.000716

C -1.172971 -0.448124 -0.000236

C -0.014156 -1.135673 -0.001492

C -2.487344 -1.175979 0.001953

C 3.752890 0.441106 0.002004

C 2.404533 -0.110925 -0.001738

C 1.287781 -0.561217 -0.002277

H -2.199365 2.859196 -0.000655

H -3.275323 1.358511 0.000890

H -0.204137 1.492047 -0.001709

H -0.050361 -2.221840 -0.001268

H -2.340172 -2.256772 0.002111

H -3.081144 -0.910452 -0.878409

H -3.078285 -0.909873 0.884075

H 3.870932 1.185982 -0.789229

H 4.495374 -0.344602 -0.157506

H 3.971475 0.925395 0.957403

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 84.5758 | 86.2251 | 109.5891 |
| 131.9927 | 174.3852 | 251.7982 |
| 279.4159 | 325.5029 | 390.0131 |
| 390.4953 | 466.9336 | 484.8079 |
| 600.8026 | 730.4574 | 796.1693 |
| 846.6078 | 864.0493 | 943.618 |
| 1012.831 | 1037.925 | 1055.365 |
| 1063.541 | 1067.933 | 1083.226 |
| 1214.071 | 1258.119 | 1358.376 |
| 1382.68 | 1422.07 | 1425.965 |
| 1464.553 | 1480.734 | 1483.409 |
| 1492.316 | 1502.553 | 1681.122 |
| 1730.795 | 2370.889 | 3040.075 |
| 3047.439 | 3099.501 | 3118.814 |
| 3121.877 | 3143.254 | 3163.637 |
| 3173.29 | 3191.658 | 3251.628 |

***p8b + H***

C -0.518382 2.025720 -0.211580

C -1.434045 1.163538 0.225688

C -1.453546 -0.294577 0.026926

C -0.366614 -1.079512 -0.088157

C -2.829673 -0.905517 -0.014350

C 3.576595 -0.038148 0.077245

C 2.166264 -0.398522 0.019136

C 0.995493 -0.676133 -0.026498

H -0.625192 3.086773 -0.015548

H 0.347518 1.707283 -0.778774

H -2.298917 1.557618 0.757604

H -0.523555 -2.146103 -0.227953

H -3.365721 -0.704937 0.919666

H -2.788956 -1.985979 -0.160222

H -3.422576 -0.468816 -0.824317

H 3.698496 1.044468 0.164883

H 4.099574 -0.367686 -0.824357

H 4.062779 -0.503710 0.938553

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 51.8472 | 60.9173 | 87.1805 |
| 107.2721 | 183.6165 | 245.2369 |
| 281.2084 | 322.0044 | 355.9538 |
| 396.1122 | 479.8417 | 499.5393 |
| 571.1055 | 725.3763 | 813.7486 |
| 847.2429 | 874.2208 | 972.8254 |
| 1022.161 | 1037.859 | 1055.913 |
| 1062.15 | 1066.254 | 1109.132 |
| 1186.118 | 1225.712 | 1352.18 |
| 1383.193 | 1416.618 | 1423.851 |
| 1468.182 | 1482.622 | 1488.008 |
| 1488.076 | 1496.637 | 1699.352 |
| 1728.51 | 2371.839 | 3040.675 |
| 3047.747 | 3100.454 | 3119.338 |
| 3120.9 | 3141.871 | 3147.641 |
| 3163.373 | 3167.539 | 3257.491 |

***p9a + H***

C -3.166799 -0.915433 -0.001091

C -2.548784 0.264461 -0.001075

C -1.095680 0.484515 0.000416

C -0.212873 -0.748845 0.001746

C -0.605587 1.724296 0.000695

C 3.845975 -0.051026 -0.001397

C 2.406774 -0.289559 0.000335

C 1.223658 -0.492237 0.001108

H -4.248628 -0.977315 -0.002264

H -2.628531 -1.857271 0.000049

H -3.150764 1.170265 -0.002206

H -0.466931 -1.358855 0.877009

H -0.467138 -1.360865 -0.872041

H 0.461625 1.910735 0.002048

H -1.269737 2.582044 -0.000180

H 4.125311 0.644413 -0.796677

H 4.391847 -0.984135 -0.160981

H 4.172847 0.373944 0.950827

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 55.9247 | 71.0647 | 93.2754 |
| 148.6809 | 209.1581 | 234.8571 |
| 296.7431 | 378.1557 | 406.8432 |
| 433.4429 | 517.2859 | 535.4846 |
| 636.3899 | 791.3547 | 802.8485 |
| 843.4381 | 939.3904 | 946.8885 |
| 964.8739 | 973.32 | 1040.576 |
| 1056.841 | 1061.479 | 1068.442 |
| 1181.211 | 1253.751 | 1283.651 |
| 1331.187 | 1394.941 | 1420.765 |
| 1439.298 | 1462.431 | 1479.71 |
| 1486.167 | 1490.059 | 1694.373 |
| 1746.703 | 2399.192 | 3034.058 |
| 3053.44 | 3065.466 | 3124.604 |
| 3127.828 | 3155.9 | 3161.76 |
| 3168.979 | 3249.825 | 3256.526 |

***p9b + H***

C -1.098374 2.025545 0.203516

C -1.728853 0.976906 -0.320833

C -1.439816 -0.434934 -0.036455

C -0.333549 -0.775343 0.944827

C -2.152934 -1.399479 -0.620375

C 3.424500 0.105477 -0.504410

C 2.100777 -0.203149 0.024332

C 1.005600 -0.456830 0.444666

H -1.387446 3.036453 -0.059325

H -0.268552 1.917655 0.893465

H -2.540244 1.148179 -1.024693

H -0.504474 -0.239346 1.885777

H -0.383453 -1.841787 1.180251

H -1.962031 -2.448883 -0.424909

H -2.948436 -1.164034 -1.319672

H 3.344368 0.634204 -1.457482

H 3.999074 -0.808834 -0.672392

H 3.987095 0.737238 0.187372

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.4297 | 88.1105 | 99.0838 |
| 155.4482 | 202.3211 | 242.911 |
| 311.1718 | 400.5742 | 409.8812 |
| 419.0822 | 486.9932 | 572.1413 |
| 658.964 | 797.559 | 813.7252 |
| 822.5602 | 949.0736 | 956.4969 |
| 962.9132 | 978.6077 | 1037.848 |
| 1057.65 | 1058.704 | 1073.364 |
| 1174.178 | 1228.725 | 1327.419 |
| 1333.715 | 1360.577 | 1417.724 |
| 1439.662 | 1468.33 | 1488.459 |
| 1489.384 | 1492.995 | 1692.639 |
| 1746.328 | 2398.526 | 3050.369 |
| 3052.548 | 3099.227 | 3125.077 |
| 3125.289 | 3156.125 | 3159.358 |
| 3172.06 | 3244.173 | 3252.486 |

***p14 + H***

C 0.799880 1.908412 0.001468

C 0.423576 0.621545 0.001277

C -3.573106 -0.276302 -0.002088

C -2.149889 0.036943 0.000546

C -0.977168 0.301789 0.001433

C 1.397151 -0.502076 0.000269

C 0.984284 -1.770185 0.002558

C 2.861805 -0.156243 -0.003386

H 0.061137 2.699644 0.002177

H 1.842846 2.198760 0.000903

H -4.079113 0.228060 -0.829196

H -4.043482 0.045644 0.930394

H -3.734776 -1.351413 -0.111025

H 1.696924 -2.587448 0.001870

H -0.069547 -2.022167 0.005448

H 3.469264 -1.061930 -0.004339

H 3.130932 0.434242 0.877890

H 3.126620 0.433320 -0.886584

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 35.5981 | 56.9775 | 94.6777 |
| 157.5253 | 223.675 | 285.0508 |
| 331.5119 | 340.7095 | 394.6484 |
| 419.568 | 450.8558 | 576.3708 |
| 617.1909 | 684.7818 | 723.5422 |
| 794.7004 | 843.347 | 939.74 |
| 950.6723 | 967.1968 | 1027.096 |
| 1058.547 | 1064.292 | 1071.472 |
| 1077.286 | 1227.941 | 1380.031 |
| 1417.963 | 1427.011 | 1432.262 |
| 1443.31 | 1483.584 | 1487.691 |
| 1489.335 | 1502.407 | 1673.194 |
| 1730.466 | 2383.278 | 3040.227 |
| 3049.844 | 3101.884 | 3120.807 |
| 3125.929 | 3138.869 | 3164.174 |
| 3179.685 | 3255.054 | 3272.4 |

***p15 + H***

C 0.825364 1.960581 -0.430338

C 0.468402 0.707183 -0.126616

C -3.471768 -0.348276 0.234660

C -2.069448 0.025720 0.106528

C -0.915836 0.349043 -0.000751

C 1.471856 -0.379956 0.069207

C 2.567065 -0.170808 0.797270

C 1.171200 -1.699450 -0.587504

H 0.082747 2.739110 -0.555468

H 1.868453 2.218162 -0.570945

H -4.031566 -0.069286 -0.661649

H -3.929385 0.154557 1.090445

H -3.576629 -1.426086 0.379947

H 3.314752 -0.947102 0.920881

H 2.739729 0.773854 1.300328

H 1.978272 -2.414596 -0.421594

H 1.029626 -1.571098 -1.664989

H 0.242991 -2.121738 -0.191695

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 64.7445 | 86.4102 | 93.0905 |
| 157.5743 | 205.9942 | 263.6055 |
| 286.1635 | 330.9649 | 400.8138 |
| 411.6426 | 488.9813 | 583.062 |
| 643.6396 | 678.5894 | 751.7362 |
| 792.9912 | 854.1053 | 953.5436 |
| 956.6991 | 979.8697 | 1037.007 |
| 1057.847 | 1062.525 | 1078.287 |
| 1089.974 | 1242.265 | 1347.943 |
| 1418.839 | 1424.489 | 1443.165 |
| 1458.232 | 1484.536 | 1485.654 |
| 1489.64 | 1504.816 | 1690.274 |
| 1733.271 | 2379.153 | 3046.603 |
| 3049.623 | 3110.393 | 3121.292 |
| 3124.935 | 3143.215 | 3152.988 |
| 3166.839 | 3243.514 | 3264.631 |

***p16 + C3H5***

C -2.399426 0.473677 0.000001

C -1.471392 -0.482327 -0.000012

C 2.564241 0.161451 0.000016

C 1.124440 -0.061610 0.000040

C -0.065584 -0.237953 -0.000009

H -2.129897 1.523631 -0.000017

H -3.453698 0.223627 0.000029

H -1.774515 -1.526164 0.000006

H 2.792614 1.229603 0.025236

H 3.022491 -0.263392 -0.896744

H 3.029335 -0.306731 0.871280

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 24.4431 | 140.0762 | 188.5809 |
| 332.0014 | 390.8488 | 545.7793 |
| 709.4461 | 726.7034 | 964.8887 |
| 1023.757 | 1054.747 | 1055.003 |
| 1058.66 | 1201.186 | 1328.813 |
| 1418.595 | 1451.104 | 1483.735 |
| 1484.151 | 1707.08 | 2378.718 |
| 3046.618 | 3118.232 | 3122.656 |
| 3157.391 | 3168.863 | 3255.855 |

***p17 + CH3***

C -1.079423 1.883732 0.000004

C -0.726736 0.411732 0.000045

C 3.268172 -0.474577 0.000007

C 1.843085 -0.170383 0.000001

C 0.663775 0.064856 0.000027

C -1.647793 -0.522189 0.000041

C -2.574777 -1.432743 -0.000029

H -0.657100 2.370616 0.882969

H -2.160694 2.023703 0.000220

H -0.657503 2.370504 -0.883218

H 3.575773 -0.899508 0.958928

H 3.856930 0.428995 -0.175812

H 3.511356 -1.196610 -0.783527

H -2.973345 -1.830171 0.928670

H -2.973241 -1.830095 -0.928808

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.5215 | 89.7159 | 136.5545 |
| 161.5731 | 198.5896 | 269.2183 |
| 303.8111 | 384.5862 | 492.9915 |
| 539.6843 | 561.1188 | 657.4269 |
| 674.8394 | 901.8971 | 935.5956 |
| 1020.834 | 1051.873 | 1054.786 |
| 1066.792 | 1067.044 | 1245.572 |
| 1331.852 | 1414.122 | 1417.196 |
| 1476.084 | 1480.393 | 1481.656 |
| 1487.752 | 1510.304 | 2083.361 |
| 2380.708 | 3052.028 | 3055.521 |
| 3123.017 | 3125.16 | 3127.226 |
| 3132.608 | 3156.875 | 3212.3 |

***p18 + H***

C 0.778109 2.038737 -0.000040

C 0.346432 0.593645 -0.000057

C -3.455595 -0.272500 0.000080

C -2.175802 0.018240 0.000005

C -0.942149 0.293244 -0.000062

C 1.361932 -0.480226 -0.000008

C 2.668660 -0.199098 0.000127

C 0.865657 -1.900984 -0.000080

H -0.089146 2.697767 -0.000361

H 1.384428 2.260804 -0.883310

H 1.383882 2.260940 0.883574

H -4.208699 0.508219 0.000090

H -3.795994 -1.302701 0.000125

H 3.407360 -0.992666 0.000212

H 3.047557 0.815729 0.000171

H 1.698728 -2.605104 0.000654

H 0.244814 -2.094848 -0.879211

H 0.243607 -2.094492 0.878267

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 54.0572 | 94.2991 | 150.0438 |
| 161.1429 | 226.1024 | 275.3264 |
| 319.9107 | 339.8626 | 411.5171 |
| 426.7535 | 503.8303 | 543.3212 |
| 588.7604 | 589.0535 | 660.1854 |
| 742.3754 | 879.1765 | 897.3839 |
| 935.4284 | 977.6106 | 1020.997 |
| 1033.705 | 1048.071 | 1071.909 |
| 1155.932 | 1161.502 | 1349.555 |
| 1405.524 | 1417.585 | 1437.519 |
| 1446.924 | 1483.88 | 1489.234 |
| 1496.151 | 1501.697 | 1697.506 |
| 1726.832 | 2230.436 | 3045.862 |
| 3054.163 | 3109.956 | 3118.132 |
| 3148.224 | 3150.448 | 3155.94 |
| 3170.916 | 3235.862 | 3255.291 |

***p19 + H***

C 0.708131 1.939638 -0.295317

C 0.260494 0.510748 -0.107184

C -3.532262 -0.324453 0.213823

C -2.255110 -0.044301 0.099027

C -1.024494 0.221986 -0.012005

C 1.295473 -0.553633 -0.028508

C 1.044653 -1.796424 -0.442797

C 2.639493 -0.158337 0.526957

H -0.149278 2.605656 -0.383555

H 1.321064 2.034551 -1.197457

H 1.318416 2.271895 0.550203

H -4.286524 0.451793 0.140188

H -3.868985 -1.341063 0.387525

H 1.798011 -2.573217 -0.371706

H 0.083799 -2.065534 -0.866514

H 3.302830 -1.022086 0.586880

H 2.538797 0.269282 1.529540

H 3.123600 0.597380 -0.099070

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 43.0416 | 94.7542 | 143.393 |
| 189.4657 | 211.8256 | 274.1318 |
| 311.1965 | 315.0394 | 404.6385 |
| 455.0491 | 503.1262 | 553.199 |
| 581.3144 | 617.5746 | 662.2658 |
| 745.2989 | 884.4459 | 901.5332 |
| 947.8422 | 974.8706 | 1021.164 |
| 1033.009 | 1050.142 | 1074.992 |
| 1143.296 | 1170.733 | 1325.051 |
| 1406.605 | 1415.947 | 1443.49 |
| 1447.453 | 1478.658 | 1485.782 |
| 1495.486 | 1505.499 | 1707.11 |
| 1730.46 | 2231.403 | 3043.268 |
| 3045.79 | 3105.096 | 3106.359 |
| 3143.418 | 3148.882 | 3160.005 |
| 3161.367 | 3233.737 | 3253.186 |

***p20 + CH3***

C -1.522330 -1.182822 -0.479668

C -0.617278 -0.573390 0.618189

C 3.286192 0.349878 -0.233449

C 1.899090 0.020283 0.072239

C 0.755498 -0.250480 0.320579

C -1.717212 0.185779 -0.011520

C -2.356035 1.331208 -0.088634

H -1.071357 -1.335081 -1.454506

H -2.219125 -1.952920 -0.165029

H -0.798436 -0.943919 1.623599

H 3.410968 1.425667 -0.380294

H 3.615271 -0.156862 -1.144200

H 3.946408 0.040602 0.580713

H -3.182430 1.466524 -0.778352

H -2.068852 2.173257 0.531655

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 86.7949 | 99.6173 | 128.7915 |
| 229.5196 | 306.7407 | 325.7515 |
| 379.5933 | 489.0371 | 545.0918 |
| 630.3792 | 719.6131 | 795.177 |
| 911.1892 | 937.684 | 945.278 |
| 1019.788 | 1055.674 | 1062.729 |
| 1065.061 | 1080.983 | 1110.476 |
| 1138.738 | 1212.947 | 1366.043 |
| 1420.348 | 1443.291 | 1475.944 |
| 1487.767 | 1492.436 | 1870.954 |
| 2395.701 | 3051.067 | 3121.84 |
| 3124.499 | 3130.902 | 3150.424 |
| 3153.576 | 3221.496 | 3240.016 |

***p21 + H***

C 0.258005 1.622261 0.614002

C -0.424064 0.770397 -0.460985

C -1.507570 -0.201404 -0.139607

C -2.473556 -0.434996 -1.025377

C -1.457659 -0.896364 1.192742

C 3.099750 -0.942414 -0.274877

C 2.032430 -0.202140 -0.153139

C 0.978482 0.522678 -0.041527

H 0.518262 2.641048 0.346818

H -0.039606 1.482653 1.648066

H -0.534581 1.259161 -1.425193

H -3.266350 -1.146360 -0.821032

H -2.501050 0.073736 -1.983257

H -2.234685 -1.658166 1.263122

H -1.607460 -0.185501 2.011730

H -0.485605 -1.373193 1.348682

H 3.875047 -0.693205 -0.991728

H 3.241118 -1.828279 0.335399

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 48.9564 | 83.5858 | 179.6182 |
| 211.8396 | 249.5325 | 286.7081 |
| 390.6299 | 407.2218 | 458.149 |
| 521.1271 | 563.4521 | 621.4303 |
| 664.9352 | 749.3689 | 789.6617 |
| 869.0079 | 929.741 | 933.2745 |
| 954.8096 | 983.2389 | 1010.147 |
| 1022.361 | 1050.753 | 1066.036 |
| 1076.426 | 1081.56 | 1126.984 |
| 1316.733 | 1333.773 | 1389.336 |
| 1421.676 | 1453.043 | 1463.023 |
| 1494.742 | 1506.543 | 1551.283 |
| 1736.881 | 2140.854 | 3046.664 |
| 3108.105 | 3133.466 | 3145.015 |
| 3151.612 | 3152.726 | 3155.855 |
| 3222.078 | 3234.83 | 3241.768 |

***p22 + H***

C -0.177482 1.810640 0.089735

C 0.425915 0.559963 0.708374

C 1.485831 -0.246086 0.027575

C 2.382444 0.298104 -0.788342

C 1.447111 -1.714534 0.345145

C -3.087384 -0.799954 -0.382311

C -2.011914 -0.111624 -0.111454

C -0.950540 0.556524 0.160736

H -0.456704 2.620450 0.755636

H 0.178467 2.118820 -0.887801

H 0.483297 0.551648 1.796127

H 3.137774 -0.307997 -1.277278

H 2.394925 1.363154 -0.992035

H 2.241352 -2.259206 -0.168142

H 0.481326 -2.139316 0.053271

H 1.556242 -1.879350 1.422469

H -3.906902 -0.860392 0.326308

H -3.193657 -1.326004 -1.325301

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 55.3009 | 78.0065 | 180.8473 |
| 188.2714 | 253.4139 | 259.7344 |
| 379.1371 | 404.2789 | 471.8754 |
| 513.4879 | 567.0165 | 619.9947 |
| 691.0513 | 726.782 | 803.2713 |
| 875.7959 | 933.1652 | 939.022 |
| 948.7068 | 987.377 | 1025.692 |
| 1029.231 | 1043.937 | 1064.729 |
| 1081.835 | 1094.973 | 1114.625 |
| 1258.09 | 1344.435 | 1398.15 |
| 1423.701 | 1442.731 | 1457.454 |
| 1483.996 | 1497.514 | 1552.921 |
| 1745.817 | 2142.246 | 3039.484 |
| 3101.926 | 3128.646 | 3135.281 |
| 3135.739 | 3147.379 | 3157.672 |
| 3225.261 | 3230.608 | 3243.412 |

***p23 + CH3***

C 0.223102 1.027096 -0.273212

C 1.224256 0.324030 0.620808

C -3.534846 -0.640265 0.032220

C -2.208075 -0.044920 -0.080360

C -1.115246 0.442356 -0.175639

C 2.330900 -0.206030 0.187246

C 3.433625 -0.736574 -0.256734

H 0.570649 0.991102 -1.309025

H 0.169897 2.085294 0.007862

H 0.984250 0.263397 1.679086

H -4.277203 0.109656 0.316184

H -3.542540 -1.427846 0.789674

H -3.845200 -1.082323 -0.917761

H 4.352516 -0.161737 -0.310694

H 3.465337 -1.771699 -0.581293

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 43.058 | 84.3034 | 112.3313 |
| 184.7114 | 215.1688 | 298.9736 |
| 341.9197 | 400.1309 | 474.3404 |
| 537.5249 | 594.488 | 784.6543 |
| 881.9182 | 886.7723 | 927.9771 |
| 1019.675 | 1030.867 | 1060.432 |
| 1064.852 | 1148.9 | 1173.967 |
| 1220.704 | 1309.845 | 1381.135 |
| 1423.208 | 1468.648 | 1484.29 |
| 1486.719 | 1492.793 | 2092.82 |
| 2398.835 | 3044.514 | 3053.996 |
| 3100.652 | 3125.793 | 3127.17 |
| 3144.286 | 3171.71 | 3226.508 |

***p23’ + CH3***

C 0.437172 -1.596888 -0.000807

C 1.729375 -0.805849 0.002011

C 1.819882 0.492416 0.000552

C 1.912504 1.789967 -0.000866

C -2.959256 0.730104 0.001083

C -1.761518 -0.101712 -0.001247

C -0.773834 -0.782577 -0.001602

H 0.430358 -2.258901 0.873130

H 0.433008 -2.257258 -0.876008

H 2.645498 -1.391726 0.005486

H 1.952507 2.346979 -0.931239

H 1.946654 2.349459 0.928252

H -3.662431 0.405315 -0.769826

H -2.703900 1.774982 -0.191610

H -3.467649 0.678386 0.967068

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 71.6104 | 88.7133 | 110.1597 |
| 184.8851 | 210.7739 | 318.0281 |
| 337.6056 | 395.8066 | 468.8656 |
| 526.5252 | 652.7826 | 773.6593 |
| 887.3851 | 887.7944 | 930.1956 |
| 959.4239 | 1025.016 | 1058.052 |
| 1068.366 | 1135.493 | 1189.547 |
| 1250.182 | 1335.02 | 1384.702 |
| 1422.67 | 1468.012 | 1490.295 |
| 1490.306 | 1491.658 | 2096.603 |
| 2404.425 | 3037.853 | 3051.625 |
| 3067.017 | 3123.973 | 3124.382 |
| 3146.194 | 3159.054 | 3229.608 |

***p24 + H***

C -0.455833 -0.613099 -0.011046

C 0.613309 0.371962 -0.009905

C -4.237955 0.326994 0.008792

C -2.963618 0.012447 0.000724

C -1.738142 -0.295975 -0.006231

C 1.931705 0.121179 -0.002885

C 2.544740 -1.250099 0.008046

C 2.923770 1.249696 0.003400

H -0.199091 -1.669201 -0.013500

H 0.286249 1.408360 -0.011984

H -5.004771 -0.440348 0.010023

H -4.559411 1.363176 0.014703

H 1.815460 -2.055996 -0.062198

H 3.247792 -1.355680 -0.824899

H 3.121378 -1.395765 0.928130

H 3.581357 1.181398 0.877384

H 2.433649 2.224338 0.017672

H 3.569542 1.201092 -0.880701

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 44.8856 | 80.0853 | 85.6518 |
| 131.61 | 221.8703 | 230.4226 |
| 245.0255 | 308.2353 | 379.4959 |
| 445.8739 | 496.9654 | 529.453 |
| 534.2236 | 587.3641 | 847.247 |
| 877.9541 | 879.8921 | 890.1731 |
| 947.045 | 975.01 | 1011.11 |
| 1034.926 | 1072.241 | 1100.325 |
| 1175.269 | 1230.956 | 1311.25 |
| 1385.271 | 1420.11 | 1427.326 |
| 1455.034 | 1471.88 | 1487.845 |
| 1494.067 | 1499.343 | 1698.07 |
| 1745.217 | 2230.562 | 3031.817 |
| 3043.923 | 3086.76 | 3097.824 |
| 3142.377 | 3149.394 | 3153.785 |
| 3167.038 | 3174.462 | 3235.194 |

***p25 + H***

C -0.292299 1.471106 0.098778

C 1.106224 1.084431 -0.022648

C -3.518779 -0.706335 -0.118363

C -2.430731 0.023975 -0.038177

C -1.367871 0.703220 0.035834

C 1.632579 -0.151700 0.008621

C 0.818518 -1.399500 0.200012

C 3.111760 -0.353815 -0.153576

H -0.470406 2.535614 0.242314

H 1.791767 1.919293 -0.139911

H -4.502879 -0.262200 -0.012533

H -3.463888 -1.775906 -0.293518

H 0.277879 -1.656805 -0.717141

H 1.457979 -2.245190 0.462898

H 0.064670 -1.271367 0.980520

H 3.531439 -0.843976 0.732046

H 3.642086 0.586547 -0.313436

H 3.314945 -1.014288 -1.004113

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 39.0281 | 84.5816 | 173.3833 |
| 187.042 | 222.7033 | 242.9259 |
| 274.4343 | 314.6049 | 400.4052 |
| 435.0179 | 468.7129 | 532.1255 |
| 606.9621 | 718.4841 | 783.2355 |
| 849.4929 | 878.0656 | 901.7263 |
| 926.9149 | 989.2975 | 1006.281 |
| 1033.675 | 1053.824 | 1101.295 |
| 1160.669 | 1231.253 | 1342.673 |
| 1391.854 | 1419.331 | 1424.023 |
| 1457.684 | 1481.426 | 1487.799 |
| 1493.104 | 1512.381 | 1702.892 |
| 1718.018 | 2226.452 | 3027.969 |
| 3040.506 | 3085.239 | 3105.798 |
| 3131.033 | 3133.681 | 3139.188 |
| 3142.402 | 3169.393 | 3226.93 |

***p26 + H***

C 0.357974 -0.015585 1.168886

C -0.799934 -0.007526 0.552637

C 3.994937 0.009830 -0.699203

C 2.696926 -0.001775 -0.036669

C 1.618722 -0.008651 0.495835

C -1.952851 0.001053 -0.052809

C -2.650635 1.290800 -0.408502

C -2.655952 -1.278023 -0.435463

H 0.379092 -0.027559 2.256890

H 4.649192 -0.765181 -0.291751

H 4.491320 0.974881 -0.567711

H 3.882607 -0.170048 -1.771173

H -2.072157 2.161086 -0.098627

H -2.812665 1.346592 -1.489932

H -3.633739 1.334331 0.071690

H -3.639049 -1.327542 0.044198

H -2.081076 -2.157063 -0.144110

H -2.818647 -1.310240 -1.517747

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 68.0243 | 74.6353 | 116.5686 |
| 160.8069 | 188.1876 | 196.4468 |
| 224.7073 | 287.7146 | 317.5154 |
| 361.9682 | 449.5224 | 472.7236 |
| 546.3714 | 597.3688 | 777.9002 |
| 806.2839 | 826.5165 | 970.716 |
| 998.7571 | 1026.988 | 1060.4 |
| 1063.614 | 1104.344 | 1190.571 |
| 1226.038 | 1252.53 | 1401.892 |
| 1415.386 | 1422.172 | 1455.261 |
| 1477.973 | 1490.079 | 1490.496 |
| 1492.295 | 1496.113 | 1524.027 |
| 2088.66 | 2384.124 | 3039.258 |
| 3041.683 | 3049.356 | 3101.947 |
| 3103.108 | 3119.052 | 3125.001 |
| 3146.94 | 3148.313 | 3149.218 |

***p27 + H***

C 0.188301 2.816832 0.000000

C 0.192882 1.477786 0.000000

C 0.196793 0.697847 1.242030

C 0.196793 -0.634782 1.246087

C 0.172470 -1.473719 0.000000

C 0.196793 -0.634782 -1.246087

C 0.196793 0.697847 -1.242030

C -1.041959 -2.419961 0.000000

H 0.186020 3.380447 0.926512

H 0.186020 3.380447 -0.926512

H 0.202542 1.247472 2.178536

H 0.199298 -1.171096 2.191463

H 1.072254 -2.107561 0.000000

H 0.199298 -1.171096 -2.191463

H 0.202542 1.247472 -2.178536

H -1.035303 -3.062432 0.884835

H -1.035303 -3.062432 -0.884835

H -1.970560 -1.843634 0.000000

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 73.3071 | 226.4699 | 233.939 |
| 272.6162 | 373.977 | 419.6608 |
| 444.6773 | 502.2021 | 606.1491 |
| 676.5457 | 696.5052 | 790.2085 |
| 802.3195 | 811.1181 | 832.3678 |
| 918.0574 | 939.2962 | 959.4121 |
| 991.5642 | 1013.471 | 1015.457 |
| 1047.438 | 1100.262 | 1132.271 |
| 1196.309 | 1230.237 | 1303.532 |
| 1337.151 | 1383.823 | 1396.846 |
| 1413.663 | 1447.69 | 1475.831 |
| 1494.304 | 1506.08 | 1686.973 |
| 1709.194 | 1776.826 | 2998.067 |
| 3041.053 | 3118.227 | 3128.293 |
| 3156.359 | 3168.833 | 3169.991 |
| 3192.273 | 3195.638 | 3246.343 |

***p28 + H***

C -2.782753 0.052398 -0.103982

C -1.458656 0.045343 0.063694

C -0.673847 -1.208425 0.364615

C 0.673863 -1.208436 -0.364644

C 1.458656 0.045343 -0.063704

C 0.670463 1.278838 -0.008144

C -0.670473 1.278844 0.008111

C 2.782744 0.052413 0.104041

H -3.363912 -0.862541 -0.062154

H -3.321832 0.976433 -0.285663

H -1.255422 -2.095000 0.101374

H -0.489406 -1.247792 1.445274

H 1.255447 -2.095002 -0.101388

H 0.489434 -1.247830 -1.445302

H 1.212376 2.219936 0.003350

H -1.212386 2.219939 -0.003432

H 3.321783 0.976461 0.285777

H 3.363928 -0.862511 0.062231

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 86.2168 | 184.0432 | 284.2885 |
| 359.9289 | 381.1289 | 434.4878 |
| 445.1158 | 555.7232 | 618.5696 |
| 707.8007 | 751.4053 | 755.203 |
| 779.0441 | 804.7479 | 851.562 |
| 930.6002 | 936.6126 | 937.2538 |
| 984.3023 | 995.2872 | 1011.836 |
| 1034.922 | 1060.428 | 1183.993 |
| 1204.621 | 1249.047 | 1309.7 |
| 1347.408 | 1362.899 | 1365.483 |
| 1428.434 | 1447.078 | 1473.123 |
| 1486.217 | 1486.268 | 1668.811 |
| 1729.002 | 1740.976 | 3039.801 |
| 3046.224 | 3103.34 | 3106.415 |
| 3152.029 | 3152.077 | 3175.983 |
| 3197.504 | 3240.684 | 3240.754 |

***p29 + CH3***

C -3.216735 -0.836561 -0.325832

C -2.335746 0.019707 0.544274

C -1.210825 0.548145 0.163604

C -0.084631 1.089406 -0.234015

C 3.593454 -0.666461 0.074816

C 2.279278 -0.046442 -0.034956

C 1.189999 0.456087 -0.116356

H -3.361494 -1.820832 0.128623

H -4.203826 -0.378972 -0.440053

H -2.779548 -0.972147 -1.315602

H -2.666956 0.202250 1.565261

H -0.108276 2.080737 -0.681487

H 3.825809 -0.900500 1.116908

H 4.370186 0.002226 -0.304180

H 3.635344 -1.596045 -0.498680

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 74.659 | 90.2196 | 143.3601 |
| 184.7718 | 209.3476 | 253.0677 |
| 302.6356 | 399.7172 | 466.6928 |
| 529.4842 | 590.7925 | 768.2329 |
| 808.6158 | 902.282 | 913.1845 |
| 1055.451 | 1062.549 | 1075.088 |
| 1095.22 | 1131.529 | 1205.637 |
| 1303.773 | 1417.663 | 1421.32 |
| 1462.578 | 1485.373 | 1487.523 |
| 1496.144 | 1514.671 | 2086.649 |
| 2385.329 | 3042.51 | 3048.134 |
| 3107.061 | 3118.255 | 3124.55 |
| 3138.994 | 3154.59 | 3155.552 |

***p30 + H***

C -3.515467 0.149903 0.355039

C -2.457390 -0.428064 -0.205656

C -1.074026 0.085843 -0.146653

C -0.018404 -0.997481 -0.007343

C -0.786899 1.382978 -0.222023

C 3.890226 0.294957 0.092178

C 2.504290 -0.158717 0.056656

C 1.364963 -0.535394 0.026647

H -4.506254 -0.279277 0.259518

H -3.421182 1.064712 0.931421

H -2.592368 -1.372310 -0.731961

H -0.229764 -1.572122 0.902810

H -0.139944 -1.706118 -0.836601

H 0.236077 1.735100 -0.156288

H -1.570234 2.118606 -0.364768

H 4.066944 1.064173 -0.663694

H 4.575663 -0.533444 -0.103069

H 4.137305 0.716523 1.069559

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 43.6038 | 70.8398 | 86.7988 |
| 120.4208 | 205.6644 | 251.2283 |
| 300.1845 | 347.1902 | 390.0596 |
| 414.7141 | 467.5733 | 589.9641 |
| 662.1289 | 777.8916 | 800.3572 |
| 859.0144 | 940.692 | 962.323 |
| 967.1976 | 971.8318 | 1043.921 |
| 1054.904 | 1057.801 | 1101.212 |
| 1177.217 | 1215.866 | 1253.324 |
| 1340.877 | 1378.685 | 1416.489 |
| 1438.261 | 1467.642 | 1469.186 |
| 1482.695 | 1491.074 | 1720.202 |
| 1736.024 | 2400.47 | 3033.697 |
| 3051.709 | 3063.345 | 3121.946 |
| 3127.127 | 3144.08 | 3158.978 |
| 3161.67 | 3246.12 | 3253.89 |

***p31 + H***

C -1.919154 1.891682 -0.108476

C -1.418861 0.864335 0.570808

C -1.302874 -0.515154 0.059918

C -0.094762 -1.298700 0.539749

C -2.213566 -1.068516 -0.739259

C 3.460972 0.584441 -0.355718

C 2.208281 -0.088971 -0.033152

C 1.176025 -0.643273 0.227088

H -1.988213 2.878523 0.334280

H -2.261852 1.779872 -1.132252

H -1.027525 1.033127 1.572521

H -0.168698 -1.425557 1.627592

H -0.110938 -2.302160 0.106150

H -2.091856 -2.076491 -1.121102

H -3.112334 -0.533644 -1.025067

H 4.198003 -0.127378 -0.735925

H 3.883381 1.069054 0.527991

H 3.303670 1.349583 -1.119929

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 48.5138 | 58.6864 | 112.179 |
| 125.7026 | 205.9813 | 242.0672 |
| 290.2486 | 381.1581 | 402.4237 |
| 406.9544 | 507.9583 | 544.3462 |
| 683.3404 | 774.0893 | 814.5131 |
| 822.123 | 936.0971 | 952.933 |
| 956.7725 | 977.4911 | 1028.594 |
| 1059.856 | 1066.441 | 1103.785 |
| 1174.123 | 1211.071 | 1282.453 |
| 1335.238 | 1346.863 | 1423.725 |
| 1447.435 | 1467.186 | 1479.198 |
| 1489.402 | 1493.334 | 1720.047 |
| 1735.117 | 2398.296 | 3033.644 |
| 3048.7 | 3099.794 | 3119.296 |
| 3123.985 | 3150.099 | 3156.488 |
| 3162.796 | 3244.537 | 3248.153 |

***p32 + H***

C 3.490332 0.070109 -0.000006

C 2.159506 -0.611053 -0.000013

C 0.939580 -0.052107 0.000013

C -0.227023 -0.939824 0.000026

C 0.661223 1.424845 0.000014

C -3.937182 0.249945 -0.000024

C -2.686618 -0.147654 0.000000

C -1.483250 -0.535574 0.000017

H 4.072128 -0.230002 0.877926

H 4.071257 -0.228222 -0.879133

H 3.417482 1.157573 0.001146

H 2.204047 -1.699052 -0.000100

H -0.030729 -2.010406 0.000052

H 0.068980 1.697741 0.878385

H 0.068642 1.697644 -0.878158

H 1.570438 2.023973 -0.000214

H -4.751932 -0.466375 -0.000007

H -4.189729 1.305007 -0.000056

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 40.5547 | 58.1485 | 73.2778 |
| 82.5733 | 206.9016 | 261.5787 |
| 270.4307 | 310.6258 | 382.5801 |
| 416.286 | 444.3345 | 534.9553 |
| 604.4239 | 608.5161 | 812.0539 |
| 837.6545 | 878.0452 | 903.3753 |
| 926.8533 | 1004.909 | 1033.293 |
| 1054.922 | 1057.815 | 1066.01 |
| 1128.48 | 1253.654 | 1328.967 |
| 1383.757 | 1423.33 | 1435.468 |
| 1453.401 | 1479.358 | 1485.924 |
| 1486.436 | 1500.21 | 1705.982 |
| 1741.263 | 2231.271 | 3037.707 |
| 3049.715 | 3089.606 | 3106.7 |
| 3142.183 | 3148.138 | 3153.376 |
| 3156.398 | 3164.964 | 3234.326 |

***p33 + H***

C -3.074403 -1.029020 0.000230

C -2.310538 0.258021 0.000092

C -0.982052 0.447891 -0.000146

C -0.031816 -0.666314 -0.000402

C -0.396757 1.834853 -0.000065

C 3.839653 -0.225236 0.000287

C 2.536043 -0.374547 0.000005

C 1.280131 -0.518552 -0.000236

H -3.724111 -1.083745 0.879890

H -3.727315 -1.082068 -0.877136

H -2.441468 -1.916401 -0.001743

H -2.932112 1.151553 0.000399

H -0.422893 -1.679258 -0.000685

H 0.236354 1.988363 -0.879038

H 0.236729 1.988105 0.878683

H -1.180799 2.593445 0.000209

H 4.291104 0.761290 0.000671

H 4.502944 -1.083856 0.000166

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 27.364 | 67.4647 | 88.9763 |
| 134.6486 | 221.376 | 249.899 |
| 257.7249 | 289.067 | 378.5048 |
| 387.1729 | 517.622 | 545.6986 |
| 557.3991 | 630.2206 | 800.2343 |
| 845.8638 | 884.7314 | 887.4078 |
| 933.1619 | 1005.257 | 1033.259 |
| 1062.35 | 1071.909 | 1072.692 |
| 1119.205 | 1264.095 | 1306.287 |
| 1395.657 | 1419.089 | 1427.22 |
| 1452.219 | 1481.619 | 1485.255 |
| 1486.736 | 1498.414 | 1700.391 |
| 1742.794 | 2231.663 | 3041.117 |
| 3051.542 | 3094.584 | 3113.516 |
| 3136.051 | 3145.678 | 3149.49 |
| 3153.69 | 3186.599 | 3234.66 |

***p34 + H***

C 2.381404 1.726735 0.006219

C 1.151688 0.881349 -0.082274

C 1.057751 -0.453526 -0.026159

C -0.253327 -1.122821 -0.123776

C 2.222145 -1.397681 0.126520

C -3.745201 0.589788 0.085433

C -2.567518 0.014841 0.013696

C -1.436302 -0.544302 -0.056526

H 2.522306 2.293512 -0.920449

H 2.278202 2.462960 0.810242

H 3.290823 1.154973 0.192231

H 0.221913 1.431467 -0.214246

H -0.232109 -2.203519 -0.257493

H 2.229367 -2.127530 -0.689376

H 2.138858 -1.960878 1.061698

H 3.184592 -0.888270 0.125624

H -4.658559 0.011543 -0.006898

H -3.839221 1.659443 0.239867

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 34.3247 | 82.6795 | 120.5346 |
| 126.7234 | 207.2199 | 234.7318 |
| 255.3662 | 330.6531 | 359.3658 |
| 416.6827 | 448.122 | 542.2675 |
| 617.8992 | 623.985 | 798.7482 |
| 862.761 | 888.9006 | 915.6421 |
| 928.9259 | 1009.099 | 1032.455 |
| 1047.678 | 1064.416 | 1070.6 |
| 1138.973 | 1231.813 | 1316.845 |
| 1386.381 | 1424.197 | 1431.861 |
| 1458.79 | 1484.963 | 1491.011 |
| 1493.763 | 1511.586 | 1707.271 |
| 1745.027 | 2228.512 | 3041.915 |
| 3048.443 | 3093.52 | 3103.44 |
| 3143.642 | 3146.708 | 3150.183 |
| 3163.394 | 3169.318 | 3234.553 |

***p35 + H***

C 0.331444 2.057960 -0.172145

C 1.450010 1.101197 0.098268

C 1.427164 -0.235701 0.002259

C 0.244324 -1.022170 -0.375217

C 2.665562 -1.058627 0.258224

C -3.498062 -0.141538 0.249227

C -2.238725 -0.436546 0.030012

C -1.020238 -0.703639 -0.175206

H -0.244750 2.260514 0.737794

H 0.725884 3.012545 -0.528609

H -0.369999 1.669109 -0.913204

H 2.395093 1.551723 0.394303

H 0.443570 -1.990350 -0.834301

H 2.937692 -1.637614 -0.631167

H 2.501023 -1.773858 1.070292

H 3.514665 -0.427308 0.524857

H -4.293839 -0.810117 -0.062073

H -3.778217 0.779745 0.749581

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.4559 | 83.4822 | 173.6614 |
| 184.2568 | 226.997 | 253.3772 |
| 294.087 | 336.8363 | 345.1566 |
| 410.5585 | 459.7634 | 555.3948 |
| 588.4428 | 643.1756 | 816.4754 |
| 848.2153 | 896.0224 | 908.1274 |
| 926.3828 | 1020.127 | 1031.618 |
| 1055.914 | 1073.329 | 1090.823 |
| 1107.337 | 1215.28 | 1337.567 |
| 1389.994 | 1415.41 | 1423.725 |
| 1457.159 | 1486.441 | 1489.249 |
| 1502.094 | 1515.2 | 1709.475 |
| 1736.995 | 2233.104 | 3035.514 |
| 3039.577 | 3096.135 | 3101.399 |
| 3132.378 | 3133.689 | 3136.281 |
| 3148.97 | 3162.58 | 3234.487 |

***p36 + H***

C -3.209410 -1.032667 -0.552868

C -2.173913 -0.333310 -0.184773

C -1.135395 0.363248 0.183448

C -0.094504 -0.241787 1.114141

C -0.909812 1.782738 -0.266849

C 3.657184 -0.307292 -0.595852

C 2.333183 -0.282482 0.015990

C 1.243336 -0.268863 0.519494

H -4.127968 -1.028349 0.026020

H -3.185926 -1.639609 -1.452830

H -0.061258 0.348370 2.038628

H -0.394183 -1.254964 1.392244

H -0.875386 2.455036 0.597321

H -1.701219 2.117320 -0.937421

H 0.050944 1.864846 -0.783467

H 3.719829 -1.088656 -1.357180

H 4.428498 -0.500997 0.153652

H 3.882658 0.649492 -1.073358

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 40.5064 | 89.787 | 102.8273 |
| 169.6601 | 186.9955 | 204.8812 |
| 245.5549 | 293.3931 | 349.3271 |
| 400.1833 | 448.7222 | 520.7303 |
| 602.3996 | 627.5838 | 778.4858 |
| 789.3288 | 890.3496 | 924.1502 |
| 1012.897 | 1028.361 | 1060.768 |
| 1065.038 | 1066.003 | 1168.895 |
| 1195.814 | 1230.135 | 1309.09 |
| 1358.249 | 1413.921 | 1424.593 |
| 1467.005 | 1480.302 | 1485.301 |
| 1489.799 | 1495.48 | 1514.814 |
| 2097.345 | 2396.94 | 3036.341 |
| 3041.66 | 3050.969 | 3105.557 |
| 3106.727 | 3122.734 | 3124.718 |
| 3134.589 | 3154.028 | 3215.115 |

***p37 + H***

C 0.904026 2.310124 -0.011042

C 1.155977 1.033209 -0.006273

C 1.418133 -0.243517 -0.000959

C 0.329862 -1.304083 -0.032117

C 2.830756 -0.770488 0.032779

C -3.518895 0.154547 0.021419

C -2.159973 -0.374046 -0.000642

C -1.038410 -0.799575 -0.016292

H 0.810884 2.860472 -0.942114

H 0.768421 2.858912 0.915691

H 0.480983 -1.922894 -0.925789

H 0.480594 -1.975501 0.822750

H 3.022538 -1.411931 -0.834133

H 2.992109 -1.377240 0.930308

H 3.558146 0.040931 0.029704

H -3.735559 0.626763 0.982812

H -4.251348 -0.640645 -0.138465

H -3.655625 0.904108 -0.761997

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 23.4549 | 72.036 | 105.5401 |
| 132.0712 | 169.9745 | 197.2597 |
| 244.1894 | 280.919 | 331.1108 |
| 388.4458 | 452.4183 | 474.5709 |
| 613.5498 | 631.442 | 768.9181 |
| 795.1401 | 893.9701 | 923.4345 |
| 992.9442 | 1029.21 | 1059.241 |
| 1062.413 | 1063.864 | 1175.058 |
| 1184.392 | 1242.708 | 1309.734 |
| 1364.685 | 1412.411 | 1422.712 |
| 1465.146 | 1476.714 | 1484.945 |
| 1489.545 | 1494.76 | 1511.342 |
| 2101.238 | 2403.915 | 3029.893 |
| 3038.644 | 3049.211 | 3059.189 |
| 3096.849 | 3120.305 | 3123.29 |
| 3143.008 | 3156.222 | 3224.514 |

***p38 + CH3***

C -2.723123 -0.942843 0.276836

C -1.536509 -0.772002 -0.296178

C -0.677952 0.420811 -0.108047

C -1.173130 1.661913 -0.029574

C 3.334241 -0.368237 0.093234

C 1.908317 -0.077541 0.022329

C 0.733318 0.173120 -0.032622

H -3.313237 -1.832121 0.088157

H -3.132742 -0.208430 0.963004

H -1.126253 -1.551446 -0.932990

H -0.524628 2.514849 0.127436

H -2.236206 1.841020 -0.139807

H 3.506056 -1.438920 0.226998

H 3.794735 0.157021 0.933682

H 3.841302 -0.053295 -0.822350

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 58.7533 | 85.6213 | 109.936 |
| 176.3665 | 281.5663 | 322.6166 |
| 354.924 | 420.3484 | 525.8466 |
| 567.7099 | 714.0173 | 738.4908 |
| 769.76 | 904.0901 | 946.3704 |
| 967.1748 | 1028.71 | 1058.913 |
| 1062.957 | 1082.545 | 1098.454 |
| 1296.222 | 1338.892 | 1424.372 |
| 1438.431 | 1461.674 | 1484.918 |
| 1487.598 | 1692.251 | 1722.055 |
| 2380.586 | 3051.575 | 3123.809 |
| 3126.731 | 3153.308 | 3171.644 |
| 3179.104 | 3247.258 | 3268.839 |

***p39 + C2H3***

C 1.132268 0.116939 0.000006

C 1.796695 1.274582 -0.000002

C 1.821464 -1.223775 -0.000002

C -2.958892 -0.044793 -0.000003

C -1.503105 0.019257 0.000003

C -0.302028 0.087385 0.000004

H 2.881162 1.292559 -0.000003

H 1.275929 2.224319 -0.000006

H 1.530025 -1.803090 0.880591

H 2.906399 -1.105518 0.000068

H 1.530131 -1.803018 -0.880677

H -3.303658 -1.081675 0.001438

H -3.369142 0.448185 -0.885041

H -3.369253 0.450666 0.883595

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 40.6061 | 114.1576 | 134.1695 |
| 169.315 | 310.0292 | 360.8824 |
| 383.2361 | 548.8619 | 579.0869 |
| 664.7475 | 742.5326 | 933.451 |
| 938.2265 | 1035.907 | 1056.124 |
| 1056.163 | 1072.148 | 1097.043 |
| 1331.673 | 1414.291 | 1420.324 |
| 1441.78 | 1477.039 | 1483.222 |
| 1486.848 | 1498.116 | 1717.304 |
| 2378.255 | 3045.836 | 3052.882 |
| 3112.028 | 3125.709 | 3125.819 |
| 3143.108 | 3165.867 | 3260.304 |

***p40 + H***

C -2.495684 -1.243580 -0.167536

C -1.405222 -0.813660 0.456445

C -0.596612 0.372097 0.073683

C 0.096112 1.118403 1.223322

C -1.049190 1.182045 -1.120339

C 3.115420 -0.775718 -0.445136

C 1.985841 -0.251834 -0.055295

C 0.869441 0.262414 0.314814

H -3.024448 -2.122968 0.180840

H -2.898214 -0.743283 -1.041624

H -1.038782 -1.358404 1.324296

H 0.200600 2.194063 1.121202

H -0.076406 0.766559 2.235857

H -0.362037 2.010352 -1.302924

H -2.050208 1.591009 -0.954213

H -1.073654 0.561291 -2.019878

H 3.742127 -0.275305 -1.175897

H 3.460380 -1.724323 -0.047401

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 76.2588 | 107.1339 | 165.5501 |
| 246.8279 | 274.6057 | 308.6594 |
| 347.71 | 358.6237 | 446.7933 |
| 465.1407 | 583.6495 | 602.4361 |
| 626.1708 | 724.4406 | 767.3785 |
| 868.7148 | 914.8325 | 948.686 |
| 953.0185 | 969.5157 | 1012.198 |
| 1021.859 | 1039.023 | 1061.205 |
| 1062.43 | 1109.865 | 1206.161 |
| 1318.159 | 1337.677 | 1384.735 |
| 1416.261 | 1457.858 | 1460.966 |
| 1488.572 | 1509.397 | 1551.572 |
| 1730.373 | 2139.715 | 3045.952 |
| 3118.032 | 3125.144 | 3138.784 |
| 3147.779 | 3157.801 | 3171.247 |
| 3215.328 | 3231.337 | 3252.272 |

***p41 + H***

C -2.376715 -1.349998 -0.080452

C -1.455621 -0.608429 -0.680169

C -0.605010 0.425421 -0.019120

C -0.214913 0.251459 1.443365

C -0.803531 1.834330 -0.547504

C 3.170003 -0.582967 -0.391003

C 1.963772 -0.270827 -0.001904

C 0.773301 0.033598 0.368266

H -2.962120 -2.075716 -0.633366

H -2.578812 -1.257735 0.982094

H -1.289497 -0.718840 -1.750422

H -0.118457 1.148530 2.047247

H -0.572649 -0.624222 1.974724

H -0.112639 2.531202 -0.067691

H -1.828196 2.168843 -0.362475

H -0.621222 1.868347 -1.625297

H 3.931364 0.178206 -0.525925

H 3.444512 -1.614128 -0.587760

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 66.0111 | 120.641 | 127.5422 |
| 231.8764 | 271.3518 | 302.3725 |
| 315.4963 | 351.7065 | 441.9432 |
| 477.5504 | 574.4598 | 605.8165 |
| 667.2436 | 712.1242 | 747.575 |
| 876.0646 | 910.599 | 953.1672 |
| 965.7536 | 976.7731 | 1011.122 |
| 1030.119 | 1042.605 | 1060.187 |
| 1069.272 | 1120.109 | 1216.383 |
| 1278.876 | 1336.572 | 1388.595 |
| 1410.628 | 1453.804 | 1459.849 |
| 1488.126 | 1506.75 | 1553.919 |
| 1735.54 | 2138.54 | 3047.023 |
| 3122.183 | 3131.312 | 3134.597 |
| 3142.091 | 3149.975 | 3162.91 |
| 3220.849 | 3225.336 | 3246.68 |

***p42 + CH3***

C 1.195538 1.199818 0.002023

C -0.193735 1.196971 -0.009046

C -0.908973 0.000002 -0.012244

C -0.193737 -1.196970 -0.009045

C 1.195536 -1.199819 0.002023

C 1.895986 -0.000001 0.008429

C -2.415550 0.000000 0.009653

H 1.731705 2.142463 0.002303

H -0.732363 2.139656 -0.017490

H -0.732367 -2.139654 -0.017490

H 1.731700 -2.142466 0.002302

H 2.980100 -0.000002 0.014617

H -2.820424 -0.884482 -0.487029

H -2.820427 0.884525 -0.486952

H -2.788313 -0.000044 1.038980

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 34.8642 | 207.7988 | 350.0785 |
| 417.0356 | 478.6255 | 533.5122 |
| 639.4238 | 717.9088 | 748.6522 |
| 808.5812 | 866.281 | 920.6975 |
| 995.496 | 1010.276 | 1013.52 |
| 1024.216 | 1064.215 | 1067.412 |
| 1121.635 | 1186.055 | 1217.239 |
| 1245.97 | 1332.672 | 1363.76 |
| 1419.204 | 1477.626 | 1499.92 |
| 1511.653 | 1547.483 | 1660.972 |
| 1684.996 | 3050.519 | 3116.919 |
| 3140.232 | 3183.009 | 3184.436 |
| 3198.008 | 3207.204 | 3220.419 |

***p43 + H***

C -2.097858 -1.232195 -0.516646

C -1.199512 -0.459379 0.081025

C 0.096804 -0.986202 0.639622

C 1.282905 -0.260390 0.040895

C 1.093620 1.176108 -0.185046

C -0.095395 1.772278 -0.078891

C -1.368433 1.030408 0.233720

C 2.433906 -0.873739 -0.235999

H -1.943747 -2.301257 -0.620366

H -3.016747 -0.822498 -0.923711

H 0.184823 -2.063313 0.485259

H 0.106811 -0.804887 1.723843

H 1.971424 1.758776 -0.448936

H -0.176061 2.843715 -0.235638

H -1.671245 1.262902 1.265410

H -2.176772 1.389534 -0.409805

H 3.281020 -0.326351 -0.636064

H 2.564274 -1.937956 -0.072071

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 102.8299 | 121.9869 | 306.5873 |
| 354.9817 | 406.641 | 439.2356 |
| 469.0592 | 542.7892 | 572.2869 |
| 688.4891 | 717.5625 | 744.8351 |
| 813.2412 | 862.5536 | 917.9593 |
| 933.2465 | 940.0491 | 947.2836 |
| 955.1106 | 1000.079 | 1013.496 |
| 1019.165 | 1030.357 | 1174 |
| 1203.474 | 1235.402 | 1299.382 |
| 1319.737 | 1339.006 | 1355.851 |
| 1413.596 | 1455.653 | 1463.359 |
| 1473.28 | 1486.64 | 1699.911 |
| 1750.795 | 1760.651 | 3009.778 |
| 3022.523 | 3089.852 | 3116.202 |
| 3147.358 | 3155.64 | 3167.103 |
| 3192.603 | 3233.452 | 3242.854 |

***p44 + CH3***

C -1.042990 1.251076 -0.000004

C 0.289724 1.243525 -0.000006

C 1.068751 0.000000 -0.000001

C 0.289724 -1.243525 -0.000006

C -1.042991 -1.251076 -0.000003

C -1.868365 0.000000 0.000006

C 2.407902 0.000000 0.000006

H -1.577451 2.196253 -0.000006

H 0.840985 2.179018 -0.000009

H 0.840984 -2.179020 -0.000011

H -1.577451 -2.196253 -0.000006

H -2.540333 0.000000 -0.869782

H -2.540289 0.000001 0.869833

H 2.971511 -0.926496 0.000008

H 2.971511 0.926496 0.000010

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 116.4393 | 305.867 | 372.729 |
| 384.6247 | 510.2396 | 558.1417 |
| 601.2898 | 686.549 | 789.3702 |
| 802.7072 | 803.9673 | 896.1845 |
| 914.7541 | 960.7094 | 964.237 |
| 975.8652 | 1013.785 | 1023.656 |
| 1027.59 | 1185.131 | 1229.457 |
| 1230.296 | 1338.353 | 1395.328 |
| 1399.501 | 1449.145 | 1458.141 |
| 1475.877 | 1686.516 | 1711.33 |
| 1778.503 | 3014.857 | 3032.297 |
| 3156.411 | 3175.788 | 3176.547 |
| 3197.461 | 3200.398 | 3246.299 |

***p45 + CH3***

C 1.831094 0.043797 -0.133275

C 1.227349 -1.144539 -0.085295

C -0.243150 -1.272168 0.199734

C -1.029444 0.013410 0.027950

C -0.271722 1.262990 0.113557

C 1.066810 1.278335 0.038837

C -2.350322 0.014089 -0.173146

H 2.899677 0.114201 -0.303620

H 1.796011 -2.060911 -0.204866

H -0.683634 -2.067411 -0.408592

H -0.350096 -1.605861 1.243053

H -0.831321 2.190100 0.187448

H 1.602697 2.220656 0.071158

H -2.906347 0.943072 -0.240169

H -2.910672 -0.909329 -0.274580

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 63.8772 | 260.4228 | 383.5535 |
| 437.1575 | 482.1043 | 552.5186 |
| 596.8266 | 674.3314 | 760.124 |
| 775.535 | 826.3803 | 906.1617 |
| 937.4333 | 954.0288 | 966.3779 |
| 985.6579 | 1006.255 | 1017.25 |
| 1036.084 | 1190.576 | 1209.371 |
| 1229.833 | 1322.024 | 1350.695 |
| 1403.023 | 1440.465 | 1448.149 |
| 1474.563 | 1664.696 | 1705.32 |
| 1747.358 | 3004.996 | 3087.622 |
| 3154.335 | 3183.136 | 3189.162 |
| 3205.166 | 3216.2 | 3242.72 |

***p46 + H***

C -2.502470 -0.950538 0.000011

C -1.144409 -0.314249 0.000013

C -0.014848 -1.027508 0.000090

C 1.319293 -0.421252 0.000019

C 1.362279 1.044575 0.000080

C 0.254372 1.783769 0.000040

C -1.120699 1.190281 -0.000108

C 2.436827 -1.160190 -0.000093

H -3.077106 -0.639834 0.879705

H -2.436399 -2.039938 0.000790

H -3.076526 -0.641052 -0.880491

H -0.064925 -2.113388 0.000191

H 2.338819 1.518849 0.000155

H 0.325327 2.867304 0.000088

H -1.682848 1.560380 0.869818

H -1.682589 1.560248 -0.870270

H 3.417683 -0.697938 -0.000158

H 2.396497 -2.243956 -0.000141

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 98.0283 | 127.8892 | 194.6462 |
| 292.8185 | 335.9744 | 420.4396 |
| 440.1147 | 487.3031 | 538.7111 |
| 584.0904 | 694.3638 | 711.4303 |
| 793.4194 | 878.2767 | 883.3785 |
| 903.435 | 930.4697 | 953.1698 |
| 974.4961 | 1006.749 | 1017.487 |
| 1048.384 | 1066.788 | 1179.861 |
| 1207.216 | 1230.381 | 1320.846 |
| 1363.617 | 1403.028 | 1418.134 |
| 1440.274 | 1461.012 | 1468.752 |
| 1478.865 | 1493.691 | 1686.984 |
| 1721.792 | 1782.071 | 3006.279 |
| 3024.211 | 3030.212 | 3086.216 |
| 3136.578 | 3161.257 | 3172.764 |
| 3177.463 | 3201.525 | 3250.752 |

***p47 + H***

C -2.572178 -0.845121 0.039428

C -1.186035 -0.270945 0.008721

C -0.082253 -1.031035 0.100009

C 1.265214 -0.465512 0.028874

C 1.382334 1.030102 0.237160

C 0.128732 1.790525 -0.088491

C -1.054072 1.181689 -0.168467

C 2.336822 -1.234813 -0.183789

H -2.555456 -1.928554 0.169087

H -3.105913 -0.617399 -0.889469

H -3.153612 -0.409490 0.858807

H -0.170551 -2.111415 0.174058

H 2.232621 1.426812 -0.324408

H 1.613517 1.214566 1.297481

H 0.207078 2.865956 -0.210291

H -1.955397 1.753608 -0.367828

H 3.332094 -0.811914 -0.270105

H 2.244236 -2.311510 -0.278004

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 86.1886 | 149.7816 | 197.4024 |
| 293.3714 | 310.4419 | 425.0958 |
| 452.6088 | 524.9006 | 547.7813 |
| 564.2832 | 697.2429 | 710.6875 |
| 762.4669 | 869.77 | 885.5038 |
| 907.9335 | 941.9996 | 958.3021 |
| 979.7316 | 1011.462 | 1024.802 |
| 1050.874 | 1070.723 | 1194.574 |
| 1206.929 | 1233.519 | 1318.658 |
| 1353.367 | 1371.354 | 1415.437 |
| 1444.778 | 1453.045 | 1461.583 |
| 1487.503 | 1495.332 | 1679.042 |
| 1708.67 | 1757.524 | 3000.718 |
| 3039.048 | 3091.619 | 3098.039 |
| 3139.132 | 3150.206 | 3173.828 |
| 3175.524 | 3199.843 | 3238.053 |

***Fragments***

***CH3***

C -0.000134 -0.000001 0.000023

H -1.080503 0.038158 -0.000046

H 0.507588 -0.954443 -0.000046

H 0.573721 0.916289 -0.000046

***Frequencies***

470.9451 1399.8856 1409.5749

3117.6199 3301.0861 3304.8947

***C2H3***

C 0.705692 -0.145170 0.000001

C -0.586151 0.030184 0.000004

H 1.596113 0.468363 -0.000011

H -1.031552 1.027946 -0.000006

H -1.281806 -0.806397 -0.000015

***Frequencies***

714.0578 840.5185 933.8993

1052.7836 1393.8374 1668.5191

3080.5313 3173.8401 3244.2107

***C3H5***

C 0.126237 -0.386841 -0.000019

C 1.338706 0.100442 -0.000011

C -1.268068 0.077619 0.000003

H 1.517336 1.179754 0.000009

H 2.219186 -0.536480 0.000075

H -1.313040 1.176378 -0.000504

H -1.802178 -0.283061 0.883344

H -1.802554 -0.283908 -0.882763

***Frequencies***

162.6044 313.5774 482.5915

894.4127 900.2700 939.9177

1051.0870 1105.6621 1389.0212

1418.5574 1456.6454 1477.9920

1768.2413 3001.6799 3066.9166

3090.8621 3119.3826 3174.2916

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm−1) for all intermediates, transition states, reactants, and products involved in the *1,3-pentadiene*  + 1-propynyl reactions at the ωB97P-D/6-311G(d,p) level.

***Intermediates***

***i20***

C 0.819905 2.575899 -0.187733

C 1.058093 1.271061 0.481816

C -0.773672 -0.210099 -0.146681

C -1.965023 -0.340969 -0.061859

C -3.410075 -0.513496 0.035009

C 0.687489 -0.015228 -0.209883

C 2.262828 -1.968326 -0.258800

C 1.408070 -1.197547 0.396726

H -0.256421 2.764670 -0.322459

H 1.266000 2.596593 -1.189486

H 1.232124 3.407387 0.386870

H 1.209451 1.232243 1.556017

H -3.841034 0.195919 0.745988

H -3.887348 -0.353815 -0.935043

H -3.657769 -1.523381 0.371328

H 0.969822 0.059997 -1.268628

H 2.491769 -1.797229 -1.306565

H 2.761128 -2.800177 0.225988

H 1.186586 -1.389977 1.444416

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 61.6271 | 71.6599 | 74.6454 |
| 119.9903 | 122.8981 | 154.9042 |
| 227.2592 | 285.7224 | 290.6561 |
| 394.4126 | 418.3753 | 447.6265 |
| 505.0071 | 545.3347 | 676.7701 |
| 811.0921 | 908.9782 | 968.1059 |
| 975.1623 | 1005.164 | 1046.474 |
| 1058.849 | 1062.989 | 1086.817 |
| 1141.531 | 1158.42 | 1189.721 |
| 1261.017 | 1291.256 | 1334.415 |
| 1382.166 | 1418.717 | 1422.583 |
| 1464.071 | 1474.8 | 1484.639 |
| 1490.106 | 1491.956 | 1741.437 |
| 2384.576 | 2989.305 | 3027.686 |
| 3048.322 | 3055.158 | 3118.582 |
| 3124.258 | 3130.016 | 3145.962 |
| 3164.684 | 3188.801 | 3237.561 |

***i21***

C -0.151325 -2.649483 -0.277013

C -0.240893 -1.330890 0.455270

C 0.716343 -0.255717 0.170449

C 1.890403 0.264354 0.226339

C 2.620191 1.476582 -0.172992

C -0.719243 -0.082905 -0.287879

C -2.464559 1.682354 -0.228631

C -1.566474 0.917861 0.384383

H 0.562814 -3.315274 0.213825

H 0.186833 -2.496894 -1.305033

H -1.124999 -3.146472 -0.303437

H -0.574186 -1.399212 1.489492

H 3.410315 1.241008 -0.891311

H 1.939130 2.203175 -0.636541

H 3.089935 1.955072 0.690799

H -0.888816 -0.209131 -1.355040

H -2.636335 1.607596 -1.298208

H -3.058117 2.405085 0.318797

H -1.413240 1.022109 1.457104

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 64.2682 | 113.4174 | 132.8276 |
| 141.4772 | 174.5187 | 202.3595 |
| 237.3665 | 269.7478 | 404.4836 |
| 423.2737 | 433.8168 | 571.4284 |
| 626.1119 | 737.6835 | 796.6776 |
| 868.5238 | 939.9051 | 993.0908 |
| 1007.669 | 1013.404 | 1035.666 |
| 1042.215 | 1050.907 | 1055.221 |
| 1127.467 | 1138.962 | 1200.149 |
| 1207.945 | 1297.099 | 1339.982 |
| 1393.81 | 1404.394 | 1423.64 |
| 1465.725 | 1469.598 | 1483.747 |
| 1485.983 | 1506.333 | 1726.333 |
| 1885.786 | 3008.069 | 3049.905 |
| 3091.037 | 3116.31 | 3123.759 |
| 3126.903 | 3138.517 | 3145.506 |
| 3152.283 | 3161.917 | 3246.968 |

***i22***

C -0.159619 2.329145 0.488600

C -0.182497 1.104551 -0.450652

C 1.010493 0.276665 -0.253753

C 1.998173 -0.384205 -0.081046

C 3.198209 -1.188332 0.122213

H 0.748028 2.915244 0.331021

H -0.189248 2.004829 1.530967

H -1.026005 2.967967 0.298464

H -0.145251 1.489741 -1.480117

H 3.387555 -1.344135 1.187048

H 3.093593 -2.167998 -0.350624

H 4.073435 -0.696862 -0.309667

C -1.476120 0.347392 -0.301929

C -2.819457 -1.631965 0.188055

C -1.610095 -0.980858 0.049536

H -2.374774 0.933182 -0.485481

H -3.758568 -1.114429 0.021942

H -2.866672 -2.677936 0.463638

H -0.696610 -1.543962 0.226669

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 68.0504 | 78.8397 | 124.116 |
| 134.9627 | 174.0736 | 205.6695 |
| 247.4832 | 303.3475 | 344.0547 |
| 386.6541 | 438.7645 | 533.1055 |
| 552.8202 | 640.3622 | 705.1532 |
| 768.2491 | 807.5017 | 904.0048 |
| 981.9815 | 1015.019 | 1028.329 |
| 1062.703 | 1066.118 | 1067.806 |
| 1098.947 | 1184.187 | 1206.767 |
| 1291.44 | 1301.094 | 1319.526 |
| 1368.972 | 1402.255 | 1427.639 |
| 1488.836 | 1491.605 | 1494.782 |
| 1499.237 | 1504.574 | 1523.112 |
| 2395.929 | 3008.907 | 3051.384 |
| 3052.619 | 3122.207 | 3126.687 |
| 3134.129 | 3143.496 | 3154.513 |
| 3160.595 | 3171.405 | 3256.527 |

***i23***

C 0.993000 -1.747945 0.887626

C 0.536868 -1.055223 -0.415427

C -0.815058 -0.498098 -0.273039

C -1.927722 -0.063659 -0.150448

C 1.177394 1.772150 0.757071

C 1.823151 1.192466 -0.313153

C 1.559088 -0.044012 -0.886234

C -3.271513 0.484925 -0.007739

H 0.275650 -2.517752 1.180413

H 1.077195 -1.021572 1.697793

H 1.970702 -2.213575 0.742098

H 0.474991 -1.829727 -1.187797

H 0.338103 1.294991 1.247415

H 1.485765 2.743952 1.122649

H 2.635870 1.757483 -0.764480

H 2.180459 -0.354298 -1.720042

H -3.776910 0.060257 0.863237

H -3.235243 1.570162 0.117102

H -3.877832 0.266453 -0.890332

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 20.3756 | 75.5571 | 93.2448 |
| 142.0468 | 218.114 | 228.5071 |
| 255.8771 | 304.3161 | 338.4661 |
| 407.1091 | 469.1385 | 529.9479 |
| 545.4335 | 657.9969 | 710.8206 |
| 750.6702 | 823.607 | 890.6292 |
| 975.6092 | 999.8792 | 1035.303 |
| 1058.022 | 1058.378 | 1087.178 |
| 1093.856 | 1168.055 | 1218.251 |
| 1248.228 | 1323.212 | 1363.475 |
| 1406.951 | 1419.486 | 1436.649 |
| 1474.353 | 1485.621 | 1486.536 |
| 1497.447 | 1501.275 | 1536.228 |
| 2390.056 | 3046.049 | 3049.282 |
| 3051.494 | 3118.474 | 3119.165 |
| 3132.229 | 3144.257 | 3150.642 |
| 3164.465 | 3187.508 | 3262.787 |

***i24***

C 0.094776 2.222176 0.275448

C -0.032079 0.862325 -0.352111

C 3.568338 -1.117734 0.111060

C 2.295225 -0.427672 -0.062187

C 1.246047 0.139087 -0.209043

C -1.165772 0.073158 0.262719

C -2.236910 -0.341962 -0.400108

C -3.371107 -1.113478 0.201015

H 0.581521 3.024873 -0.264684

H -0.071190 2.336285 1.340390

H -0.230461 0.981921 -1.423958

H 4.242456 -0.536190 0.745025

H 4.060125 -1.274796 -0.852144

H 3.421212 -2.094297 0.579064

H -1.060672 -0.144578 1.324777

H -2.315242 -0.117249 -1.463259

H -4.317875 -0.577632 0.079468

H -3.212383 -1.290203 1.267140

H -3.488597 -2.083539 -0.292574

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.3996 | 115.8803 | 137.7841 |
| 143.8381 | 145.1109 | 186.4264 |
| 224.6973 | 238.0275 | 282.6959 |
| 339.8481 | 405.0146 | 433.693 |
| 496.6389 | 539.644 | 583.923 |
| 773.6345 | 853.7216 | 893.071 |
| 971.2131 | 1012.429 | 1064.465 |
| 1067.375 | 1074.265 | 1080.57 |
| 1116.978 | 1159.386 | 1182.296 |
| 1267.341 | 1304.871 | 1335.271 |
| 1371.436 | 1427.213 | 1429.5 |
| 1455.423 | 1492.263 | 1492.47 |
| 1493.813 | 1504.677 | 1773.005 |
| 2383.219 | 3040.137 | 3047.827 |
| 3048.056 | 3099.666 | 3119.408 |
| 3121.271 | 3127.124 | 3149.52 |
| 3152.919 | 3154.811 | 3268.903 |

***i25***

C -0.907226 1.925355 -0.235887

C -0.059510 0.874868 0.479638

C -2.606639 -1.743369 0.053153

C -2.351557 -0.321089 -0.219626

C -1.447263 0.575150 -0.039744

C 1.097545 0.259027 -0.196923

C 2.188747 -0.184181 0.421374

C 3.357478 -0.827209 -0.259563

H -1.309411 2.732627 0.368047

H -0.607841 2.211372 -1.240294

H 0.028816 0.991929 1.556615

H -3.472346 -1.871389 0.708828

H -1.736173 -2.206728 0.537243

H -2.809456 -2.288891 -0.872764

H 1.014503 0.157681 -1.278927

H 2.254925 -0.081391 1.503780

H 4.278939 -0.263576 -0.080505

H 3.203023 -0.893423 -1.339137

H 3.525569 -1.839527 0.122583

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 56.199 | 100.8618 | 114.5029 |
| 156.3729 | 173.0883 | 208.0209 |
| 223.1963 | 306.9608 | 398.9201 |
| 426.9732 | 473.2353 | 514.5843 |
| 669.7229 | 815.9553 | 835.6638 |
| 874.4498 | 932.7572 | 962.0659 |
| 1003.678 | 1016.932 | 1050.525 |
| 1051.903 | 1064.044 | 1074.057 |
| 1088.791 | 1112.99 | 1192.101 |
| 1202.894 | 1279.533 | 1338.513 |
| 1388.546 | 1402.388 | 1424.84 |
| 1461.689 | 1468.276 | 1477.393 |
| 1482.597 | 1503.718 | 1763.779 |
| 1890.263 | 3009.799 | 3037.926 |
| 3091.711 | 3095.869 | 3116.593 |
| 3123.288 | 3123.821 | 3138.855 |
| 3146.76 | 3153.784 | 3213.089 |

***i26***

C 0.783721 1.767006 -0.000096

C -0.687449 1.453456 -0.000274

C 3.281800 -1.510823 -0.000493

C 2.398059 -0.350095 0.000509

C 1.671722 0.605667 0.000542

H 1.019318 2.391844 -0.872417

H 1.019017 2.392820 0.871597

H -1.347509 2.317394 -0.001206

H 3.267437 -2.010642 -0.972180

H 2.974251 -2.234989 0.757899

H 4.312293 -1.216001 0.212529

C -1.239379 0.189727 0.000535

C -2.595858 -0.080178 0.000004

C -3.176246 -1.454783 0.000019

H -0.551970 -0.655200 0.001369

H -3.293622 0.754677 -0.001407

H -3.817324 -1.618096 0.874478

H -2.395009 -2.218588 0.007301

H -3.805097 -1.623075 -0.882444

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 14.3533 | 66.9179 | 82.6359 |
| 94.1157 | 178.3895 | 198.5457 |
| 205.9781 | 230.4258 | 289.6887 |
| 398.4999 | 428.5639 | 465.4981 |
| 617.4967 | 723.7462 | 759.522 |
| 765.7547 | 922.8525 | 944.4333 |
| 982.1777 | 999.5814 | 1029.348 |
| 1054.539 | 1066.903 | 1124.495 |
| 1170.611 | 1206.503 | 1229.251 |
| 1290.432 | 1305.987 | 1365.759 |
| 1414.156 | 1420.141 | 1449.944 |
| 1461.548 | 1478.699 | 1488.541 |
| 1491.65 | 1507.632 | 1542.479 |
| 2398.699 | 3011.924 | 3023.599 |
| 3033.443 | 3052.771 | 3072.78 |
| 3122.881 | 3124.165 | 3126.282 |
| 3154.832 | 3161.271 | 3167.718 |

***i27***

C 0.364919 -0.535112 0.000037

C -0.431619 0.741973 0.000027

C -1.817467 0.774725 0.000005

C -2.655043 -0.321427 -0.000003

C -4.145119 -0.235343 -0.000031

C 4.437675 0.092250 -0.000031

C 2.996220 -0.132548 -0.000004

C 1.810952 -0.321364 0.000016

H 0.092869 -1.143378 0.873862

H 0.092850 -1.143401 -0.873766

H 0.122267 1.673146 0.000040

H -2.283681 1.758501 -0.000006

H -2.223562 -1.319425 0.000011

H -4.572350 -0.732968 -0.878440

H -4.486670 0.802536 -0.000040

H -4.572383 -0.732963 0.878365

H 4.901992 -0.352819 -0.883580

H 4.901519 -0.349530 0.885415

H 4.664042 1.161383 -0.001961

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 24.8633 | 36.389 | 76.97 |
| 140.8897 | 167.2414 | 170.5048 |
| 203.3407 | 294.5801 | 351.5471 |
| 357.468 | 388.8216 | 496.8977 |
| 625.116 | 625.5604 | 748.8879 |
| 810.5873 | 913.8713 | 922.047 |
| 973.3505 | 1016.223 | 1032.358 |
| 1058.839 | 1059.281 | 1141.465 |
| 1175.905 | 1201.759 | 1227.354 |
| 1240.861 | 1321.737 | 1354.088 |
| 1417.855 | 1420.628 | 1460.313 |
| 1479.34 | 1479.656 | 1486.476 |
| 1486.708 | 1490.044 | 1540.731 |
| 2398.924 | 3006.04 | 3020.888 |
| 3029.623 | 3046.576 | 3072.415 |
| 3118.013 | 3118.768 | 3119.733 |
| 3145.974 | 3165.996 | 3206.782 |

***i28***

C -0.280515 -0.102275 0.286462

C 0.516895 0.947722 -0.204633

C 1.877279 1.034791 -0.095660

C 2.769526 0.014274 0.544332

C 3.249140 -1.048533 -0.455479

C -4.322876 -0.219982 -0.121040

C -2.874991 -0.172900 0.023645

C -1.669923 -0.135715 0.143949

H 0.184680 -0.939113 0.798355

H 2.255816 -0.477452 1.376276

H -0.003441 1.752265 -0.717241

H 2.364150 1.892234 -0.551898

H 3.639432 0.518655 0.976300

H 3.787294 -0.588241 -1.288389

H 2.398578 -1.594743 -0.870857

H 3.918560 -1.765841 0.026588

H -4.701099 0.704254 -0.564616

H -4.807417 -0.354230 0.850058

H -4.623764 -1.052071 -0.764029

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 32.8456 | 73.6851 | 76.5192 |
| 92.4233 | 193.033 | 230.4234 |
| 250.8673 | 260.4682 | 311.9489 |
| 438.0762 | 465.2514 | 511.5753 |
| 570.4458 | 754.0072 | 766.7842 |
| 797.5528 | 851.9902 | 884.4976 |
| 991.7406 | 1024.646 | 1051.354 |
| 1059.584 | 1081.29 | 1089.682 |
| 1183.461 | 1205.622 | 1248.479 |
| 1294.74 | 1341.302 | 1362.085 |
| 1409.602 | 1424.716 | 1480.438 |
| 1483.291 | 1486.367 | 1499.558 |
| 1500.504 | 1510.314 | 1538.487 |
| 2263.173 | 3043.338 | 3047.495 |
| 3052.649 | 3090.102 | 3110.558 |
| 3121.304 | 3124.409 | 3131.883 |
| 3160.972 | 3177.85 | 3184.167 |

***i29***

C -0.574044 -1.028895 0.001693

C 0.631068 -0.296969 0.000931

C -4.249695 0.703767 -0.002438

C -2.933256 0.081969 0.002436

C -1.835299 -0.431910 0.002331

H -0.527469 -2.114745 0.001093

H 0.543394 0.786319 0.002030

H -4.327616 1.459515 0.784010

H -5.032311 -0.040955 0.162381

H -4.445481 1.194810 -0.960120

C 1.866860 -0.869849 -0.001353

C 3.178620 -0.146336 -0.002577

C 3.098947 1.376482 0.001524

H 1.926212 -1.957102 -0.002774

H 3.756142 -0.479923 -0.875204

H 3.760219 -0.484392 0.865578

H 2.575312 1.744976 0.887786

H 2.572032 1.749663 -0.880821

H 4.100350 1.812280 0.000761

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 68.2755 | 70.7396 | 114.4539 |
| 130.8553 | 178.5903 | 194.5496 |
| 244.3266 | 295.5154 | 317.648 |
| 349.0081 | 440.7527 | 492.6136 |
| 607.9911 | 708.1082 | 753.6637 |
| 813.2417 | 841.1242 | 914.515 |
| 980.7129 | 1037.161 | 1047.255 |
| 1064.047 | 1092.724 | 1104.976 |
| 1179.274 | 1207.701 | 1286.338 |
| 1291.369 | 1316.576 | 1382.353 |
| 1417.604 | 1423.545 | 1451.835 |
| 1475.597 | 1481.383 | 1491.919 |
| 1502.291 | 1515.942 | 1571.204 |
| 2259.306 | 3017.253 | 3039.61 |
| 3042.247 | 3053.848 | 3110.219 |
| 3118.936 | 3126.501 | 3133.69 |
| 3152.24 | 3169.395 | 3182.933 |

***i40***

C 0.344476 2.562043 -0.091431

C 0.313944 1.067097 0.007940

C -0.877523 0.375327 -0.004197

C -1.931015 -0.238723 -0.007443

C -3.182299 -0.981173 -0.031389

C 1.639844 0.352947 0.072231

C 2.043305 -2.089083 -0.307160

C 1.560792 -1.100727 0.432663

H -0.656527 2.979522 -0.201033

H 0.948290 2.883384 -0.949884

H 0.806907 3.003375 0.800834

H 2.270005 0.874312 0.808450

H -3.683631 -0.874571 -0.998370

H -3.003625 -2.045705 0.139889

H -3.869384 -0.623637 0.741296

H 2.158054 0.468625 -0.891079

H 2.531776 -1.899534 -1.258843

H 1.964246 -3.123558 0.007900

H 1.064749 -1.328469 1.373560

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 45.0288 | 66.4954 | 102.5475 |
| 114.1477 | 126.8054 | 154.0473 |
| 222.4392 | 283.1353 | 301.8119 |
| 381.2598 | 415.9285 | 445.0243 |
| 578.7677 | 611.3687 | 702.3301 |
| 887.4736 | 931.4344 | 966.068 |
| 977.8544 | 1013.814 | 1045.779 |
| 1047.672 | 1054.919 | 1062.999 |
| 1130.317 | 1203.694 | 1249.349 |
| 1323.835 | 1342.301 | 1403.422 |
| 1413.047 | 1430.431 | 1453.691 |
| 1474.583 | 1485.058 | 1486.273 |
| 1489.148 | 1503.183 | 1743.659 |
| 2181.894 | 2997.597 | 3012.731 |
| 3025.715 | 3037.903 | 3060.118 |
| 3101.123 | 3118.541 | 3143.28 |
| 3146.393 | 3168.959 | 3237.788 |

***i41***

C 2.269161 -1.135475 0.500105

C 1.306516 -0.436929 -0.473179

C -0.081518 -0.940228 -0.354895

C -1.206452 -0.336675 -0.051504

C -1.168845 1.157041 0.226596

C 0.201794 1.753220 0.080579

C 1.289799 1.062017 -0.238030

C -2.546621 -1.011896 0.037677

H 2.303162 -2.210217 0.307765

H 1.942971 -0.978484 1.531116

H 3.281207 -0.734781 0.393141

H 1.671363 -0.617936 -1.493535

H -1.552631 1.347658 1.238609

H -1.869075 1.668161 -0.448951

H 0.285664 2.823631 0.247440

H 2.248187 1.568440 -0.327832

H -2.464449 -2.081319 -0.158099

H -2.983780 -0.872944 1.032395

H -3.245630 -0.578657 -0.686146

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 89.0066 | 140.3472 | 205.6705 |
| 236.784 | 260.7957 | 319.4656 |
| 375.0423 | 460.7289 | 472.9061 |
| 514.5093 | 585.0046 | 709.6539 |
| 756.7211 | 858.4705 | 909.3967 |
| 913.6869 | 930.5669 | 995.7788 |
| 1009.797 | 1019.627 | 1067.356 |
| 1086.233 | 1101.84 | 1159.734 |
| 1190.338 | 1209.968 | 1216.857 |
| 1319.427 | 1337.82 | 1364.246 |
| 1404.358 | 1414.323 | 1419.372 |
| 1473.097 | 1491.027 | 1493.082 |
| 1496.38 | 1506.895 | 1745.633 |
| 1795.311 | 3013.708 | 3021.111 |
| 3031.855 | 3037.381 | 3048.587 |
| 3088.529 | 3126.681 | 3137.906 |
| 3147.106 | 3155.478 | 3183.907 |

***i42***

C 2.163141 -1.176475 0.611760

C 1.334113 -0.489470 -0.433043

C -0.088073 -1.003857 -0.355617

C -1.148009 -0.263146 -0.041115

C -1.033164 1.212954 0.230959

C 0.349711 1.759517 0.040005

C 1.398238 1.007395 -0.269215

C -2.531361 -0.838959 0.058641

H 2.712830 -2.083185 0.387102

H -0.217463 -2.066970 -0.544018

H 2.052484 -0.878889 1.648623

H 1.741760 -0.751152 -1.418771

H -1.376901 1.420633 1.254546

H -1.736940 1.755645 -0.415819

H 0.475811 2.831597 0.162309

H 2.376135 1.463669 -0.392365

H -2.536971 -1.912536 -0.138843

H -2.950584 -0.672251 1.057307

H -3.207736 -0.354317 -0.654319

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 75.1484 | 87.1535 | 147.3901 |
| 201.9444 | 265.8765 | 330.527 |
| 367.0088 | 459.6481 | 475.5775 |
| 511.969 | 530.3716 | 586.2863 |
| 723.2036 | 755.6057 | 857.671 |
| 872.8089 | 918.937 | 955.7514 |
| 977.198 | 1013.557 | 1029.688 |
| 1055.175 | 1075.386 | 1097.373 |
| 1121.49 | 1187.12 | 1217.191 |
| 1237.066 | 1304.856 | 1335.611 |
| 1350.609 | 1412.519 | 1424.049 |
| 1434.103 | 1454.606 | 1473.15 |
| 1485.658 | 1498.73 | 1741.602 |
| 1781.916 | 3012.512 | 3024.807 |
| 3031.559 | 3032.67 | 3087.376 |
| 3134.031 | 3149.348 | 3161.792 |
| 3164.883 | 3186.345 | 3263.799 |

***i43***

C 2.275786 -0.980177 0.528621

C 1.260316 -0.356644 -0.447559

C -0.076138 -1.020382 -0.328735

C -1.262313 -0.378756 -0.025038

C -1.277052 1.119996 0.205295

C 0.059596 1.779910 0.047536

C 1.177996 1.131260 -0.249470

C -2.456834 -1.075926 0.074912

H 2.375645 -2.055297 0.355842

H 1.952535 -0.825460 1.561240

H 3.262342 -0.524128 0.405019

H -0.100772 -2.096304 -0.486164

H 1.644521 -0.542038 -1.462809

H -1.667607 1.324655 1.209804

H -1.993849 1.582090 -0.484671

H 0.087597 2.856960 0.188124

H 2.110366 1.681783 -0.346613

H -3.386556 -0.570153 0.309672

H -2.492370 -2.147788 -0.082815

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 70.0778 | 132.5585 | 261.2191 |
| 274.4211 | 343.7674 | 408.6712 |
| 469.8981 | 481.3361 | 507.3989 |
| 545.5132 | 575.3951 | 717.878 |
| 752.0301 | 761.0988 | 809.9405 |
| 861.4819 | 921.8451 | 932.5121 |
| 974.5356 | 1014.088 | 1019.47 |
| 1030.787 | 1057.279 | 1086.44 |
| 1158.529 | 1203.358 | 1236.833 |
| 1244.765 | 1311.143 | 1334.889 |
| 1376.46 | 1408.355 | 1426.379 |
| 1431.08 | 1471.692 | 1479.916 |
| 1502.55 | 1508.33 | 1525.162 |
| 1765.876 | 2988.375 | 3032.529 |
| 3041.537 | 3058.611 | 3117.334 |
| 3129.72 | 3156.438 | 3161.912 |
| 3165.402 | 3186.702 | 3254.86 |

***i43***

C 2.565186 -0.759358 0.109206

C 1.211799 -0.349731 -0.361916

C 0.092885 -1.017976 0.483655

C -1.249553 -0.446376 0.121738

C -1.360573 1.038803 0.352469

C -0.097468 1.763472 -0.034388

C 1.034897 1.150193 -0.362808

C -2.235067 -1.175294 -0.389805

H 2.927738 -1.763490 -0.078805

H 0.301717 -0.816255 1.541596

H 3.134658 -0.125200 0.779511

H 1.082848 -0.711016 -1.393438

H 0.111731 -2.101046 0.340986

H -1.568783 1.231005 1.414895

H -2.210873 1.447880 -0.201926

H -0.141111 2.848995 -0.046982

H 1.899442 1.740863 -0.654402

H -3.185519 -0.730210 -0.666813

H -2.124494 -2.243928 -0.543528

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 103.9618 | 127.157 | 169.5772 |
| 283.5481 | 303.7394 | 401.4039 |
| 427.2387 | 445.0614 | 507.5187 |
| 546.9724 | 561.3932 | 691.2014 |
| 743.9486 | 748.6496 | 844.1054 |
| 883.0906 | 932.2701 | 942.737 |
| 952.9451 | 976.3863 | 1010.533 |
| 1011.787 | 1050.804 | 1100.329 |
| 1126.433 | 1170.175 | 1226.392 |
| 1242.431 | 1281.153 | 1304.769 |
| 1331.911 | 1353.686 | 1361.77 |
| 1419.467 | 1459.249 | 1462.656 |
| 1473.733 | 1498.726 | 1746.607 |
| 1755.791 | 3000.942 | 3015.503 |
| 3039.922 | 3083.814 | 3112.176 |
| 3149.289 | 3150.397 | 3157.439 |
| 3185.226 | 3235.324 | 3260.322 |

***i30***

C -2.487474 -0.952693 -0.209095

C -1.171384 -0.267632 -0.083352

C 0.015237 -1.041040 0.394640

C 1.336845 -0.401551 0.027613

C 1.352425 1.062609 -0.025456

C 0.242914 1.802209 0.002934

C -1.140074 1.220078 0.041835

C 2.436455 -1.120902 -0.201901

H -2.966310 -1.100032 0.773829

H -2.382910 -1.944017 -0.661054

H -3.186371 -0.370877 -0.817844

H -0.021905 -2.069967 0.023384

H -0.021213 -1.117714 1.498446

H 2.322653 1.545499 -0.098866

H -1.635960 1.539484 0.978273

H 0.319877 2.885117 -0.027567

H -1.744746 1.674330 -0.755471

H 3.383979 -0.643094 -0.428319

H 2.423254 -2.205201 -0.168118

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 79.4057 | 93.8658 | 176.1463 |
| 248.8528 | 300.3684 | 311.4142 |
| 412.4887 | 447.0551 | 479.0285 |
| 550.7268 | 665.3452 | 706.5412 |
| 792.0506 | 847.4082 | 871.1036 |
| 894.454 | 922.8413 | 936.2658 |
| 960.6553 | 1002.119 | 1009.902 |
| 1021.254 | 1028.195 | 1168.008 |
| 1187.315 | 1198.469 | 1241.474 |
| 1302.457 | 1334.236 | 1342.396 |
| 1401.6 | 1416.749 | 1430.599 |
| 1450.221 | 1459.394 | 1469.511 |
| 1487.737 | 1495.112 | 1700.63 |
| 1750.893 | 2919.809 | 2927.767 |
| 2962.281 | 3025.068 | 3060.466 |
| 3078.118 | 3108.928 | 3153.85 |
| 3168.558 | 3191.707 | 3240.987 |

***i44***

C 2.570450 -1.014346 0.010424

C 1.259348 -0.286741 -0.011609

C 0.026741 -0.985166 -0.008752

C -1.183887 -0.361273 -0.000416

C -1.273442 1.138380 0.010120

C 0.055862 1.825036 -0.000581

C 1.221995 1.135573 -0.009302

C -2.479494 -1.109809 -0.000479

H 2.436884 -2.082559 -0.173900

H 3.070146 -0.905901 0.980812

H 3.257644 -0.624536 -0.747730

H 0.052278 -2.072770 -0.015069

H -1.860856 1.464059 0.886788

H -1.880307 1.475017 -0.848612

H 0.062994 2.910037 -0.001648

H 2.163158 1.678907 -0.016144

H -2.323402 -2.190336 -0.010600

H -3.077502 -0.858476 0.884247

H -3.086482 -0.843372 -0.874578

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 102.931 | 116.0062 | 130.0723 |
| 194.7818 | 276.2467 | 301.8438 |
| 399.9382 | 430.1645 | 486.0878 |
| 532.3924 | 548.824 | 693.2966 |
| 715.9051 | 871.9445 | 880.193 |
| 929.3859 | 940.6525 | 971.4278 |
| 994.484 | 1006.453 | 1033.661 |
| 1045.747 | 1051.247 | 1162.291 |
| 1191.543 | 1205.092 | 1260.657 |
| 1282.746 | 1335.71 | 1420.465 |
| 1425.24 | 1435.637 | 1447.421 |
| 1455.954 | 1476.691 | 1491.096 |
| 1493.807 | 1500.359 | 1557.749 |
| 1650.739 | 2946.638 | 2951.201 |
| 3015.827 | 3023.499 | 3065.289 |
| 3079.909 | 3126.291 | 3130.617 |
| 3164.143 | 3172.125 | 3199.686 |

***i45***

C -2.380457 -1.229975 -0.155197

C -1.300099 -0.468342 0.026778

C 0.048910 -1.037559 0.032866

C 1.171614 -0.311141 0.011980

C 1.142499 1.195412 -0.062076

C -0.220188 1.767171 -0.236230

C -1.401252 1.021353 0.280194

C 2.534291 -0.937725 0.034823

H -2.294524 -2.301846 -0.300556

H -3.378731 -0.805630 -0.164668

H 0.120597 -2.122674 0.046472

H 1.800891 1.523915 -0.877777

H 1.619673 1.594284 0.852893

H -0.323715 2.810174 -0.512020

H -1.475804 1.162435 1.374597

H -2.330289 1.416721 -0.138215

H 2.477967 -2.023566 0.129393

H 3.086750 -0.699130 -0.880976

H 3.125275 -0.549849 0.872030

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 89.7496 | 137.6758 | 148.9918 |
| 199.0044 | 296.7488 | 365.4709 |
| 408.9666 | 425.9451 | 460.8736 |
| 526.88 | 544.2211 | 667.879 |
| 717.5063 | 850.1153 | 866.3741 |
| 883.9525 | 902.1825 | 919.6709 |
| 928.9226 | 988.4182 | 1008.732 |
| 1046.399 | 1062.44 | 1122.612 |
| 1178.105 | 1189.779 | 1229.615 |
| 1313.969 | 1332.766 | 1350.812 |
| 1399.713 | 1406.948 | 1422.114 |
| 1453.919 | 1457.058 | 1463.511 |
| 1484.527 | 1493.822 | 1709.469 |
| 1758.18 | 2929.437 | 2933.343 |
| 3030.237 | 3033.733 | 3090.081 |
| 3090.552 | 3134.466 | 3153.451 |
| 3164.447 | 3204.943 | 3241.532 |

***i31***

C -2.593336 -0.710666 -0.117123

C -1.230166 -0.114940 0.014043

C -0.118872 -1.014692 0.489701

C 1.242375 -0.509800 0.081965

C 1.468574 0.959801 0.335176

C 0.291513 1.781073 -0.107108

C -0.962258 1.218993 -0.251005

C 2.156511 -1.292155 -0.479182

H -2.920368 -1.162970 0.827817

H -2.601559 -1.513057 -0.865526

H -3.335267 0.034680 -0.410917

H -0.270732 -2.033292 0.118019

H -0.167766 -1.080958 1.589352

H 2.383658 1.294374 -0.161595

H 1.632160 1.115801 1.414054

H 0.441271 2.837581 -0.297092

H -1.781954 1.853862 -0.577921

H 3.126360 -0.905903 -0.776126

H 1.968149 -2.345803 -0.658865

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 96.4348 | 131.4849 | 180.1724 |
| 278.7265 | 316.9265 | 384.5447 |
| 435.6697 | 457.2317 | 477.6432 |
| 565.6806 | 655.0619 | 688.2445 |
| 740.3267 | 848.5894 | 888.4527 |
| 916.7675 | 938.4153 | 941.423 |
| 946.8391 | 991.9668 | 1010.85 |
| 1021.234 | 1041.957 | 1159.928 |
| 1176.765 | 1209.453 | 1239.146 |
| 1305.14 | 1314.646 | 1352.852 |
| 1358.19 | 1421.729 | 1453.239 |
| 1463.859 | 1477.486 | 1481.182 |
| 1483.851 | 1490.352 | 1527.517 |
| 1755.176 | 2976.726 | 2981.521 |
| 3016.765 | 3064.256 | 3076.174 |
| 3088.244 | 3129.688 | 3148.2 |
| 3167.114 | 3205.381 | 3233.558 |

***i32***

C 2.228030 -1.105781 0.519544

C 1.259958 -0.388108 -0.447879

C -0.123747 -0.958546 -0.342887

C -1.223181 -0.223433 -0.029867

C -1.092062 1.177006 0.193013

C 0.168234 1.803104 0.080226

C 1.285889 1.094575 -0.231066

C -2.586964 -0.853125 0.086298

H 2.242174 -2.181775 0.324855

H 1.914401 -0.945959 1.554034

H 3.246137 -0.723800 0.403391

H -0.223366 -2.027762 -0.513165

H 1.639685 -0.593221 -1.464061

H -1.968973 1.763433 0.444135

H 0.240769 2.873479 0.244518

H 2.246792 1.593424 -0.312977

H -2.998449 -0.706450 1.089433

H -2.549813 -1.925873 -0.111986

H -3.286300 -0.399656 -0.622476

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 85.9816 | 114.2778 | 174.0151 |
| 248.4061 | 288.2139 | 358.7597 |
| 417.4039 | 469.5766 | 503.6676 |
| 560.7307 | 615.7196 | 701.1058 |
| 749.3744 | 787.3221 | 818.1258 |
| 874.4487 | 955.449 | 970.7935 |
| 982.4908 | 1004.982 | 1056.894 |
| 1065.063 | 1077.435 | 1095.725 |
| 1144.149 | 1189.234 | 1212.73 |
| 1289.56 | 1329.652 | 1337.855 |
| 1378.729 | 1401.469 | 1420.146 |
| 1449.491 | 1488.381 | 1496.472 |
| 1501.277 | 1503.436 | 1583.228 |
| 1641.794 | 2944.394 | 3038.905 |
| 3041.423 | 3105.163 | 3118.466 |
| 3127.024 | 3132.417 | 3161.83 |
| 3170.182 | 3186.214 | 3201.231 |

***i46***

C 1.591786 -1.265282 0.954498

C 1.251769 -0.693908 -0.385836

C -0.221125 -0.902436 -0.771123

C -1.166588 0.027620 -0.048210

C -0.739578 1.248949 0.294056

C 0.634382 1.673089 0.024842

C 1.575215 0.790062 -0.324639

C -2.566128 -0.453853 0.176625

H 2.590418 -1.631837 1.160709

H -0.499032 -1.945879 -0.591711

H 0.934505 -1.068317 1.794893

H 1.880724 -1.167186 -1.145343

H -0.341451 -0.727864 -1.850329

H -1.417648 1.953303 0.766415

H 0.882155 2.723687 0.135596

H 2.603850 1.096686 -0.481634

H -2.573674 -1.326427 0.839534

H -3.022091 -0.772178 -0.768116

H -3.196158 0.320562 0.618705

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 72.0074 | 113.5476 | 141.2423 |
| 183.6913 | 272.9584 | 334.7886 |
| 341.2647 | 442.3473 | 501.2474 |
| 525.3302 | 562.3106 | 606.3918 |
| 747.004 | 756.3054 | 850.708 |
| 854.0787 | 886.2659 | 948.0129 |
| 964.8402 | 1002.922 | 1017.98 |
| 1044.426 | 1071.324 | 1108.918 |
| 1125.974 | 1182.207 | 1205.035 |
| 1256.171 | 1300.703 | 1334.326 |
| 1350.562 | 1400.577 | 1414.871 |
| 1426.928 | 1454.339 | 1478.35 |
| 1483.509 | 1489.066 | 1678.561 |
| 1744.715 | 3012.566 | 3029.397 |
| 3076.06 | 3082.671 | 3084.686 |
| 3133.185 | 3151.689 | 3177.712 |
| 3189.483 | 3210.462 | 3262.951 |

***i35***

C -2.457205 -0.960788 0.105921

C -1.193820 -0.238687 -0.359256

C 0.049324 -1.030566 -0.079215

C 1.307678 -0.424675 -0.014947

C 1.356465 1.047522 -0.122276

C 0.257709 1.791720 -0.003278

C -1.088735 1.168588 0.244280

C 2.472462 -1.145733 0.145095

H -2.437213 -1.113060 1.189467

H -2.549012 -1.940527 -0.370883

H -3.352344 -0.382517 -0.139219

H -1.258949 -0.114521 -1.453852

H -0.023900 -2.112803 -0.015885

H 2.326857 1.511647 -0.267978

H 0.326468 2.874336 -0.042919

H -1.258229 1.109818 1.329809

H -1.885397 1.802037 -0.156898

H 3.436644 -0.653350 0.191299

H 2.451802 -2.225341 0.239112

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 127.6151 | 147.4309 | 270.0247 |
| 276.5751 | 323.4568 | 396.2373 |
| 447.3198 | 454.8029 | 532.2385 |
| 556.053 | 596.9184 | 691.1269 |
| 712.68 | 765.9744 | 801.267 |
| 877.1029 | 892.9122 | 934.0126 |
| 957.6913 | 1007.516 | 1019.353 |
| 1028.981 | 1077.428 | 1109.683 |
| 1182.438 | 1193.827 | 1238.738 |
| 1274.452 | 1314.286 | 1337.99 |
| 1361.483 | 1374.36 | 1413.272 |
| 1450.093 | 1452.656 | 1484.685 |
| 1503.243 | 1512.218 | 1526.815 |
| 1726.102 | 2959.792 | 3010.96 |
| 3040.424 | 3090.278 | 3117.557 |
| 3118.17 | 3159.723 | 3172.25 |
| 3173.394 | 3196.149 | 3258.09 |

***i8***

C 2.549259 -0.989396 -0.000009

C 1.268948 -0.215171 -0.000002

C 0.000001 -1.018373 0.000024

C -1.268949 -0.215172 0.000009

C -1.223843 1.145347 0.000009

C 0.000001 1.852482 0.000000

C 1.223844 1.145348 -0.000008

C -2.549260 -0.989395 -0.000017

H 2.613056 -1.641975 -0.879422

H 2.612986 -1.642107 0.879309

H 3.420073 -0.330862 0.000074

H 0.000006 -1.703959 0.867206

H 0.000002 -1.704027 -0.867101

H 0.000000 2.935517 0.000000

H -2.155453 1.704163 0.000010

H 2.155454 1.704164 -0.000018

H -3.420069 -0.330855 0.000160

H -2.612956 -1.642197 0.879237

H -2.613099 -1.641882 -0.879495

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 105.322 | 121.3122 | 146.1784 |
| 233.321 | 271.5806 | 308.6448 |
| 395.1505 | 463.7989 | 492.2639 |
| 514.9125 | 529.5915 | 699.5178 |
| 730.1448 | 864.4786 | 876.2869 |
| 910.5745 | 921.8337 | 943.6904 |
| 997.9289 | 1011.912 | 1041.236 |
| 1065.802 | 1078.291 | 1128.882 |
| 1170.816 | 1221.361 | 1244.254 |
| 1315.34 | 1337.058 | 1398.717 |
| 1414.088 | 1417.337 | 1444.038 |
| 1463.725 | 1481.334 | 1481.776 |
| 1482.105 | 1489.225 | 1570.73 |
| 1652.126 | 2940.093 | 2940.697 |
| 3018.134 | 3019.617 | 3069.454 |
| 3069.581 | 3127.566 | 3127.888 |
| 3175.596 | 3177.772 | 3220.278 |

***i47***

C 0.490914 1.557239 0.004289

C -0.861957 0.899175 -0.001488

C 3.728803 -0.991462 -0.006044

C 2.578188 -0.094738 -0.001669

C 1.635877 0.648932 0.001381

C -1.091154 -0.457392 0.011263

H 0.566906 2.226367 -0.863393

H 0.563848 2.216832 0.879767

H -1.702446 1.587586 -0.013943

H 3.423882 -2.015384 -0.236051

H 4.222645 -0.997122 0.968757

H 4.460961 -0.680896 -0.755452

H -0.221143 -1.109539 0.021995

C -2.343607 -1.057719 0.009826

C -3.635333 -0.303426 -0.010285

H -2.388939 -2.141524 0.010628

H -3.765029 0.243098 -0.953146

H -3.681724 0.439662 0.794225

H -4.489341 -0.972740 0.102984

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 56.2899 | 71.1939 | 83.9522 |
| 93.0912 | 159.3542 | 192.9491 |
| 202.6581 | 250.1153 | 358.4737 |
| 392.5047 | 397.8448 | 536.1504 |
| 618.841 | 664.842 | 744.1128 |
| 762.8033 | 923.3807 | 945.8802 |
| 978.7234 | 994.7356 | 1024.357 |
| 1054.034 | 1066.556 | 1094.471 |
| 1171.716 | 1204.309 | 1229.703 |
| 1252.643 | 1322.343 | 1373.123 |
| 1407.346 | 1420.032 | 1457.319 |
| 1471.079 | 1487.049 | 1490.683 |
| 1491.411 | 1498.835 | 1533.789 |
| 2399.249 | 3016.266 | 3022.707 |
| 3038.282 | 3052.903 | 3072.495 |
| 3124.179 | 3126.638 | 3136.179 |
| 3165.551 | 3182.886 | 3197.272 |

***i48***

C 0.122267 -0.375176 0.269604

C -0.578717 0.955118 0.158330

C 4.205809 -0.038632 -0.180003

C 2.761023 -0.160811 -0.019280

C 1.572308 -0.266041 0.109294

C -1.931493 1.171227 -0.043017

C -2.981158 0.274437 -0.165986

C -2.927714 -1.220125 -0.077778

H -0.088267 -0.832041 1.246935

H -0.265846 -1.076839 -0.475565

H 0.058593 1.827503 0.253034

H 4.719430 -0.193030 0.772192

H 4.472668 0.953951 -0.551243

H 4.582207 -0.777617 -0.891713

H -2.214111 2.219047 -0.117458

H -3.958148 0.705477 -0.361625

H -3.925454 -1.629823 0.091267

H -2.283996 -1.568053 0.733413

H -2.551025 -1.668550 -1.006220

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 24.6732 | 39.8995 | 81.1194 |
| 105.6415 | 139.5495 | 183.003 |
| 211.6389 | 293.7922 | 331.7931 |
| 393.9892 | 458.1484 | 502.7424 |
| 596.9484 | 681.6527 | 706.2627 |
| 820.1357 | 895.69 | 924.7751 |
| 979.8558 | 1010.098 | 1020.65 |
| 1058.849 | 1059.362 | 1095.913 |
| 1176.608 | 1201.511 | 1231.433 |
| 1264.38 | 1312.1 | 1403.024 |
| 1419.869 | 1424.391 | 1461.235 |
| 1464.949 | 1486.245 | 1486.763 |
| 1491.919 | 1497.234 | 1525.644 |
| 2398.292 | 3007.257 | 3019.859 |
| 3047.421 | 3076.12 | 3093.551 |
| 3119.877 | 3120.578 | 3128.472 |
| 3148.903 | 3178.571 | 3194.852 |

***i49***

C 0.599593 1.696066 -0.360796

C -0.019359 0.684989 0.565663

C -3.785614 -0.756677 -0.156333

C -2.446132 -0.241006 0.101616

C -1.343841 0.185936 0.321148

C 1.130120 0.288936 -0.404566

C 2.444798 -0.046852 0.123823

C 3.034336 -1.402836 -0.049824

H 1.236067 2.451643 0.085920

H -0.001536 2.035783 -1.194828

H 0.271069 0.749189 1.608632

H -4.333160 -0.100746 -0.837971

H -4.356777 -0.828434 0.772759

H -3.744220 -1.752982 -0.604200

H 0.785266 -0.318272 -1.236146

H 2.894420 0.634212 0.841424

H 2.803373 -1.815579 -1.037430

H 2.641202 -2.117889 0.689917

H 4.120891 -1.388263 0.067537

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 34.4042 | 58.6586 | 82.6037 |
| 95.8463 | 118.7059 | 225.6906 |
| 279.7611 | 314.4983 | 329.1903 |
| 435.8239 | 483.4039 | 509.73 |
| 531.5854 | 720.1706 | 768.1159 |
| 829.0304 | 919.5921 | 954.2209 |
| 985.4229 | 1009.887 | 1056.637 |
| 1058.354 | 1077.978 | 1090.597 |
| 1095.211 | 1136.789 | 1194.777 |
| 1222.826 | 1233.171 | 1304.093 |
| 1384.161 | 1412.771 | 1421.258 |
| 1458.05 | 1480.588 | 1484.697 |
| 1486.927 | 1490.692 | 1496.14 |
| 2384.879 | 2978.594 | 3044.584 |
| 3061.803 | 3112.256 | 3115.718 |
| 3118.093 | 3142.183 | 3159.83 |
| 3168.195 | 3171.716 | 3238.369 |

***i50***

C -0.316171 2.063560 -0.014528

C -0.204935 0.585467 -0.245907

C 3.701029 -0.729892 -0.044892

C 2.322179 -0.260930 -0.123842

C 1.185868 0.120359 -0.192808

C -1.046519 -0.139556 0.796000

C -2.236286 -0.703889 0.607112

C -3.024475 -0.793371 -0.664483

H -1.237637 2.566688 -0.282025

H 0.406826 2.577305 0.606397

H -0.600163 0.356876 -1.241678

H 4.315291 -0.038805 0.537651

H 4.141739 -0.816841 -1.041107

H 3.750927 -1.711114 0.433681

H -0.609325 -0.150127 1.790567

H -2.708408 -1.159641 1.474950

H -2.520032 -0.335346 -1.516441

H -3.994837 -0.300416 -0.546765

H -3.228527 -1.839063 -0.915142

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 31.2331 | 97.632 | 102.1026 |
| 130.5582 | 134.8187 | 179.4816 |
| 229.5377 | 239.8022 | 296.9853 |
| 342.0035 | 442.7446 | 495.6487 |
| 526.5853 | 549.425 | 567.7985 |
| 738.8394 | 779.6526 | 924.022 |
| 982.4565 | 1004.302 | 1019.317 |
| 1056.956 | 1065.542 | 1075.753 |
| 1101.358 | 1132.701 | 1183.391 |
| 1254.517 | 1299.465 | 1339.457 |
| 1411.935 | 1423.149 | 1437.64 |
| 1450.315 | 1488.79 | 1491.768 |
| 1492.087 | 1504.926 | 1748.177 |
| 2396.116 | 3042.451 | 3050.717 |
| 3062.169 | 3098.034 | 3121.969 |
| 3123.725 | 3138.311 | 3157.365 |
| 3162.077 | 3188.707 | 3281.551 |

***i51***

C -0.719578 1.770636 -0.062627

C 0.779163 1.708469 0.043162

C -3.111967 -1.494972 -0.014883

C -2.254795 -0.319638 -0.034751

C -1.535879 0.665899 -0.052519

C 1.321340 0.355994 0.399367

C 2.206007 -0.318526 -0.324327

C 2.757660 -1.665646 0.028461

H 1.098673 2.442554 0.796834

H -1.177122 2.748966 -0.173274

H 1.224930 2.049120 -0.901874

H -3.596036 -1.612357 0.959872

H -2.534701 -2.401342 -0.214941

H -3.898587 -1.418917 -0.770865

H 0.939055 -0.084091 1.319306

H 2.570976 0.124315 -1.250811

H 2.549037 -2.393712 -0.762044

H 2.326601 -2.041376 0.959402

H 3.845466 -1.626458 0.147103

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 45.1422 | 74.6629 | 113.9629 |
| 117.5632 | 174.8196 | 194.4465 |
| 209.647 | 270.9545 | 285.0917 |
| 402.643 | 407.9032 | 489.6401 |
| 580.4343 | 613.1492 | 770.4473 |
| 790.2599 | 920.8001 | 953.8909 |
| 988.6483 | 1016.017 | 1044.504 |
| 1055.096 | 1073.655 | 1106.147 |
| 1127.379 | 1214.564 | 1236.509 |
| 1313.766 | 1345.59 | 1367.373 |
| 1416.871 | 1417.825 | 1439.349 |
| 1473.691 | 1482.178 | 1488.51 |
| 1489.842 | 1498.534 | 1779.179 |
| 2172.144 | 3003.524 | 3030.654 |
| 3036.911 | 3037.382 | 3097.64 |
| 3101.316 | 3117.938 | 3121.178 |
| 3141.792 | 3150.118 | 3172.325 |

***i52***

C 0.714014 1.953719 -0.143547

C -0.182050 0.731234 -0.340012

C 2.613536 -1.621560 0.023089

C 2.310075 -0.182862 0.011515

C 1.313441 0.616146 -0.133373

C -1.073786 0.293109 0.751060

C -2.218514 -0.379403 0.634114

C -2.878042 -0.845615 -0.628696

H 0.885445 2.587242 -1.007989

H 0.635534 2.482888 0.801995

H -0.520282 0.564657 -1.357405

H 3.306654 -1.885652 -0.780479

H 1.695562 -2.210917 -0.106689

H 3.075392 -1.918197 0.968897

H -0.727295 0.547407 1.750949

H -2.746530 -0.625552 1.552380

H -3.002256 -1.933346 -0.618220

H -2.314663 -0.583507 -1.525285

H -3.879608 -0.413643 -0.723053

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 36.8151 | 88.5085 | 114.5561 |
| 117.715 | 169.7113 | 196.6581 |
| 250.9944 | 321.2789 | 390.489 |
| 459.0069 | 524.1373 | 578.0235 |
| 660.4868 | 765.8732 | 830.0037 |
| 857.7593 | 924.5518 | 949.1602 |
| 1012.195 | 1020.363 | 1047.884 |
| 1049.331 | 1057.787 | 1065.646 |
| 1078.46 | 1085.315 | 1178.597 |
| 1200.678 | 1295.485 | 1328.968 |
| 1400.274 | 1413.039 | 1454.55 |
| 1466.58 | 1467.766 | 1479.658 |
| 1486.991 | 1496.108 | 1752.625 |
| 1890.069 | 3004.317 | 3038.763 |
| 3086.455 | 3093.642 | 3110.908 |
| 3116.487 | 3131.972 | 3145.718 |
| 3166.993 | 3172.888 | 3206.206 |

***i53***

C 0.167934 2.511006 0.000526

C -0.060704 1.024839 -0.000256

C 3.247966 -1.351441 0.001208

C 2.058350 -0.510872 -0.002312

C 1.072645 0.190263 -0.001637

C -1.366133 0.486693 0.000530

C -1.690731 -0.838439 -0.000425

C -3.089668 -1.359260 0.000325

H 0.745576 2.818631 0.878520

H -0.779306 3.054074 0.005292

H 0.737779 2.820815 -0.881823

H 3.748434 -1.314993 0.972986

H 3.962401 -1.019959 -0.757086

H 2.991468 -2.393099 -0.207197

H -2.180005 1.210463 0.002078

H -0.885709 -1.569265 -0.001830

H -3.279215 -1.984764 -0.879544

H -3.822829 -0.549018 0.003585

H -3.276549 -1.989616 0.877262

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 54.4557 | 78.0702 | 91.9737 |
| 105.8017 | 126.9992 | 193.2825 |
| 198.3711 | 213.2118 | 299.9285 |
| 351.3307 | 382.3057 | 452.3688 |
| 550.7509 | 620.5002 | 684.0299 |
| 793.4691 | 937.2837 | 964.085 |
| 990.4432 | 1034.564 | 1039.462 |
| 1052.333 | 1055.718 | 1060.32 |
| 1134.717 | 1238.48 | 1265.604 |
| 1361.097 | 1383.009 | 1414.444 |
| 1417.146 | 1424.817 | 1477.409 |
| 1480.631 | 1485.936 | 1487.946 |
| 1489.331 | 1497.388 | 1573.487 |
| 2286.025 | 3027.612 | 3031.065 |
| 3045.327 | 3079.614 | 3087.418 |
| 3114.359 | 3119.806 | 3123.265 |
| 3133.849 | 3153.795 | 3177.595 |

***i54***

C 0.815531 2.438578 0.002468

C 0.657742 0.939709 -0.000070

C -3.210143 -0.333404 -0.001316

C -1.826681 0.119793 -0.000750

C -0.664776 0.457950 -0.000020

C 1.795897 0.108752 -0.003137

H 0.334664 2.883126 -0.874971

H 1.868895 2.725464 -0.000197

H 0.340369 2.879366 0.884933

H -3.739249 0.023795 -0.889185

H -3.744029 0.036176 0.878566

H -3.259869 -1.425525 0.006132

H 2.743762 0.642430 -0.006594

C 1.883431 -1.258975 -0.002280

C 0.752587 -2.240004 0.004035

H 2.887002 -1.673371 -0.007338

H 0.100399 -2.095945 0.871141

H 1.129333 -3.264012 0.024213

H 0.117194 -2.125889 -0.880292

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 34.1982 | 69.4468 | 82.9976 |
| 104.5485 | 151.9286 | 200.217 |
| 250.711 | 289.7711 | 306.6979 |
| 324.3871 | 409.1065 | 534.7067 |
| 574.7658 | 635.8128 | 681.1763 |
| 706.7788 | 932.4593 | 960.5133 |
| 987.4712 | 1029.258 | 1038.608 |
| 1047.473 | 1053.54 | 1058.188 |
| 1114.215 | 1233.873 | 1263.133 |
| 1341.268 | 1406.208 | 1414.125 |
| 1419.395 | 1470.483 | 1479.383 |
| 1481.098 | 1483.227 | 1486.655 |
| 1496.555 | 1506.267 | 1539.001 |
| 2277.43 | 3031.436 | 3037.509 |
| 3040.123 | 3090.369 | 3094.515 |
| 3110.037 | 3114.626 | 3128.183 |
| 3130.235 | 3151.641 | 3179.969 |

***i55***

C -1.832174 -1.027459 0.294101

C -1.976529 0.427496 -0.093876

C -0.944234 1.201752 -0.405272

C 0.501322 0.774355 -0.398992

C 1.309176 1.643816 0.578317

C 2.045808 -1.299279 -0.182349

C 0.660216 -0.716427 -0.098432

C -0.409926 -1.412159 0.205409

H -2.222355 -1.185851 1.307074

H -2.446687 -1.652008 -0.366265

H -2.984839 0.832025 -0.113842

H -1.126255 2.240512 -0.671216

H 0.910820 0.949109 -1.405496

H 2.380118 1.441459 0.504479

H 0.989283 1.452946 1.606257

H 1.156258 2.705640 0.365251

H 2.505336 -1.061272 -1.147883

H 2.019234 -2.383358 -0.068929

H 2.697139 -0.891775 0.597145

**Frequencies**

|  |  |  |
| --- | --- | --- |
| 63.2272 | 171.6267 | 216.8506 |
| 234.264 | 295.3513 | 315.9419 |
| 345.9251 | 448.276 | 491.5675 |
| 547.5946 | 585.6176 | 702.57 |
| 742.9648 | 830.7838 | 910.5149 |
| 920.0297 | 968.0207 | 980.5797 |
| 1006.253 | 1023.086 | 1048.66 |
| 1100.551 | 1120.489 | 1135.096 |
| 1185.898 | 1213.218 | 1217.628 |
| 1322.557 | 1343.922 | 1356.852 |
| 1406.857 | 1409.229 | 1419.42 |
| 1482.017 | 1486.027 | 1494.755 |
| 1502.479 | 1517.252 | 1746.614 |
| 1792.768 | 2998.561 | 3029.498 |
| 3041.133 | 3048.409 | 3055.457 |
| 3101.394 | 3123.094 | 3135.159 |
| 3146.202 | 3157.58 | 3185.183 |

***i56***

C 1.802012 0.843880 0.326858

C 1.868122 -0.573047 -0.160113

C 0.793044 -1.272431 -0.498857

C -0.620226 -0.767255 -0.390429

C -1.361395 -1.539469 0.716301

C -1.919911 1.367834 -0.296189

C -0.695825 0.733940 -0.149160

C 0.437005 1.438327 0.218254

H 2.156297 0.894121 1.367926

H 2.514954 1.461289 -0.237098

H 2.852570 -1.025493 -0.234881

H 0.907579 -2.297701 -0.842281

H -1.130934 -0.978886 -1.338270

H -2.412183 -1.244996 0.769014

H -0.899774 -1.339254 1.686899

H -1.316197 -2.616967 0.533148

H -2.023377 2.431859 -0.116936

H -2.805653 0.822915 -0.602383

H 0.339760 2.502442 0.414868

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 60.0934 | 194.6038 | 241.9102 |
| 265.7611 | 281.857 | 385.6939 |
| 459.3989 | 509.9832 | 544.8379 |
| 566.5693 | 616.3426 | 709.1111 |
| 747.5971 | 754.4479 | 788.4498 |
| 858.7707 | 901.5408 | 935.5996 |
| 955.7088 | 993.389 | 1016.622 |
| 1033.654 | 1093.513 | 1102.582 |
| 1143.97 | 1208.148 | 1216.48 |
| 1248.952 | 1323.887 | 1343.717 |
| 1385.841 | 1407.678 | 1429.245 |
| 1437.184 | 1459.144 | 1482.403 |
| 1496.794 | 1505.535 | 1528.299 |
| 1763.894 | 2997.556 | 3026.35 |
| 3037.27 | 3045.019 | 3123.147 |
| 3130.025 | 3155.346 | 3161.859 |
| 3175.329 | 3187.244 | 3252.009 |

***i57***

C 1.752409 -1.004388 -0.246496

C 2.023679 0.352115 0.047820

C 1.022097 1.211520 0.364237

C -0.422837 0.805771 0.393032

C -1.247973 1.697726 -0.564225

C -2.033471 -1.186282 0.191679

C -0.630693 -0.663922 0.113161

C 0.421450 -1.475082 -0.192817

H 2.558327 -1.682614 -0.497892

H 3.048911 0.707057 0.024206

H 1.242833 2.250627 0.589880

H -0.817490 1.007279 1.405358

H -2.319914 1.520721 -0.450533

H -0.968543 1.498426 -1.602045

H -1.058695 2.753936 -0.355565

H -2.515084 -0.875752 1.126426

H -2.055334 -2.276598 0.140942

H -2.654314 -0.801958 -0.625546

H 0.231342 -2.525873 -0.393576

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 68.8902 | 139.9691 | 220.6518 |
| 251.4679 | 321.5845 | 366.3992 |
| 400.3251 | 490.313 | 495.6913 |
| 575.5934 | 631.7645 | 685.3003 |
| 745.4153 | 789.1081 | 844.576 |
| 928.6815 | 956.4442 | 976.9808 |
| 986.1119 | 1025.324 | 1034.06 |
| 1060.452 | 1077.568 | 1114.829 |
| 1131.919 | 1191.853 | 1208.821 |
| 1293.82 | 1321.809 | 1344.886 |
| 1406.581 | 1412.707 | 1431.17 |
| 1437.083 | 1475.914 | 1492.745 |
| 1508.903 | 1516.525 | 1566.035 |
| 1637.747 | 2936.352 | 3029.681 |
| 3047.922 | 3083.334 | 3126.505 |
| 3130.74 | 3135.441 | 3169.965 |
| 3172.158 | 3194.202 | 3222.089 |

***i58***

C -1.308249 -1.310338 0.381411

C -1.953805 -0.234350 -0.072245

C -1.196830 0.843568 -0.797966

C 0.257387 0.978069 -0.284676

C 0.336006 1.709843 1.018427

C 2.390701 -0.463001 -0.275685

C 0.901650 -0.393327 -0.131794

C 0.140476 -1.439577 0.210170

H -1.846652 -2.115964 0.869364

H -3.029731 -0.142981 0.031532

H -1.171174 0.593132 -1.868979

H 0.816439 1.548861 -1.034212

H 0.077294 1.198339 1.938586

H -1.704900 1.807813 -0.713121

H 0.513519 2.778591 1.050072

H 2.696783 -0.199230 -1.294174

H 2.773517 -1.460378 -0.050495

H 2.872221 0.254656 0.398042

H 0.598670 -2.408155 0.387537

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 89.6451 | 125.3166 | 180.7035 |
| 213.6583 | 242.9299 | 297.906 |
| 348.3659 | 480.2059 | 494.9519 |
| 502.7249 | 574.1649 | 621.4298 |
| 713.226 | 753.7958 | 845.1915 |
| 888.584 | 896.1875 | 930.7735 |
| 981.6005 | 1002.608 | 1039.888 |
| 1052.988 | 1063.464 | 1090.864 |
| 1118.27 | 1183.364 | 1201.356 |
| 1237.609 | 1291.254 | 1339.996 |
| 1353.699 | 1396.654 | 1410.362 |
| 1431.897 | 1455.443 | 1474.048 |
| 1481.838 | 1493.719 | 1696.68 |
| 1747.803 | 3004.104 | 3031.83 |
| 3059.444 | 3088.961 | 3093.9 |
| 3133.922 | 3152.468 | 3170.453 |
| 3181.997 | 3202.987 | 3265.023 |

***i59***

C -2.022653 -0.661433 0.000005

C -1.887146 0.826609 0.000000

C -0.671401 1.431055 -0.000008

C 0.547628 0.707058 -0.000010

C 1.861521 1.430596 0.000007

C 0.493786 -0.726292 -0.000002

C -0.704259 -1.367649 0.000004

H -2.622008 -0.985653 0.867627

H -2.622011 -0.985658 -0.867614

H -2.793943 1.421946 0.000001

H -0.621468 2.516678 -0.000010

H 2.387207 -1.279324 -0.880057

H 2.465914 1.177242 -0.878964

H 2.465728 1.177529 0.879193

H 1.712881 2.512095 -0.000177

H -0.725904 -2.453750 0.000007

C 1.779671 -1.512588 -0.000003

H 1.583451 -2.585996 0.000056

H 2.387266 -1.279233 0.879985

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.2713 | 109.5737 | 167.7462 |
| 244.2136 | 264.5107 | 327.458 |
| 408.7265 | 423.5626 | 487.0681 |
| 566.9463 | 594.7329 | 714.3908 |
| 719.4709 | 766.9211 | 807.3322 |
| 920.2611 | 937.6841 | 962.6552 |
| 987.2894 | 1001.107 | 1030.136 |
| 1063.116 | 1084.44 | 1166.138 |
| 1191.368 | 1194.318 | 1255.596 |
| 1272.941 | 1324.997 | 1395.355 |
| 1419.066 | 1431.439 | 1446.477 |
| 1460.895 | 1477.354 | 1489.389 |
| 1498.722 | 1505.552 | 1566.236 |
| 1648.432 | 2957.822 | 2959.2 |
| 3020.934 | 3041.013 | 3069.693 |
| 3099.751 | 3130.199 | 3137.737 |
| 3169.509 | 3178.975 | 3193.834 |

***i60***

C -1.575512 -1.013503 0.295140

C -1.875962 0.149739 -0.389549

C -0.910114 1.079560 -0.727819

C 0.531111 0.895165 -0.337638

C 0.856333 1.715838 0.928794

C 1.920295 -1.147467 -0.648525

C 0.841466 -0.572543 -0.130015

C -0.166014 -1.337208 0.694845

H -2.362614 -1.705122 0.573164

H 0.020829 -2.411905 0.614559

H -2.908962 0.343246 -0.662455

H -1.186561 1.994058 -1.241822

H 1.168456 1.269284 -1.146086

H 1.911164 1.605039 1.192941

H 0.247988 1.382514 1.773907

H 0.646947 2.776221 0.764936

H 2.131843 -2.200916 -0.495029

H 2.629803 -0.582341 -1.244888

H -0.028515 -1.087566 1.759383

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 91.0635 | 131.6959 | 252.5526 |
| 257.8567 | 306.7181 | 412.5811 |
| 473.3233 | 481.9346 | 555.8515 |
| 605.1137 | 631.3471 | 729.4709 |
| 732.043 | 760.9625 | 858.8677 |
| 920.3038 | 936.9372 | 950.2305 |
| 954.3111 | 973.701 | 1000.525 |
| 1034.922 | 1083.832 | 1088.757 |
| 1152.203 | 1169.714 | 1212.964 |
| 1308.624 | 1315.529 | 1323.471 |
| 1344.235 | 1391.593 | 1410.921 |
| 1454.938 | 1465.158 | 1475.279 |
| 1499.207 | 1506.956 | 1521.494 |
| 1751.572 | 2986.544 | 3045.805 |
| 3060.223 | 3086.485 | 3125.651 |
| 3131.219 | 3147.414 | 3175.555 |
| 3197.401 | 3210.798 | 3232.955 |

***i61***

C -1.919300 -0.812792 0.001771

C -2.020385 0.538926 0.002150

C -0.805224 1.406514 -0.003172

C 0.503512 0.665832 -0.005757

C 1.720470 1.540356 0.002859

C 1.859097 -1.457230 0.000074

C 0.547693 -0.704742 -0.001942

C -0.656943 -1.451743 -0.000208

H -2.817764 -1.421498 0.004168

H -2.991185 1.022798 0.004835

H -0.829566 2.093834 0.861282

H -0.835252 2.088367 -0.871673

H 2.650940 0.984065 -0.107726

H 1.779426 2.110132 0.939209

H 1.670912 2.278418 -0.806561

H 2.438023 -1.256784 -0.906346

H 1.686355 -2.533605 0.050385

H 2.481355 -1.181698 0.856055

H -0.606761 -2.534757 0.001722

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 76.1446 | 104.2886 | 141.1477 |
| 177.8148 | 299.1417 | 327.0682 |
| 394.3357 | 472.5252 | 503.8742 |
| 541.1058 | 566.1281 | 665.4653 |
| 722.4155 | 768.496 | 818.5197 |
| 909.383 | 931.5392 | 981.2972 |
| 987.3593 | 1019.131 | 1037.005 |
| 1062.995 | 1094.28 | 1161.686 |
| 1189.927 | 1203.673 | 1211.542 |
| 1272.417 | 1323.222 | 1409.572 |
| 1422.969 | 1427.139 | 1442.054 |
| 1442.982 | 1481.665 | 1487.554 |
| 1502.352 | 1511.524 | 1586.075 |
| 1634.398 | 2947.326 | 2947.561 |
| 3022.332 | 3047.17 | 3069.973 |
| 3109.399 | 3136.677 | 3153.588 |
| 3176.141 | 3199.785 | 3208.929 |

***i62***

C -1.200191 -1.327331 0.270486

C -1.781641 -0.338072 -0.400183

C -1.041183 0.876226 -0.890938

C 0.298940 1.077048 -0.160419

C 0.105964 1.635402 1.212652

C 2.239264 -0.433428 -0.614467

C 1.031953 -0.254845 -0.090556

C 0.267380 -1.350633 0.608317

H -1.793873 -2.173280 0.605156

H -2.844033 -0.395495 -0.619678

H -0.858751 0.777947 -1.967824

H 0.921778 1.769052 -0.738922

H -0.826298 1.483836 1.745514

H -1.661313 1.769978 -0.763826

H 0.952818 2.042472 1.752439

H 2.741254 -1.394796 -0.569074

H 2.767490 0.378463 -1.104401

H 0.695563 -2.325388 0.355544

H 0.382454 -1.238991 1.695720

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 111.3348 | 142.075 | 156.3536 |
| 231.8951 | 322.2327 | 393.4236 |
| 414.9299 | 454.6158 | 525.3066 |
| 558.0892 | 600.2061 | 680.9849 |
| 740.2909 | 765.5063 | 831.2974 |
| 905.7759 | 919.2996 | 934.0283 |
| 958.6378 | 972.7456 | 1006.418 |
| 1020.273 | 1026.323 | 1090.917 |
| 1115.438 | 1182.244 | 1222.746 |
| 1241.685 | 1291.582 | 1306.495 |
| 1336.441 | 1355.15 | 1372.53 |
| 1421.874 | 1456.598 | 1457.916 |
| 1471.067 | 1484.838 | 1741.568 |
| 1750.463 | 3015.826 | 3037.901 |
| 3051.564 | 3081.504 | 3086.17 |
| 3143.203 | 3152.897 | 3164.274 |
| 3188.552 | 3229.083 | 3265.375 |

***i63***

C -1.318810 -1.258443 0.368974

C -1.962024 -0.014033 -0.172566

C -0.988800 0.908767 -0.820427

C 0.437618 0.924087 -0.372353

C 0.589894 1.732838 0.940135

C 2.235294 -0.807331 -0.385818

C 0.959639 -0.487011 -0.163303

C -0.001737 -1.469369 0.349149

H -1.980299 -2.019050 0.773055

H -2.752690 -0.292468 -0.881086

H -2.496138 0.495303 0.650749

H -1.362306 1.729573 -1.423038

H 1.049946 1.413433 -1.136214

H 1.642211 1.795978 1.228638

H 0.041355 1.250137 1.753742

H 0.198475 2.745933 0.814451

H 2.609022 -1.807764 -0.193086

H 2.943505 -0.079647 -0.768570

H 0.400481 -2.408456 0.718618

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 82.3352 | 123.6349 | 222.5261 |
| 242.9635 | 269.955 | 356.2719 |
| 380.3199 | 459.3873 | 510.8141 |
| 582.0144 | 608.4186 | 718.332 |
| 740.9081 | 810.0308 | 855.4109 |
| 881.0453 | 914.2015 | 933.3452 |
| 950.2216 | 991.301 | 1005.877 |
| 1018.463 | 1054.442 | 1076.669 |
| 1142.624 | 1194.638 | 1198.178 |
| 1306.792 | 1321.578 | 1329.906 |
| 1378.179 | 1389.04 | 1410.064 |
| 1418.412 | 1457.493 | 1468.775 |
| 1492.115 | 1500.838 | 1698.62 |
| 1749.966 | 2938.416 | 3041.592 |
| 3041.691 | 3067.832 | 3124.089 |
| 3127.038 | 3146.894 | 3164.378 |
| 3189.582 | 3197.886 | 3234.044 |

***i64***

C -1.075899 -1.428539 0.347428

C -1.884584 -0.218881 -0.025383

C -1.076318 0.751498 -0.887512

C 0.314031 1.006533 -0.279676

C 0.220996 1.727603 1.026117

C 2.380832 -0.396084 -0.312871

C 1.063219 -0.305440 -0.125339

C 0.257193 -1.461267 0.280974

H -1.614454 -2.310109 0.682916

H -2.791808 -0.528839 -0.553442

H -2.223067 0.282739 0.891088

H -0.949936 0.325030 -1.888009

H 0.881814 1.634131 -0.985746

H 0.990424 1.609837 1.779005

H -1.610567 1.699386 -1.002223

H -0.548202 2.477512 1.180392

H 2.908327 -1.332695 -0.164214

H 2.969481 0.462885 -0.618036

H 0.791170 -2.372421 0.535839

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 98.2183 | 177.2873 | 204.3675 |
| 238.8654 | 346.6837 | 365.0863 |
| 402.4627 | 475.6262 | 487.9737 |
| 595.226 | 625.8673 | 722.1366 |
| 733.7147 | 789.939 | 824.231 |
| 867.3449 | 909.8303 | 934.8445 |
| 967.278 | 979.6897 | 995.7219 |
| 1015.978 | 1035.797 | 1103.311 |
| 1123.435 | 1181.317 | 1206.441 |
| 1256.081 | 1293.541 | 1317.782 |
| 1348.105 | 1382.188 | 1387.546 |
| 1420.526 | 1455.36 | 1468.24 |
| 1477.426 | 1503.679 | 1697.014 |
| 1747.833 | 2970.897 | 3029.836 |
| 3052.747 | 3082.118 | 3101.997 |
| 3141.061 | 3147.972 | 3167.242 |
| 3190.67 | 3235.975 | 3255.938 |

***i65***

C 2.011360 0.442048 -0.033643

C 1.842855 -0.872713 -0.043279

C 0.496850 -1.523457 0.031937

C -0.668145 -0.578470 0.019343

C -2.028759 -1.211903 -0.005811

C -1.580021 1.676858 -0.038922

C -0.507725 0.807262 0.009319

C 0.882296 1.421353 0.057993

H 3.013618 0.857937 -0.086665

H 2.704905 -1.530656 -0.103781

H 0.441765 -2.150526 0.936139

H 0.386092 -2.236999 -0.798858

H -2.545442 -1.014020 -0.952507

H -2.669964 -0.831486 0.795958

H -1.956849 -2.295455 0.111076

H -1.419891 2.749286 -0.048723

H -2.605472 1.332334 -0.073800

H 0.975329 2.158234 -0.748562

H 0.983643 1.995482 0.988105

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 60.5878 | 115.9373 | 135.6738 |
| 282.8607 | 351.939 | 385.7926 |
| 403.9908 | 496.4661 | 503.9493 |
| 519.1581 | 553.2676 | 675.8239 |
| 703.146 | 752.4286 | 821.1042 |
| 919.8121 | 928.7955 | 946.336 |
| 973.3148 | 1015.225 | 1019.244 |
| 1035.725 | 1041.7 | 1162.869 |
| 1196.972 | 1226.53 | 1227.289 |
| 1244.486 | 1293.841 | 1388.829 |
| 1402.523 | 1413.687 | 1428.887 |
| 1455.806 | 1473.443 | 1482.28 |
| 1493.617 | 1503.537 | 1544.57 |
| 1772.289 | 2985.799 | 3006.48 |
| 3029.598 | 3030.394 | 3058.637 |
| 3088.311 | 3124.104 | 3165.371 |
| 3165.918 | 3190.24 | 3259.912 |

***i66***

C 1.903267 0.697262 -0.007386

C 1.852314 -0.773847 0.296754

C 0.582337 -1.413678 -0.268316

C -0.655629 -0.595633 -0.027407

C -1.979865 -1.288921 0.053539

C -1.648113 1.642781 0.094342

C -0.558074 0.810994 -0.021258

C 0.786977 1.408837 -0.151445

H 2.872387 1.182272 -0.067288

H 2.734706 -1.280518 -0.103370

H 1.884709 -0.911808 1.386303

H 0.454065 -2.419128 0.143896

H 0.705203 -1.543809 -1.356097

H -2.652024 -0.972282 -0.753110

H -2.492626 -1.066262 0.996796

H -1.864096 -2.372226 -0.015045

H -1.524422 2.719444 0.089674

H -2.655036 1.260150 0.202744

H 0.837844 2.477387 -0.337440

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 69.4271 | 122.7323 | 150.8837 |
| 283.936 | 344.1133 | 366.3408 |
| 412.5518 | 479.1818 | 504.8045 |
| 587.5145 | 604.7714 | 704.9733 |
| 716.4977 | 776.8796 | 806.2429 |
| 864.9555 | 910.0058 | 968.3573 |
| 981.0095 | 1004.047 | 1012.93 |
| 1049.411 | 1066.047 | 1174.299 |
| 1196.973 | 1199.756 | 1250.451 |
| 1284.487 | 1332.793 | 1359.669 |
| 1394.786 | 1415.035 | 1428.345 |
| 1459.243 | 1477.101 | 1484.967 |
| 1490.027 | 1502.934 | 1547.189 |
| 1731.69 | 2974.224 | 3023.633 |
| 3023.906 | 3074.669 | 3077.983 |
| 3096.246 | 3127.666 | 3167.181 |
| 3176.594 | 3199.892 | 3261.617 |

***Transition states***

***i55 – i27***

C 1.999966 -0.831286 0.168726

C 1.936847 0.631898 -0.221120

C 0.816654 1.367767 -0.161642

C -0.446491 0.954907 0.429155

C -1.696495 1.664492 -0.005016

C -1.956790 -1.549842 -0.174029

C -0.537030 -1.197090 -0.040191

C 0.672484 -1.445129 0.011165

H 2.745112 -1.338401 -0.451305

H 2.337439 -0.951452 1.206891

H 2.832881 1.057196 -0.661719

H 0.830385 2.351401 -0.632131

H -0.419884 0.656416 1.473139

H -1.803313 1.655132 -1.093851

H -1.675977 2.716741 0.311214

H -2.591162 1.214898 0.430539

H -2.508101 -1.309922 0.739514

H -2.060214 -2.620190 -0.364608

H -2.422042 -1.006116 -0.999967

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -648.673 | 70.1328 | 120.8732 |
| 147.9855 | 188.4376 | 226.5611 |
| 251.0372 | 304.6995 | 373.1673 |
| 407.0212 | 449.4957 | 509.0002 |
| 682.5443 | 709.7382 | 774.0343 |
| 806.7474 | 894.053 | 924.2519 |
| 971.1432 | 981.0407 | 1002.239 |
| 1042.535 | 1069.209 | 1115.446 |
| 1141.975 | 1162.154 | 1211.621 |
| 1245.021 | 1321.16 | 1338.503 |
| 1406.564 | 1418.153 | 1432.409 |
| 1466.883 | 1480.117 | 1482.011 |
| 1494.584 | 1502.259 | 1662.632 |
| 2098.952 | 3009.402 | 3030.41 |
| 3048.14 | 3085.071 | 3086.987 |
| 3116.332 | 3128.844 | 3129.987 |
| 3133.105 | 3159.493 | 3190.768 |

***i55 – i56***

C -1.845114 -0.884311 0.262048

C -1.864741 0.604726 -0.017375

C -0.799789 1.342367 -0.326476

C 0.623652 0.837706 -0.438882

C 1.563629 1.595802 0.510421

C 1.669131 -1.704854 -0.122356

C 0.623801 -0.632327 -0.171139

C -0.435081 -1.354460 0.136190

H -2.246358 -1.084687 1.262321

H -2.504664 -1.409060 -0.439138

H -2.836591 1.087883 0.044899

H -0.939858 2.406197 -0.504286

H 0.974755 1.019300 -1.465037

H 2.593388 1.246326 0.396795

H 1.259742 1.440046 1.548968

H 1.544953 2.669654 0.304770

H 2.087634 -2.066097 -1.062454

H 0.493402 -2.417353 0.197844

H 2.360669 -1.720108 0.720728

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2272.91 | 80.9049 | 167.0635 |
| 223.7253 | 248.1264 | 289.3499 |
| 393.5442 | 452.6943 | 471.839 |
| 503.5254 | 576.462 | 595.3902 |
| 714.2869 | 765.2025 | 835.8305 |
| 902.6916 | 940.4823 | 959.3893 |
| 973.4055 | 1014.029 | 1024.302 |
| 1049.393 | 1079.714 | 1086.851 |
| 1117.069 | 1129.428 | 1199.06 |
| 1219.367 | 1236.875 | 1316.546 |
| 1337.258 | 1393.264 | 1404.042 |
| 1423.196 | 1441.236 | 1475.69 |
| 1493.505 | 1507.424 | 1730.606 |
| 1798.703 | 1874.791 | 3011.336 |
| 3041.403 | 3046.304 | 3067.844 |
| 3078.862 | 3124.692 | 3129.703 |
| 3154.183 | 3172.636 | 3178.66 |

***i55 – i57***

C -1.389600 -1.186113 0.521738

C -1.901806 -0.198254 -0.434918

C -1.078930 0.777688 -0.840747

C 0.340649 0.916509 -0.321219

C 0.397739 1.898919 0.862660

C 2.252757 -0.841446 -0.430095

C 0.872833 -0.470196 0.012046

C 0.021840 -1.290857 0.664766

H -2.048803 -1.616865 1.270179

H -0.731929 -2.263326 0.140100

H -2.926295 -0.258669 -0.785532

H -1.433581 1.534660 -1.535415

H 0.964129 1.333552 -1.122600

H 1.427324 2.019456 1.210534

H -0.203300 1.520410 1.692703

H 0.012152 2.882551 0.577797

H 2.346146 -0.758409 -1.519749

H 2.497896 -1.862663 -0.135675

H 3.003368 -0.168191 0.002265

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1846.2 | 90.7592 | 144.4263 |
| 188.4574 | 233.9316 | 260.3305 |
| 321.0926 | 409.4825 | 464.6354 |
| 512.5208 | 563.9235 | 606.4394 |
| 717.6033 | 741.1045 | 810.0811 |
| 839.0832 | 910.9249 | 951.7275 |
| 985.1747 | 1013.127 | 1023.45 |
| 1035.623 | 1090.552 | 1099.165 |
| 1151.897 | 1187.083 | 1212.386 |
| 1223.668 | 1320.973 | 1338.783 |
| 1385.524 | 1402.384 | 1408.181 |
| 1413.133 | 1476.709 | 1484.731 |
| 1491.257 | 1496.493 | 1590.434 |
| 1669.029 | 2107.541 | 3018.369 |
| 3032.737 | 3044.878 | 3068.898 |
| 3121.391 | 3136.463 | 3139.696 |
| 3167.996 | 3172.407 | 3203.817 |

***i57 – p42***

C -1.579692 1.058189 -0.469344

C -2.006828 -0.130836 0.122447

C -1.090969 -0.963237 0.734826

C 0.291545 -0.662436 0.686941

C 0.948891 -1.960035 -0.943629

C 2.150756 1.008005 0.300977

C 0.704836 0.612423 0.208993

C -0.235011 1.427201 -0.398909

H -2.295738 1.716351 -0.947913

H -3.059862 -0.389759 0.119639

H -1.417195 -1.880808 1.211695

H 0.962040 -1.203920 1.346923

H 2.025779 -1.824243 -0.960008

H 0.400501 -1.515218 -1.766162

H 0.604497 -2.936329 -0.618885

H 2.542949 0.844273 1.308922

H 2.293737 2.060510 0.048888

H 2.763767 0.412376 -0.384650

H 0.078356 2.381123 -0.812257

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -576.404 | 85.7262 | 121.6788 |
| 128.5931 | 190.2386 | 218.8043 |
| 352.9577 | 401.1366 | 487.9325 |
| 522.7612 | 558.47 | 584.7065 |
| 638.3069 | 693.9742 | 738.9179 |
| 797.9556 | 860.9046 | 883.2599 |
| 947.7206 | 982.2728 | 992.4044 |
| 1010.342 | 1029.678 | 1053.781 |
| 1066.118 | 1100.838 | 1179.238 |
| 1194.852 | 1226.839 | 1325.71 |
| 1345.598 | 1419.889 | 1425.386 |
| 1431.607 | 1456.432 | 1493.174 |
| 1506.587 | 1533.495 | 1608.943 |
| 1639.367 | 3038.607 | 3089.198 |
| 3099.336 | 3136.433 | 3177.287 |
| 3181.492 | 3189.656 | 3206.647 |
| 3216.657 | 3245.086 | 3255.774 |

***i57 – p89***

C 1.962322 -0.696804 -0.027879

C 1.958242 0.694061 -0.032178

C 0.755437 1.374634 -0.010596

C -0.474631 0.689367 0.070426

C -1.762530 1.456378 -0.135118

C -1.754052 -1.496066 -0.008591

C -0.462717 -0.729367 -0.011290

C 0.756611 -1.391195 -0.030851

H 2.899994 -1.240495 -0.043415

H 2.892633 1.242961 -0.059604

H 0.745917 2.459692 -0.017039

H -0.616343 0.717779 1.895451

H -2.581612 1.056487 0.463944

H -2.060654 1.406631 -1.188051

H -1.632255 2.506758 0.129838

H -2.297419 -1.330852 0.928714

H -1.575692 -2.567468 -0.111702

H -2.412532 -1.181180 -0.823663

H 0.765872 -2.476354 -0.058009

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -902.203 | 152.4408 | 168.4286 |
| 198.5697 | 257.0256 | 329.5618 |
| 381.2164 | 427.9521 | 469.3768 |
| 481.9117 | 541.0198 | 551.481 |
| 600.3995 | 721.9146 | 750.9676 |
| 767.4685 | 840.6054 | 876.4618 |
| 956.1207 | 1003.28 | 1011.976 |
| 1021.598 | 1048.539 | 1073.48 |
| 1081.791 | 1152.662 | 1189.471 |
| 1215.513 | 1248.193 | 1313.935 |
| 1324.104 | 1417.791 | 1427.138 |
| 1473.083 | 1482.613 | 1498.328 |
| 1501.931 | 1515.21 | 1526.96 |
| 1625.846 | 1663.915 | 3040.144 |
| 3047.403 | 3100.918 | 3123.703 |
| 3140.016 | 3153.713 | 3185.924 |
| 3191.693 | 3205.033 | 3219.57 |

***i56 – p92***

C 1.693149 0.724329 0.411086

C 1.814638 -0.628941 -0.133677

C 0.736642 -1.299828 -0.540252

C -0.660113 -0.753527 -0.403728

C -1.380742 -1.505552 0.734519

C -1.794269 1.468538 -0.387076

C -0.694785 0.744273 -0.139938

C 0.492810 1.352703 0.437812

H 2.552182 1.169515 0.899323

H 2.553341 1.708501 -1.204107

H 2.802192 -1.069690 -0.208134

H 0.833106 -2.306768 -0.935319

H -1.206195 -0.953709 -1.331913

H -2.416092 -1.165856 0.817920

H -0.878629 -1.318552 1.687373

H -1.378550 -2.583823 0.551817

H -1.840522 2.524591 -0.143972

H -2.673838 1.026044 -0.843375

H 0.409031 2.357776 0.837909

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -637.469 | 74.6023 | 183.8475 |
| 249.965 | 256.9286 | 275.5698 |
| 309.9347 | 386.6152 | 418.3131 |
| 494.0268 | 542.3589 | 586.8882 |
| 678.6169 | 699.427 | 751.1266 |
| 776.0074 | 847.3973 | 875.3501 |
| 925.0327 | 942.2589 | 961.7538 |
| 1000.12 | 1004.424 | 1017.203 |
| 1033.974 | 1091.523 | 1123.079 |
| 1186.742 | 1213.406 | 1308.083 |
| 1327.265 | 1353.325 | 1395.506 |
| 1415.001 | 1440.276 | 1472.932 |
| 1489.117 | 1506.763 | 1587.743 |
| 1677.753 | 1725.872 | 3045.581 |
| 3058.387 | 3127.569 | 3132.873 |
| 3152.807 | 3177.927 | 3188.536 |
| 3203.755 | 3216.21 | 3241.431 |

***i56 – i60***

C -1.722837 -0.880754 0.346788

C -1.916219 0.449845 -0.150618

C -0.874170 1.207343 -0.551761

C 0.572523 0.813023 -0.384334

C 1.197936 1.616527 0.773119

C 1.976551 -1.249779 -0.346826

C 0.766436 -0.685642 -0.157120

C -0.360638 -1.452213 0.317725

H -2.498170 -1.412971 0.881706

H -1.278327 -1.666232 -0.591463

H -2.930237 0.823516 -0.240538

H -1.059119 2.193739 -0.966574

H 1.112286 1.083106 -1.300294

H 2.269995 1.420522 0.853105

H 0.724396 1.340398 1.719191

H 1.050742 2.690022 0.620666

H 2.144890 -2.306176 -0.167898

H 2.825276 -0.659901 -0.675192

H -0.199222 -2.416122 0.785466

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1867.87 | 41.0282 | 199.7926 |
| 249.4347 | 284.5468 | 374.0914 |
| 391.1589 | 494.7679 | 499.8633 |
| 559.467 | 637.3523 | 661.6015 |
| 686.6065 | 740.1532 | 756.7631 |
| 856.9842 | 860.7152 | 901.5351 |
| 930.4013 | 946.2036 | 968.5576 |
| 1014.044 | 1031.845 | 1091.15 |
| 1108.333 | 1140.843 | 1198.491 |
| 1237.459 | 1307.513 | 1323.984 |
| 1345.062 | 1384.223 | 1398.86 |
| 1411.947 | 1455.883 | 1469.264 |
| 1500.506 | 1501.607 | 1626.874 |
| 1628.493 | 2164.326 | 3034.668 |
| 3042.807 | 3120.072 | 3132.472 |
| 3151.51 | 3174.495 | 3198.871 |
| 3201.709 | 3224.5 | 3240.91 |

***i56 – i63***

C -1.541060 -1.032849 0.403076

C -1.907600 0.266918 -0.203637

C -0.919001 1.131828 -0.640747

C 0.536038 0.857937 -0.367782

C 0.993450 1.666485 0.865271

C 2.040942 -1.129396 -0.443037

C 0.824830 -0.626858 -0.149193

C -0.215703 -1.440964 0.423318

H -2.324886 -1.611045 0.876946

H -1.983192 -0.862817 -0.875545

H -2.946465 0.574362 -0.156977

H -1.193299 2.069898 -1.108698

H 1.132031 1.195548 -1.223060

H 2.063100 1.522900 1.041991

H 0.450193 1.335767 1.754647

H 0.800412 2.733614 0.722090

H 2.280601 -2.170158 -0.253050

H 2.819898 -0.508989 -0.873262

H 0.030230 -2.437687 0.771305

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1907.87 | 68.5834 | 177.7784 |
| 253.2398 | 280.9042 | 365.5492 |
| 401.8366 | 496.7523 | 539.4906 |
| 562.3296 | 641.4241 | 658.6207 |
| 679.8589 | 735.6887 | 742.693 |
| 819.1699 | 869.5061 | 879.7464 |
| 928.1142 | 954.3367 | 996 |
| 1007.072 | 1027.671 | 1082.467 |
| 1097.844 | 1124.394 | 1168.828 |
| 1209.05 | 1310.113 | 1319.86 |
| 1331.757 | 1378.116 | 1405.955 |
| 1410.777 | 1447.632 | 1497.637 |
| 1501.011 | 1519.382 | 1543.17 |
| 1621.672 | 1862.624 | 3039.429 |
| 3045.382 | 3121.042 | 3125.906 |
| 3151.111 | 3191.62 | 3200.36 |
| 3211.851 | 3222.282 | 3241.644 |

***i60 – i62***

C -0.897526 -1.587065 0.182785

C -1.668556 -0.694487 -0.455384

C -1.249366 0.678002 -0.701002

C 0.174300 1.069503 -0.269420

C -0.351301 1.769179 0.983793

C 2.349168 -0.097643 -0.525083

C 1.100093 -0.097205 -0.071288

C 0.501382 -1.281973 0.646741

H -1.285079 -2.579140 0.391826

H -2.675010 -0.971544 -0.754155

H -1.643267 1.178537 -1.583369

H 0.618158 1.784815 -0.962731

H -0.363997 1.187683 1.902884

H -1.612659 1.443731 0.342814

H -0.177929 2.835600 1.101441

H 3.002571 -0.953809 -0.391592

H 2.762323 0.762109 -1.042698

H 1.143086 -2.158093 0.520061

H 0.482635 -1.079756 1.728665

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2087.37 | 111.5735 | 134.5583 |
| 259.5418 | 362.4591 | 377.3579 |
| 457.558 | 491.1287 | 526.8496 |
| 573.0746 | 625.7845 | 697.1887 |
| 735.075 | 761.7134 | 860.1434 |
| 900.5105 | 916.1838 | 928.6873 |
| 936.018 | 941.4242 | 965.1615 |
| 994.8417 | 1006.237 | 1051.326 |
| 1085.363 | 1110.511 | 1186.513 |
| 1209.876 | 1262.099 | 1308.066 |
| 1322.861 | 1329.403 | 1340.623 |
| 1363.119 | 1430.499 | 1433.936 |
| 1461.944 | 1479.495 | 1671.512 |
| 1746.661 | 1806.575 | 3001.882 |
| 3093.5 | 3105.271 | 3115.203 |
| 3152.489 | 3155.804 | 3175.838 |
| 3198.011 | 3225.264 | 3237.53 |

***i56 – i59***

C -1.945739 -0.469195 0.412671

C -1.715283 0.821396 -0.338132

C -0.496973 1.287495 -0.638716

C 0.703773 0.566169 -0.198791

C 1.645164 1.343358 0.701946

C 0.456159 -0.873681 0.111306

C -0.745453 -1.380753 0.350961

H -2.225919 -0.237452 1.450260

H -2.815484 -0.983211 -0.010888

H -2.595695 1.393826 -0.615508

H -0.380285 2.239848 -1.148332

H 1.579376 -0.081765 -1.084890

H 2.571871 0.798532 0.896969

H 1.159783 1.541821 1.664186

H 1.904670 2.304294 0.250042

H -0.906367 -2.454280 0.379502

C 1.682600 -1.436880 -0.506782

H 1.588965 -2.266203 -1.203518

H 2.613596 -1.402862 0.055396

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2270.95 | 125.7351 | 216.943 |
| 226.1106 | 257.9471 | 292.8471 |
| 422.5774 | 433.8952 | 461.5098 |
| 518.6717 | 548.6731 | 621.3228 |
| 726.9369 | 762.7291 | 811.1977 |
| 844.5057 | 888.8586 | 914.5954 |
| 962.4769 | 981.9821 | 1011.058 |
| 1016.457 | 1064.403 | 1072.084 |
| 1147.634 | 1161.74 | 1184.824 |
| 1219.603 | 1266.431 | 1307.201 |
| 1363.82 | 1381.431 | 1414.467 |
| 1421.736 | 1443.822 | 1477.333 |
| 1491.149 | 1500.936 | 1662.531 |
| 1694.181 | 1829.338 | 3010.845 |
| 3034.954 | 3068.442 | 3106.518 |
| 3115.279 | 3131.839 | 3163.799 |
| 3182.166 | 3187.069 | 3213.005 |

***i57 – i58***

C 1.310330 -1.411544 -0.252056

C 1.971774 -0.296327 0.128419

C 1.255576 0.914585 0.471579

C -0.283157 0.902502 0.419772

C -0.294030 1.881925 -0.753113

C -2.402064 -0.498894 0.198258

C -0.907892 -0.432301 0.114875

C -0.141269 -1.477131 -0.236796

H 1.862954 -2.298708 -0.540785

H 3.056204 -0.272772 0.139253

H 1.689819 1.561954 1.231399

H -0.745008 1.332336 1.313463

H -0.497920 1.467070 -1.736733

H 1.170546 1.738882 -0.560104

H -0.593969 2.911944 -0.578573

H -2.742460 -0.279455 1.217149

H -2.779280 -1.483869 -0.083510

H -2.864101 0.248122 -0.457140

H -0.612400 -2.422398 -0.490046

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2084.12 | 99.8991 | 164.9029 |
| 212.0589 | 251.5604 | 327.9831 |
| 382.8004 | 480.7927 | 532.575 |
| 554.875 | 576.6157 | 641.7938 |
| 726.5055 | 756.3375 | 855.6675 |
| 887.3802 | 896.2784 | 913.5612 |
| 939.9425 | 974.5201 | 984.8209 |
| 1041.697 | 1052.466 | 1064.798 |
| 1082.813 | 1134.586 | 1182.209 |
| 1205.865 | 1261.778 | 1321.402 |
| 1337.796 | 1343.285 | 1405.089 |
| 1415.492 | 1424.92 | 1449.948 |
| 1477.146 | 1494.862 | 1583.609 |
| 1718.996 | 1807.511 | 3029.538 |
| 3071.341 | 3083.943 | 3117.191 |
| 3134.572 | 3147.653 | 3178.683 |
| 3190.25 | 3208.712 | 3235.828 |

***i41 – i43***

C 2.187308 -1.141839 0.488991

C 1.219883 -0.436048 -0.469867

C -0.194040 -0.895848 -0.304165

C -1.252110 -0.173893 0.007003

C -1.238984 1.297707 0.240164

C 0.168582 1.816365 0.062997

C 1.224084 1.067737 -0.252256

C -2.286442 -1.256264 0.023428

H 2.187020 -2.220033 0.311812

H 1.892059 -0.962472 1.525819

H 3.207500 -0.771678 0.352649

H 1.554002 -0.637425 -1.496073

H -1.113452 -1.969394 -0.306083

H -1.606040 1.539324 1.246292

H -1.919548 1.812409 -0.450863

H 0.312136 2.883996 0.204312

H 2.194306 1.549457 -0.356251

H -2.673309 -1.590043 0.986932

H -3.004370 -1.301646 -0.796315

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2257.96 | 92.3213 | 132.5987 |
| 230.9418 | 265.1303 | 332.8925 |
| 390.4603 | 430.9313 | 474.9883 |
| 509.0347 | 542.0029 | 595.6059 |
| 710.8333 | 765.7961 | 869.0018 |
| 910.1581 | 933.3812 | 944.2134 |
| 980.1544 | 993.0431 | 1022.653 |
| 1061.891 | 1073.543 | 1083.93 |
| 1109.986 | 1144.697 | 1211.094 |
| 1212.909 | 1238.213 | 1321.575 |
| 1332.7 | 1396.219 | 1406.242 |
| 1423.284 | 1440.948 | 1473.643 |
| 1491.931 | 1507.831 | 1730.244 |
| 1798.856 | 1876.092 | 3027.244 |
| 3030.138 | 3047.911 | 3050.411 |
| 3079.8 | 3126.091 | 3134.692 |
| 3147.35 | 3173.291 | 3180.721 |

***i41 – i23***

C 1.985871 -1.222011 0.730263

C 1.250896 -0.620339 -0.481585

C -0.184054 -0.956234 -0.466198

C -1.318186 -0.556852 -0.192448

C -0.715195 1.379247 0.674807

C 0.466938 1.749623 -0.078664

C 1.390010 0.892169 -0.543046

C -2.778072 -0.642163 -0.059486

H 1.884417 -2.309818 0.743779

H 1.571015 -0.823606 1.658886

H 3.048821 -0.970776 0.692747

H 1.707623 -1.030022 -1.389356

H -0.595453 0.855261 1.616362

H -1.564566 2.057385 0.645328

H 0.583165 2.803427 -0.326678

H 2.258505 1.274278 -1.071130

H -3.127535 -1.630756 -0.365926

H -3.084403 -0.474419 0.976307

H -3.270837 0.108408 -0.682175

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -662.454 | 89.9775 | 120.1652 |
| 138.1145 | 212.8344 | 250.9961 |
| 265.6432 | 321.1738 | 373.71 |
| 477.8076 | 493.9038 | 541.5471 |
| 623.1213 | 682.6367 | 711.9462 |
| 758.9769 | 852.8472 | 882.9627 |
| 954.9622 | 983.049 | 1022.281 |
| 1033.95 | 1058.302 | 1073.939 |
| 1092.174 | 1120.868 | 1182.087 |
| 1246.496 | 1321.863 | 1348.897 |
| 1396.947 | 1407 | 1411.872 |
| 1477.602 | 1487.312 | 1491.165 |
| 1497.178 | 1501.064 | 1652.383 |
| 2118.723 | 3049.107 | 3053.131 |
| 3055.153 | 3124.259 | 3131.02 |
| 3131.965 | 3133.758 | 3135.517 |
| 3145.224 | 3190.141 | 3222.425 |

***i41 – i44***

C 2.559755 -0.911906 0.274711

C 1.227995 -0.352331 -0.155834

C 0.005073 -1.041944 0.086846

C -1.190572 -0.410137 0.132431

C -1.162308 1.049267 0.551755

C 0.002780 1.741933 -0.122903

C 1.117714 1.085912 -0.462658

C -2.494721 -1.026177 -0.263086

H 2.511544 -1.999435 0.358108

H 2.822490 -0.509668 1.258519

H 3.358121 -0.637605 -0.420691

H 0.751688 -1.231677 -1.011923

H -1.079863 1.168586 1.642605

H -2.103519 1.537733 0.275828

H -0.082920 2.807481 -0.316301

H 1.951785 1.597248 -0.933588

H -2.360347 -2.069286 -0.552227

H -3.221776 -0.987738 0.557579

H -2.941490 -0.483350 -1.105482

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1752.67 | 126.4231 | 142.2104 |
| 172.6486 | 214.0421 | 271.7403 |
| 309.3883 | 378.1212 | 470.9068 |
| 479.4508 | 515.3939 | 605.9577 |
| 674.5021 | 751.5409 | 850.6986 |
| 879.5642 | 918.6179 | 938.0802 |
| 977.5817 | 997.9389 | 1014.994 |
| 1037.714 | 1048.517 | 1124.87 |
| 1184.127 | 1196.959 | 1209.219 |
| 1246.176 | 1334.431 | 1366.081 |
| 1408.862 | 1410.546 | 1414.783 |
| 1466.414 | 1479.26 | 1484.354 |
| 1488.506 | 1501.019 | 1580.754 |
| 1681.477 | 2100.421 | 2991.661 |
| 3019.773 | 3042.949 | 3065.905 |
| 3069.213 | 3110.118 | 3138.924 |
| 3143.699 | 3169.886 | 3193.105 |

***i41 – i42***

C 1.780639 -1.479600 0.452658

C 1.387572 -0.311625 -0.461328

C 0.009904 -0.879953 -0.507412

C -1.111558 -0.259555 -0.154244

C -1.076671 1.253883 -0.050400

C 0.307008 1.797832 0.211246

C 1.424858 1.094928 0.052711

C -2.398318 -0.953698 0.173517

H 2.567415 -2.159574 0.132572

H 0.563275 -2.008338 0.059439

H 1.711505 -1.295962 1.521758

H 1.913381 -0.386480 -1.419155

H -1.743870 1.565113 0.764038

H -1.493839 1.717845 -0.955034

H 0.364903 2.827437 0.553524

H 2.390566 1.546423 0.261745

H -2.305841 -2.033016 0.044594

H -2.698108 -0.748151 1.207628

H -3.209989 -0.598565 -0.471599

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2069.87 | 120.1379 | 140.6607 |
| 197.2562 | 268.3864 | 330.4794 |
| 384.8618 | 439.1739 | 476.1277 |
| 503.5716 | 566.1955 | 642.9064 |
| 710.252 | 762.1869 | 869.3337 |
| 896.0747 | 918.748 | 949.2919 |
| 985.4364 | 1007.069 | 1008.438 |
| 1055.092 | 1077.899 | 1084.795 |
| 1137.008 | 1184.744 | 1203.802 |
| 1226.769 | 1242.506 | 1271.11 |
| 1347.156 | 1368.808 | 1413.066 |
| 1416.611 | 1433.269 | 1476.116 |
| 1487.4 | 1492.429 | 1713.003 |
| 1750.229 | 1893.042 | 3018.931 |
| 3029.702 | 3046.228 | 3056.489 |
| 3085.282 | 3113.369 | 3138.774 |
| 3165.011 | 3189.278 | 3226.753 |

***i26 – i27***

C 0.556434 1.487746 0.427320

C -0.543035 1.240851 -0.570014

C 3.620089 -1.232251 -0.090192

C 2.546507 -0.262680 0.098632

C 1.665016 0.536490 0.262223

H 0.940105 2.507340 0.325026

H 0.157736 1.390089 1.444277

H -0.501912 1.775529 -1.514921

H 3.327599 -2.000133 -0.810742

H 3.866320 -1.728754 0.851722

H 4.524748 -0.746201 -0.463905

C -1.379922 0.037077 -0.463767

C -2.591489 -0.001754 0.084922

C -3.433825 -1.233502 0.214472

H -0.951560 -0.893667 -0.848757

H -3.018141 0.921285 0.474651

H -3.654085 -1.445172 1.265867

H -2.933781 -2.105951 -0.212313

H -4.395676 -1.106226 -0.292487

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -206.265 | 29.9783 | 85.4792 |
| 106.2903 | 149.3765 | 206.0593 |
| 213.2746 | 235.263 | 267.007 |
| 386.4025 | 398.1949 | 414.5719 |
| 519.0292 | 596.5429 | 749.7042 |
| 800.2959 | 880.4503 | 955.8666 |
| 995.9542 | 1030.236 | 1061.593 |
| 1063.619 | 1080.828 | 1120.346 |
| 1137.158 | 1167.345 | 1228.167 |
| 1302.709 | 1314.745 | 1336.229 |
| 1378.653 | 1422.841 | 1423.958 |
| 1471.609 | 1486.48 | 1489.103 |
| 1492.242 | 1503.413 | 1753.069 |
| 2389.274 | 3037.238 | 3038.108 |
| 3053.261 | 3077.394 | 3090.735 |
| 3097.197 | 3125.069 | 3126.21 |
| 3127.374 | 3150.299 | 3173.77 |

***i23 – i22***

C -0.952475 -1.840494 -0.815870

C -0.476750 -1.127452 0.461383

C 0.863384 -0.548808 0.265784

C 1.941432 -0.048281 0.089369

C -1.429447 -0.045627 0.909595

C 3.250658 0.557082 -0.127671

H -0.242617 -2.618084 -1.104599

H -1.033708 -1.127611 -1.639332

H -1.930768 -2.299234 -0.651023

H -0.402933 -1.869422 1.264030

H -1.585360 0.097055 1.973972

H 3.735718 0.128866 -1.008435

H 3.158585 1.634901 -0.284173

H 3.905138 0.394216 0.732201

C -1.331859 2.074929 -0.371133

C -1.956791 0.949795 -0.037039

H -0.366556 2.328063 0.054857

H -1.764423 2.770248 -1.082931

H -2.921989 0.734136 -0.501076

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -220.614 | 57.2186 | 70.0446 |
| 96.9033 | 136.2264 | 203.8132 |
| 255.1284 | 280.7871 | 309.3108 |
| 321.2251 | 411.0365 | 500.8419 |
| 535.2539 | 566.2176 | 707.2389 |
| 732.039 | 881.6223 | 958.1269 |
| 975.3099 | 1023.812 | 1035.484 |
| 1056.007 | 1060.265 | 1072.91 |
| 1105.723 | 1154.782 | 1186.641 |
| 1320.054 | 1323.481 | 1336.508 |
| 1358.337 | 1415.263 | 1418.588 |
| 1453.556 | 1485.467 | 1490.078 |
| 1502.787 | 1508.625 | 1706.9 |
| 2383.921 | 3051.766 | 3052.619 |
| 3055.668 | 3099.531 | 3122.514 |
| 3125.869 | 3134.12 | 3144.704 |
| 3151.683 | 3186.573 | 3243.347 |

***i27 – p67***

C 0.383360 0.799988 0.733918

C -0.493402 0.952385 -0.482993

C -1.701134 0.414511 -0.679889

C -2.434585 -0.447976 0.232944

C -3.656468 -0.930674 -0.034206

C 4.075839 -0.723727 -0.289575

C 2.774490 -0.180212 0.082772

C 1.701027 0.260673 0.389496

H 0.515744 1.783646 1.201065

H -0.083135 0.162256 1.488129

H -0.069282 1.567822 -1.271443

H -2.202779 0.633003 -1.619973

H -1.970907 -0.705485 1.180536

H -4.146173 -0.730126 -0.982097

H -5.043770 0.632273 0.807693

H -4.161334 -1.603478 0.648176

H 4.028056 -1.205068 -1.269442

H 4.407610 -1.469227 0.437279

H 4.831210 0.064571 -0.334728

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -431.65 | 21.5575 | 85.4697 |
| 106.0349 | 120.502 | 175.8886 |
| 185.2829 | 224.0796 | 258.9202 |
| 277.0812 | 374.0184 | 388.3777 |
| 401.63 | 517.7204 | 617.3967 |
| 667.9939 | 785.5561 | 832.1995 |
| 916.4187 | 942.1792 | 958.1979 |
| 1000.76 | 1030.517 | 1040.838 |
| 1059.366 | 1068.351 | 1171.916 |
| 1175.232 | 1242.421 | 1300.618 |
| 1323.165 | 1339.086 | 1403.231 |
| 1424.398 | 1474.781 | 1477.765 |
| 1489.347 | 1493.949 | 1656.87 |
| 1731.614 | 2398.888 | 3037.93 |
| 3052.375 | 3110.544 | 3124.488 |
| 3125.943 | 3157.689 | 3161.48 |
| 3187.046 | 3190.89 | 3255.218 |

***i27 – p62***

C 0.390653 -0.259463 -0.185089

C -0.429711 0.780519 0.105680

C -1.880247 0.760396 0.004666

C -2.647428 -0.334245 0.056621

C -4.137128 -0.336977 -0.063481

C 4.465305 -0.048165 0.020335

C 3.011981 -0.122533 -0.048798

C 1.811283 -0.178769 -0.099035

H 0.050471 -1.421311 1.506885

H -0.015173 -1.144450 -0.666801

H 0.025603 1.702769 0.454929

H -2.364516 1.730572 -0.088589

H -2.174180 -1.301065 0.218606

H -4.456605 -0.948303 -0.914222

H -4.532818 0.671813 -0.200851

H -4.600096 -0.771455 0.828415

H 4.856019 0.636099 -0.737443

H 4.913146 -1.030801 -0.146412

H 4.789898 0.311552 1.000090

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -633.309 | 65.9431 | 77.5511 |
| 77.9833 | 144.2622 | 173.5288 |
| 196.3186 | 213.1493 | 308.5085 |
| 320.5516 | 327.6663 | 353.5749 |
| 374.0305 | 491.2644 | 501.8118 |
| 629.3672 | 796.3884 | 852.7737 |
| 893.5276 | 930.6576 | 987.6675 |
| 1005.933 | 1054.627 | 1061.295 |
| 1074.779 | 1077.744 | 1138.548 |
| 1213.37 | 1308.373 | 1322.751 |
| 1354.099 | 1362.738 | 1420.492 |
| 1422.234 | 1485.037 | 1486.189 |
| 1486.293 | 1495.345 | 1629.379 |
| 1724.995 | 2376.064 | 3037.027 |
| 3047.761 | 3095.714 | 3119.127 |
| 3122.874 | 3126.67 | 3149.805 |
| 3157.426 | 3179.257 | 3187.342 |

***i27 – i28***

C -0.073494 0.316852 -0.793705

C 0.676483 1.395817 -0.063225

C 1.735724 0.935858 0.597776

C 1.923165 -0.540747 0.492062

C 3.157976 -1.056563 -0.199525

C -3.918483 -0.479484 0.355486

C -2.553210 -0.188356 -0.063148

C -1.425325 0.057943 -0.411556

H 0.080806 0.305697 -1.875600

H 0.766194 -0.612739 -0.332018

H 0.360414 2.433226 -0.087407

H 2.419767 1.567684 1.158493

H 1.629296 -1.106186 1.379166

H 4.061838 -0.829927 0.381772

H 3.279590 -0.591067 -1.181906

H 3.116781 -2.140289 -0.332599

H -4.213158 0.158574 1.192531

H -4.015075 -1.520648 0.675605

H -4.623479 -0.312250 -0.463030

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1927.95 | 28.0236 | 56.5201 |
| 89.8093 | 124.1275 | 183.6263 |
| 221.625 | 227.7892 | 320.3097 |
| 414.6718 | 458.3901 | 515.8068 |
| 600.6941 | 673.216 | 738.3825 |
| 812.7076 | 844.5452 | 905.5483 |
| 940.1271 | 998.4403 | 1015.219 |
| 1052.329 | 1057.623 | 1070.406 |
| 1099.665 | 1130.893 | 1162.588 |
| 1201.257 | 1297.114 | 1342.306 |
| 1369.936 | 1400.816 | 1414.705 |
| 1420.382 | 1483.941 | 1485.018 |
| 1489.62 | 1493.338 | 1637.701 |
| 1708.31 | 2335.45 | 3013.008 |
| 3042.571 | 3082.801 | 3090.111 |
| 3099.314 | 3111.746 | 3117.814 |
| 3124.266 | 3164.393 | 3201.086 |

***i27 – p70***

C -0.438956 1.008657 -0.271366

C 0.489404 0.396151 0.759179

C 1.610473 -0.191078 0.434492

C 2.631461 -0.741888 -0.194969

C 3.954726 -0.069990 -0.412807

C -4.212708 -0.637194 -0.064528

C -2.880516 -0.049059 -0.146208

C -1.782822 0.432060 -0.213108

H -0.507574 2.088495 -0.095367

H -0.016282 0.873878 -1.270431

H 0.179724 0.461042 1.796719

H 2.376462 -0.422068 2.255328

H 2.542057 -1.785972 -0.488735

H 4.736801 -0.560630 0.176120

H 3.916359 0.981466 -0.125713

H 4.248684 -0.137664 -1.464371

H -4.169841 -1.630171 0.389657

H -4.655783 -0.738615 -1.058340

H -4.876987 -0.015714 0.541024

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -706.3 | 36.5476 | 76.6762 |
| 94.9757 | 104.6284 | 125.2396 |
| 174.1632 | 199.6647 | 231.6612 |
| 278.212 | 335.3519 | 401.9397 |
| 464.0072 | 521.1897 | 559.3156 |
| 577.0155 | 717.7112 | 785.4796 |
| 857.5759 | 901.4405 | 953.5129 |
| 1044.07 | 1051.467 | 1061.411 |
| 1067.832 | 1106.064 | 1160.098 |
| 1174.901 | 1224.928 | 1299.14 |
| 1345.369 | 1403.388 | 1424.439 |
| 1446.684 | 1479.039 | 1481.43 |
| 1490.459 | 1492.665 | 1502.298 |
| 2024.157 | 2398.661 | 3041.584 |
| 3046.574 | 3049.615 | 3098.564 |
| 3104.487 | 3120.266 | 3124.386 |
| 3141.267 | 3159.288 | 3192.353 |

***i23 – p11b***

C -0.736503 2.253538 1.013372

C -0.542803 0.777685 -0.835683

C 0.762571 0.313316 -0.493132

C 1.882619 -0.044381 -0.235921

C -1.114972 -1.860130 0.766973

C -1.936104 -1.206778 -0.070385

C -1.697959 0.041197 -0.758630

C 3.228785 -0.504719 0.077954

H 0.182223 2.809245 0.871681

H -0.743746 1.481935 1.772293

H -1.671632 2.758506 0.804522

H -0.559521 1.654901 -1.474310

H -0.127322 -1.492289 1.013612

H -1.432364 -2.788867 1.227114

H -2.917598 -1.640007 -0.249465

H -2.567813 0.483942 -1.234545

H 3.752140 0.217230 0.710056

H 3.197967 -1.460831 0.606712

H 3.813862 -0.642141 -0.834956

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -454.654 | 60.3109 | 65.504 |
| 79.1273 | 100.6977 | 124.9136 |
| 133.3906 | 217.7852 | 237.9251 |
| 328.8582 | 347.492 | 462.6498 |
| 486.3893 | 495.4361 | 531.7371 |
| 626.8207 | 678.9869 | 764.5301 |
| 814.1997 | 836.1372 | 935.0248 |
| 949.1405 | 957.0774 | 1040.984 |
| 1050.702 | 1055.796 | 1095.589 |
| 1161.451 | 1264.177 | 1341.877 |
| 1412.261 | 1415.673 | 1421.889 |
| 1431.557 | 1467.35 | 1482.877 |
| 1485.362 | 1518.792 | 1664.389 |
| 2369.804 | 3052.201 | 3107.381 |
| 3124.819 | 3125.783 | 3151.935 |
| 3170.296 | 3174.654 | 3191.362 |
| 3268.586 | 3277.441 | 3284.892 |

***i23 – p12b***

C 0.750425 -2.401990 0.026327

C 0.643756 -0.893417 -0.053400

C -0.694225 -0.384393 -0.019001

C -1.842384 -0.029327 0.037111

C 0.949174 2.242880 -0.196249

C 1.843978 1.336397 0.211984

C 1.745000 -0.110053 0.137236

C -3.221366 0.434979 0.096056

H 0.119669 -2.878394 -0.725497

H 0.410053 -2.741756 1.009539

H 1.780751 -2.729615 -0.121295

H 0.773425 -0.819930 -2.049441

H 0.008523 1.963065 -0.652776

H 1.157451 3.301463 -0.090457

H 2.782508 1.700195 0.623950

H 2.689071 -0.640899 0.227566

H -3.837957 -0.086071 -0.640487

H -3.650177 0.254025 1.084969

H -3.279473 1.507456 -0.106452

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -797.355 | 67.3379 | 74.8498 |
| 82.5379 | 150.8688 | 179.5288 |
| 221.9535 | 236.7976 | 311.8458 |
| 323.3858 | 358.6326 | 393.4491 |
| 434.3968 | 527.0753 | 579.8926 |
| 640.4893 | 658.3615 | 698.8963 |
| 889.6687 | 959.9726 | 962.2734 |
| 1014.92 | 1040.94 | 1054.183 |
| 1056.235 | 1059.487 | 1072.193 |
| 1141.012 | 1234.427 | 1346.223 |
| 1407.719 | 1409.231 | 1422.441 |
| 1460.072 | 1481.389 | 1483.925 |
| 1487.983 | 1495.865 | 1596.312 |
| 1689.245 | 2371.67 | 3051.426 |
| 3053.282 | 3121.705 | 3127.507 |
| 3128.098 | 3151.45 | 3155.104 |
| 3172.029 | 3179.229 | 3268.214 |

***i23 – p51***

C -0.862395 2.229992 0.561554

C -0.605897 1.092724 -0.444083

C 0.738601 0.541084 -0.280675

C 1.843893 0.100801 -0.122623

C -0.989650 -2.375645 0.296927

C -1.507964 -1.205385 -0.020314

C -1.705187 0.046363 -0.334531

C 3.181096 -0.447764 0.070128

H -0.118312 3.019832 0.441939

H -0.802819 1.847063 1.582441

H -1.855618 2.660296 0.408156

H -0.676271 1.516450 -1.454167

H -0.716195 -3.089999 -0.472182

H -0.905145 -2.683675 1.333602

H -3.382434 -1.788271 -0.047005

H -2.710811 0.409849 -0.519155

H 3.877460 0.326845 0.400705

H 3.169053 -1.236418 0.826425

H 3.566113 -0.874985 -0.859053

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -827.114 | 53.9123 | 76.1408 |
| 99.0737 | 115.8236 | 137.5999 |
| 198.8685 | 265.8817 | 308.0634 |
| 313.7698 | 330.5654 | 356.5741 |
| 474.7501 | 500.4999 | 523.465 |
| 591.4954 | 666.8415 | 728.2389 |
| 865.8591 | 900.6914 | 914.5277 |
| 990.8491 | 1025.279 | 1062.058 |
| 1063.384 | 1078.9 | 1093.305 |
| 1132.899 | 1209.922 | 1306.445 |
| 1325.468 | 1378.732 | 1413.879 |
| 1423.798 | 1472.18 | 1489.657 |
| 1492.645 | 1501.346 | 1504.03 |
| 2016.765 | 2399.06 | 3035.007 |
| 3050.635 | 3052.229 | 3123.022 |
| 3126.18 | 3130.922 | 3144.006 |
| 3151.437 | 3190.087 | 3240.644 |

***i60 – p92***

C -1.521994 -1.100060 0.259769

C -1.923136 0.190485 -0.272464

C -1.009187 1.109280 -0.605092

C 0.463803 0.893877 -0.379329

C 0.901375 1.693936 0.866356

C 2.034085 -1.040039 -0.523570

C 0.822945 -0.571940 -0.212949

C -0.216958 -1.451009 0.328996

H -2.287288 -1.792740 0.591166

H -2.980596 0.394988 -0.397779

H -1.315415 2.076992 -0.990818

H 1.015673 1.290682 -1.237854

H 1.978471 1.589331 1.018958

H 0.389168 1.320402 1.756672

H 0.663160 2.754691 0.749194

H 2.302257 -2.075048 -0.340332

H 2.790357 -0.401634 -0.968642

H 0.067514 -2.455441 0.623778

H 0.071105 -1.049398 2.425349

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -539.357 | 91.7519 | 182.6301 |
| 248.4347 | 263.7779 | 288.5515 |
| 291.1251 | 378.9163 | 408.5593 |
| 487.2556 | 538.6738 | 594.4689 |
| 690.212 | 709.2114 | 749.3814 |
| 769.1191 | 843.6976 | 876.6406 |
| 929.9407 | 946.6879 | 962.7575 |
| 994.9451 | 1011.199 | 1017.429 |
| 1036.727 | 1089.157 | 1118.393 |
| 1187.067 | 1208.075 | 1310.733 |
| 1321.774 | 1348.635 | 1396.57 |
| 1415.738 | 1441.361 | 1472.4 |
| 1495.545 | 1502.967 | 1584.172 |
| 1695.313 | 1728.213 | 3045.871 |
| 3062.666 | 3128.763 | 3134.206 |
| 3152.799 | 3181.757 | 3190.975 |
| 3204.48 | 3216.316 | 3241.635 |

***i60 – p45***

C -1.680753 -0.793477 0.478701

C -1.931251 0.287201 -0.276380

C -0.860161 1.032101 -0.898154

C 0.439933 0.625972 -0.783422

C 1.219079 1.895933 1.100983

C 1.859535 -1.357351 -0.550754

C 0.744937 -0.699956 -0.224864

C -0.278113 -1.269943 0.733658

H -2.491692 -1.331834 0.957862

H -2.952050 0.622808 -0.424618

H -1.095944 1.940024 -1.441667

H 1.209984 1.106659 -1.376417

H 2.199230 1.443072 1.183201

H 0.465476 1.601121 1.820460

H 1.155682 2.900822 0.702563

H 2.059440 -2.355483 -0.175799

H 2.603939 -0.913450 -1.203551

H -0.233603 -2.362884 0.722384

H 0.000304 -0.973729 1.756977

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -426.696 | 84.3232 | 102.431 |
| 131.032 | 133.9118 | 271.3754 |
| 387.538 | 442.3999 | 456.472 |
| 478.762 | 487.739 | 555.4402 |
| 596.9006 | 680.1701 | 723.4316 |
| 774.3275 | 777.3318 | 822.3496 |
| 900.8317 | 933.4964 | 939.1143 |
| 957.8238 | 972.4066 | 992.1449 |
| 998.2941 | 1034.153 | 1170.663 |
| 1198.212 | 1216.871 | 1314.201 |
| 1342.814 | 1395.102 | 1416.252 |
| 1423.873 | 1435.983 | 1451.064 |
| 1466.835 | 1501.226 | 1674.701 |
| 1719.279 | 2997.751 | 3086.336 |
| 3104.722 | 3152.319 | 3180.793 |
| 3190.386 | 3202.992 | 3213.558 |
| 3239.799 | 3275.63 | 3277.953 |

***i60 – p91***

C -2.052852 -0.218885 0.070541

C -1.696293 1.058250 0.244640

C -0.314042 1.470211 0.095344

C 0.700649 0.579820 -0.078949

C 2.136939 1.025909 -0.045324

C 1.303354 -1.777545 0.328613

C 0.387028 -0.863596 0.002972

C -1.038458 -1.254083 -0.315701

H -3.090598 -0.523771 0.153414

H -2.438206 1.811648 0.484481

H -0.085002 2.530487 0.132872

H 0.541361 0.608675 -2.157353

H 2.737008 0.496103 -0.788128

H 2.573378 0.826630 0.939273

H 2.214212 2.096863 -0.238299

H 1.035963 -2.823918 0.430331

H 2.341754 -1.521317 0.500166

H -1.114146 -1.400328 -1.405144

H -1.273669 -2.221565 0.135576

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -596.191 | 110.1633 | 180.4688 |
| 247.3335 | 305.0586 | 341.75 |
| 356.4798 | 385.2942 | 426.726 |
| 482.798 | 504.8166 | 522.7963 |
| 605.5943 | 699.9361 | 725.1769 |
| 761.9676 | 831.9702 | 884.3678 |
| 926.1948 | 941.621 | 963.4952 |
| 991.483 | 1002.562 | 1020.11 |
| 1058.981 | 1093.309 | 1170.031 |
| 1198.178 | 1224.289 | 1302.528 |
| 1347.112 | 1400.112 | 1421.266 |
| 1439.806 | 1450.19 | 1462.776 |
| 1493.787 | 1504.798 | 1592.098 |
| 1698.439 | 1724.852 | 2991.683 |
| 3046.878 | 3095.938 | 3116.683 |
| 3148.678 | 3165.956 | 3184.873 |
| 3193.726 | 3214.972 | 3252.272 |

***i63 – p92***

C -1.339391 -1.278090 0.298357

C -1.879515 -0.052856 -0.297148

C -1.045765 0.919202 -0.726570

C 0.421360 0.892949 -0.401950

C 0.667151 1.772931 0.844510

C 2.227993 -0.823617 -0.332432

C 0.941796 -0.511983 -0.149935

C -0.018194 -1.493111 0.355596

H -2.036143 -2.024455 0.662119

H -2.932200 -0.022912 -0.554206

H -2.523338 0.741808 1.418851

H -1.439012 1.801506 -1.220887

H 0.980351 1.331130 -1.234916

H 1.736048 1.816368 1.067384

H 0.146388 1.354569 1.709632

H 0.298479 2.789254 0.681458

H 2.611182 -1.807546 -0.083412

H 2.934198 -0.104394 -0.734554

H 0.371446 -2.427885 0.745967

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -704.703 | 80.8786 | 187.0485 |
| 239.073 | 254.0354 | 318.1027 |
| 342.4554 | 387.9266 | 411.2764 |
| 506.5267 | 526.1854 | 591.4929 |
| 689.7235 | 711.1465 | 748.0169 |
| 786.496 | 837.6965 | 875.9343 |
| 926.0169 | 942.2297 | 962.9668 |
| 1002.103 | 1006.218 | 1017.911 |
| 1030.77 | 1083.482 | 1113.63 |
| 1186.172 | 1208.229 | 1307.134 |
| 1323.999 | 1349.009 | 1392.866 |
| 1413.862 | 1438.19 | 1473.834 |
| 1488.578 | 1501.453 | 1607.162 |
| 1683.387 | 1727.646 | 3047.165 |
| 3064.707 | 3129.721 | 3136.903 |
| 3149.253 | 3178.851 | 3188.676 |
| 3203.848 | 3213.175 | 3238.068 |

***i63 – p44***

C -1.515650 -1.006305 0.508042

C -1.982414 0.271883 -0.119959

C -0.894775 1.017278 -0.824274

C 0.420765 0.664873 -0.727560

C 1.169835 1.824428 1.057289

C 2.032161 -1.176571 -0.401017

C 0.802784 -0.676125 -0.234525

C -0.254519 -1.433536 0.442455

H -2.260783 -1.603948 1.024593

H -2.804242 0.057108 -0.817369

H -2.435600 0.914222 0.651497

H -1.166341 1.933598 -1.338151

H 1.146129 1.178217 -1.349936

H 2.232523 1.634916 0.958004

H 0.659411 1.289329 1.849903

H 0.835786 2.838219 0.866475

H 2.289815 -2.166319 -0.040660

H 2.810002 -0.610506 -0.902222

H 0.024175 -2.380390 0.895159

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -543.241 | 86.711 | 127.0801 |
| 136.0797 | 163.3504 | 310.3749 |
| 362.0672 | 378.7669 | 498.1422 |
| 522.3617 | 553.9525 | 584.8938 |
| 609.7129 | 698.6608 | 739.0523 |
| 782.3972 | 805.7419 | 866.408 |
| 896.4431 | 905.2197 | 948.1201 |
| 956.5025 | 968.3961 | 990.5966 |
| 1020.798 | 1022.63 | 1166.43 |
| 1206.341 | 1210.323 | 1324.839 |
| 1378.992 | 1387.898 | 1418.087 |
| 1429.144 | 1436.271 | 1456.696 |
| 1466.208 | 1553.672 | 1688.308 |
| 1752.352 | 2992.696 | 3025.71 |
| 3093.351 | 3156.449 | 3176.827 |
| 3182.662 | 3198.52 | 3201.621 |
| 3245.851 | 3256.395 | 3261.518 |

***i63 – p90***

C -1.951483 -0.591295 -0.000535

C -1.857785 0.900058 0.064781

C -0.454200 1.405431 0.088928

C 0.643141 0.621157 -0.066785

C 2.024510 1.212421 0.064620

C 1.539120 -1.689519 0.080393

C 0.494533 -0.857239 -0.006225

C -0.877117 -1.377058 -0.026751

H -2.944627 -1.028879 -0.019715

H -2.385819 1.342256 -0.793543

H -2.400338 1.270566 0.945770

H -0.321158 2.481672 0.153074

H 0.594001 0.657863 -1.962286

H 2.706047 0.816297 -0.690626

H 2.441814 0.977549 1.049009

H 1.989660 2.297062 -0.047037

H 1.385452 -2.761544 0.135575

H 2.563629 -1.340502 0.098955

H -0.992971 -2.456074 -0.059737

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -882.197 | 88.9677 | 207.8301 |
| 264.087 | 306.8398 | 348.3443 |
| 397.6477 | 415.8812 | 455.0253 |
| 478.5698 | 520.2005 | 572.3268 |
| 610.6723 | 711.1345 | 737.442 |
| 795.0924 | 813.0424 | 835.4868 |
| 912.7638 | 916.3929 | 964.911 |
| 968.9442 | 1009.488 | 1011.477 |
| 1065.608 | 1092.002 | 1173.479 |
| 1202.921 | 1217.186 | 1308.536 |
| 1385.729 | 1394.505 | 1417.054 |
| 1441.338 | 1457.796 | 1470.349 |
| 1490.746 | 1513.463 | 1633.591 |
| 1690.768 | 1759.764 | 3005.06 |
| 3029.387 | 3051.728 | 3122.2 |
| 3145.387 | 3169.178 | 3176.825 |
| 3178.335 | 3201.869 | 3257.743 |

***i59 – p89***

C 1.945607 0.605740 -0.043523

C 1.880897 -0.795142 -0.094064

C 0.649909 -1.423396 -0.044448

C -0.540953 -0.696698 0.003725

C -1.863900 -1.410559 0.065417

C -0.487091 0.710620 -0.029648

C 0.746685 1.339405 -0.078588

C -1.755431 1.522292 -0.016323

H 2.388580 0.827305 1.729388

H 2.887228 1.110527 -0.225475

H 2.793361 -1.378149 -0.134759

H 0.602992 -2.507937 -0.051250

H -2.485266 -1.175419 -0.804981

H -2.433849 -1.117257 0.952800

H -1.725580 -2.492394 0.097708

H 0.792095 2.423123 -0.108262

H -2.415937 1.248252 -0.844679

H -1.540857 2.589137 -0.094845

H -2.317111 1.359238 0.909071

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -922.567 | 97.4069 | 163.3641 |
| 181.2285 | 251.9813 | 328.8149 |
| 343.3888 | 392.9145 | 425.3748 |
| 452.4356 | 512.2259 | 558.6361 |
| 594.3974 | 725.3581 | 753.645 |
| 801.6425 | 841.2384 | 879.9568 |
| 964.2487 | 1012.974 | 1018.896 |
| 1045.965 | 1050.738 | 1063.508 |
| 1074.301 | 1147.973 | 1186.776 |
| 1212.982 | 1258.451 | 1314.475 |
| 1327.722 | 1419.089 | 1430.018 |
| 1471.67 | 1482.195 | 1500.392 |
| 1505.744 | 1508.839 | 1532.101 |
| 1620.779 | 1664.283 | 3038.481 |
| 3046.371 | 3095.488 | 3105.561 |
| 3138.241 | 3141.269 | 3184.667 |
| 3190.216 | 3203.048 | 3216.304 |

***i59 – p90***

C 1.960764 -0.759366 -0.063851

C 1.916282 0.733445 -0.000903

C 0.771467 1.410269 0.071188

C -0.539112 0.754274 0.097645

C -1.664928 1.486790 0.169376

C -0.547330 -0.721225 0.031279

C 0.606592 -1.394040 -0.041769

C -1.868930 -1.435940 0.044386

H 2.500632 -1.075642 -0.967714

H 2.563756 -1.147455 0.769435

H 2.863210 1.263991 -0.016457

H 0.780742 2.495207 0.114621

H -1.617091 2.568320 0.229472

H -2.648596 1.037509 0.212698

H -2.186513 1.747123 -2.237777

H 0.581169 -2.479635 -0.091939

H -2.424393 -1.218882 0.962286

H -1.727750 -2.515761 -0.021914

H -2.493993 -1.120024 -0.796820

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -305.656 | 81.506 | 100.2686 |
| 145.9496 | 200.5688 | 252.7962 |
| 317.1345 | 349.5888 | 410.8423 |
| 425.0422 | 490.5259 | 571.1206 |
| 609.4146 | 723.5827 | 735.6721 |
| 801.056 | 835.8363 | 842.8175 |
| 906.0866 | 918.131 | 971.9805 |
| 972.4758 | 1013.943 | 1017.422 |
| 1071.606 | 1090.68 | 1177.762 |
| 1197.571 | 1217.568 | 1303.928 |
| 1382.203 | 1394.295 | 1421.352 |
| 1446.569 | 1458.792 | 1468.417 |
| 1485.177 | 1506.831 | 1661.587 |
| 1716.693 | 1767.401 | 3013.519 |
| 3031.03 | 3042.251 | 3103.247 |
| 3139.228 | 3171.263 | 3171.633 |
| 3178.205 | 3201.177 | 3264.5 |

***i58 – p91***

C -1.748586 -1.015073 -0.124387

C -2.041530 0.284750 -0.037332

C -0.973901 1.275239 0.317540

C 0.427898 0.814544 -0.036084

C 1.437737 1.717834 -0.120629

C 2.086598 -1.144619 0.090647

C 0.673621 -0.642561 0.054580

C -0.378645 -1.481730 0.039692

H -2.522938 -1.746225 -0.328404

H -3.059438 0.640636 -0.152613

H -1.172555 2.251829 -0.128209

H -1.004253 1.421610 1.409024

H -0.005591 0.751094 -1.913793

H 2.471594 1.417982 -0.234142

H 1.228185 2.781491 -0.130243

H 2.613738 -0.887248 -0.834266

H 2.110757 -2.229758 0.201168

H 2.646316 -0.699437 0.919153

H -0.204965 -2.552281 0.088166

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -852.6 | 115.2765 | 189.6519 |
| 240.8575 | 337.5072 | 342.9298 |
| 397.2302 | 423.2048 | 477.582 |
| 482.3932 | 510.5467 | 525.7552 |
| 589.7565 | 666.9608 | 725.4236 |
| 739.8048 | 827.6523 | 867.22 |
| 895.931 | 936.1205 | 960.9433 |
| 991.8483 | 1001.857 | 1023.427 |
| 1069.943 | 1088.596 | 1170.702 |
| 1195.638 | 1223.015 | 1306.61 |
| 1338.825 | 1395.372 | 1418.825 |
| 1438.976 | 1446.099 | 1466.199 |
| 1487.837 | 1502.69 | 1596.877 |
| 1668.015 | 1734.562 | 2995.926 |
| 3040.772 | 3100.908 | 3108.363 |
| 3139.643 | 3169.29 | 3183.451 |
| 3194.091 | 3213.208 | 3264.736 |

***i44 – p1***

C 2.571276 -0.988934 0.057746

C 1.251869 -0.267261 -0.006475

C 0.047639 -0.973064 -0.019363

C -1.182711 -0.331769 -0.054609

C -1.206299 1.076774 -0.031085

C -0.001768 1.794717 -0.090875

C 1.208427 1.129110 -0.056436

C -2.472451 -1.101413 -0.046174

H 2.450437 -2.057262 -0.131526

H 3.028190 -0.874488 1.045703

H 3.276482 -0.590467 -0.676473

H 0.074782 -2.059372 -0.010249

H -1.651154 1.278065 1.781992

H -2.146099 1.593434 -0.195778

H -0.027712 2.877331 -0.139435

H 2.136630 1.691430 -0.079720

H -2.303894 -2.168385 -0.202153

H -2.980732 -0.973949 0.915751

H -3.152826 -0.745295 -0.824489

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -813.404 | 130.2682 | 146.1397 |
| 192.1847 | 210.2601 | 281.8157 |
| 339.1612 | 375.3894 | 417.5071 |
| 459.0084 | 523.5133 | 544.3855 |
| 563.8394 | 723.1647 | 740.1261 |
| 810.679 | 896.5279 | 932.4744 |
| 961.7882 | 1005.676 | 1018.746 |
| 1027.746 | 1038.664 | 1071.678 |
| 1073.983 | 1122.841 | 1188.085 |
| 1199.543 | 1286.895 | 1313.801 |
| 1348.486 | 1425.873 | 1427.933 |
| 1463.881 | 1495.778 | 1498.296 |
| 1498.994 | 1520.146 | 1530.435 |
| 1631.7 | 1669.819 | 3042.011 |
| 3043.34 | 3106.603 | 3106.818 |
| 3135.89 | 3138.341 | 3178.488 |
| 3183.47 | 3189.62 | 3213.181 |

***i44 – i32***

C 2.554331 -1.023593 -0.022257

C 1.229715 -0.322594 0.012474

C 0.051566 -0.987909 0.076594

C -1.231111 -0.333792 0.144937

C -1.209876 1.180504 0.071905

C 0.056966 1.833636 -0.066084

C 1.222548 1.144571 -0.060067

C -2.510978 -1.053462 -0.154580

H 2.436936 -2.108498 0.013996

H 3.180873 -0.719836 0.824492

H 3.106856 -0.768442 -0.933763

H 0.051573 -2.075480 0.074332

H -1.292408 0.498095 1.153870

H -2.142588 1.695437 -0.117411

H 0.064742 2.913466 -0.174335

H 2.169241 1.665883 -0.147544

H -2.485000 -2.079817 0.220424

H -3.369053 -0.553240 0.304724

H -2.700135 -1.091736 -1.236315

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2649.02 | 135.388 | 139.0415 |
| 180.0321 | 193.1311 | 265.5705 |
| 373.0116 | 389.6796 | 418.454 |
| 472.5566 | 537.1573 | 609.9229 |
| 687.2009 | 703.8616 | 764.8061 |
| 839.5881 | 875.3774 | 961.7865 |
| 972.493 | 977.6797 | 1031.792 |
| 1052.018 | 1061.235 | 1072.368 |
| 1137.486 | 1183.212 | 1210.635 |
| 1268.646 | 1295.083 | 1333.81 |
| 1398.886 | 1420.017 | 1426.279 |
| 1456.139 | 1477.724 | 1484.802 |
| 1497.176 | 1501.538 | 1592.285 |
| 1642.022 | 2200.072 | 3005.927 |
| 3024.949 | 3078.188 | 3078.497 |
| 3119.904 | 3130.043 | 3169.692 |
| 3184.537 | 3205.102 | 3221.885 |

***i44 – p48***

C 2.580437 -0.932217 -0.000739

C 1.221315 -0.297129 -0.014546

C 0.089982 -1.008290 -0.160159

C -1.232480 -0.393495 -0.134161

C -1.294781 1.116003 -0.244546

C -0.009805 1.814178 0.092471

C 1.146343 1.156801 0.176980

C -2.345851 -1.134222 -0.030850

H 2.520739 -2.011307 -0.151367

H 3.084172 -0.744924 0.953545

H 3.214765 -0.509019 -0.786690

H 0.136937 -2.089741 -0.252854

H -2.112086 1.504569 0.370345

H -1.554660 1.379088 -1.280852

H -0.044235 2.890442 0.227168

H 2.067756 1.689765 0.391330

H -2.615419 -1.141448 2.437501

H -3.330146 -0.679699 -0.003505

H -2.298772 -2.217504 -0.011331

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -285.166 | 55.5996 | 95.5616 |
| 131.1956 | 171.9012 | 209.3735 |
| 294.0776 | 305.719 | 424.7324 |
| 458.3531 | 526.7927 | 547.3947 |
| 555.6475 | 700.6811 | 711.5805 |
| 763.4032 | 866.4372 | 884.6174 |
| 895.9389 | 941.2144 | 955.851 |
| 975.5056 | 1013.077 | 1026.281 |
| 1051.983 | 1072.072 | 1194.169 |
| 1206.672 | 1230.22 | 1318.415 |
| 1349.019 | 1373.51 | 1418.757 |
| 1446.219 | 1446.598 | 1457.528 |
| 1489.135 | 1498.158 | 1672.73 |
| 1679.165 | 1752.193 | 3002.854 |
| 3039.746 | 3086.233 | 3098.748 |
| 3140.4 | 3157.851 | 3176.172 |
| 3177.563 | 3201.572 | 3247.522 |

***i44 – p46***

C 2.439600 -1.011851 0.176390

C 1.284075 -0.328040 0.110320

C -0.014306 -1.001846 0.084340

C -1.177297 -0.347736 0.007889

C -1.226806 1.154310 -0.055406

C 0.115367 1.816683 -0.024655

C 1.257586 1.134851 0.049906

C -2.500402 -1.052466 -0.025136

H 2.923395 -1.366514 -2.224589

H 2.451525 -2.094119 0.240251

H 3.395397 -0.501584 0.211146

H -0.009283 -2.087858 0.127918

H -1.844026 1.530367 0.773726

H -1.768210 1.459685 -0.962901

H 0.132601 2.901429 -0.068542

H 2.209556 1.656192 0.067077

H -2.381730 -2.134921 0.046011

H -3.139056 -0.720881 0.800998

H -3.037066 -0.825225 -0.952987

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -289.866 | 94.8668 | 113.8081 |
| 129.308 | 149.949 | 208.9093 |
| 294.1842 | 341.5081 | 420.3231 |
| 443.5712 | 487.6937 | 538.146 |
| 589.8688 | 710.6859 | 716.0306 |
| 801.0208 | 882.3129 | 885.405 |
| 905.4548 | 931.1049 | 952.4072 |
| 974.445 | 1010.542 | 1017.781 |
| 1051.433 | 1070.194 | 1179.569 |
| 1203.263 | 1231.298 | 1319.134 |
| 1361.649 | 1402.113 | 1423.045 |
| 1441.017 | 1457.92 | 1465.898 |
| 1483.318 | 1495.794 | 1664.855 |
| 1716.76 | 1771.165 | 3007.258 |
| 3025.629 | 3034.867 | 3091.908 |
| 3136.477 | 3162.004 | 3175.011 |
| 3178.985 | 3202.096 | 3252.451 |

***i42 – p46***

C -2.421531 -1.136642 -0.190329

C -1.300544 -0.401691 0.068038

C 0.035405 -1.021374 0.044487

C 1.166906 -0.316212 -0.000944

C 1.155854 1.188577 -0.009352

C -0.213447 1.793648 -0.052193

C -1.328643 1.070497 -0.005321

C 2.518699 -0.963906 -0.043501

H -2.379897 -2.218084 -0.245780

H -3.392347 -0.663149 -0.276019

H -1.474207 -0.451940 1.902168

H 0.072955 -2.107124 0.055779

H 1.747622 1.550173 -0.862179

H 1.692606 1.556487 0.877939

H -0.274745 2.875434 -0.120452

H -2.301696 1.549873 -0.032762

H 2.445084 -2.052252 -0.010449

H 3.055814 -0.681939 -0.955804

H 3.132615 -0.634865 0.802251

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1032.25 | 86.1258 | 131.5271 |
| 199.6325 | 289.7893 | 338.9441 |
| 389.9388 | 441.6174 | 444.2318 |
| 472.591 | 506.2286 | 550.6103 |
| 585.3708 | 633.2826 | 711.0316 |
| 775.9906 | 855.6448 | 875.334 |
| 887.1441 | 927.8453 | 952.7319 |
| 969.5903 | 1009.442 | 1016.842 |
| 1047.588 | 1068.539 | 1176.549 |
| 1205.891 | 1233.377 | 1317.918 |
| 1350.582 | 1394.25 | 1416.804 |
| 1433.224 | 1460.431 | 1462.017 |
| 1479.804 | 1493.786 | 1578.38 |
| 1723.731 | 1774.213 | 3006.534 |
| 3028.09 | 3033.831 | 3090.965 |
| 3136.891 | 3160.131 | 3178.314 |
| 3179.195 | 3204.384 | 3257.458 |

***i26 – p58***

C -0.688290 1.600667 -0.078365

C 0.654344 1.391352 -0.125260

C -3.486956 -1.376847 -0.003892

C -2.482898 -0.321489 -0.027543

C -1.655793 0.552277 -0.041052

C 1.295288 0.104113 -0.014028

C 2.623722 -0.064009 -0.043591

C 3.320559 -1.381002 0.064509

H -0.886039 2.197710 1.872163

H -1.070158 2.600676 -0.254547

H 1.297897 2.261134 -0.224475

H -3.255301 -2.116512 0.766534

H -3.533087 -1.892752 -0.966533

H -4.476347 -0.963975 0.207029

H 0.645564 -0.761378 0.096878

H 3.258200 0.814332 -0.155550

H 3.918238 -1.580765 -0.831286

H 2.609242 -2.199769 0.191574

H 4.011939 -1.389076 0.913550

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -733.384 | 60.5379 | 64.6562 |
| 92.4232 | 133.8134 | 180.2078 |
| 186.5572 | 210.3493 | 286.439 |
| 307.0579 | 322.2651 | 390.2932 |
| 428.9263 | 472.6301 | 560.625 |
| 647.3312 | 784.636 | 793.7256 |
| 864.9401 | 952.7709 | 982.6634 |
| 1023.173 | 1056.045 | 1059.187 |
| 1066.165 | 1089.111 | 1139.73 |
| 1188.531 | 1247.315 | 1299.366 |
| 1332.313 | 1416.712 | 1419.209 |
| 1436.349 | 1482.018 | 1483.163 |
| 1488.619 | 1492.053 | 1595.676 |
| 1709.536 | 2374.927 | 3038.113 |
| 3051.113 | 3095.84 | 3122.613 |
| 3127 | 3130.575 | 3154.677 |
| 3171.235 | 3179.374 | 3196.844 |

***i26 – p66***

C 0.756373 1.745721 0.064527

C -0.706700 1.392189 0.004240

C 3.334921 -1.465862 -0.028903

C 2.421588 -0.328953 0.003859

C 1.672983 0.608909 0.031307

C -1.214613 0.160602 -0.055400

C -2.639925 -0.116529 -0.112435

C -3.162887 -1.349737 -0.159421

H 0.990924 2.422596 -0.766432

H 0.939815 2.329082 0.975598

H -1.382395 2.245416 0.013572

H 3.305309 -1.961021 -1.002522

H 3.068296 -2.200867 0.734356

H 4.362552 -1.143677 0.155998

H -0.539047 -0.692161 -0.062591

H -3.307666 0.742561 -0.103325

H -3.449992 -1.882361 2.010875

H -2.527036 -2.228438 -0.202193

H -4.231196 -1.509179 -0.239978

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -460.324 | 63.1107 | 80.283 |
| 95.8616 | 130.5196 | 175.4787 |
| 190.7384 | 220.1168 | 230.8339 |
| 286.6533 | 297.8531 | 399.2311 |
| 428.9736 | 474.424 | 622.8897 |
| 681.8778 | 768.1662 | 839.3094 |
| 949.8199 | 960.0107 | 976.6611 |
| 1000.957 | 1011.981 | 1051.84 |
| 1055.553 | 1065.349 | 1174.948 |
| 1193.707 | 1243.214 | 1288.611 |
| 1315.868 | 1345.541 | 1375.985 |
| 1416.948 | 1455.435 | 1463.924 |
| 1487.464 | 1491.29 | 1662.055 |
| 1741.58 | 2400.118 | 3033.71 |
| 3054.764 | 3060.205 | 3127.474 |
| 3128.264 | 3152.782 | 3159.272 |
| 3161.526 | 3170.901 | 3252.182 |

***i26 – p71***

C -0.732998 1.875004 -0.143303

C 0.749530 1.712505 0.096430

C -2.861782 -1.642156 0.069140

C -2.118002 -0.390034 -0.000960

C -1.500664 0.636688 -0.063869

C 1.383961 0.557731 0.154680

C 2.037922 -0.507256 0.537246

C 2.717520 -1.528323 -0.325060

H -1.123854 2.598879 0.581367

H -0.879896 2.331251 -1.130859

H 1.331177 2.631164 0.123154

H -2.744993 -2.110199 1.049717

H -2.505880 -2.346348 -0.686952

H -3.927900 -1.472639 -0.100809

H 1.038251 0.150064 -1.778050

H 2.079618 -0.673462 1.613122

H 3.781869 -1.590967 -0.079417

H 2.614068 -1.284082 -1.382935

H 2.284617 -2.518619 -0.154164

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -700.038 | 39.01 | 63.9897 |
| 92.7965 | 134.5883 | 144.4588 |
| 166.6448 | 214.8182 | 240.1689 |
| 312.3927 | 352.7889 | 399.5619 |
| 465.9734 | 535.5596 | 554.0418 |
| 639.747 | 689.6221 | 770.8972 |
| 875.332 | 890.6296 | 955.3649 |
| 982.4265 | 1066.372 | 1067.674 |
| 1068.617 | 1100.195 | 1159.551 |
| 1191.196 | 1246.697 | 1299.443 |
| 1363.927 | 1414.686 | 1429.624 |
| 1456.274 | 1476.687 | 1488.162 |
| 1492.709 | 1495.033 | 1509.297 |
| 2025.228 | 2403.999 | 3027.018 |
| 3044.206 | 3049.295 | 3060.783 |
| 3106.117 | 3120.116 | 3123.491 |
| 3137.8 | 3153.059 | 3157.763 |

***i57 – p92***

C -1.435327 -1.244619 0.369550

C -1.963683 -0.042028 -0.266408

C -1.146972 0.942171 -0.648255

C 0.332591 0.909254 -0.372023

C 0.639499 1.876364 0.791910

C 2.146608 -0.790545 -0.177242

C 0.848512 -0.480039 -0.038067

C -0.112950 -1.449534 0.474096

H -2.133613 -1.991873 0.730137

H -3.033041 0.034568 -0.429047

H -1.542312 1.839863 -1.113927

H 0.866590 1.274191 -1.255885

H 1.716328 1.920917 0.972977

H 0.148107 1.533314 1.705933

H 0.279561 2.883893 0.565754

H 2.862285 -0.073420 -0.565448

H 2.180195 -1.625078 -2.452332

H 2.533175 -1.753683 0.137716

H 0.273050 -2.368843 0.902749

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -341.02 | 75.2243 | 122.1266 |
| 148.2039 | 213.5066 | 244.9626 |
| 269.138 | 385.1294 | 398.7726 |
| 485.9235 | 532.36 | 593.2865 |
| 688.6154 | 713.7967 | 748.7213 |
| 785.5087 | 849.7743 | 876.048 |
| 917.6896 | 944.3029 | 966.6132 |
| 1012.139 | 1014.271 | 1022.855 |
| 1033.637 | 1085.824 | 1118.964 |
| 1194.527 | 1215.481 | 1305.979 |
| 1326.215 | 1347.645 | 1394.79 |
| 1414.941 | 1441.607 | 1477.296 |
| 1489.165 | 1503.764 | 1652.721 |
| 1670.78 | 1737.585 | 3047.313 |
| 3059.93 | 3129.169 | 3135.945 |
| 3149.576 | 3179.502 | 3184.215 |
| 3200.822 | 3213.02 | 3239.513 |

***i57 – i61***

C -1.951552 -0.753869 0.070204

C -2.012495 0.598437 0.060270

C -0.830535 1.393942 -0.085371

C 0.521152 0.697067 -0.138237

C 1.736348 1.530313 0.147020

C 1.826098 -1.472434 -0.008867

C 0.508884 -0.749302 -0.046970

C -0.664181 -1.432893 0.006439

H -2.855779 -1.343400 0.160760

H -2.965373 1.106989 0.161243

H -0.836440 2.463194 0.080643

H -0.176099 1.108173 -1.155844

H 2.646720 1.090729 -0.265222

H 1.882184 1.662440 1.228222

H 1.630106 2.529582 -0.285559

H 2.436263 -1.225530 -0.883867

H 1.677270 -2.552872 0.012466

H 2.404284 -1.190174 0.876945

H -0.645446 -2.516699 0.043283

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2578.99 | 129.585 | 160.3242 |
| 211.2737 | 227.9527 | 306.1681 |
| 320.2891 | 387.488 | 485.12 |
| 498.4871 | 544.3036 | 627.6194 |
| 666.9581 | 715.7621 | 757.3442 |
| 815.6946 | 829.0173 | 942.7006 |
| 976.0321 | 977.5816 | 1040.534 |
| 1052.674 | 1064.576 | 1089.822 |
| 1164.971 | 1177.858 | 1187.83 |
| 1245.893 | 1285.944 | 1339.588 |
| 1388.156 | 1417.766 | 1431.457 |
| 1449.221 | 1479.743 | 1489.282 |
| 1501.428 | 1508.19 | 1602.11 |
| 1624.12 | 2207.358 | 3002.992 |
| 3036.722 | 3079.658 | 3095.086 |
| 3127.405 | 3142.058 | 3187.973 |
| 3195.263 | 3216.683 | 3224.988 |

***i60 – i65***

C -2.014931 -0.309450 0.161600

C -1.738274 1.007780 0.226903

C -0.420278 1.503811 -0.044800

C 0.721708 0.555771 -0.151887

C 2.109791 1.099356 0.011961

C 1.381650 -1.769731 0.263005

C 0.439298 -0.860036 -0.051202

C -0.991392 -1.295986 -0.326836

H -3.010362 -0.674043 0.389067

H -2.508541 1.725044 0.487316

H -0.179176 2.552655 0.073267

H 0.089845 1.103457 -1.178274

H 2.836763 0.540337 -0.581585

H 2.415656 1.040943 1.063720

H 2.159523 2.148820 -0.288264

H 1.133867 -2.822151 0.340955

H 2.410573 -1.494078 0.461055

H -1.113232 -1.428666 -1.414353

H -1.160352 -2.281414 0.114635

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1847.83 | 112.2591 | 163.6331 |
| 206.6018 | 287.6738 | 340.2404 |
| 411.8862 | 484.8128 | 490.6468 |
| 504.0791 | 583.2446 | 676.1754 |
| 702.0131 | 720.3827 | 787.7469 |
| 826.0289 | 859.2834 | 928.0052 |
| 957.3779 | 961.068 | 984.0233 |
| 1011.949 | 1044.993 | 1090.985 |
| 1157.575 | 1179.944 | 1217.175 |
| 1243.414 | 1267.392 | 1343.418 |
| 1378.155 | 1404.516 | 1418.43 |
| 1447.007 | 1461.807 | 1483.867 |
| 1487.636 | 1510.248 | 1627.216 |
| 1641.817 | 2113.394 | 2971.442 |
| 3027.813 | 3086.92 | 3099.891 |
| 3130.867 | 3164.66 | 3192.779 |
| 3210.375 | 3224.647 | 3250.574 |

***i63 – i66***

C -1.914720 -0.656664 -0.021367

C -1.899005 0.830060 0.206471

C -0.560077 1.436853 -0.080164

C 0.677386 0.600992 -0.150114

C 2.000326 1.282946 0.051455

C 1.601745 -1.677155 0.132552

C 0.552750 -0.845151 -0.038899

C -0.811175 -1.396468 -0.121182

H -2.887174 -1.137467 -0.065696

H -2.680453 1.308821 -0.394784

H -2.181570 1.022986 1.255883

H -0.417434 2.506250 0.011207

H 0.081492 0.991192 -1.192061

H 2.798389 0.801297 -0.517924

H 2.281387 1.263694 1.111495

H 1.950324 2.329226 -0.260081

H 1.448719 -2.748436 0.192710

H 2.618260 -1.318336 0.233118

H -0.895327 -2.471704 -0.246379

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1937.58 | 95.5769 | 152.805 |
| 178.6183 | 276.5919 | 344.0032 |
| 371.8422 | 413.2542 | 479.1491 |
| 515.9629 | 606.8483 | 620.5796 |
| 683.6586 | 713.1391 | 783.4806 |
| 822.2699 | 853.4916 | 904.5774 |
| 938.4088 | 973.9034 | 1002.193 |
| 1018.289 | 1035.933 | 1084.721 |
| 1152.514 | 1192.806 | 1207.877 |
| 1249.723 | 1263.362 | 1358.834 |
| 1375.217 | 1410.277 | 1418.924 |
| 1444.46 | 1461.387 | 1477.799 |
| 1489.19 | 1508.708 | 1633.282 |
| 1743.941 | 2206.18 | 2950.614 |
| 3024.768 | 3048.532 | 3098.407 |
| 3127.753 | 3169.196 | 3174.699 |
| 3197.315 | 3211.888 | 3258.601 |

***i22 – p12a***

C 0.011388 2.462021 -0.148999

C 0.207816 0.977399 0.062630

C -0.983568 0.179304 0.037677

C -2.005183 -0.454273 -0.005594

C -3.238420 -1.228610 -0.046040

C 1.443451 0.404550 -0.025184

C 2.939973 -1.534276 -0.054645

C 1.709469 -1.013547 0.001967

H -0.760331 2.855388 0.513811

H -0.308801 2.643381 -1.179937

H 0.939978 3.006791 0.029387

H 0.247240 1.153940 2.043616

H -3.177313 -2.019466 -0.797768

H -3.432905 -1.695584 0.922905

H -4.089896 -0.589701 -0.291967

H 2.302277 1.068725 -0.083534

H 3.819876 -0.901547 -0.122978

H 3.102427 -2.605253 -0.035893

H 0.847888 -1.672086 0.071490

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -842.787 | 38.2006 | 79.2918 |
| 114.4109 | 153.5891 | 201.3979 |
| 202.797 | 217.705 | 301.8623 |
| 343.7145 | 395.9521 | 396.4519 |
| 442.8788 | 470.2454 | 582.9638 |
| 626.8769 | 677.3833 | 684.9146 |
| 895.0792 | 946.3382 | 952.5153 |
| 1040.087 | 1042.021 | 1053.789 |
| 1058.116 | 1060.476 | 1065.004 |
| 1186.103 | 1249.569 | 1327.978 |
| 1378.273 | 1417.038 | 1420.165 |
| 1455.131 | 1483.343 | 1483.704 |
| 1484.475 | 1499.963 | 1594.629 |
| 1679.121 | 2371.09 | 3047.065 |
| 3047.499 | 3119.5 | 3121.689 |
| 3123.429 | 3149.118 | 3149.434 |
| 3166.334 | 3178.814 | 3245.029 |

***i22 – p51***

C 0.132824 2.188725 0.002906

C 0.169382 0.684100 0.322080

C -1.163771 0.083264 0.200673

C -2.257534 -0.397891 0.081512

C -3.584799 -0.986070 -0.058751

C 1.140719 -0.033920 -0.591718

C 3.220115 -1.376920 0.219371

C 2.269543 -0.573280 -0.175784

H -0.562927 2.702288 0.669403

H -0.195440 2.352605 -1.026533

H 1.128671 2.620463 0.126105

H 0.516223 0.553142 1.351947

H -3.808663 -1.190372 -1.108651

H -3.654613 -1.927221 0.492022

H -4.352112 -0.309384 0.325313

H 0.925071 -0.007584 -1.657522

H 2.999504 -2.427705 0.381040

H 4.231271 -1.033926 0.397483

H 3.214145 1.139641 0.047656

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -755.859 | 45.5504 | 92.7904 |
| 109.601 | 113.7112 | 143.4732 |
| 201.7214 | 257.3249 | 295.2384 |
| 302.938 | 354.919 | 404.2594 |
| 485.2115 | 521.0052 | 529.1748 |
| 551.378 | 671.3943 | 767.2522 |
| 871.3403 | 904.7654 | 919.6897 |
| 1015.993 | 1021.358 | 1058.791 |
| 1064.86 | 1090.617 | 1099.452 |
| 1152.516 | 1195.636 | 1271.174 |
| 1336.931 | 1386.05 | 1411.412 |
| 1421.858 | 1476.411 | 1488.709 |
| 1490.904 | 1497.058 | 1503.09 |
| 2009.099 | 2392.801 | 3051.129 |
| 3052.827 | 3074.526 | 3122.825 |
| 3125.708 | 3135.66 | 3143.339 |
| 3154.145 | 3164.649 | 3248.086 |

***i22 – p11a***

C -0.047722 2.490482 0.787739

C -0.199351 0.777410 -0.828285

C 1.005293 0.108844 -0.446203

C 2.025745 -0.447077 -0.134019

C 3.261773 -1.123572 0.238242

C -1.446434 0.241039 -0.631559

C -2.956001 -1.398273 0.394095

C -1.723226 -0.920285 0.169449

H 0.925107 2.884149 0.518737

H -0.101771 1.854470 1.661793

H -0.916377 3.095386 0.557181

H -0.089542 1.574032 -1.555541

H 3.070364 -1.899833 0.983120

H 3.723792 -1.596694 -0.632107

H 3.980751 -0.417446 0.661371

H -2.294382 0.760518 -1.069371

H -3.833870 -0.918324 -0.028098

H -3.119015 -2.281027 1.000584

H -0.865522 -1.426640 0.605581

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -459.116 | 31.1864 | 75.7164 |
| 89.3454 | 96.8847 | 107.7155 |
| 159.1556 | 210.362 | 238.2858 |
| 331.3089 | 343.7246 | 445.2314 |
| 477.7449 | 488.4891 | 520.9179 |
| 647.619 | 663.3789 | 765.9889 |
| 808.497 | 840.6676 | 922.3735 |
| 943.0231 | 948.6316 | 1040.763 |
| 1054.799 | 1058.685 | 1120.656 |
| 1194.561 | 1252.336 | 1320.568 |
| 1393.024 | 1414.744 | 1418.869 |
| 1419.098 | 1469.533 | 1483.781 |
| 1485.35 | 1529.146 | 1649.165 |
| 2372.078 | 3046.018 | 3099.043 |
| 3117.188 | 3121.368 | 3147.94 |
| 3166.41 | 3172.785 | 3191.933 |
| 3243.904 | 3268.07 | 3275.615 |

***i25 – i24***

C -0.655416 1.762053 -0.398259

C 0.090969 0.746163 0.416683

C -3.597064 -0.993537 -0.119000

C -2.240815 -0.556824 0.191163

C -1.218008 0.132435 0.247817

C 1.252824 0.055905 -0.218476

C 2.419103 -0.145055 0.381960

C 3.597296 -0.828850 -0.240286

H -1.137390 2.596405 0.090759

H -0.545874 1.763917 -1.474251

H 0.298392 1.059502 1.440819

H -4.133947 -0.242010 -0.710811

H -4.167587 -1.174124 0.796054

H -3.584800 -1.926635 -0.688754

H 1.095879 -0.291862 -1.238518

H 2.547976 0.204715 1.405525

H 4.467482 -0.165137 -0.265178

H 3.380208 -1.145971 -1.262813

H 3.886320 -1.712540 0.337550

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -700.876 | 55.3394 | 70.7605 |
| 93.8991 | 131.3711 | 172.325 |
| 204.5231 | 222.3892 | 302.7348 |
| 357.0691 | 411.8085 | 442.7523 |
| 462.4775 | 631.1452 | 678.2832 |
| 741.46 | 844.5476 | 893.1707 |
| 962.4513 | 1005.797 | 1033.048 |
| 1056.463 | 1073.726 | 1075.431 |
| 1100.003 | 1157.017 | 1204.153 |
| 1215.957 | 1277.789 | 1338.779 |
| 1388.144 | 1413.39 | 1421.518 |
| 1444.449 | 1478.64 | 1479.544 |
| 1485.102 | 1498.477 | 1774.592 |
| 2095.793 | 3016.668 | 3035.504 |
| 3088.344 | 3095.993 | 3101.81 |
| 3113.229 | 3122.094 | 3143.788 |
| 3148.58 | 3167.433 | 3290.284 |

***i25 – i26***

C -0.962762 1.916603 -0.205328

C 0.019825 1.022477 0.497868

C -2.512248 -1.838029 0.046787

C -2.284985 -0.412378 -0.192833

C -1.560564 0.602529 -0.122400

C 1.146091 0.424759 -0.176312

C 2.138061 -0.245182 0.430167

C 3.300188 -0.869817 -0.275536

H -1.420391 2.700877 0.393704

H -0.677810 2.256745 -1.199901

H 0.009527 1.034872 1.581838

H -3.341001 -1.990209 0.743452

H -1.617631 -2.314679 0.467947

H -2.765464 -2.354858 -0.882838

H 1.166562 0.523067 -1.261955

H 2.111471 -0.347808 1.513951

H 4.249389 -0.446682 0.070886

H 3.236735 -0.719336 -1.356044

H 3.346972 -1.947760 -0.085516

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -701.11 | 54.6974 | 94.5143 |
| 121.4832 | 143.4689 | 168.4809 |
| 204.0315 | 220.5273 | 294.7982 |
| 377.387 | 438.2329 | 464.2463 |
| 472.0977 | 705.7474 | 787.2157 |
| 834.6956 | 905.7316 | 964.1279 |
| 988.679 | 1021.363 | 1036.351 |
| 1058.58 | 1061.39 | 1076.946 |
| 1124.287 | 1166.714 | 1204.992 |
| 1216.75 | 1287.194 | 1326.995 |
| 1400.986 | 1411.594 | 1422.974 |
| 1466.799 | 1477.254 | 1480.043 |
| 1484.682 | 1499.935 | 1680.433 |
| 2023.66 | 3016.697 | 3031.102 |
| 3086.175 | 3093.835 | 3099.914 |
| 3119.087 | 3121.157 | 3137.907 |
| 3151.468 | 3174.465 | 3201.897 |

***i21 – i20***

C -0.200508 2.479859 -0.122719

C 0.182483 1.181716 0.508042

C -0.578096 -0.340575 -0.185881

C -1.692570 -0.873460 -0.203070

C -3.113210 -1.093619 0.045532

C 0.813072 0.076603 -0.293727

C 2.994501 -1.121553 -0.172439

C 1.836529 -0.780276 0.375020

H -1.018522 2.962473 0.417774

H -0.525699 2.331299 -1.156544

H 0.645262 3.181293 -0.140070

H 0.269833 1.112493 1.586196

H -3.543459 -0.295343 0.662988

H -3.670889 -1.132013 -0.894178

H -3.275209 -2.043985 0.561422

H 1.109190 0.373716 -1.302029

H 3.267326 -0.797354 -1.172289

H 3.709543 -1.739863 0.357938

H 1.579408 -1.124893 1.374252

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -691.94 | 68.2826 | 72.4299 |
| 93.1778 | 113.4864 | 148.1398 |
| 169.9794 | 232.5035 | 273.5478 |
| 355.167 | 405.1755 | 420.0963 |
| 509.5641 | 633.8991 | 705.2862 |
| 803.904 | 892.3163 | 957.819 |
| 965.3427 | 1026.958 | 1032.562 |
| 1037.66 | 1056.512 | 1075.041 |
| 1123.751 | 1171.898 | 1195.485 |
| 1217.173 | 1290.153 | 1333.524 |
| 1392.315 | 1412.502 | 1422.629 |
| 1466.405 | 1478.554 | 1479.95 |
| 1484.882 | 1495.764 | 1738.823 |
| 2094.605 | 3003.027 | 3014.624 |
| 3079.021 | 3086.806 | 3089.562 |
| 3112.092 | 3117.705 | 3145.65 |
| 3163.716 | 3194.782 | 3237.916 |

***i22 – i21***

C -0.209450 2.656187 0.301885

C -0.283081 1.330579 -0.429182

C 0.783071 0.367936 -0.240835

C 1.861866 -0.260113 -0.195499

C 2.647445 -1.443077 0.155537

C -0.865223 0.142498 0.288462

C -2.282633 -1.877777 0.231774

C -1.607395 -0.896069 -0.382621

H 0.495642 3.328017 -0.192437

H 0.128460 2.508709 1.330344

H -1.192533 3.133447 0.323463

H -0.618244 1.423640 -1.463309

H 3.422584 -1.194804 0.885279

H 2.008863 -2.225936 0.584406

H 3.144832 -1.857017 -0.725671

H -0.925340 0.208937 1.370202

H -2.321038 -1.947095 1.314495

H -2.819226 -2.630462 -0.332739

H -1.591601 -0.868421 -1.471164

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -677.938 | 64.3133 | 114.7092 |
| 121.1741 | 140.812 | 183.2409 |
| 187.8126 | 225.2432 | 273.6728 |
| 389.5294 | 411.9428 | 462.9856 |
| 524.7569 | 674.8537 | 697.3104 |
| 848.8798 | 885.4552 | 891.8357 |
| 972.0638 | 1011.092 | 1022.244 |
| 1029.713 | 1057.559 | 1102.946 |
| 1108.608 | 1168.607 | 1216.348 |
| 1228.119 | 1295.331 | 1326.205 |
| 1399.461 | 1407.947 | 1423.533 |
| 1469.1 | 1476.075 | 1482.235 |
| 1488.833 | 1504.753 | 1647.155 |
| 2017.117 | 3018.006 | 3054.919 |
| 3095.505 | 3105.709 | 3120.708 |
| 3135.952 | 3140.167 | 3149.832 |
| 3159.008 | 3182.929 | 3248.809 |

***i25 – p80***

C -0.808367 1.748552 -0.348654

C 0.090721 0.806825 0.451531

C -3.187760 -1.352078 0.068501

C -2.216387 -0.464691 0.082601

C -1.298631 0.428147 0.078612

C 1.228140 0.128533 -0.206629

C 2.372731 -0.172503 0.397579

C 3.531034 -0.860652 -0.255781

H -1.198166 2.624717 0.158432

H -0.582460 1.885979 -1.401678

H 0.242289 1.073110 1.494361

H -4.725452 -0.432231 -0.997665

H -3.887345 -1.423248 0.894201

H -3.216902 -2.131596 -0.684973

H 1.083450 -0.135335 -1.253784

H 2.495200 0.091646 1.447155

H 4.431197 -0.238877 -0.215074

H 3.320808 -1.088042 -1.303437

H 3.768503 -1.798911 0.255902

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -535.825 | 55.7384 | 97.247 |
| 154.044 | 165.3685 | 202.409 |
| 211.9318 | 232.9843 | 284.4196 |
| 349.5621 | 403.0078 | 439.0292 |
| 472.3919 | 585.9455 | 654.7479 |
| 695.7424 | 825.3926 | 878.6398 |
| 901.0098 | 938.9723 | 953.3081 |
| 986.6819 | 1003.502 | 1027.891 |
| 1039.024 | 1059.94 | 1073.933 |
| 1106.938 | 1123.276 | 1198.095 |
| 1274.718 | 1337.326 | 1344.174 |
| 1401.678 | 1423.34 | 1461.261 |
| 1484.478 | 1498.556 | 1531.624 |
| 1770.056 | 2103.357 | 3034.501 |
| 3094.662 | 3120.71 | 3124.874 |
| 3140.908 | 3145.46 | 3146.852 |
| 3153.094 | 3216.857 | 3232.961 |

***i21 – p57***

C -0.259929 2.514033 -0.166706

C 0.054582 1.181932 0.470783

C -0.616286 -0.043791 0.004421

C -1.669517 -0.766663 -0.082053

C -2.778825 -1.471484 -0.146266

C 0.831436 0.118899 -0.308450

C 2.932774 -1.197033 -0.184529

C 1.822314 -0.736147 0.378184

H -1.145826 2.960981 0.290690

H -0.458354 2.394394 -1.234622

H 0.577289 3.206745 -0.046041

H 0.270151 1.213856 1.536844

H -3.432369 -1.401427 -1.008879

H -2.984321 -2.250491 0.579756

H -4.192449 -0.316682 0.868964

H 1.063123 0.371750 -1.340890

H 3.182953 -0.969063 -1.216193

H 3.627708 -1.819530 0.366550

H 1.592800 -0.989016 1.411520

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -532.061 | 70.063 | 101.6295 |
| 135.9221 | 186.5264 | 203.7211 |
| 216.9787 | 233.923 | 291.0935 |
| 337.4394 | 396.2953 | 424.8611 |
| 487.6786 | 586.9315 | 637.5285 |
| 687.5167 | 757.81 | 849.3569 |
| 885.3485 | 900.4299 | 948.8351 |
| 1004.596 | 1019.351 | 1029.159 |
| 1043.608 | 1047.332 | 1101.115 |
| 1127.104 | 1148.173 | 1205.904 |
| 1291.643 | 1314.728 | 1337.877 |
| 1412.539 | 1423.162 | 1463.994 |
| 1493.085 | 1501.4 | 1536.081 |
| 1733.729 | 2100.148 | 3045.364 |
| 3122.007 | 3124.159 | 3137.283 |
| 3143.254 | 3147.543 | 3148.037 |
| 3159.408 | 3233.744 | 3241.38 |

***i63 – i64***

C 1.105246 1.417276 0.365270

C 1.891791 0.355215 -0.344373

C 1.139572 -0.942932 -0.536873

C -0.387725 -0.974061 -0.353402

C -0.255257 -1.815086 0.924977

C -2.350504 0.551055 -0.408930

C -1.057934 0.358302 -0.137388

C -0.227011 1.425437 0.430407

H 1.665157 2.247749 0.784844

H 2.180427 0.758028 -1.327385

H 2.837400 0.172869 0.177065

H 1.517522 -1.594618 -1.323135

H -0.893501 -1.517890 -1.152580

H -0.424303 -1.292607 1.864302

H 1.103516 -1.711535 0.605071

H -0.601113 -2.845999 0.891634

H -2.832530 1.502529 -0.209984

H -2.962275 -0.234921 -0.838979

H -0.739373 2.265158 0.891009

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2133.45 | 72.7119 | 89.8653 |
| 230.0865 | 347.3123 | 359.4505 |
| 383.3599 | 486.4488 | 514.5417 |
| 615.3928 | 630.2951 | 712.4955 |
| 744.4671 | 760.1385 | 823.8544 |
| 873.2638 | 895.8865 | 924.7138 |
| 939.6483 | 957.258 | 984.1451 |
| 993.3272 | 1023.289 | 1051.707 |
| 1072.265 | 1126.85 | 1193.341 |
| 1222.346 | 1247.587 | 1305.307 |
| 1322.826 | 1345.659 | 1365.214 |
| 1374.104 | 1423.073 | 1426.966 |
| 1468.096 | 1474.564 | 1697.935 |
| 1747.844 | 1832.969 | 2997.278 |
| 3066.295 | 3097.106 | 3106.511 |
| 3145.049 | 3153.082 | 3170.068 |
| 3194.572 | 3217.584 | 3241.159 |

***i44 – i42***

C 2.546173 -1.093085 0.131794

C 1.286540 -0.331332 -0.099767

C -0.008563 -1.004834 -0.049101

C -1.174022 -0.345796 -0.007476

C -1.228092 1.160885 -0.009704

C 0.121986 1.814321 0.040808

C 1.266025 1.123504 -0.000261

C -2.496654 -1.049374 0.044635

H 2.504151 -2.166560 0.247800

H 3.469750 -0.557042 0.297229

H 1.960018 -0.704650 -1.075227

H -0.008514 -2.092182 -0.041695

H -1.844032 1.504154 0.835480

H -1.776064 1.500878 -0.903385

H 0.149572 2.896678 0.115388

H 2.218290 1.644069 0.043768

H -2.379895 -2.134769 0.028193

H -3.047930 -0.777152 0.952197

H -3.125705 -0.759155 -0.805317

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1901.63 | 94.6846 | 157.5561 |
| 208.965 | 272.435 | 325.7562 |
| 389.7556 | 394.3652 | 445.6912 |
| 480.5318 | 515.5395 | 535.3167 |
| 599.9757 | 695.331 | 760.0535 |
| 864.4184 | 874.7863 | 924.9794 |
| 954.0732 | 963.7108 | 991.5061 |
| 1001.541 | 1037.806 | 1068.51 |
| 1147.336 | 1164.272 | 1202.68 |
| 1230.428 | 1266.938 | 1331.045 |
| 1353.33 | 1418.105 | 1426.802 |
| 1432.429 | 1449.497 | 1473.732 |
| 1481.767 | 1498.085 | 1676.316 |
| 1747.826 | 2214.912 | 2975.978 |
| 2995.256 | 3022.161 | 3076.085 |
| 3126.365 | 3160.201 | 3167.561 |
| 3175.074 | 3191.316 | 3299.586 |

***i61 – p89***

C 1.917690 -0.789016 -0.029208

C 1.971248 0.589043 -0.086818

C 0.778131 1.330545 -0.039689

C -0.471931 0.681226 -0.059672

C -1.735262 1.495017 -0.068191

C -1.833217 -1.441287 0.030123

C -0.514027 -0.715272 0.003073

C 0.682919 -1.431336 0.028750

H 2.831206 -1.372742 -0.036919

H 2.922493 1.105512 -0.136376

H 0.812999 2.399097 -0.225889

H 0.769378 1.838126 1.735994

H -2.267151 1.396376 0.884630

H -2.421125 1.168295 -0.855173

H -1.522113 2.554102 -0.221106

H -2.461444 -1.097822 0.857542

H -1.687144 -2.516810 0.141532

H -2.397019 -1.272653 -0.893052

H 0.646616 -2.515006 0.078625

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -875.241 | 133.9551 | 170.2394 |
| 176.7251 | 249.2751 | 306.1203 |
| 319.4907 | 391.037 | 428.3219 |
| 507.6452 | 518.9267 | 528.3246 |
| 591.8561 | 731.2204 | 757.0609 |
| 777.0609 | 840.7193 | 903.6292 |
| 986.8827 | 1011.346 | 1016.806 |
| 1024.164 | 1058.725 | 1076.477 |
| 1080.768 | 1146.164 | 1190.155 |
| 1212.88 | 1248.932 | 1311.154 |
| 1326.048 | 1420.027 | 1429.409 |
| 1467.88 | 1486.642 | 1503.329 |
| 1503.946 | 1506.322 | 1535.776 |
| 1639.095 | 1652.832 | 3042.019 |
| 3045.498 | 3102.054 | 3106.267 |
| 3137.915 | 3140.503 | 3183.328 |
| 3187.79 | 3201.423 | 3219.364 |

***i61 – p91***

C -1.873760 -0.881211 -0.073711

C -2.049256 0.439722 -0.031669

C -0.886577 1.363687 0.176087

C 0.471710 0.748018 -0.093559

C 1.525828 1.526303 -0.378554

C 1.943440 -1.348625 0.054840

C 0.582273 -0.716180 0.020645

C -0.539572 -1.460776 0.033637

H -2.720002 -1.550406 -0.183716

H -3.040430 0.876090 -0.094163

H -0.907119 1.687593 1.228708

H -1.007185 2.277589 -0.412271

H 2.519858 1.123444 -0.526168

H 2.257006 2.035289 1.971542

H 1.410168 2.597643 -0.502210

H 2.477142 -1.183372 -0.886851

H 1.866538 -2.425431 0.212847

H 2.556620 -0.922180 0.854747

H -0.457110 -2.541899 0.091234

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -291.42 | 60.6646 | 98.5363 |
| 136.5172 | 178.9797 | 255.6071 |
| 320.6706 | 346.4931 | 422.0123 |
| 477.1714 | 497.1547 | 526.3931 |
| 599.5422 | 707.1316 | 721.8685 |
| 775.8809 | 833.0751 | 897.6493 |
| 918.1677 | 939.3839 | 957.4924 |
| 988.3545 | 1004.672 | 1023.237 |
| 1072.418 | 1090.937 | 1170.212 |
| 1195.856 | 1224.383 | 1302.999 |
| 1345.457 | 1401.655 | 1422 |
| 1439.192 | 1445.457 | 1454.569 |
| 1492.274 | 1510.261 | 1670.974 |
| 1678.899 | 1740.919 | 2991.085 |
| 3044.205 | 3090.434 | 3104.668 |
| 3140.747 | 3163.197 | 3179.58 |
| 3189.79 | 3212.92 | 3251.578 |

***i58 – i61***

C 1.847176 -0.899921 0.100222

C 2.033868 0.426820 0.052119

C 0.886233 1.353093 -0.226163

C -0.458655 0.729789 0.075447

C -1.618187 1.651856 0.071000

C -1.968273 -1.306747 -0.069958

C -0.593666 -0.706686 -0.031256

C 0.529215 -1.480758 -0.029440

H 2.692411 -1.563830 0.249207

H 3.025743 0.855020 0.147974

H 0.895164 1.643038 -1.292932

H 0.997875 2.293052 0.326007

H -2.630982 1.276332 0.065748

H -1.435976 2.715056 0.003433

H -0.925776 1.113508 1.161915

H -2.539858 -1.054037 0.831309

H -1.918772 -2.394178 -0.141089

H -2.538607 -0.928653 -0.925705

H 0.432514 -2.559980 -0.077686

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1886 | 110.2806 | 182.7969 |
| 229.0476 | 307.3228 | 312.1633 |
| 391.4825 | 422.5516 | 477.5337 |
| 499.7301 | 535.9729 | 558.5266 |
| 626.1857 | 715.2539 | 724.9999 |
| 807.2525 | 831.9661 | 925.8088 |
| 953.9181 | 986.7969 | 994.4701 |
| 1006.88 | 1056.427 | 1083.248 |
| 1163.806 | 1170.543 | 1195.641 |
| 1235.455 | 1258.851 | 1304.709 |
| 1364.547 | 1415.275 | 1427.657 |
| 1439.626 | 1456.351 | 1481.05 |
| 1485.505 | 1503.106 | 1580.299 |
| 1697.482 | 2219.586 | 2932.001 |
| 3026.924 | 3056.321 | 3082.433 |
| 3138.074 | 3180.661 | 3186.539 |
| 3192.01 | 3208.552 | 3306.054 |

***i65 – p94***

C 1.892781 0.500765 0.232669

C 1.804002 -0.736786 -0.239263

C 0.501192 -1.427180 -0.535388

C -0.703260 -0.654870 -0.052156

C -1.805038 -1.267017 0.402457

C -1.521216 1.603045 -0.593810

C -0.577876 0.819799 -0.074370

C 0.698900 1.369785 0.519125

H 2.869724 0.929581 0.435334

H 2.710027 -1.303993 -0.431454

H 0.501186 -2.428451 -0.093194

H 0.416621 -1.574175 -1.621360

H -1.900111 -2.347608 0.376767

H -2.665079 -0.697855 0.736051

H -1.288242 -1.533316 2.525502

H -1.413352 2.682929 -0.605378

H -2.419856 1.185313 -1.033737

H 0.875087 2.383875 0.148236

H 0.577086 1.458453 1.607644

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -436.69 | 90.6785 | 100.0636 |
| 164.2462 | 204.4834 | 303.2061 |
| 327.3354 | 387.1232 | 429.5378 |
| 477.8041 | 556.745 | 614.8632 |
| 665.9761 | 725.0617 | 735.2061 |
| 807.8369 | 845.2916 | 924.7283 |
| 937.3654 | 943.2813 | 947.2653 |
| 977.2686 | 982.2623 | 996.6657 |
| 1026.528 | 1038.503 | 1198.065 |
| 1204.553 | 1228.791 | 1249.13 |
| 1335.063 | 1350.204 | 1360.593 |
| 1420.481 | 1444.889 | 1460.116 |
| 1472.406 | 1476.791 | 1678.954 |
| 1727.71 | 1760.528 | 3018.246 |
| 3019.307 | 3082.571 | 3086.141 |
| 3153.245 | 3154.456 | 3169.248 |
| 3193.037 | 3243.862 | 3247.162 |

***i65 – p91***

C 2.031177 0.333674 -0.107281

C 1.739692 -0.958497 -0.249295

C 0.367446 -1.434640 -0.083736

C -0.690374 -0.586521 -0.007993

C -2.097601 -1.103666 0.019465

C -1.425904 1.754219 -0.182394

C -0.446616 0.861614 0.008527

C 0.971301 1.317256 0.291129

H 3.048131 0.694054 -0.219181

H 2.509934 -1.682941 -0.488007

H 0.423514 -1.956228 2.001867

H 0.182727 -2.499113 -0.183682

H -2.641601 -0.811740 -0.884788

H -2.647086 -0.699224 0.874950

H -2.110348 -2.192583 0.085124

H -1.215606 2.818253 -0.202979

H -2.458849 1.459663 -0.321595

H 1.149755 2.292600 -0.169171

H 1.064700 1.476621 1.376936

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -528.051 | 84.9352 | 162.0033 |
| 192.1585 | 236.0055 | 258.4387 |
| 345.5232 | 348.4012 | 426.9111 |
| 489.78 | 499.3102 | 521.4254 |
| 602.5372 | 703.8086 | 724.4145 |
| 758.3789 | 832.0498 | 911.0075 |
| 919.275 | 943.8715 | 964.9204 |
| 984.2217 | 1006.984 | 1022.335 |
| 1062.773 | 1085.81 | 1173.268 |
| 1197.271 | 1232.449 | 1305.061 |
| 1351.897 | 1399.335 | 1417.883 |
| 1433.531 | 1455.782 | 1466.582 |
| 1482.793 | 1501.13 | 1622.318 |
| 1685.459 | 1729.115 | 2994.564 |
| 3043.084 | 3089.166 | 3104.362 |
| 3141.877 | 3166.463 | 3188.375 |
| 3195.608 | 3216.827 | 3255.892 |

***i66 – p93***

C 1.820496 0.776256 0.169077

C 1.872784 -0.724419 0.108102

C 0.611266 -1.303373 -0.544660

C -0.627734 -0.665112 0.025763

C -1.625185 -1.377404 0.563195

C -1.753828 1.532884 -0.193439

C -0.635592 0.816693 -0.031210

C 0.679785 1.463229 0.086112

H 2.759629 1.308369 0.286791

H 2.760013 -1.043972 -0.446908

H 1.985941 -1.126016 1.123475

H 0.573784 -2.388141 -0.423596

H 0.649692 -1.090610 -1.620139

H -2.472234 -0.899222 1.041262

H -1.575339 -2.459966 0.608567

H -2.985657 -1.636802 -1.244209

H -1.722780 2.617113 -0.213039

H -2.718438 1.058048 -0.328922

H 0.693443 2.548668 0.119076

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -373.146 | 99.9384 | 150.5166 |
| 159.427 | 215.915 | 294.2311 |
| 346.1682 | 379.7846 | 432.1884 |
| 480.0022 | 560.5635 | 636.774 |
| 698.9195 | 735.0875 | 772.9096 |
| 787.7895 | 822.6353 | 880.9626 |
| 899.1813 | 937.9104 | 945.0298 |
| 974.8504 | 989.8999 | 1008.289 |
| 1049.056 | 1056.974 | 1185.013 |
| 1196.473 | 1233.791 | 1270.897 |
| 1339.628 | 1350.537 | 1368.669 |
| 1419.096 | 1450.17 | 1466.993 |
| 1484.306 | 1498.317 | 1681.539 |
| 1696.289 | 1744.362 | 3032.341 |
| 3042.631 | 3083.983 | 3114.119 |
| 3157.148 | 3158.935 | 3175.232 |
| 3197.947 | 3247.589 | 3249.468 |

***i66 – p90***

C -1.921327 -0.658696 0.000514

C -1.864959 0.829733 -0.129005

C -0.470355 1.374403 -0.056825

C 0.643528 0.612860 -0.058235

C 2.005492 1.241916 -0.053270

C 1.600710 -1.666382 0.000752

C 0.531581 -0.855205 -0.004326

C -0.825756 -1.413051 0.053246

H -2.902453 -1.121094 0.041638

H -2.316852 1.131559 -1.085194

H -2.489804 1.298297 0.640464

H -0.384541 1.767781 2.031769

H -0.366782 2.452395 -0.141694

H 2.593241 0.915964 -0.916965

H 2.561128 0.958648 0.846352

H 1.931252 2.329931 -0.080285

H 1.476383 -2.742714 0.045189

H 2.615887 -1.292396 -0.039684

H -0.910953 -2.491842 0.141312

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -483.179 | 87.1012 | 179.4866 |
| 195.1063 | 249.3655 | 326.4438 |
| 341.9851 | 353.5698 | 417.3765 |
| 438.7442 | 489.9442 | 569.9656 |
| 609.6856 | 718.232 | 724.946 |
| 796.5573 | 834.3837 | 878.1226 |
| 908.354 | 917.6054 | 966.1606 |
| 975.3632 | 1009.992 | 1017.689 |
| 1063.438 | 1087.18 | 1178.762 |
| 1204.083 | 1217.75 | 1306.983 |
| 1382.643 | 1394.863 | 1415.621 |
| 1445.499 | 1463.405 | 1466.293 |
| 1479.777 | 1502.186 | 1666.751 |
| 1676.401 | 1757.76 | 3014.663 |
| 3041.92 | 3056.717 | 3103.471 |
| 3141.651 | 3168.033 | 3174.956 |
| 3176.043 | 3200.127 | 3257.754 |

***i62 – p94***

C -1.722525 -0.842877 0.250617

C -1.889937 0.385427 -0.224721

C -0.749912 1.297778 -0.594717

C 0.558963 0.809805 -0.000675

C 1.260474 1.547309 0.887718

C 1.866724 -1.228869 -0.579142

C 0.768521 -0.666193 -0.088284

C -0.377188 -1.474532 0.482228

H -2.591878 -1.444080 0.500628

H -2.893199 0.772979 -0.375654

H -0.673990 1.345846 -1.686928

H -0.953539 2.316797 -0.253085

H 1.607028 1.331213 -1.491145

H 1.028365 2.593622 1.056355

H 2.114821 1.126572 1.405063

H 1.983845 -2.307745 -0.600082

H 2.674016 -0.627107 -0.981168

H -0.360902 -2.485381 0.063215

H -0.225281 -1.589809 1.564666

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -916.499 | 90.731 | 107.606 |
| 265.1762 | 331.1706 | 386.392 |
| 432.0202 | 466.0749 | 498.4603 |
| 538.6567 | 572.0273 | 626.6255 |
| 655.3217 | 697.9304 | 724.3357 |
| 763.5581 | 847.6608 | 919.5345 |
| 924.253 | 936.8285 | 947.0019 |
| 971.9985 | 979.4963 | 993.4957 |
| 1026.028 | 1036.757 | 1189.386 |
| 1197.138 | 1229.291 | 1246.748 |
| 1324.691 | 1345.073 | 1352.577 |
| 1413.509 | 1439.958 | 1456.617 |
| 1471.99 | 1479.226 | 1633.741 |
| 1740.875 | 1757.86 | 3018.23 |
| 3046.231 | 3085.087 | 3093.946 |
| 3154.006 | 3154.663 | 3163.97 |
| 3188.74 | 3245.954 | 3254.186 |

***i24 – p83***

C 0.181566 2.060936 -0.190338

C -0.003767 0.724683 0.001591

C -3.768356 -0.899359 0.010880

C -2.434538 -0.313006 0.016281

C -1.337446 0.177190 0.030272

C 1.096235 -0.253226 -0.235554

C 2.332524 -0.133406 0.236192

C 3.449268 -1.087182 -0.048972

H -0.645199 2.755052 -0.108254

H 1.172874 2.455246 -0.376497

H 0.113491 0.702890 1.845822

H -4.463204 -0.280613 -0.562091

H -4.155431 -0.993798 1.028658

H -3.750245 -1.895276 -0.438312

H 0.826588 -1.111262 -0.847174

H 2.560540 0.704307 0.893522

H 4.287918 -0.572872 -0.529452

H 3.125438 -1.897763 -0.705421

H 3.834320 -1.525696 0.877091

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1084.65 | 53.0968 | 81.0607 |
| 84.5229 | 146.3999 | 179.561 |
| 209.0603 | 222.9421 | 306.3341 |
| 362.1149 | 395.7056 | 431.1275 |
| 472.5286 | 494.5317 | 585.7814 |
| 589.9186 | 675.227 | 766.4909 |
| 828.8732 | 893.5948 | 921.0573 |
| 987.5423 | 1005.162 | 1053.218 |
| 1058.238 | 1074.595 | 1078.55 |
| 1133.717 | 1271.127 | 1333.33 |
| 1352.095 | 1413.528 | 1421.576 |
| 1424.814 | 1483.899 | 1485.194 |
| 1488.151 | 1499.739 | 1577.324 |
| 1757.073 | 2384.779 | 3038.869 |
| 3053.244 | 3097.672 | 3124.949 |
| 3128.681 | 3129.34 | 3155.143 |
| 3160.557 | 3170.36 | 3274.144 |

***i24 – i53***

C 0.108783 2.535780 0.156220

C -0.055385 1.073489 -0.112935

C 3.251369 -1.327183 0.038149

C 2.071993 -0.472106 -0.010022

C 1.098838 0.236307 -0.049441

C -1.394403 0.478710 -0.060134

C -1.664931 -0.827451 0.004364

C -3.045344 -1.403394 0.052308

H 1.101101 2.936021 0.297448

H -0.770765 3.133896 0.348195

H 0.024098 1.871543 -1.062199

H 3.957641 -0.978455 0.795847

H 3.766567 -1.341193 -0.926119

H 2.972695 -2.354814 0.284839

H -2.217956 1.191204 -0.080779

H -0.835574 -1.530784 0.032787

H -3.210371 -2.101342 -0.775454

H -3.809022 -0.623703 -0.003360

H -3.203940 -1.967281 0.977743

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1886.36 | 70.021 | 81.1181 |
| 110.6754 | 137.5683 | 192.8035 |
| 195.2386 | 212.4672 | 304.1911 |
| 346.4242 | 378.1488 | 421.9614 |
| 446.9638 | 542.1935 | 616.3591 |
| 642.6813 | 674.6049 | 831.0033 |
| 916.1869 | 988.4166 | 996.7801 |
| 1038.999 | 1053.556 | 1062.974 |
| 1066.439 | 1131.443 | 1174.392 |
| 1240.461 | 1335.623 | 1350.473 |
| 1370.804 | 1418.358 | 1422.03 |
| 1425.426 | 1483.855 | 1484.265 |
| 1490.234 | 1500.264 | 1725.25 |
| 2226.032 | 2356.426 | 3035.697 |
| 3047.59 | 3093.102 | 3118.526 |
| 3120.554 | 3121.532 | 3152.591 |
| 3172.206 | 3181.332 | 3312.782 |

***i24 – p76'***

C -0.077131 2.175335 0.424417

C 0.370937 1.269573 -0.484235

C 3.504421 -1.258418 0.255916

C 2.385999 -0.361381 -0.006152

C 1.463748 0.382118 -0.211999

C -1.224097 -0.384813 -0.539528

C -2.336457 -0.192692 0.124416

C -3.477618 -1.172740 0.216598

H -0.817794 2.914824 0.145308

H 0.251697 2.144130 1.455941

H 0.122856 1.409867 -1.531910

H 4.308243 -0.736180 0.780960

H 3.911321 -1.655540 -0.677344

H 3.188971 -2.102760 0.874379

H -0.831952 -1.203890 -1.129778

H -2.459457 0.747183 0.665119

H -3.662682 -1.447350 1.259706

H -3.270779 -2.084100 -0.347583

H -4.399244 -0.728079 -0.171394

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -404.233 | 31.308 | 40.2178 |
| 72.2661 | 119.1558 | 137.7181 |
| 148.1111 | 193.8192 | 211.5912 |
| 279.1884 | 337.5515 | 416.0307 |
| 421.852 | 545.2494 | 611.6168 |
| 685.5833 | 724.83 | 854.5564 |
| 882.5898 | 917.1181 | 932.2989 |
| 975.5019 | 1043.045 | 1055.941 |
| 1058.969 | 1063.926 | 1117.111 |
| 1189.708 | 1283.235 | 1291.006 |
| 1406.578 | 1417.829 | 1434.018 |
| 1484.576 | 1485.715 | 1486.736 |
| 1490.239 | 1571.688 | 1707.96 |
| 2381.503 | 3037.545 | 3045.601 |
| 3102.395 | 3110.702 | 3117.382 |
| 3119.918 | 3134.812 | 3160.409 |
| 3171.786 | 3222.06 | 3262.388 |

***i24 – i49***

C 0.454582 1.729359 -0.444016

C -0.049105 0.681364 0.481647

C -3.851959 -0.747509 -0.157085

C -2.504306 -0.239572 0.072266

C -1.395616 0.178265 0.266533

C 1.071501 -0.091846 -0.146829

C 2.297788 -0.292929 0.434270

C 3.436201 -0.982733 -0.244574

H 1.175759 2.451709 -0.090878

H 0.017176 1.840035 -1.426324

H 0.139260 0.901209 1.533229

H -4.591381 0.051466 -0.061682

H -4.101143 -1.528960 0.565010

H -3.940915 -1.173080 -1.159700

H 0.831459 -0.581054 -1.085369

H 2.481777 0.126263 1.421192

H 3.126467 -1.415907 -1.198938

H 3.843868 -1.787985 0.375967

H 4.263162 -0.290091 -0.445779

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -620.909 | 30.9774 | 72.6258 |
| 101.4861 | 140.3848 | 171.4596 |
| 225.8155 | 258.2777 | 323.3951 |
| 332.345 | 424.5795 | 504.6534 |
| 550.9474 | 581.65 | 645.3572 |
| 722.0038 | 750.7462 | 920.9125 |
| 942.6903 | 989.3868 | 1034.423 |
| 1057.848 | 1058.625 | 1066.138 |
| 1095.824 | 1162.239 | 1186.738 |
| 1216.196 | 1284.795 | 1303.112 |
| 1389.546 | 1418.624 | 1420.269 |
| 1450.142 | 1480.214 | 1485.589 |
| 1486.116 | 1490.789 | 1553.467 |
| 2397.461 | 3015.954 | 3047.522 |
| 3070.855 | 3103.934 | 3115.05 |
| 3120.359 | 3121.045 | 3152.855 |
| 3174.93 | 3186.562 | 3300.346 |

***i26 – i51***

C -0.783481 1.662131 -0.038894

C 0.692984 1.438284 -0.000726

C -3.455483 -1.410085 -0.000207

C -2.500232 -0.310088 -0.014892

C -1.714987 0.608874 -0.037277

C 1.307708 0.143699 0.036043

C 2.635183 -0.078287 -0.036083

C 3.269091 -1.432773 -0.005395

H -0.032823 1.716701 1.040871

H -1.113860 2.666718 -0.270969

H 1.300103 2.313283 -0.204725

H -4.368186 -1.129627 0.532276

H -3.029376 -2.283056 0.501289

H -3.733082 -1.708788 -1.015206

H 0.635195 -0.708141 0.125062

H 3.306305 0.773986 -0.130909

H 3.840998 -1.626516 -0.919748

H 2.518586 -2.220584 0.095811

H 3.971446 -1.524496 0.830832

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1899.29 | 14.8655 | 60.0113 |
| 101.3931 | 140.9841 | 175.3859 |
| 194.1904 | 214.2174 | 280.4855 |
| 325.6377 | 417.1796 | 432.6248 |
| 463.8449 | 630.4405 | 632.8219 |
| 767.8351 | 793.9642 | 865.7521 |
| 951.1495 | 984.5627 | 1005.223 |
| 1050.039 | 1055.662 | 1056.231 |
| 1122.146 | 1180.153 | 1216.658 |
| 1254.033 | 1296.826 | 1322.923 |
| 1394.114 | 1413.103 | 1422.915 |
| 1433.796 | 1480.983 | 1482.163 |
| 1486.468 | 1500.26 | 1664.446 |
| 2158.358 | 2309.706 | 3024.263 |
| 3038.943 | 3078.035 | 3106.561 |
| 3115.037 | 3115.48 | 3144.307 |
| 3152.364 | 3190.56 | 3207.861 |

***i20 – p56***

C 1.935434 2.014396 -0.182456

C 1.082238 1.182570 0.421308

C -0.983820 0.007076 -0.168418

C -2.180786 0.043883 -0.083038

C -3.635449 0.087354 0.008517

C 0.482596 -0.037417 -0.241360

C 1.813571 -2.164504 -0.181543

C 1.013229 -1.295602 0.417093

H 2.324025 2.888177 0.327114

H 2.169683 1.914170 -1.237600

H 3.800473 1.105091 0.130635

H 0.813360 1.334488 1.463629

H -3.961462 0.927077 0.627116

H -4.082628 0.202591 -0.981836

H -4.025035 -0.832525 0.451355

H 0.783981 -0.044323 -1.294664

H 2.130866 -2.028715 -1.211113

H 2.180947 -3.042849 0.336573

H 0.703704 -1.449719 1.448177

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -555.122 | 19.5252 | 58.089 |
| 64.1833 | 107.2126 | 120.6593 |
| 194.2709 | 274.502 | 284.0213 |
| 288.1595 | 348.1583 | 399.7415 |
| 437.6573 | 501.0328 | 508.4644 |
| 672.2954 | 711.9374 | 839.7523 |
| 924.2463 | 962.8754 | 972.5236 |
| 978.812 | 1021.32 | 1036.452 |
| 1058.38 | 1058.91 | 1121.175 |
| 1162.424 | 1186.241 | 1278.067 |
| 1309.436 | 1314.088 | 1332.13 |
| 1419.933 | 1451.064 | 1454.851 |
| 1485.569 | 1485.78 | 1673.447 |
| 1735.53 | 2391.629 | 3048.598 |
| 3058.28 | 3121.905 | 3122.471 |
| 3146.42 | 3149.53 | 3166.463 |
| 3171.24 | 3238.959 | 3244.197 |

***i20 – p52***

C -0.455767 2.487324 -0.009515

C -1.175632 1.195097 -0.172558

C 0.807246 -0.219565 0.020326

C 1.995392 -0.401782 0.015162

C 3.436226 -0.618965 0.026843

C -0.622684 -0.043765 -0.011503

C -2.632033 -1.518510 0.178927

C -1.419763 -1.270504 -0.299876

H -0.694313 3.172582 -0.828228

H 0.625121 2.345329 0.030536

H -0.769881 2.979268 0.919659

H -2.244234 1.234981 -0.361925

H 3.907542 -0.168903 -0.850472

H 3.886241 -0.176543 0.919167

H 3.665819 -1.687158 0.026105

H -0.750758 -0.113824 1.842644

H -3.110123 -0.845402 0.883783

H -3.176163 -2.410877 -0.107066

H -0.937157 -1.985436 -0.961044

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1018.14 | 39.8905 | 75.8256 |
| 93.1071 | 104.1372 | 152.7733 |
| 186.1962 | 224.6894 | 287.8987 |
| 357.8082 | 387.8319 | 449.3025 |
| 485.1192 | 491.9889 | 566.6703 |
| 598.3199 | 702.3454 | 718.3526 |
| 827.8035 | 932.9502 | 960.1001 |
| 1014.472 | 1025.086 | 1049.788 |
| 1056.042 | 1058.19 | 1104.576 |
| 1142.632 | 1235.327 | 1320.311 |
| 1371.041 | 1413.404 | 1420.131 |
| 1450.227 | 1478.124 | 1483.864 |
| 1484.667 | 1485.668 | 1607.125 |
| 1723.441 | 2379.393 | 3025.837 |
| 3047.121 | 3088.988 | 3119.115 |
| 3123.169 | 3140.89 | 3150.11 |
| 3171.203 | 3182.479 | 3244.258 |

***i20 – p55***

C 2.439122 1.607038 0.055804

C 0.998410 1.316237 0.307477

C -1.142466 0.266389 -0.246145

C -2.323279 0.102240 -0.088549

C -3.756239 -0.088129 0.099176

C 0.264053 0.450851 -0.445164

C 2.111760 -2.055958 -0.104901

C 0.955345 -1.600704 0.309040

H 2.642102 2.681537 0.098320

H 2.758742 1.234274 -0.920449

H 3.067667 1.130662 0.818203

H 0.542824 1.746434 1.194677

H -4.009676 -0.110790 1.162048

H -4.322212 0.723296 -0.365803

H -4.085149 -1.029659 -0.347705

H 0.658093 0.121917 -1.403490

H 2.710923 -1.517069 -0.836616

H 2.527067 -2.996864 0.258893

H 0.229383 -1.971525 1.021501

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -439.308 | 26.7367 | 36.3346 |
| 76.9504 | 100.4483 | 108.65 |
| 146.4725 | 190.3021 | 227.802 |
| 266.1204 | 288.3003 | 346.3028 |
| 389.8076 | 480.67 | 516.8319 |
| 743.1554 | 797.5262 | 818.1608 |
| 909.0538 | 930.9505 | 941.0516 |
| 962.2251 | 1042.846 | 1055.645 |
| 1058.178 | 1091.075 | 1133.27 |
| 1198.669 | 1293.588 | 1315.076 |
| 1397.293 | 1414.673 | 1419.554 |
| 1479.936 | 1484.327 | 1485.796 |
| 1488.306 | 1601.57 | 1666.725 |
| 2379.793 | 3024.1 | 3045.714 |
| 3085.284 | 3086.66 | 3117.238 |
| 3119.734 | 3120.073 | 3155.674 |
| 3166.164 | 3178.282 | 3227.48 |

***i28 – p62***

C -0.441044 -0.257617 -0.204714

C 0.379502 0.783637 0.013676

C 1.833520 0.745159 -0.053836

C 2.606398 -0.348580 0.088186

C 4.091454 -0.360758 -0.113933

C -4.509091 -0.093942 0.083502

C -3.057030 -0.147932 -0.018774

C -1.856296 -0.183987 -0.100153

H -0.029439 -1.221731 -0.492820

H -0.068774 1.745182 0.247537

H 2.327868 1.704431 -0.192054

H 2.130904 -1.316139 0.234265

H 2.609661 -0.376877 2.232959

H 4.497182 0.652616 -0.149394

H 4.338129 -0.857960 -1.058468

H 4.599500 -0.909420 0.682465

H -4.817266 0.213487 1.086202

H -4.950103 -1.072069 -0.123089

H -4.922144 0.622601 -0.631322

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -554.66 | 17.6207 | 57.9122 |
| 74.8069 | 97.4317 | 173.9806 |
| 180.2781 | 215.9292 | 297.9989 |
| 310.5401 | 323.8618 | 350.9459 |
| 367.7778 | 483.4311 | 500.1522 |
| 628.2023 | 804.5761 | 857.0527 |
| 889.074 | 925.5661 | 994.0412 |
| 1006.323 | 1053.522 | 1057.991 |
| 1063.268 | 1076.485 | 1133.352 |
| 1217.839 | 1306.911 | 1318.576 |
| 1341.235 | 1359.447 | 1418.795 |
| 1420.311 | 1483.284 | 1483.841 |
| 1484.635 | 1497.179 | 1655.945 |
| 1702.033 | 2368.379 | 3037.944 |
| 3045.257 | 3103.936 | 3116.396 |
| 3121.267 | 3130.583 | 3151.205 |
| 3160.265 | 3164.122 | 3179.194 |

***i28 – p10b***

C 0.235239 -0.038070 0.238013

C -0.486213 -1.019450 -0.339857

C -1.924190 -1.173406 -0.244253

C -2.728682 -0.543419 0.641097

C -3.165812 1.694365 -0.349503

C 4.289759 0.322463 -0.051700

C 2.842531 0.190427 0.049432

C 1.646331 0.073376 0.128827

H -0.265170 0.731995 0.819797

H 0.042917 -1.746065 -0.949860

H -2.381516 -1.830825 -0.978395

H -2.325689 0.008312 1.482381

H -3.792047 -0.745517 0.661735

H -3.813282 1.384211 -1.158635

H -2.132388 1.914722 -0.582777

H -3.615552 2.173858 0.511079

H 4.605050 0.354306 -1.097945

H 4.792311 -0.522494 0.426502

H 4.631591 1.239781 0.433786

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -316.226 | 34.4931 | 53.9666 |
| 68.648 | 90.4149 | 106.9324 |
| 135.5282 | 230.8644 | 244.6229 |
| 302.6584 | 321.5832 | 410.326 |
| 433.2614 | 466.7155 | 507.691 |
| 564.642 | 690.1544 | 709.9888 |
| 835.5559 | 878.9647 | 904.5886 |
| 984.1552 | 990.3963 | 1016.852 |
| 1053.542 | 1058.006 | 1081.604 |
| 1219.149 | 1300.722 | 1322.495 |
| 1341.515 | 1411.28 | 1418.382 |
| 1419.263 | 1448.865 | 1483.303 |
| 1484.179 | 1581.41 | 1672.928 |
| 2361.117 | 3044.708 | 3105.446 |
| 3115.239 | 3120.883 | 3161.813 |
| 3162.307 | 3169.172 | 3183.231 |
| 3256.091 | 3278.204 | 3284.263 |

***i28 – p75***

C 0.541509 0.975612 0.543677

C -0.548498 0.744877 -0.175577

C -1.662703 0.299312 -0.684659

C -2.451929 -0.838309 -0.083251

C -3.851941 -0.398924 0.349805

C 4.177655 -0.741876 -0.151724

C 2.878223 -0.131020 0.092614

C 1.799765 0.367196 0.284916

H 0.496195 1.717090 1.338104

H -0.227362 2.315636 -1.479227

H -2.069122 0.765263 -1.578478

H -1.903472 -1.252189 0.766141

H -2.534025 -1.634978 -0.831151

H -4.414766 0.011366 -0.493572

H -3.794610 0.372792 1.121436

H -4.417414 -1.243138 0.751774

H 4.090612 -1.564768 -0.865185

H 4.601092 -1.137602 0.774947

H 4.880393 -0.010676 -0.559598

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -676.741 | 22.9131 | 48.0666 |
| 55.8433 | 103.1194 | 123.0575 |
| 180.3763 | 233.0412 | 247.3007 |
| 295.7836 | 374.2865 | 400.961 |
| 437.7849 | 496.8686 | 547.8252 |
| 579.9048 | 773.7587 | 807.3243 |
| 811.6808 | 892.6947 | 907.1474 |
| 1019.222 | 1053.711 | 1057.916 |
| 1088.487 | 1107.809 | 1146.458 |
| 1211.005 | 1278.851 | 1316.432 |
| 1357.357 | 1417.329 | 1417.686 |
| 1455.491 | 1482.733 | 1484.015 |
| 1490.113 | 1501.917 | 1509.294 |
| 2018.038 | 2367.217 | 3043.834 |
| 3046.535 | 3046.901 | 3100.208 |
| 3118.109 | 3123.091 | 3123.396 |
| 3127.825 | 3150.788 | 3164.16 |

***i28 – p73***

C -0.405633 -0.235799 0.231052

C 0.456316 0.867683 -0.160537

C 1.785434 0.919588 -0.003561

C 2.685512 -0.125423 0.582766

C 3.663177 -0.684266 -0.457457

C -4.272987 -0.218916 -0.286324

C -2.965679 -0.227046 -0.118982

C -1.716754 -0.233519 0.052628

H 0.042229 -1.112473 0.691353

H -0.046281 1.713338 -0.620326

H 2.292401 1.814462 -0.359948

H 2.111188 -0.943465 1.023483

H 3.256227 0.327175 1.402101

H 4.268036 0.114286 -0.896358

H 3.123105 -1.178434 -1.268802

H 4.342564 -1.410562 -0.004857

H -5.116810 0.757792 1.764890

H -4.878245 -1.073810 -0.004957

H -4.770722 0.617877 -0.764087

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -416.986 | 28.1036 | 59.5736 |
| 88.229 | 128.7598 | 162.0007 |
| 204.251 | 246.8039 | 263.625 |
| 272.0476 | 312.1851 | 444.4471 |
| 495.8503 | 548.8352 | 583.5605 |
| 620.6914 | 789.3338 | 811.5847 |
| 881.6123 | 882.516 | 893.5122 |
| 945.8706 | 1026.346 | 1034.366 |
| 1036.517 | 1077.02 | 1098.679 |
| 1176.353 | 1279.47 | 1291.085 |
| 1309.85 | 1346.356 | 1415.555 |
| 1427.994 | 1465.762 | 1493.907 |
| 1502.964 | 1511.646 | 1676.455 |
| 1722.097 | 2155.96 | 3043.952 |
| 3044.532 | 3099.966 | 3123.441 |
| 3127.903 | 3147.029 | 3149.998 |
| 3167.423 | 3184.834 | 3234.797 |

***i32 – i46***

C 1.713527 -1.352083 0.705071

C 1.335061 -0.476427 -0.489505

C -0.123430 -0.967447 -0.432992

C -1.184526 -0.044474 -0.057262

C -0.881669 1.240321 0.239510

C 0.467968 1.765599 0.106529

C 1.497593 0.995995 -0.268293

C -2.578005 -0.595396 0.045427

H 2.302631 -2.249073 0.531472

H 0.280604 -1.680748 0.614544

H 1.844521 -0.851974 1.660818

H 1.853440 -0.785767 -1.400129

H -0.380979 -1.749886 -1.146359

H -1.669415 1.919534 0.549419

H 0.623671 2.823640 0.290169

H 2.487066 1.420245 -0.405009

H -2.630855 -1.380504 0.807329

H -2.893548 -1.045297 -0.901924

H -3.296247 0.183309 0.308761

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2067.58 | 113.8235 | 155.9103 |
| 186.4156 | 306.4653 | 315.2591 |
| 376.3981 | 496.8198 | 516.4395 |
| 551.9153 | 574.3348 | 640.3661 |
| 751.5521 | 764.6443 | 867.9395 |
| 878.0117 | 891.6811 | 911.2746 |
| 937.2668 | 987.9683 | 1008.848 |
| 1036.272 | 1064.018 | 1073.869 |
| 1086.38 | 1119.603 | 1198.395 |
| 1201.705 | 1264.143 | 1313.186 |
| 1333.22 | 1351.543 | 1409.926 |
| 1420.168 | 1427.97 | 1446.527 |
| 1484.125 | 1504.929 | 1615.945 |
| 1711.299 | 1802.317 | 3036.919 |
| 3084.116 | 3094.269 | 3116.895 |
| 3136.672 | 3140.215 | 3174.525 |
| 3188.156 | 3203.476 | 3236.081 |

***i40 – p39***

C -0.621885 1.979504 -0.917444

C -0.306022 1.035420 0.211783

C 0.963533 0.385115 0.167670

C 2.038574 -0.154361 0.093355

C 3.337148 -0.811221 0.023622

C -1.197216 0.740826 1.180991

C -1.707432 -1.889732 -0.635010

C -2.448736 -1.183482 0.177990

H -0.637521 1.440048 -1.869607

H 0.139326 2.760542 -0.996984

H -1.595757 2.449812 -0.771280

H 3.226604 -1.897320 0.079066

H 3.847595 -0.568380 -0.911483

H 3.976984 -0.495119 0.851748

H -2.137948 1.275038 1.243175

H -0.935232 0.086554 2.002473

H -0.676139 -1.611894 -0.846972

H -2.086408 -2.786243 -1.128819

H -3.469294 -1.265444 0.530944

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -217.495 | 29.8809 | 42.4948 |
| 60.4565 | 88.6166 | 118.884 |
| 151.9119 | 169.189 | 209.7074 |
| 270.1477 | 311.9894 | 368.7445 |
| 384.7903 | 564.1677 | 581.7369 |
| 666.0592 | 767.7432 | 794.6094 |
| 881.7655 | 894.8866 | 940.2772 |
| 952.1478 | 1029.027 | 1052.472 |
| 1058.834 | 1066.696 | 1082.415 |
| 1096.801 | 1336.22 | 1395.226 |
| 1411.261 | 1420.828 | 1429.159 |
| 1480.495 | 1483.525 | 1484.167 |
| 1497.182 | 1624.975 | 1669.685 |
| 2350.279 | 3041.593 | 3045.199 |
| 3081.291 | 3107.402 | 3116.201 |
| 3120.971 | 3138.206 | 3164.443 |
| 3166.127 | 3222.813 | 3262.493 |

***i43 – i43***

C 1.971790 -1.051431 0.702565

C 1.302066 -0.424355 -0.527311

C -0.037467 -1.097938 -0.217075

C -1.248351 -0.307381 0.006729

C -1.060792 1.122441 0.462748

C 0.209548 1.757873 -0.030685

C 1.254752 1.071675 -0.478844

C -2.471445 -0.835329 -0.138951

H 2.573401 -1.945120 0.555802

H 0.597339 -1.466053 0.917732

H 2.288698 -0.382499 1.499116

H 1.742836 -0.757823 -1.469822

H -0.184532 -2.050771 -0.722755

H -1.054234 1.145485 1.561823

H -1.923992 1.720597 0.157660

H 0.262626 2.841798 0.016743

H 2.151868 1.598924 -0.791730

H -3.366599 -0.251663 0.048249

H -2.608018 -1.866204 -0.447870

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2165.52 | 60.7954 | 118.64 |
| 262.4279 | 315.0911 | 369.255 |
| 445.2902 | 502.3564 | 515.5107 |
| 534.493 | 618.4768 | 687.8781 |
| 725.4465 | 754.0378 | 861.4746 |
| 876.5846 | 891.2934 | 912.1135 |
| 925.4888 | 941.8443 | 974.3769 |
| 1009.8 | 1023.531 | 1040.565 |
| 1067.506 | 1132.87 | 1199.38 |
| 1223.497 | 1262.349 | 1296.673 |
| 1323.583 | 1340.933 | 1354.521 |
| 1381.374 | 1417.684 | 1430.209 |
| 1459.5 | 1469.655 | 1672.154 |
| 1754.213 | 1793.176 | 3020.33 |
| 3083.238 | 3084.957 | 3116.316 |
| 3147.839 | 3154.058 | 3164.483 |
| 3188.572 | 3229.87 | 3241.776 |

***i43 – i31***

C 2.596336 -0.766865 -0.063852

C 1.226432 -0.192119 -0.067011

C 0.107313 -1.002160 0.545173

C -1.235661 -0.492414 0.089302

C -1.442680 0.985937 0.304999

C -0.219407 1.786510 -0.062007

C 0.989476 1.224933 -0.239242

C -2.144971 -1.275499 -0.478828

H 2.738201 -1.784809 0.270671

H 3.450519 -0.124994 -0.232828

H 1.712764 -0.712444 -1.103252

H 0.185630 -0.906854 1.639450

H 0.219639 -2.064090 0.309282

H -1.688150 1.165990 1.362487

H -2.307571 1.330536 -0.269571

H -0.340264 2.857306 -0.185394

H 1.834073 1.848874 -0.519910

H -3.097941 -0.882891 -0.818855

H -1.967919 -2.336562 -0.623277

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1921.19 | 108.8761 | 122.9647 |
| 295.7295 | 303.0672 | 377.5359 |
| 402.3093 | 431.5755 | 455.5412 |
| 498.5672 | 569.2789 | 607.9886 |
| 685.4042 | 734.915 | 746.5165 |
| 846.1497 | 913.8467 | 926.5536 |
| 933.6758 | 945.8867 | 976.3568 |
| 982.8839 | 1005.185 | 1020.259 |
| 1164.086 | 1182.212 | 1212.474 |
| 1224.983 | 1268.991 | 1305.697 |
| 1337.573 | 1352.874 | 1357.46 |
| 1430.365 | 1451.157 | 1463.071 |
| 1472.454 | 1487.258 | 1660.465 |
| 1756.941 | 2218.157 | 2989.824 |
| 3002.9 | 3081.66 | 3093.389 |
| 3145.814 | 3162.973 | 3174.16 |
| 3197.318 | 3231.175 | 3296.881 |

***i64 – p93***

C -1.544331 -1.119233 0.257015

C -1.932040 0.326814 0.123833

C -0.872198 1.115395 -0.656258

C 0.499078 0.816740 -0.087707

C 1.152708 1.695918 0.703156

C 2.098448 -1.085635 -0.218111

C 0.849632 -0.635961 -0.075305

C -0.283924 -1.544053 0.142833

H -2.334310 -1.837807 0.453141

H -2.900272 0.408296 -0.379350

H -2.064305 0.763246 1.122276

H -0.909795 0.804755 -1.704222

H -1.074429 2.187963 -0.618086

H 1.416008 1.273009 -1.685874

H 2.042722 1.406188 1.249247

H 0.831275 2.730010 0.768348

H 2.321666 -2.145464 -0.158907

H 2.921790 -0.408139 -0.413002

H -0.054590 -2.601968 0.229686

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -891.223 | 101.2717 | 195.4092 |
| 280.3845 | 336.2005 | 376.6336 |
| 415.0825 | 455.8093 | 464.7037 |
| 512.0301 | 574.4008 | 636.0287 |
| 676.1316 | 722.8035 | 741.2856 |
| 773.9955 | 818.8253 | 880.613 |
| 897.159 | 915.3183 | 936.3984 |
| 973.9305 | 986.5555 | 1010.721 |
| 1045.309 | 1052.616 | 1183.375 |
| 1195.167 | 1231.371 | 1269.696 |
| 1333.399 | 1355.329 | 1366.393 |
| 1414.998 | 1445.161 | 1462.444 |
| 1480.905 | 1499.063 | 1634.052 |
| 1691.578 | 1742.101 | 3030.593 |
| 3062.348 | 3083.899 | 3118.625 |
| 3150.807 | 3154.329 | 3168.282 |
| 3190.99 | 3246.208 | 3248.613 |

***i64 – i66***

C 1.779517 -0.854866 -0.130965

C 1.845371 0.634281 -0.330522

C 0.725436 1.325352 0.451109

C -0.620130 0.680058 0.173755

C -1.736537 1.522462 -0.327356

C -1.815954 -1.494487 -0.016167

C -0.675169 -0.781771 0.092510

C 0.621861 -1.479432 0.087199

H 2.701358 -1.425040 -0.188031

H 2.815290 1.022004 -0.006439

H 1.758779 0.863819 -1.400522

H 0.964545 1.243406 1.517615

H 0.688070 2.390422 0.208619

H -1.500410 1.105671 0.949336

H -2.602096 1.063569 -0.783665

H -1.588920 2.591394 -0.393169

H -1.784462 -2.575539 -0.083226

H -2.795294 -1.031090 -0.026135

H 0.596770 -2.558197 0.208234

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1880.06 | 69.7722 | 158.6233 |
| 301.8543 | 327.4739 | 373.2424 |
| 416.4202 | 430.0289 | 467.1663 |
| 526.0853 | 602.9086 | 642.5552 |
| 693.4922 | 696.4871 | 734.0221 |
| 798.7535 | 847.7477 | 866.8094 |
| 898.0906 | 962.8746 | 986.1467 |
| 1011.214 | 1035.409 | 1050.448 |
| 1168.919 | 1185.903 | 1195.874 |
| 1220.402 | 1273.558 | 1293.178 |
| 1355.289 | 1367.034 | 1396.92 |
| 1433.22 | 1442.369 | 1465.447 |
| 1481.234 | 1496.705 | 1629.061 |
| 1728.041 | 2251.904 | 3032.579 |
| 3042.679 | 3090.995 | 3102.079 |
| 3167.49 | 3175.085 | 3175.797 |
| 3198.286 | 3255.557 | 3299.282 |

***i62 – i65***

C -1.967778 -0.449391 -0.106563

C -1.812783 0.844819 0.140793

C -0.471404 1.498855 0.287200

C 0.678272 0.609530 -0.124648

C 2.000317 1.262137 -0.242867

C 1.563123 -1.640764 0.357427

C 0.538992 -0.833844 0.031455

C -0.830561 -1.416731 -0.260770

H -2.968571 -0.859785 -0.208758

H -2.685414 1.480882 0.256860

H -0.449851 2.432374 -0.288638

H -0.323380 1.801156 1.335680

H 1.133052 0.954956 -1.246338

H 2.075585 2.329438 -0.083886

H 2.898645 0.676444 -0.371694

H 1.424605 -2.714043 0.430476

H 2.550500 -1.255932 0.581261

H -0.842736 -1.811623 -1.286082

H -1.001512 -2.281526 0.388949

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1883.03 | 76.8589 | 121.3506 |
| 287.0946 | 344.1362 | 385.6645 |
| 404.7238 | 448.9249 | 500.8074 |
| 509.7121 | 563.4202 | 666.447 |
| 668.1427 | 707.555 | 730.5337 |
| 822.4576 | 869.8529 | 916.1518 |
| 930.7502 | 962.2312 | 976.8588 |
| 995.9974 | 1025.02 | 1038.265 |
| 1190.357 | 1190.514 | 1211.893 |
| 1234.395 | 1259.173 | 1260.229 |
| 1345.741 | 1371.683 | 1412.895 |
| 1425.86 | 1451.339 | 1463.483 |
| 1468.56 | 1486.483 | 1652.593 |
| 1766.174 | 2228.233 | 2992.909 |
| 3023.357 | 3045.822 | 3074.392 |
| 3162.41 | 3165.079 | 3183.499 |
| 3192.231 | 3251.228 | 3302.61 |

***i61 – i59***

C -2.011353 -0.644016 -0.000131

C -1.922340 0.782179 -0.054903

C -0.726571 1.414570 -0.016087

C 0.544131 0.678759 0.014760

C 1.795675 1.508304 0.030869

C 0.536136 -0.684816 -0.010799

C -0.708401 -1.411342 0.017710

C 1.804373 -1.501899 -0.048880

H -1.446067 -1.137740 1.047764

H -2.925053 -1.175901 -0.225996

H -2.841743 1.353609 -0.127010

H -0.685901 2.498523 -0.035674

H 1.890703 2.086258 -0.896581

H 2.701587 0.913441 0.147657

H 1.765068 2.233641 0.851910

H -0.739159 -2.472419 -0.192055

H 2.466541 -1.180072 -0.856448

H 1.584039 -2.560195 -0.198386

H 2.360082 -1.409577 0.889579

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2559.64 | 68.1267 | 122.8508 |
| 158.777 | 194.3903 | 334.1495 |
| 347.1179 | 388.4631 | 468.6198 |
| 500.8913 | 537.6963 | 602.387 |
| 634.0805 | 720.7755 | 736.8569 |
| 779.4976 | 822.5083 | 919.078 |
| 966.4483 | 980.5958 | 1000.439 |
| 1035.019 | 1063.956 | 1103.264 |
| 1161.339 | 1183.232 | 1203.817 |
| 1222.336 | 1264.875 | 1343.537 |
| 1397.196 | 1412.937 | 1422.911 |
| 1452.771 | 1482.752 | 1489.368 |
| 1504.298 | 1515.478 | 1604.237 |
| 1621.661 | 2215.431 | 3027.613 |
| 3050.342 | 3076.621 | 3115.2 |
| 3138.953 | 3151.44 | 3184.207 |
| 3204.168 | 3214.806 | 3232.175 |

***i23 – p13b***

C 0.583254 1.658267 -0.292408

C 0.177777 0.222179 -0.033441

C -1.241300 0.001712 0.017798

C -2.435542 -0.137973 0.040558

C 3.292306 -0.065715 0.387545

C 2.450020 -0.877266 -0.257360

C 0.997486 -0.861777 -0.173080

C -3.880605 -0.319441 0.080868

H 0.328737 2.300820 0.552083

H 0.026660 2.021504 -1.160977

H 1.648745 1.747398 -0.495964

H 0.443704 0.307406 1.909897

H 2.940313 0.700011 1.070097

H 4.364756 -0.177040 0.277417

H 2.867987 -1.680178 -0.861392

H 0.514704 -1.834827 -0.191377

H -4.395287 0.632974 -0.066562

H -4.208417 -1.008903 -0.701187

H -4.192279 -0.729078 1.045088

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -858.267 | 81.1469 | 87.1037 |
| 93.4495 | 123.0161 | 175.7035 |
| 245.9518 | 261.7752 | 309.7831 |
| 328.6366 | 375.5354 | 441.6256 |
| 481.5075 | 542.3448 | 566.281 |
| 575.8526 | 637.9993 | 784.3345 |
| 884.8722 | 908.8469 | 968.844 |
| 1012.989 | 1043.938 | 1052.655 |
| 1060.504 | 1064.799 | 1071.263 |
| 1112.151 | 1286.863 | 1333.7 |
| 1376.753 | 1418.807 | 1421.61 |
| 1460.693 | 1485.881 | 1487.333 |
| 1492.58 | 1498.24 | 1611.606 |
| 1694.987 | 2375.612 | 3051.814 |
| 3062.111 | 3123.412 | 3127.546 |
| 3128.618 | 3154.833 | 3164.446 |
| 3177.989 | 3185.04 | 3252.489 |

***i23 – p10b***

C -0.457646 2.134455 0.363590

C -0.211548 -0.123193 -0.361863

C 1.207587 -0.194599 -0.230568

C 2.405599 -0.249732 -0.132110

C -3.246131 -0.138869 -0.511005

C -2.494558 -0.869544 0.325244

C -1.054970 -0.815531 0.463306

C 3.855884 -0.326992 -0.012139

H 0.084222 2.626668 -0.434809

H 0.044305 2.028445 1.316022

H -1.538896 2.197946 0.366227

H -0.583663 0.255523 -1.308360

H -2.817764 0.594523 -1.186426

H -4.322272 -0.259347 -0.541756

H -3.001422 -1.565625 0.988751

H -0.620348 -1.329592 1.314607

H 4.290474 0.666068 0.129288

H 4.142349 -0.946680 0.841113

H 4.297713 -0.763890 -0.911384

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -434.399 | 73.194 | 81.353 |
| 91.9073 | 104.6961 | 119.3062 |
| 145.9493 | 244.3191 | 265.6693 |
| 280.3398 | 322.0877 | 470.2711 |
| 473.0821 | 495.0972 | 513.4364 |
| 566.83 | 635.745 | 759.9232 |
| 831.1159 | 856.0304 | 928.1155 |
| 943.3733 | 1010.658 | 1036.586 |
| 1059.328 | 1063.072 | 1078.766 |
| 1211.78 | 1281.354 | 1321.475 |
| 1341.321 | 1408.229 | 1423.439 |
| 1425.418 | 1457.033 | 1484.093 |
| 1490.451 | 1556.487 | 1670.931 |
| 2373.225 | 3046.915 | 3103.126 |
| 3116.913 | 3122.185 | 3159.158 |
| 3171.034 | 3177.049 | 3196.76 |
| 3250.264 | 3273.772 | 3283.01 |

***i22 – p10a***

C -0.105740 2.321913 0.341135

C -0.122346 0.149364 -0.567129

C 1.246095 -0.149783 -0.289086

C 2.401814 -0.400035 -0.067126

C 3.799782 -0.710830 0.203331

C -1.155306 -0.479741 0.077115

C -3.568699 -0.868710 0.344049

C -2.532859 -0.314892 -0.302029

H 0.668304 2.758117 -0.278916

H 0.159991 2.066735 1.358899

H -1.130819 2.618736 0.154710

H -0.323310 0.646067 -1.512032

H 4.044508 -0.517037 1.250834

H 4.012727 -1.762682 -0.004434

H 4.460107 -0.100977 -0.418026

H -0.934995 -1.089626 0.948939

H -3.417515 -1.492792 1.219445

H -4.589296 -0.715809 0.014707

H -2.726141 0.305560 -1.175687

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -463.285 | 77.1538 | 90.311 |
| 95.4546 | 106.829 | 137.7538 |
| 141.1876 | 231.1453 | 246.662 |
| 294.5719 | 351.5192 | 429.6709 |
| 471.4328 | 477.4695 | 508.1363 |
| 553.0914 | 636.4882 | 779.3521 |
| 823.5596 | 859.0443 | 912.3985 |
| 943.0451 | 964.7813 | 1025.568 |
| 1064.884 | 1066.722 | 1193.241 |
| 1196.992 | 1281.054 | 1286.234 |
| 1328.487 | 1412.299 | 1420.349 |
| 1426.128 | 1448.604 | 1490.381 |
| 1492.942 | 1558.951 | 1653.015 |
| 2373.699 | 3047.017 | 3102.287 |
| 3118.534 | 3121.815 | 3150.433 |
| 3162.617 | 3170.114 | 3178.692 |
| 3254.103 | 3273.669 | 3276.793 |

***i22 – p13a***

C 0.294432 1.968816 -0.129570

C 0.099917 0.485007 0.097240

C -1.259366 0.028962 0.052584

C -2.410125 -0.314690 -0.016119

C -3.801629 -0.740031 -0.089252

C 1.106659 -0.436219 0.049511

C 3.458385 -1.101182 -0.074293

C 2.517866 -0.149878 -0.056937

H -0.473360 2.534696 0.398445

H 0.199742 2.189656 -1.197516

H 1.269245 2.314852 0.213218

H 0.123376 0.680329 2.090810

H -4.213503 -0.554349 -1.084634

H -3.893393 -1.808325 0.120646

H -4.412412 -0.196445 0.635889

H 0.828825 -1.483713 0.124652

H 3.199384 -2.153017 -0.000581

H 4.510032 -0.857042 -0.164693

H 2.825223 0.888653 -0.135212

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -802.1 | 53.3202 | 84.2582 |
| 102.447 | 125.0733 | 137.4017 |
| 232.6133 | 245.1222 | 319.057 |
| 347.2357 | 390.9437 | 408.6733 |
| 430.3745 | 447.7475 | 567.3875 |
| 585.3752 | 669.892 | 747.2375 |
| 907.2396 | 920.825 | 947.4886 |
| 1009.569 | 1029.899 | 1053.434 |
| 1055.542 | 1060.185 | 1072.013 |
| 1209.782 | 1271.138 | 1338.615 |
| 1359.123 | 1419.793 | 1422.854 |
| 1453.575 | 1482.952 | 1484.351 |
| 1488.736 | 1501.566 | 1600.691 |
| 1676.926 | 2374.231 | 3052.321 |
| 3057.309 | 3121.985 | 3129.123 |
| 3133.499 | 3156.81 | 3161.719 |
| 3181.581 | 3192.147 | 3252.942 |

***i22 – i40***

C -0.047697 2.511735 0.154452

C -0.126594 1.033795 -0.121146

C 1.038962 0.241302 -0.055721

C 2.038168 -0.437378 -0.015185

C 3.244811 -1.252111 0.042164

C -1.475883 0.389664 -0.105140

C -2.923769 -1.592350 0.100170

C -1.708149 -1.021049 0.003254

H 0.862054 2.943424 -0.265036

H -0.050310 2.697728 1.235060

H -0.907234 3.035905 -0.273037

H -0.846566 0.742814 -1.186870

H 3.532076 -1.460839 1.076666

H 3.087584 -2.209225 -0.462034

H 4.082036 -0.747763 -0.447355

H -2.309549 1.075788 0.003855

H -3.833220 -0.999370 0.103346

H -3.032314 -2.665881 0.190049

H -0.823653 -1.654225 0.008267

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1888.45 | 77.4451 | 119.1902 |
| 125.6842 | 146.8035 | 170.8521 |
| 198.4122 | 202.8065 | 304.6798 |
| 328.2525 | 374.2137 | 440.4662 |
| 528.9557 | 606.2964 | 614.9477 |
| 672.8307 | 797.5803 | 870.0327 |
| 920.3792 | 1016.107 | 1028.814 |
| 1044.446 | 1053.868 | 1060.202 |
| 1062.849 | 1153.966 | 1231.967 |
| 1255.861 | 1308.289 | 1354.388 |
| 1376.043 | 1423.097 | 1426.173 |
| 1479.145 | 1487.134 | 1489.887 |
| 1492.217 | 1499.883 | 1635.898 |
| 2151.685 | 2312.698 | 3030.994 |
| 3042.683 | 3099.456 | 3110.471 |
| 3118.757 | 3140.749 | 3149.982 |
| 3161.839 | 3194.522 | 3248.003 |

***i50 – i54***

C -0.742142 2.449387 -0.230715

C -0.575209 0.973313 -0.076109

C 3.238440 -0.487011 0.150523

C 1.882059 0.038856 0.061694

C 0.755331 0.460375 -0.001488

C -1.712234 0.185973 0.440032

C -1.910342 -1.129524 0.304769

C -1.051142 -2.099309 -0.446013

H -1.730494 2.871312 -0.109907

H 0.130757 3.081037 -0.306127

H -0.783708 1.457888 -1.202026

H 3.948547 0.303922 0.404898

H 3.554115 -0.933841 -0.796280

H 3.301824 -1.256495 0.924286

H -2.456160 0.762073 0.986254

H -2.788823 -1.547276 0.790209

H -0.394016 -1.600885 -1.159195

H -1.674359 -2.817199 -0.986790

H -0.416248 -2.672894 0.238513

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1897.41 | 42.2928 | 76.4064 |
| 92.8183 | 124.9533 | 147.9953 |
| 241.4041 | 286.2079 | 314.2588 |
| 351.4057 | 388.3736 | 448.1398 |
| 522.6485 | 541.2383 | 618.1881 |
| 636.6538 | 702.4231 | 769.2143 |
| 900.7886 | 966.7214 | 992.344 |
| 1041.301 | 1053.882 | 1057.98 |
| 1062.931 | 1120.755 | 1183.506 |
| 1242.558 | 1275.763 | 1363.045 |
| 1408.622 | 1420.684 | 1422.373 |
| 1445.189 | 1484.004 | 1488.746 |
| 1491.615 | 1508.348 | 1713.885 |
| 2232.11 | 2352.647 | 3044.414 |
| 3047.538 | 3103.485 | 3115.654 |
| 3123.039 | 3148.122 | 3155.901 |
| 3172.441 | 3180.262 | 3304.383 |

***i50 – p85***

C 0.574815 1.693315 -0.350575

C 0.145049 0.413096 -0.168071

C -3.857223 -0.393267 0.215294

C -2.436664 -0.099105 0.079969

C -1.264792 0.149630 -0.014125

C 0.984543 -0.763072 -0.528672

C 2.267155 -0.963021 -0.227485

C 3.156487 -0.087819 0.600658

H 1.601985 1.899285 -0.622256

H -0.095309 2.528883 -0.193024

H 0.404425 0.278270 1.676893

H -4.451418 0.220258 -0.466335

H -4.196398 -0.193815 1.235037

H -4.057485 -1.443889 -0.008049

H 0.459193 -1.524640 -1.097582

H 2.720679 -1.875223 -0.607233

H 2.582674 0.592089 1.234733

H 3.814265 0.517669 -0.033082

H 3.801163 -0.697420 1.238940

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1037.93 | 70.5485 | 96.837 |
| 112.6067 | 161.0802 | 197.1946 |
| 247.3367 | 281.538 | 327.5424 |
| 353.9621 | 427.8242 | 455.3333 |
| 509.4099 | 546.5822 | 562.2248 |
| 592.6741 | 666.1539 | 766.1176 |
| 788.251 | 885.9443 | 904.5538 |
| 972.5493 | 1011.55 | 1052.368 |
| 1067.501 | 1076.026 | 1080.404 |
| 1118.466 | 1280.851 | 1289.872 |
| 1407.13 | 1418.711 | 1426.255 |
| 1448.254 | 1487.981 | 1489.419 |
| 1494.563 | 1502.966 | 1577.773 |
| 1743.886 | 2383.785 | 3034.272 |
| 3051.29 | 3097.56 | 3124.331 |
| 3124.538 | 3125.509 | 3163.025 |
| 3174.039 | 3188.28 | 3277.651 |

***i26 – p59***

C -0.583071 0.730845 0.098097

C 0.467230 -0.118304 -0.044883

C -4.487663 -0.468403 0.011595

C -3.093938 -0.045399 0.042703

C -1.942931 0.304055 0.059772

C 1.846267 0.287297 0.085162

C 2.883289 -0.544000 -0.074805

C 4.320885 -0.156110 0.046548

H -0.400544 1.747494 0.436572

H -0.571537 1.654703 -1.724379

H 0.268724 -1.155950 -0.299695

H -4.572629 -1.544373 0.182384

H -4.940745 -0.242642 -0.957338

H -5.066355 0.044845 0.783641

H 2.033456 1.334150 0.320238

H 2.680035 -1.587168 -0.312467

H 4.819142 -0.739254 0.828071

H 4.432948 0.903779 0.285046

H 4.857099 -0.355474 -0.887199

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -746.876 | 42.459 | 67.4798 |
| 75.2688 | 123.8349 | 181.0244 |
| 188.774 | 214.3964 | 301.2491 |
| 316.13 | 328.3749 | 377.927 |
| 403.9855 | 445.8739 | 498.9875 |
| 586.7643 | 811.3429 | 816.1785 |
| 897.7684 | 953.668 | 964.5777 |
| 1027.287 | 1055.368 | 1059.037 |
| 1069.817 | 1111.176 | 1191.181 |
| 1208.487 | 1262.823 | 1310.986 |
| 1347.213 | 1366.701 | 1421.537 |
| 1422.526 | 1482.582 | 1483.719 |
| 1488.351 | 1492.556 | 1622.594 |
| 1719.322 | 2376.575 | 3038.701 |
| 3051.048 | 3096.53 | 3121.835 |
| 3125.626 | 3129.685 | 3147.857 |
| 3152.64 | 3168.981 | 3178.603 |

***i26 – i47***

C -0.651154 1.665728 0.180037

C 0.768993 1.221087 -0.075469

C -3.497140 -1.306746 -0.018218

C -2.485200 -0.258502 0.054177

C -1.657821 0.609513 0.111854

C 1.160344 -0.017581 -0.355222

H -0.699822 2.144490 1.165695

H -0.909302 2.452014 -0.539968

H 1.511387 2.014592 -0.020544

H -3.336085 -2.059904 0.757118

H -3.470178 -1.807789 -0.988962

H -4.497503 -0.888726 0.119038

H 0.394652 -0.797630 -0.403530

C 2.556488 -0.419222 -0.582458

C 3.367076 -1.004342 0.523558

H 2.915658 -0.502247 -1.604152

H 2.968135 -1.979062 0.845653

H 3.345613 -0.359362 1.410018

H 4.407922 -1.155987 0.230077

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -227.462 | 45.4063 | 78.2081 |
| 105.2774 | 115.6084 | 154.2141 |
| 197.681 | 223.8489 | 268.523 |
| 385.1998 | 385.6379 | 405.3118 |
| 477.3204 | 631.5186 | 760.0224 |
| 791.4507 | 934.8134 | 969.6002 |
| 974.0122 | 993.0054 | 1004.008 |
| 1058.883 | 1064.773 | 1107.623 |
| 1145.4 | 1175.31 | 1241.893 |
| 1278.462 | 1345.495 | 1353.602 |
| 1381.441 | 1404.718 | 1420.635 |
| 1477.377 | 1478.248 | 1483.641 |
| 1487.596 | 1493.946 | 1752.104 |
| 2399.378 | 2983.782 | 3036.457 |
| 3049.132 | 3051.133 | 3063.723 |
| 3087.99 | 3119.799 | 3124.775 |
| 3125.813 | 3163.134 | 3175.454 |

***i27 – p63***

C 0.424882 1.774779 -0.000612

C -0.926508 1.716409 -0.145133

C -1.804504 0.562955 -0.186523

C -1.506298 -0.705441 0.128124

C -2.483647 -1.833804 0.061980

C 3.089490 -1.319466 -0.074594

C 2.130389 -0.223702 -0.040464

C 1.326893 0.672131 -0.011201

H 0.892630 2.752567 -0.059794

H 0.521039 2.129656 2.034404

H -1.426797 2.676946 -0.226958

H -2.827506 0.780803 -0.488812

H -0.502674 -0.950009 0.460780

H -2.130546 -2.611462 -0.623763

H -3.466852 -1.498969 -0.276804

H -2.599355 -2.307682 1.042421

H 3.206461 -1.765355 0.916703

H 4.069660 -0.967433 -0.405271

H 2.759762 -2.102224 -0.762377

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -681.488 | 40.8668 | 60.9302 |
| 75.7392 | 147.4066 | 184.3783 |
| 190.5036 | 212.1257 | 284.771 |
| 299.6759 | 322.5214 | 394.5599 |
| 399.5174 | 506.924 | 570.2239 |
| 677.5444 | 760.9364 | 836.8752 |
| 868.2452 | 914.1283 | 990.7455 |
| 1007.442 | 1045.821 | 1055.183 |
| 1059.418 | 1071.263 | 1140.882 |
| 1175.745 | 1278.604 | 1359.571 |
| 1363.241 | 1419.219 | 1421.877 |
| 1463.484 | 1481.512 | 1484.255 |
| 1485.553 | 1497.038 | 1600.017 |
| 1715.694 | 2369.151 | 3033.97 |
| 3048.193 | 3091.911 | 3118.544 |
| 3125.76 | 3126.116 | 3147.149 |
| 3173.455 | 3191.231 | 3209.729 |

***i51 – i49***

C 0.617668 1.645536 -0.380354

C -0.118601 0.826496 0.622116

C -3.760031 -0.817519 -0.179401

C -2.458306 -0.229346 0.109027

C -1.385803 0.266948 0.358695

C 1.235737 0.296355 -0.492713

C 2.452723 -0.064309 0.077937

C 3.010180 -1.447700 0.020118

H 1.261863 2.421188 0.026678

H 0.037225 1.983842 -1.233436

H 0.235521 0.845171 1.644435

H -4.563422 -0.087670 -0.044656

H -3.959471 -1.665798 0.480563

H -3.803029 -1.177159 -1.210965

H 0.763940 -0.390093 -1.188051

H 2.980201 0.669642 0.683099

H 2.456261 -2.070441 -0.687032

H 2.966647 -1.942393 0.999667

H 4.062856 -1.445052 -0.282859

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -636.694 | 31.0526 | 67.2573 |
| 101.7015 | 125.3151 | 151.6665 |
| 224.6161 | 268.9138 | 298.9496 |
| 329.0584 | 470.1778 | 475.5618 |
| 536.5989 | 664.565 | 729.9173 |
| 804.8913 | 860.1235 | 936.643 |
| 1006.494 | 1023.095 | 1031.211 |
| 1051.585 | 1055.615 | 1074.38 |
| 1136.908 | 1182.285 | 1201.365 |
| 1228.289 | 1275.706 | 1325.824 |
| 1393.025 | 1416.974 | 1421.637 |
| 1478.61 | 1481.783 | 1482.525 |
| 1486.164 | 1489.616 | 1527.061 |
| 2317.498 | 3008.689 | 3040 |
| 3065.677 | 3108.233 | 3113.482 |
| 3114.294 | 3115.112 | 3154.81 |
| 3180.561 | 3196.126 | 3210.303 |

***i28 – i29***

C -0.488266 -0.823521 -0.202021

C 0.546164 -0.325672 0.484675

C -4.315495 0.594521 -0.003316

C -2.949241 0.092657 -0.070879

C -1.818777 -0.316503 -0.120386

H -0.329569 -1.668539 -0.867743

H 0.356766 0.523903 1.145678

H -4.683422 0.583192 1.025899

H -4.985535 -0.019285 -0.610196

H -4.370983 1.622572 -0.370672

C 1.921048 -0.834926 0.395234

C 2.931852 -0.169025 -0.482712

C 3.349408 1.223989 0.024300

H 2.254487 -1.558089 1.134915

H 2.515571 -0.059138 -1.492128

H 3.819318 -0.802744 -0.568451

H 3.792332 1.160448 1.021702

H 2.486633 1.892973 0.078924

H 4.084231 1.675581 -0.647289

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -261.257 | 29.2906 | 47.7186 |
| 75.345 | 101.4178 | 192.1654 |
| 216.2347 | 256.7633 | 280.0457 |
| 319.0405 | 406.1406 | 496.8438 |
| 520.945 | 548.1284 | 788.8562 |
| 819.0437 | 861.2438 | 906.8928 |
| 980.3585 | 996.8463 | 1047.871 |
| 1055.256 | 1058.648 | 1118.873 |
| 1142.637 | 1206.115 | 1274.803 |
| 1287.648 | 1328.031 | 1339.739 |
| 1376.873 | 1409.341 | 1419.44 |
| 1484.181 | 1484.466 | 1487.205 |
| 1502.48 | 1508.704 | 1709.151 |
| 2376.933 | 3026.452 | 3042.288 |
| 3045.602 | 3085.306 | 3091.632 |
| 3117.087 | 3121.029 | 3121.175 |
| 3124.904 | 3160.196 | 3162.815 |

***i46 – p3***

C 2.302233 -1.141484 0.430802

C 1.285507 -0.407841 -0.096483

C -0.086959 -1.027387 -0.324724

C -1.253676 -0.128150 0.010111

C -1.077076 1.190302 0.137487

C 0.244328 1.802696 0.016601

C 1.353811 1.065138 -0.101721

C -2.590920 -0.794439 0.109237

H 3.263944 -0.687301 0.641436

H 2.204719 -2.210117 0.584691

H 1.910359 -0.489288 -1.825601

H -0.163098 -1.961840 0.240645

H -0.194421 -1.309974 -1.379489

H -1.927391 1.835159 0.335502

H 0.317748 2.883827 0.060709

H 2.334410 1.526034 -0.141553

H -2.603022 -1.525102 0.925362

H -2.817757 -1.344088 -0.811723

H -3.388979 -0.070324 0.282163

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1043.92 | 2.8064 | 164.5115 |
| 208.2094 | 299.5194 | 349.1665 |
| 401.1164 | 442.0477 | 459.7755 |
| 497.3512 | 520.8204 | 568.3627 |
| 601.6951 | 645.864 | 733.2284 |
| 778.6745 | 866.7306 | 872.324 |
| 885.8368 | 930.4575 | 948.915 |
| 977.7673 | 996.9777 | 1012.84 |
| 1069.15 | 1082.195 | 1182.036 |
| 1204.386 | 1244.121 | 1318.533 |
| 1335.797 | 1371.474 | 1418.677 |
| 1426.981 | 1455.573 | 1469.548 |
| 1482.61 | 1498.557 | 1592.528 |
| 1683.764 | 1753.847 | 3032.025 |
| 3036.057 | 3079.445 | 3089.924 |
| 3135.188 | 3156.031 | 3183.545 |
| 3195.261 | 3214.354 | 3252.762 |

***i46 – i8***

C 2.504129 -1.100319 -0.062013

C 1.265707 -0.290618 -0.058315

C -0.024002 -1.012370 0.255773

C -1.258162 -0.184726 -0.003396

C -1.166562 1.154853 -0.054263

C 0.103936 1.840955 0.053087

C 1.269445 1.145570 0.047080

C -2.555166 -0.927303 -0.090553

H 3.470289 -0.614188 -0.074113

H 2.433932 -2.175397 0.023378

H 1.746800 -0.637670 -1.149096

H -0.009114 -1.308116 1.321501

H -0.074927 -1.956839 -0.300451

H -2.067105 1.747952 -0.183389

H 0.116419 2.923472 0.100430

H 2.223089 1.664366 0.067024

H -2.724617 -1.519152 0.817484

H -2.550336 -1.632559 -0.929575

H -3.400377 -0.248129 -0.217596

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1923.02 | 100.265 | 160.4954 |
| 207.3102 | 273.589 | 338.902 |
| 389.7862 | 418.985 | 454.8873 |
| 485.2579 | 509.7905 | 551.1014 |
| 608.8231 | 721.8751 | 743.3296 |
| 858.2369 | 878.1892 | 921.3654 |
| 942.095 | 949.6715 | 976.6657 |
| 1003.918 | 1061.991 | 1079.723 |
| 1163.351 | 1171.66 | 1190.125 |
| 1248.294 | 1267.435 | 1323.928 |
| 1345.187 | 1403.611 | 1419.802 |
| 1443.167 | 1463.503 | 1482.038 |
| 1486.101 | 1492.988 | 1577.809 |
| 1715.075 | 2219.542 | 2927.681 |
| 3026.18 | 3040.194 | 3079.342 |
| 3134.908 | 3177.311 | 3181.324 |
| 3185.96 | 3214.767 | 3299.286 |

***i43 – p43***

C 2.500788 -0.816940 -0.051465

C 1.262391 -0.267186 -0.028605

C 0.081996 -1.002558 0.583663

C -1.232448 -0.449948 0.103113

C -1.377217 1.038866 0.288661

C -0.110944 1.777391 -0.055399

C 1.068050 1.179601 -0.225787

C -2.172793 -1.204344 -0.451924

H 2.655694 -1.863684 0.183921

H 3.362180 -0.241038 -0.370612

H 0.792705 -0.734993 -1.804074

H 0.147762 -0.854260 1.670809

H 0.155543 -2.074190 0.391441

H -1.639038 1.256155 1.334799

H -2.205343 1.418222 -0.316902

H -0.187250 2.853685 -0.176417

H 1.941446 1.762233 -0.502463

H -3.106489 -0.778380 -0.804577

H -2.036140 -2.273038 -0.579463

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -943.487 | 105.0668 | 133.6113 |
| 326.6864 | 328.0199 | 398.3069 |
| 428.9727 | 443.359 | 456.3744 |
| 512.7863 | 544.5876 | 569.2341 |
| 643.11 | 702.0127 | 741.7473 |
| 784.7106 | 859.9835 | 879.9815 |
| 920.3994 | 937.8576 | 939.2927 |
| 950.7662 | 999.0535 | 1010.103 |
| 1017.357 | 1026.677 | 1176.732 |
| 1205.42 | 1238.495 | 1299.056 |
| 1317.063 | 1337.993 | 1359.038 |
| 1400.355 | 1454.854 | 1460.581 |
| 1469.639 | 1486.124 | 1609.791 |
| 1729.824 | 1759.817 | 3007.091 |
| 3023.643 | 3091.109 | 3124.171 |
| 3149.249 | 3155.322 | 3169.464 |
| 3192.862 | 3235.767 | 3250.377 |

***i20 – p54***

C 0.957234 2.051723 0.709309

C 1.195869 1.254176 -0.527758

C -0.935925 0.028089 -0.485855

C -2.054845 -0.171429 -0.092116

C -3.411112 -0.406409 0.387754

C 0.390557 0.252436 -0.982464

C 2.462807 -1.552804 0.522401

C 1.284883 -1.646207 -0.039594

H 1.685538 1.785956 1.485186

H -0.042408 1.878219 1.111010

H 1.077119 3.122356 0.515570

H 2.126470 1.427364 -1.060831

H -4.063028 0.437210 0.146504

H -3.835542 -1.302810 -0.071202

H -3.422202 -0.544299 1.471955

H 0.613564 -0.191710 -1.947199

H 3.017018 -0.615874 0.517588

H 2.937329 -2.400591 1.016938

H 0.569332 -2.453271 -0.135579

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -434.595 | 45.4317 | 82.2247 |
| 88.0829 | 93.2088 | 109.6301 |
| 134.9277 | 197.3907 | 221.1702 |
| 266.1079 | 343.9467 | 356.8756 |
| 416.3729 | 517.2518 | 602.767 |
| 719.8921 | 791.9487 | 799.6389 |
| 909.2754 | 916.7702 | 946.1862 |
| 950.5987 | 1047.667 | 1052.544 |
| 1058.456 | 1087.256 | 1101.287 |
| 1171.472 | 1258.261 | 1390.436 |
| 1399.607 | 1415.633 | 1438.022 |
| 1480.281 | 1484.908 | 1489.397 |
| 1489.836 | 1581.808 | 1671.354 |
| 2378.403 | 3031.504 | 3050.515 |
| 3088.966 | 3095.992 | 3120.806 |
| 3125.026 | 3138.966 | 3173.682 |
| 3175.347 | 3191.172 | 3228.673 |

***i20 – p53***

C 2.478547 -1.434451 -0.129401

C 1.006740 -1.250170 0.007573

C -1.106873 -0.076263 0.040737

C -2.308243 -0.057590 0.011080

C -3.765221 -0.044139 -0.011626

C 0.334642 -0.060951 0.040694

C 2.014634 1.802702 0.192724

C 0.947651 1.238543 -0.358540

H 2.941589 -1.561373 0.857838

H 2.957890 -0.579954 -0.610004

H 2.698787 -2.339269 -0.701540

H 0.413294 -2.145407 0.168104

H -4.152588 -0.820885 -0.675728

H -4.170927 -0.217851 0.988278

H -4.137903 0.920546 -0.364594

H 0.478605 0.204759 1.895509

H 2.512254 1.358511 1.048476

H 2.408000 2.740058 -0.183546

H 0.439740 1.734775 -1.182242

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -973.727 | 54.9598 | 77.7853 |
| 105.4467 | 124.7403 | 193.9196 |
| 210.8763 | 240.8866 | 299.8534 |
| 334.2505 | 405.7076 | 430.0644 |
| 473.9674 | 509.9587 | 519.2085 |
| 569.1114 | 728.2473 | 755.0862 |
| 832.5555 | 933.6977 | 973.8319 |
| 989.5589 | 1029.341 | 1054.298 |
| 1056.272 | 1061.378 | 1104.115 |
| 1139.457 | 1260.157 | 1335.234 |
| 1353.127 | 1414.822 | 1419.834 |
| 1458.076 | 1475.529 | 1483.453 |
| 1486.861 | 1493.335 | 1607.789 |
| 1728.772 | 2382.693 | 3022.497 |
| 3049.75 | 3092.696 | 3121.933 |
| 3123.796 | 3139.469 | 3151.133 |
| 3164.769 | 3188.261 | 3246.692 |

***i40 – p49***

C -0.549728 2.328425 -0.400714

C -0.390332 1.060505 0.010682

C 0.890158 0.427263 -0.005134

C 1.947661 -0.146651 0.002418

C 3.231396 -0.834252 0.003020

C -1.545073 0.225121 0.527313

C -1.732140 -2.218308 -0.002776

C -1.840672 -0.948246 -0.366169

H -0.282622 3.488614 1.524732

H -1.532407 2.786174 -0.417389

H 0.280551 2.900997 -0.795097

H 3.812393 -0.569139 0.890188

H 3.089842 -1.917645 0.000374

H 3.817496 -0.563688 -0.878692

H -2.429752 0.865498 0.602888

H -1.306135 -0.131467 1.534460

H -1.415607 -2.494355 0.998846

H -1.953323 -3.025929 -0.691478

H -2.148061 -0.702202 -1.380673

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -406.423 | 33.74 | 48.7313 |
| 60.8679 | 114.9912 | 133.429 |
| 157.647 | 223.9563 | 246.3977 |
| 316.2391 | 349.7461 | 394.0397 |
| 438.3622 | 568.6378 | 600.7756 |
| 643.6699 | 732.3038 | 782.8881 |
| 918.7324 | 945.3402 | 949.1915 |
| 964.977 | 976.3001 | 1041.957 |
| 1053.923 | 1057.459 | 1083.426 |
| 1132.256 | 1243.981 | 1312.25 |
| 1334.56 | 1341.75 | 1417.99 |
| 1442.66 | 1454.172 | 1482.31 |
| 1482.796 | 1483.738 | 1664.694 |
| 1738.558 | 2369.241 | 3047.057 |
| 3048.128 | 3098.321 | 3119.289 |
| 3123.535 | 3142.778 | 3158.375 |
| 3160.564 | 3235.783 | 3257.668 |

***i40 – p50***

C -0.223922 2.550779 0.102111

C -0.233273 1.050468 -0.007033

C 0.874771 0.342769 0.076736

C 1.935923 -0.338014 0.151695

C 3.042656 -1.049905 0.212100

C -1.586578 0.406224 -0.213009

C -2.219155 -1.949188 0.336702

C -1.559703 -1.078542 -0.413999

H 0.781675 2.935467 0.268382

H -0.865835 2.874812 0.928536

H -0.625836 3.000328 -0.812382

H 4.004001 -0.578721 0.385347

H 3.012177 -2.132915 0.160604

H 3.733159 -1.176899 -2.037075

H -2.050138 0.886916 -1.086479

H -2.225960 0.661236 0.641581

H -2.829932 -1.628092 1.175795

H -2.170494 -3.014695 0.142778

H -0.947135 -1.434982 -1.238911

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -368.754 | 36.3281 | 77.1832 |
| 92.6951 | 127.4912 | 147.3141 |
| 160.2883 | 214.4195 | 226.9791 |
| 306.4079 | 376.8117 | 411.0406 |
| 425.0189 | 555.7382 | 573.7382 |
| 596.5217 | 632.4943 | 734.6214 |
| 880.2168 | 904.5933 | 935.3421 |
| 959.3042 | 996.3756 | 1033.917 |
| 1034.337 | 1047.461 | 1126.648 |
| 1161.315 | 1209.5 | 1261.23 |
| 1329.191 | 1358.145 | 1412.914 |
| 1445.808 | 1454.19 | 1475.531 |
| 1488.708 | 1489.913 | 1719.681 |
| 1746.038 | 2191.595 | 3016.325 |
| 3037.873 | 3056.496 | 3095.861 |
| 3146.676 | 3148.767 | 3157.387 |
| 3171.401 | 3235.654 | 3240.07 |

***i53 – p82***

C 0.084520 2.428453 -0.177933

C -0.063421 1.092212 -0.109372

C 3.223925 -1.341621 0.040362

C 2.048040 -0.483102 -0.015474

C 1.088424 0.240357 -0.060855

C -1.397012 0.477759 -0.069843

C -1.638691 -0.830154 0.008700

C -3.002541 -1.440834 0.054447

H 1.063903 2.885845 -0.230503

H 0.137830 3.056690 2.133312

H -0.781721 3.077811 -0.236829

H 3.702225 -1.277289 1.021049

H 3.956622 -1.043555 -0.713559

H 2.955832 -2.385423 -0.139281

H -2.229617 1.177321 -0.106792

H -0.793365 -1.514172 0.046656

H -3.139165 -2.152185 -0.766461

H -3.786623 -0.683366 -0.012706

H -3.145389 -2.000106 0.984919

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -382.64 | 79.9315 | 109.258 |
| 113.0521 | 122.8832 | 135.8928 |
| 188.4983 | 205.9088 | 211.8894 |
| 218.9841 | 313.541 | 388.9082 |
| 397.4874 | 455.0025 | 623.9136 |
| 646.1045 | 676.5823 | 753.2916 |
| 856.6109 | 926.4862 | 927.8379 |
| 1008.972 | 1012.513 | 1057.907 |
| 1063.339 | 1074.854 | 1085.743 |
| 1136.177 | 1303.746 | 1337.618 |
| 1367.273 | 1421.448 | 1421.895 |
| 1440.946 | 1484.453 | 1487.732 |
| 1490.127 | 1498.341 | 1649.621 |
| 1748.303 | 2378.8 | 3040.502 |
| 3052.342 | 3100.568 | 3123.762 |
| 3127.636 | 3128.05 | 3163.674 |
| 3168.163 | 3169.762 | 3268.068 |

***i53 – p86***

C 0.149837 2.500690 -0.044567

C 0.006925 1.000554 0.004871

C 3.156574 -1.299068 0.188340

C 2.091687 -0.522934 0.132892

C 1.077469 0.222409 0.070855

C -1.360689 0.465754 -0.023416

C -1.693466 -0.826304 0.012840

C -3.093396 -1.346243 -0.016332

H 1.196408 2.802386 -0.026625

H -0.362113 2.957393 0.808879

H -0.314936 2.895875 -0.953723

H 3.060199 -2.377372 0.250592

H 4.154568 -0.876721 0.229426

H 3.678561 -1.732135 -2.182911

H -2.150686 1.212951 -0.079002

H -0.896847 -1.566162 0.068266

H -3.240525 -2.018920 -0.867656

H -3.824748 -0.537983 -0.085848

H -3.309523 -1.928463 0.885701

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -365.932 | 35.5011 | 74.7027 |
| 112.4982 | 130.1924 | 157.9593 |
| 161.384 | 178.6927 | 198.1131 |
| 230.6495 | 305.5986 | 377.4702 |
| 436.2956 | 469.8005 | 557.6145 |
| 599.977 | 623.0446 | 736.1143 |
| 828.9437 | 856.9317 | 933.8628 |
| 1008.484 | 1016.274 | 1035.519 |
| 1052.553 | 1071.67 | 1101.32 |
| 1174.294 | 1238.672 | 1334.475 |
| 1361.463 | 1410.04 | 1417.965 |
| 1448.756 | 1481.43 | 1485.487 |
| 1492.922 | 1493.053 | 1694.71 |
| 1732.838 | 2160.702 | 3038.469 |
| 3041.398 | 3097.437 | 3103.232 |
| 3128.318 | 3151.908 | 3153.298 |
| 3156.178 | 3163.255 | 3239.311 |

***i53 – p88***

C 0.013915 2.299939 -0.059437

C -0.025012 0.797180 0.083670

C 3.579017 -1.126527 -0.058546

C 2.290582 -0.448452 -0.011910

C 1.217890 0.095681 0.031039

C -1.165845 0.129025 0.183989

C -2.218561 -0.545779 0.553930

C -3.247990 -1.191518 -0.327418

H 0.673139 2.729769 0.699258

H -0.983814 2.725820 0.048150

H 0.411380 2.573893 -1.040994

H 4.110771 -1.013653 0.889874

H 4.208595 -0.714752 -0.851255

H 3.446271 -2.194358 -0.248070

H -1.612654 0.572165 -1.862287

H -2.363665 -0.654488 1.629095

H -3.300843 -2.265275 -0.125115

H -3.014270 -1.043920 -1.382305

H -4.238883 -0.772506 -0.128248

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -527.801 | 57.871 | 92.5154 |
| 100.5609 | 120.761 | 149.2959 |
| 154.6799 | 182.6298 | 228.5547 |
| 273.1973 | 297.7758 | 371.3872 |
| 460.3482 | 478.0067 | 489.4643 |
| 572.3388 | 607.0486 | 676.1201 |
| 823.2983 | 872.4283 | 1003.031 |
| 1054.141 | 1056.767 | 1061.159 |
| 1064.504 | 1068.227 | 1105.122 |
| 1232 | 1294.971 | 1406.064 |
| 1410.744 | 1420.06 | 1439.668 |
| 1482.923 | 1486.862 | 1488.209 |
| 1491.001 | 1492.618 | 1512.187 |
| 2028.121 | 2367.776 | 3046.89 |
| 3051.194 | 3052.404 | 3110.85 |
| 3121.406 | 3123.469 | 3125.895 |
| 3128.476 | 3149.821 | 3153.062 |

***i53 – p12a***

C 0.161495 2.503743 -0.043748

C -0.109365 1.023072 0.009665

C 3.238536 -1.326507 -0.019973

C 2.037973 -0.501128 -0.011006

C 1.042304 0.175448 -0.000516

C -1.359473 0.523287 0.063605

C -1.697522 -0.883671 0.117466

C -2.956628 -1.342856 0.163937

H 0.779121 2.811476 0.804960

H -0.769078 3.073649 -0.025198

H 0.711443 2.759547 -0.954043

H 3.739121 -1.291393 0.951118

H 3.944806 -0.976912 -0.777096

H 2.994057 -2.368874 -0.237870

H -2.188897 1.226760 0.066694

H -0.870152 -1.587961 0.109521

H -3.168628 -2.402443 0.238291

H -3.511661 -1.606946 -2.054686

H -3.804058 -0.665230 0.201730

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -367.19 | 78.7441 | 97.9086 |
| 105.1915 | 132.4796 | 158.1846 |
| 177.4349 | 204.7996 | 230.473 |
| 280.501 | 306.7367 | 370.1766 |
| 392.9105 | 462.1125 | 593.2645 |
| 619.1588 | 677.4165 | 722.6434 |
| 915.8686 | 948.8868 | 952.7457 |
| 1041.446 | 1047.178 | 1056.97 |
| 1060.635 | 1064.136 | 1071.701 |
| 1185.851 | 1255.263 | 1325.285 |
| 1378.779 | 1417.799 | 1423.991 |
| 1459.249 | 1480.609 | 1486.313 |
| 1490.27 | 1497.216 | 1656.213 |
| 1698.147 | 2367.997 | 3045.607 |
| 3050.087 | 3110.843 | 3123.066 |
| 3123.695 | 3141.634 | 3156.163 |
| 3171.591 | 3187.577 | 3253.248 |

***i53 – i54***

C 0.369066 2.541430 0.256965

C 0.432693 1.066535 -0.045157

C -3.160799 -0.895482 -0.021172

C -1.880379 -0.199918 -0.034338

C -0.816286 0.362136 -0.046912

C 1.580238 0.421634 -0.300035

H -0.257681 3.057174 -0.476127

H 1.365202 2.987516 0.240496

H -0.076135 2.712569 1.241151

H -3.825177 -0.504792 -0.796248

H -3.659530 -0.772856 0.943712

H -3.023085 -1.964688 -0.199363

H 2.502511 1.007087 -0.277679

C 1.686084 -1.014551 -0.585414

C 1.787636 -2.009236 0.519654

H 1.569486 -1.356646 -1.609082

H 0.840218 -2.067419 1.076212

H 2.555947 -1.723922 1.248366

H 2.018728 -3.009315 0.147016

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -242.065 | 69.9868 | 91.9464 |
| 122.6563 | 128.6786 | 149.1504 |
| 180.7098 | 187.2968 | 304.5033 |
| 314.5049 | 353.0573 | 419.7422 |
| 482.9155 | 607.1665 | 630.8362 |
| 649.9328 | 837.0431 | 922.5731 |
| 990.5672 | 1014.651 | 1061.027 |
| 1063.246 | 1066.191 | 1071.999 |
| 1105.92 | 1153.574 | 1219.533 |
| 1339.645 | 1391.112 | 1408.063 |
| 1420.041 | 1426.937 | 1475.677 |
| 1478.848 | 1487.465 | 1490.034 |
| 1491.5 | 1500.955 | 1710.388 |
| 2375.12 | 2995.202 | 3048.431 |
| 3049.804 | 3054.78 | 3097.922 |
| 3114.031 | 3120.202 | 3125.041 |
| 3126.515 | 3142.868 | 3182.176 |

***i54 – p87***

C -0.928847 -2.365592 0.294132

C -0.607486 -0.926961 -0.031038

C 3.120401 0.207466 -0.271569

C 1.863322 -0.180296 -0.186949

C 0.653624 -0.523529 -0.096526

C -1.749900 -0.046382 -0.292764

C -1.810811 1.284513 -0.163053

C -0.724850 2.201788 0.303699

H -1.484048 -2.822523 -0.531779

H -1.562735 -2.421149 1.184653

H -0.023272 -2.945300 0.469196

H 3.373905 1.217138 -0.576635

H 3.934570 -0.486642 -0.093981

H 3.594631 1.026797 1.975692

H -2.655956 -0.564818 -0.598890

H -2.759054 1.754184 -0.412367

H -0.099589 2.526484 -0.535578

H -0.061804 1.713035 1.020530

H -1.149366 3.096743 0.763564

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -369.083 | 45.2278 | 74.2422 |
| 104.0268 | 120.9096 | 135.3467 |
| 160.5343 | 185.5847 | 256.3357 |
| 296.5459 | 312.8616 | 364.7561 |
| 497.5633 | 523.3996 | 559.6774 |
| 591.9835 | 652.3116 | 729.8193 |
| 749.9379 | 859.3713 | 932.4095 |
| 992.6322 | 1004.524 | 1033.177 |
| 1050.916 | 1064.2 | 1087.795 |
| 1160.466 | 1223.025 | 1299.727 |
| 1403.867 | 1407.695 | 1445.465 |
| 1457.439 | 1485.234 | 1486.206 |
| 1487.995 | 1498.366 | 1694.513 |
| 1719.472 | 2172.283 | 3040.788 |
| 3043.047 | 3102.731 | 3107.157 |
| 3138.184 | 3150.163 | 3155.527 |
| 3160.49 | 3181.577 | 3237.358 |

***i54 – p84***

C -0.776356 -2.331881 -0.272566

C -0.609925 -1.005086 -0.104045

C 3.225485 0.412183 0.064983

C 1.860097 -0.090268 -0.003098

C 0.724026 -0.481282 -0.057108

C -1.791318 -0.144402 0.072004

C -1.907276 1.186861 0.097537

C -0.867698 2.251410 -0.070217

H -1.768865 -2.765502 -0.319937

H -0.748481 -3.154075 1.990087

H 0.070125 -2.990530 -0.418498

H 3.765091 0.197505 -0.860840

H 3.768785 -0.054099 0.890673

H 3.233078 1.494061 0.220975

H -2.709633 -0.713356 0.194075

H -2.914906 1.565118 0.258743

H -1.225207 3.006078 -0.777264

H 0.084176 1.864536 -0.425191

H -0.696367 2.765054 0.882241

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -360.284 | 50.5411 | 66.5412 |
| 80.2933 | 120.7931 | 133.289 |
| 147.6699 | 187.5279 | 250.7723 |
| 305.4416 | 333.2753 | 353.6426 |
| 413.633 | 532.6337 | 619.7326 |
| 641.0412 | 713.9394 | 740.7816 |
| 807.02 | 902.2903 | 928.626 |
| 979.8398 | 1021.935 | 1053.589 |
| 1058.289 | 1078.163 | 1079.994 |
| 1122.821 | 1295.573 | 1361.287 |
| 1410.569 | 1416.043 | 1428.884 |
| 1462.986 | 1480.307 | 1487.866 |
| 1493.24 | 1498.543 | 1636.302 |
| 1742.12 | 2377.128 | 3043.902 |
| 3050.188 | 3097.41 | 3122.834 |
| 3124.769 | 3147.41 | 3170.404 |
| 3176.196 | 3184.374 | 3270.553 |

***i54 – p88***

C -0.129992 -2.240935 0.357874

C -0.101726 -0.779673 -0.022797

C 3.556317 1.044126 0.032005

C 2.250768 0.398491 0.007028

C 1.163855 -0.117638 -0.017895

C -1.191455 -0.139540 -0.423702

C -2.274543 0.574547 -0.557188

C -2.953892 1.278205 0.587726

H 0.469624 -2.825686 -0.345676

H -1.151085 -2.622885 0.352916

H 0.300529 -2.376643 1.353551

H 4.209310 0.633922 -0.742669

H 4.044346 0.896542 0.998778

H 3.458482 2.118735 -0.139477

H -1.117101 -0.996680 -2.340614

H -2.724037 0.678600 -1.540870

H -3.011046 2.353311 0.393669

H -2.416779 1.122359 1.524020

H -3.978233 0.912931 0.708062

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -559.876 | 59.2324 | 102.7604 |
| 115.6323 | 127.129 | 150.1994 |
| 153.7791 | 180.828 | 204.5605 |
| 257.7116 | 304.8666 | 346.3962 |
| 413.5254 | 490.932 | 509.3978 |
| 564.0395 | 620.0303 | 666.6027 |
| 836.6709 | 879.7277 | 996.1451 |
| 1056.038 | 1057.966 | 1061.977 |
| 1064.527 | 1066.551 | 1109.024 |
| 1233.053 | 1300.388 | 1408.68 |
| 1412.822 | 1420.21 | 1432.344 |
| 1480.775 | 1488.404 | 1489.502 |
| 1493.158 | 1494.816 | 1508.723 |
| 2029.92 | 2369.786 | 3048.434 |
| 3049.522 | 3050.347 | 3112.022 |
| 3117.182 | 3120.854 | 3126.693 |
| 3146.55 | 3156.534 | 3165.823 |

***i54 – p12b***

C -0.822484 -2.443536 -0.023055

C -0.683721 -0.941169 -0.003383

C 3.200080 0.328293 0.009466

C 1.815396 -0.121847 -0.004577

C 0.659381 -0.459238 -0.010563

C -1.765377 -0.137805 0.043866

C -1.836733 1.317161 0.082113

C -0.900981 2.202447 -0.289300

H -0.362524 -2.858927 -0.924244

H -1.871815 -2.742611 0.003076

H -0.309639 -2.886270 0.835636

H 3.693988 0.095972 -0.937537

H 3.758658 -0.160574 0.811581

H 3.253473 1.408397 0.167352

H -2.728463 -0.639662 0.093756

H -2.782286 1.709188 0.450027

H -1.101739 3.265702 -0.227051

H 0.042023 1.897747 -0.723883

H 0.414951 2.445208 1.623873

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -289.489 | 54.8906 | 67.5592 |
| 83.9254 | 154.8187 | 160.9089 |
| 178.2617 | 210.7193 | 243.7018 |
| 272.4511 | 314.8119 | 349.45 |
| 370.2234 | 528.729 | 590.8954 |
| 634.0991 | 674.8159 | 716.4383 |
| 901.3527 | 961.7186 | 964.3436 |
| 1019.38 | 1038.87 | 1054.769 |
| 1056.984 | 1072.625 | 1073.194 |
| 1144.337 | 1244.646 | 1348.283 |
| 1414.02 | 1418.387 | 1427.015 |
| 1466.076 | 1479.313 | 1479.859 |
| 1488.02 | 1502.036 | 1661.019 |
| 1703.986 | 2365.431 | 3047.804 |
| 3050.291 | 3114.996 | 3122.163 |
| 3125.778 | 3138.919 | 3149.756 |
| 3171.932 | 3179.616 | 3274.48 |

***i40 – p12a***

C -0.008758 2.472293 0.102070

C -0.188253 0.980272 0.048807

C 1.000838 0.197551 0.020418

C 2.028820 -0.430658 0.000842

C 3.266329 -1.198507 -0.019352

C -1.421033 0.408806 -0.023016

C -2.889489 -1.559761 0.111504

C -1.673809 -1.027732 -0.003221

H 0.599522 2.757217 0.964968

H -0.971726 2.981641 0.165910

H 0.512133 2.823887 -0.793952

H 3.780204 -1.127554 0.942841

H 3.066885 -2.253577 -0.221008

H 3.943131 -0.825475 -0.792183

H -1.714422 0.776940 -2.018838

H -2.286285 1.057986 0.082576

H -3.777112 -0.937661 0.179640

H -3.036605 -2.632909 0.137079

H -0.803592 -1.674082 -0.075337

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -667.503 | 80.5817 | 105.8845 |
| 112.0831 | 118.9631 | 162.1249 |
| 190.1157 | 211.6824 | 289.3554 |
| 306.5873 | 330.3088 | 394.738 |
| 402.9932 | 459.6247 | 588.0375 |
| 619.7779 | 681.497 | 704.485 |
| 928.1377 | 947.0588 | 951.8282 |
| 1040.737 | 1043.209 | 1057.474 |
| 1061.027 | 1064.279 | 1067.629 |
| 1178.715 | 1246.829 | 1316.895 |
| 1377.835 | 1419.672 | 1425.467 |
| 1452.134 | 1478.084 | 1486.701 |
| 1489.89 | 1496.718 | 1613.222 |
| 1717.338 | 2353.197 | 3045.197 |
| 3050.469 | 3109.823 | 3122.023 |
| 3126.226 | 3143.135 | 3152.726 |
| 3176.196 | 3184.86 | 3247.376 |

***i47 – p60***

C 0.502343 0.948231 0.036135

C -0.644266 0.219976 0.004603

C 4.232103 -0.718450 0.035565

C 2.901521 -0.125406 0.033789

C 1.800938 0.360533 0.023980

C -1.954443 0.815207 0.125993

C -3.129304 0.168881 0.089313

C -3.356363 -1.299702 -0.084050

H 0.547951 1.653358 -1.887866

H 0.449597 2.010678 0.260202

H -0.561332 -0.851659 -0.142645

H 4.321685 -1.472808 0.821485

H 4.996321 0.043617 0.206160

H 4.441565 -1.201203 -0.922513

H -1.972793 1.894609 0.258994

H -4.030464 0.767225 0.199406

H -3.880212 -1.709597 0.785677

H -2.433082 -1.863809 -0.217054

H -3.994413 -1.486029 -0.953809

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -736.313 | 61.4539 | 70.2686 |
| 97.9794 | 112.3534 | 123.3138 |
| 186.0452 | 223.5329 | 312.4785 |
| 323.3808 | 358.2276 | 372.9848 |
| 412.2363 | 498.3122 | 511.7121 |
| 627.3834 | 754.4902 | 815.4519 |
| 897.6473 | 940.2308 | 980.6314 |
| 1031.787 | 1048.417 | 1056.302 |
| 1062.461 | 1065.679 | 1172.52 |
| 1203.012 | 1261.15 | 1283.81 |
| 1318.854 | 1406.743 | 1423.71 |
| 1445.09 | 1482.891 | 1483.236 |
| 1489.379 | 1493.199 | 1612.876 |
| 1703.808 | 2375.746 | 3046.739 |
| 3047.929 | 3101.216 | 3119.862 |
| 3122.702 | 3147.481 | 3159.307 |
| 3167.464 | 3181.598 | 3199.326 |

***i51 – p76'***

C -0.655922 1.618403 0.509680

C 0.204651 2.117481 -0.398534

C -3.221670 -1.472317 -0.219313

C -2.304216 -0.370488 0.039369

C -1.548552 0.546112 0.243739

C 2.220651 0.642293 -0.229396

C 1.899452 -0.595095 0.053805

C 2.861906 -1.754785 0.120076

H -0.654801 2.010215 1.522670

H 0.829923 2.966855 -0.153780

H 0.182611 1.790623 -1.430661

H -2.690156 -2.427719 -0.234409

H -3.716489 -1.346837 -1.185728

H -3.992192 -1.526254 0.553589

H 3.147250 1.152278 -0.464821

H 0.852284 -0.825198 0.258181

H 2.831874 -2.219884 1.110137

H 3.887590 -1.441053 -0.083199

H 2.584310 -2.522649 -0.608533

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -208.024 | 40.7744 | 64.2382 |
| 101.8548 | 108.8876 | 118.6484 |
| 152.0355 | 185.8778 | 212.9364 |
| 242.5187 | 332.6823 | 408.8738 |
| 412.4473 | 546.6623 | 675.0456 |
| 716.0864 | 730.5223 | 861.576 |
| 909.361 | 911.1668 | 947.651 |
| 976.1309 | 1051.248 | 1058.322 |
| 1064.511 | 1070.947 | 1108.147 |
| 1201.293 | 1303.331 | 1314.585 |
| 1402.865 | 1423.688 | 1439.867 |
| 1484.301 | 1488.005 | 1492.432 |
| 1492.921 | 1616.371 | 1702.698 |
| 2350.824 | 3043.706 | 3048.938 |
| 3109.159 | 3116.28 | 3119.095 |
| 3124.379 | 3139.105 | 3167.786 |
| 3181.288 | 3222.1 | 3266.822 |

***i51 – p78***

C 0.762456 -1.719519 -0.115331

C -0.739712 -1.701614 0.014377

C 3.049818 1.420028 0.173272

C 2.278830 0.355724 0.084748

C 1.539865 -0.664034 -0.016495

C -1.313901 -0.369595 0.391114

C -2.212688 0.294052 -0.325075

C -2.796711 1.622097 0.045716

H 1.223235 -2.687343 -0.303339

H -1.016447 -2.454143 0.765485

H -1.176912 -2.050543 -0.929094

H 2.630592 2.396037 0.392781

H 3.176462 2.201770 -2.012136

H 4.129051 1.336635 0.103163

H -0.943895 0.064663 1.318727

H -2.565713 -0.144016 -1.258383

H -2.606159 2.364464 -0.735729

H -2.374898 1.996229 0.981382

H -3.883050 1.553411 0.163187

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -388.068 | 44.1582 | 80.6433 |
| 113.2609 | 139.3633 | 173.5502 |
| 192.5583 | 210.3008 | 265.1828 |
| 280.0362 | 294.0545 | 390.5442 |
| 488.3508 | 522.5711 | 577.216 |
| 628.8706 | 786.4745 | 828.4697 |
| 856.5424 | 888.9298 | 936.6948 |
| 973.5045 | 1015.163 | 1032.906 |
| 1035.955 | 1076.156 | 1113.94 |
| 1140.247 | 1226.735 | 1299.165 |
| 1332.461 | 1347.226 | 1379.889 |
| 1420.693 | 1452.644 | 1470.627 |
| 1490.049 | 1498.502 | 1705.885 |
| 1779.987 | 2187.865 | 3022.302 |
| 3037.37 | 3060.11 | 3098.554 |
| 3121.931 | 3142.19 | 3148.954 |
| 3149.727 | 3151.795 | 3236.907 |

***i51 – p58***

C -0.700270 1.605276 -0.147778

C 0.639892 1.404040 -0.032644

C -3.527650 -1.326627 0.047162

C -2.513602 -0.283621 -0.023191

C -1.672561 0.578326 -0.077702

C 1.272434 0.092763 0.038931

C 2.589453 -0.094346 -0.059665

C 3.270178 -1.424366 -0.016382

H -1.069706 2.618118 -0.271819

H 0.806873 1.922178 1.918801

H 1.294150 2.258021 -0.182484

H -4.022236 -1.321913 1.022107

H -3.081851 -2.312957 -0.102539

H -4.291748 -1.178099 -0.720151

H 0.610462 -0.761058 0.163697

H 3.233313 0.776265 -0.179322

H 3.822856 -1.609645 -0.943376

H 2.552355 -2.235615 0.122430

H 3.998291 -1.463959 0.800275

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -746.556 | 64.473 | 96.6387 |
| 114.6888 | 136.9246 | 181.0166 |
| 210.2182 | 212.3537 | 273.2793 |
| 288.768 | 363.5371 | 412.1458 |
| 431.4733 | 472.3743 | 539.4245 |
| 650.3003 | 785.414 | 798.0433 |
| 847.4776 | 953.6134 | 986.7315 |
| 1024.227 | 1056.389 | 1061.652 |
| 1071.251 | 1080.836 | 1139.561 |
| 1188.164 | 1246.914 | 1298.619 |
| 1333.057 | 1418.228 | 1420.753 |
| 1434.289 | 1483.543 | 1484.505 |
| 1490.746 | 1497.856 | 1591.893 |
| 1744.651 | 2349.805 | 3040.205 |
| 3046.926 | 3099.337 | 3119.22 |
| 3121.805 | 3129.358 | 3153.879 |
| 3174.68 | 3181.247 | 3196.911 |

***i47 – p68***

C 0.540954 1.589360 0.021063

C -0.828564 0.978867 -0.129991

C 3.670128 -1.089320 0.083193

C 2.559774 -0.143627 0.059463

C 1.650378 0.639716 0.042284

C -1.094780 -0.322646 -0.228621

C -2.436115 -0.896952 -0.348133

C -3.559291 -0.375821 0.165269

H 0.698839 2.311397 -0.789647

H 0.558069 2.181627 0.944850

H -1.642920 1.699024 -0.168253

H 3.317206 -2.107164 -0.100028

H 4.172271 -1.075307 1.053567

H 4.407511 -0.843324 -0.684720

H -0.262199 -1.022057 -0.244008

H -2.500445 -1.848284 -0.870681

H -4.523648 -0.835453 -0.014706

H -3.553764 0.561351 0.712456

H -3.685824 -1.299266 2.174012

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -469.282 | 56.1227 | 74.9325 |
| 90.2922 | 145.7041 | 166.4958 |
| 198.9696 | 224.7347 | 242.5523 |
| 257.6873 | 305.0724 | 392.7192 |
| 399.3814 | 536.0896 | 640.8246 |
| 694.0204 | 763.0793 | 832.1932 |
| 963.9069 | 975.6048 | 982.6599 |
| 1006.177 | 1020.969 | 1038.38 |
| 1051.831 | 1064.023 | 1104.017 |
| 1177.694 | 1242.533 | 1302.394 |
| 1315.613 | 1351.481 | 1378.089 |
| 1416.375 | 1455.844 | 1467.361 |
| 1486.22 | 1490.795 | 1665.457 |
| 1741.735 | 2399.407 | 3031.732 |
| 3054.528 | 3059.161 | 3127.187 |
| 3128.215 | 3156.106 | 3165.265 |
| 3170.73 | 3179.359 | 3250.186 |

***i47 – p71***

C 0.495505 1.888677 -0.269725

C -0.979318 1.584424 -0.141913

C 2.923993 -1.412261 0.125382

C 2.070424 -0.238839 -0.018232

C 1.366871 0.726052 -0.133432

C -1.474000 0.469475 0.360396

C -1.971479 -0.723211 0.549756

C -2.239521 -1.689997 -0.571449

H 0.667537 2.364994 -1.241752

H 0.767351 2.639525 0.483512

H -1.659094 2.396799 -0.387979

H 2.335419 -2.330136 0.052565

H 3.428444 -1.410276 1.094735

H 3.688406 -1.437250 -0.655108

H -1.251547 1.035223 2.249700

H -2.200159 -1.049728 1.559385

H -1.691888 -2.622936 -0.408770

H -1.935367 -1.272452 -1.531871

H -3.303946 -1.939680 -0.619112

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -747.176 | 28.4267 | 58.351 |
| 89.1878 | 93.6078 | 140.7065 |
| 157.4521 | 205.8575 | 225.5673 |
| 291.2073 | 320.1432 | 396.4524 |
| 468.0297 | 478.2203 | 586.929 |
| 648.0682 | 711.831 | 762.4254 |
| 885.2881 | 890.8304 | 956.1864 |
| 977.8888 | 1054.455 | 1062.268 |
| 1063.686 | 1107.638 | 1146.655 |
| 1188.456 | 1242.56 | 1299.579 |
| 1360.661 | 1411.241 | 1418.62 |
| 1447.383 | 1478.049 | 1483.413 |
| 1484.83 | 1492.552 | 1505.352 |
| 2029.372 | 2405.707 | 3031.067 |
| 3046.299 | 3053.539 | 3064.728 |
| 3109.26 | 3125.152 | 3127.237 |
| 3147.835 | 3164.955 | 3185.424 |

***i47 – p61***

C 0.458392 1.396454 -0.102886

C -0.812153 0.910287 -0.104164

C 3.825852 -0.917023 -0.009684

C 2.622092 -0.097198 -0.043768

C 1.627537 0.579602 -0.062385

C -1.152575 -0.482169 0.062867

C -2.391787 -0.997174 0.083520

C -3.690577 -0.268393 -0.060177

H 0.616368 2.448562 -0.315459

H 0.566086 2.091162 1.829186

H -1.613388 1.633734 -0.209071

H 3.662272 -1.871392 -0.516289

H 4.120307 -1.126910 1.021985

H 4.657576 -0.407821 -0.502566

H -0.314236 -1.162879 0.181230

H -2.480020 -2.072394 0.219977

H -4.254291 -0.661597 -0.912374

H -3.568805 0.805355 -0.204178

H -4.312555 -0.422135 0.827611

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -722.306 | 43.5918 | 75.4675 |
| 116.2242 | 119.4627 | 170.751 |
| 210.5343 | 231.715 | 259.7892 |
| 322.04 | 370.2661 | 404.0998 |
| 411.0979 | 554.814 | 564.0046 |
| 680.0445 | 759.7968 | 784.4269 |
| 841.0199 | 942.1861 | 990.5533 |
| 1028.832 | 1031.301 | 1055.918 |
| 1062.465 | 1063.765 | 1146.144 |
| 1183.257 | 1258.808 | 1298.482 |
| 1381.916 | 1419.363 | 1421.502 |
| 1479.365 | 1486.022 | 1487.309 |
| 1490.744 | 1495.221 | 1593.561 |
| 1701.428 | 2372.662 | 3046.194 |
| 3048.714 | 3100.915 | 3120.446 |
| 3124.004 | 3144.321 | 3164.807 |
| 3184.945 | 3192.163 | 3206.694 |

***i29 – p10a***

C 0.608284 -0.732193 -0.511003

C -0.479081 -0.414796 0.221016

C 4.376604 0.648289 0.226124

C 3.030323 0.157402 -0.035651

C 1.914281 -0.245051 -0.245010

C -1.802245 -0.912213 -0.048934

C -2.894269 -0.560753 0.670322

C -3.793620 1.483661 -0.359048

H 0.500748 -1.403430 -1.360193

H -0.361757 0.257102 1.068309

H 4.375443 1.732479 0.365451

H 5.045408 0.412620 -0.605269

H 4.787984 0.192576 1.130843

H -1.918338 -1.573192 -0.904889

H -2.793746 0.019083 1.581347

H -3.855889 -1.024044 0.490874

H -4.135757 1.062902 -1.295454

H -2.868726 2.045104 -0.366355

H -4.537033 1.732727 0.388444

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -333.888 | 47.0606 | 81.9299 |
| 87.0642 | 91.0399 | 99.4784 |
| 146.1298 | 219.4466 | 243.5907 |
| 304.3812 | 350.6787 | 410.6322 |
| 443.7574 | 456.0347 | 476.3452 |
| 551.6218 | 716.9319 | 730.4918 |
| 823.4596 | 872.0199 | 909.3653 |
| 944.902 | 974.7312 | 1018.409 |
| 1050.618 | 1056.233 | 1194.188 |
| 1213.683 | 1279.538 | 1297.553 |
| 1328.488 | 1414.475 | 1415.846 |
| 1416.667 | 1451.325 | 1482.921 |
| 1488.368 | 1592.697 | 1647.773 |
| 2361.004 | 3050.116 | 3108.193 |
| 3120.059 | 3125.633 | 3161.082 |
| 3164.181 | 3169.213 | 3176.098 |
| 3258.439 | 3280.137 | 3285.481 |

***i29 – p72***

C 0.618262 -1.005676 -0.002995

C -0.630875 -0.263243 0.013595

C 4.141748 0.660262 0.172820

C 2.951542 0.096359 0.122388

C 1.814656 -0.445246 0.061261

C -1.827797 -0.855275 -0.051934

C -3.161527 -0.171243 -0.042323

C -3.125864 1.350815 0.029357

H 0.554689 -2.090205 -0.075107

H -0.548879 0.817334 0.083235

H 4.248678 1.735075 0.270175

H 4.694920 1.044408 -2.155601

H 5.045293 0.060268 0.179714

H -1.860533 -1.942162 -0.120114

H -3.741543 -0.567803 0.800830

H -3.711654 -0.485780 -0.938339

H -2.595455 1.775542 -0.827194

H -2.627297 1.694757 0.939529

H -4.139083 1.758039 0.029861

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -379.17 | 65.8514 | 69.292 |
| 107.9532 | 151.5603 | 175.4659 |
| 202.442 | 214.1207 | 269.6654 |
| 310.9262 | 319.9826 | 342.9316 |
| 492.4462 | 533.3157 | 591.6027 |
| 608.747 | 750.7108 | 864.335 |
| 881.9056 | 887.7854 | 903.3962 |
| 951.8497 | 1015.173 | 1032.841 |
| 1036.797 | 1107.32 | 1112.347 |
| 1180.609 | 1263.491 | 1294.971 |
| 1344.753 | 1351.467 | 1384.176 |
| 1424.998 | 1452.82 | 1476.623 |
| 1504.288 | 1516.561 | 1682.497 |
| 1730.678 | 2159.138 | 3030.257 |
| 3054.356 | 3055.621 | 3127.579 |
| 3135.149 | 3146.048 | 3147.487 |
| 3148.788 | 3189.163 | 3234.851 |

***i29 – p74***

C -0.399049 -0.773228 0.743817

C 0.704237 -0.756682 0.026568

C -4.099085 0.551279 -0.363194

C -2.777994 0.078893 0.027803

C -1.678593 -0.304379 0.328496

C 1.924774 -0.948742 -0.428230

C 3.007583 0.096607 -0.449514

C 2.715401 1.324469 0.403984

H -0.329491 -1.178465 1.751670

H 0.129668 0.500924 -1.407397

H -4.386467 0.138285 -1.333395

H -4.112912 1.641381 -0.441735

H -4.852053 0.253654 0.370593

H 2.137462 -1.895537 -0.921929

H 3.168916 0.395331 -1.493463

H 3.942541 -0.376719 -0.128877

H 2.576837 1.047981 1.452400

H 1.803099 1.824290 0.069181

H 3.538755 2.039576 0.344577

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -769.773 | 30.67 | 48.9259 |
| 75.4657 | 106.7871 | 137.8708 |
| 187.0924 | 251.5717 | 272.4826 |
| 305.2016 | 376.6453 | 407.7848 |
| 452.4375 | 484.1413 | 505.0227 |
| 649.5698 | 723.6414 | 806.0388 |
| 816.3709 | 868.4215 | 897.4526 |
| 1007.789 | 1054.572 | 1058.619 |
| 1094.32 | 1103.85 | 1128.148 |
| 1211.774 | 1292.962 | 1302.204 |
| 1370.82 | 1416.836 | 1422.751 |
| 1461.763 | 1483.003 | 1484.18 |
| 1484.682 | 1501.45 | 1508.405 |
| 2004.891 | 2381.953 | 3029.186 |
| 3046.698 | 3049.575 | 3065.292 |
| 3119.433 | 3121.878 | 3126.197 |
| 3131.149 | 3143.028 | 3144.445 |

***i49 – p77***

C 0.626683 1.539442 -0.448938

C -0.068969 0.653274 0.550741

C -3.871329 -0.693774 -0.175036

C -2.519723 -0.209695 0.080676

C -1.406258 0.185146 0.299788

C 1.081036 0.109945 -0.295947

C 2.367824 -0.185716 0.352327

C 3.177856 -1.192429 0.005085

H 1.274951 2.316472 -0.061008

H 0.082839 1.797713 -1.348396

H 0.166951 0.832027 1.594849

H -4.436283 0.017927 -0.782236

H -4.410579 -0.840094 0.764154

H -3.850153 -1.650059 -0.703799

H 0.783784 -0.572787 -1.084201

H 2.672901 0.493280 1.147132

H 2.886762 -1.913599 -0.751702

H 4.099077 -1.384737 0.541330

H 4.407033 -0.333304 -1.528290

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -483.468 | 63.1984 | 97.883 |
| 107.8222 | 114.4762 | 181.8521 |
| 239.1563 | 266.6159 | 309.0964 |
| 327.0914 | 360.4201 | 443.1214 |
| 507.9107 | 528.4887 | 687.6039 |
| 752.8808 | 841.0294 | 883.9615 |
| 939.4604 | 955.4844 | 966.0728 |
| 1009.585 | 1023.529 | 1055.83 |
| 1061.478 | 1074.701 | 1110.41 |
| 1113.403 | 1198.94 | 1231.465 |
| 1240.074 | 1317.002 | 1335.812 |
| 1413.135 | 1424.088 | 1473.786 |
| 1487.668 | 1489.745 | 1504.686 |
| 1685.855 | 2393.717 | 3052.995 |
| 3124.636 | 3126.553 | 3151.518 |
| 3152.902 | 3164.136 | 3167.623 |
| 3190.297 | 3248.133 | 3254.338 |

***i49 – p79***

C -0.739801 1.864668 0.178337

C -0.106912 0.731807 -0.663652

C 3.622017 -0.716892 0.232247

C 2.298967 -0.194286 -0.086430

C 1.202413 0.228559 -0.335367

C -1.288224 0.506905 0.205635

C -2.369116 -0.257633 0.348002

C -2.471973 -1.654556 -0.173428

H -1.286944 2.634872 -0.355477

H -0.156309 2.208825 1.024064

H -0.321849 0.771720 -1.728536

H 4.183377 -0.010851 0.849300

H 4.195906 -0.898730 -0.679967

H 3.546587 -1.660370 0.778699

H -0.334783 -0.152003 1.838404

H -3.193559 0.120323 0.948512

H -1.605208 -1.911655 -0.784879

H -3.378199 -1.781221 -0.774153

H -2.533246 -2.372337 0.651964

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -765.091 | 65.5116 | 82.2901 |
| 93.7383 | 121.483 | 170.7249 |
| 198.1281 | 283.4134 | 296.4731 |
| 334.7871 | 397.6419 | 448.3587 |
| 473.1485 | 525.3088 | 542.2157 |
| 700.6182 | 745.2103 | 813.2487 |
| 917.4789 | 954.6503 | 971.3015 |
| 1045.805 | 1054.545 | 1055.811 |
| 1057.049 | 1063.298 | 1102.148 |
| 1121.144 | 1140.597 | 1215.277 |
| 1336.758 | 1383.871 | 1415.671 |
| 1418.286 | 1460.33 | 1479.669 |
| 1486.485 | 1487.689 | 1495.119 |
| 1805.449 | 2394.17 | 3038.354 |
| 3051.702 | 3098.109 | 3123.861 |
| 3124.855 | 3133.822 | 3136.19 |
| 3149.245 | 3166.797 | 3230.178 |

***i49 – i50***

C 0.606946 1.676759 0.024561

C 0.139972 0.317413 0.403840

C -3.870102 -0.478984 -0.040730

C -2.448127 -0.198923 0.121509

C -1.277700 0.030703 0.259007

C 1.017572 -0.068079 -0.752333

C 2.305478 -0.537495 -0.672050

C 3.095898 -0.697106 0.587727

H 1.477530 2.096657 0.507016

H 0.025735 2.279200 -0.658730

H 0.521249 -0.019345 1.367398

H -4.368375 0.334580 -0.573733

H -4.355827 -0.593213 0.931538

H -4.024246 -1.401386 -0.606035

H 0.531802 -0.030166 -1.720318

H 2.822939 -0.720231 -1.608387

H 2.469387 -0.965259 1.443028

H 3.625576 0.228833 0.851517

H 3.854606 -1.475395 0.477527

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -612.645 | 57.6966 | 69.3084 |
| 94.9323 | 130.8484 | 159.1972 |
| 258.3995 | 283.0177 | 326.709 |
| 366.2595 | 488.1689 | 521.1382 |
| 547.5722 | 581.6779 | 656.2957 |
| 681.3974 | 768.0427 | 915.2776 |
| 943.1636 | 989.1783 | 1014.872 |
| 1032.05 | 1060.505 | 1065.335 |
| 1092.569 | 1157.991 | 1189.278 |
| 1222.386 | 1262.987 | 1347.924 |
| 1408.064 | 1425.292 | 1430.669 |
| 1462.439 | 1486.451 | 1486.764 |
| 1490.053 | 1502.886 | 1543.363 |
| 2397.5 | 3012.322 | 3049.459 |
| 3083.684 | 3117.274 | 3120.012 |
| 3124.818 | 3125.148 | 3181.75 |
| 3182.985 | 3213.899 | 3306.85 |

***i29 – p60***

C -0.560134 -0.946603 -0.064451

C 0.577071 -0.228660 -0.027086

C -4.312137 0.654147 0.051261

C -2.972193 0.084252 0.013149

C -1.860710 -0.378061 -0.019844

C 1.889028 -0.832935 -0.084410

C 3.068846 -0.179670 -0.063380

C 3.272254 1.306653 -0.070979

H -0.503863 -2.030541 -0.137698

H 0.501345 0.851795 0.043407

H -4.389676 1.412007 0.834941

H -5.058768 -0.118676 0.249081

H -4.558478 1.128302 -0.902542

H 1.912158 -1.918847 -0.138192

H 3.969583 -0.776927 -0.174557

H 3.500445 -0.509675 2.066802

H 2.406805 1.854665 0.303066

H 3.474325 1.652101 -1.090903

H 4.133978 1.581055 0.541040

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -512.886 | 64.933 | 74.329 |
| 94.3254 | 105.6365 | 122.2715 |
| 194.7726 | 207.4705 | 272.6061 |
| 298.6348 | 322.838 | 358.2957 |
| 410.1959 | 500.058 | 510.2742 |
| 629.192 | 768.5853 | 817.9533 |
| 889.8514 | 939.6307 | 973.3032 |
| 1017.989 | 1047.996 | 1053.56 |
| 1057.968 | 1063.788 | 1170.315 |
| 1209.849 | 1263.909 | 1297.698 |
| 1336.294 | 1404.087 | 1421.467 |
| 1445.451 | 1481.842 | 1485.278 |
| 1491.806 | 1494.38 | 1658.736 |
| 1680.438 | 2368.196 | 3046.972 |
| 3049.483 | 3111.75 | 3121.241 |
| 3124.287 | 3146.056 | 3158.903 |
| 3163.02 | 3186.701 | 3193.799 |

***i47 – i48***

C -0.112665 1.889546 -0.133648

C -1.410110 1.168585 -0.377251

C 3.042366 -0.749513 0.174240

C 1.943077 0.202248 0.063358

C 1.031365 0.977933 -0.025057

H 0.071725 2.611278 -0.934549

H -0.177387 2.473265 0.798339

H -2.053212 1.518323 -1.178624

H 2.793516 -1.689026 -0.326339

H 3.260524 -0.971372 1.221908

H 3.951619 -0.353222 -0.284639

C -1.907477 0.161441 0.570910

C -1.729429 -1.155010 0.473586

C -0.996533 -1.859615 -0.625584

H -2.455464 0.539068 1.438165

H -2.145758 -1.786215 1.255931

H -0.147827 -2.420027 -0.220474

H -0.612081 -1.154748 -1.364804

H -1.649211 -2.581020 -1.128249

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -224.914 | 48.9385 | 63.5769 |
| 128.0855 | 153.0838 | 190.841 |
| 204.0287 | 235.7266 | 284.0927 |
| 361.462 | 393.4041 | 450.1594 |
| 556.1002 | 629.5601 | 720.8304 |
| 770.2634 | 859.7106 | 938.8198 |
| 992.4449 | 999.4694 | 1059.553 |
| 1064.869 | 1075.196 | 1087.87 |
| 1116.192 | 1175.9 | 1226.16 |
| 1261.987 | 1324.026 | 1347.238 |
| 1403.054 | 1421.459 | 1437.746 |
| 1463.9 | 1485.133 | 1488.925 |
| 1490.751 | 1492.82 | 1739.727 |
| 2396.505 | 2983.556 | 3041.62 |
| 3049.114 | 3086.028 | 3090.305 |
| 3100.917 | 3120.013 | 3123.054 |
| 3136.821 | 3167.547 | 3183.37 |

***i50 – i52***

C 0.484592 1.782203 -0.065402

C -0.283132 0.512813 -0.296086

C 3.605155 -0.788844 0.027318

C 2.176952 -0.537244 -0.124992

C 1.093466 0.049021 -0.202416

C -1.211651 0.064695 0.786047

C -2.442441 -0.414525 0.632741

C -3.193089 -0.631967 -0.646170

H 0.775988 2.395494 -0.906000

H 0.575275 2.174174 0.938572

H -0.697354 0.426596 -1.299362

H 4.152177 0.135816 0.248378

H 4.024033 -1.219623 -0.886116

H 3.792794 -1.495786 0.840067

H -0.804709 0.149700 1.791058

H -2.980700 -0.691629 1.536601

H -3.435836 -1.692089 -0.770536

H -2.638111 -0.311480 -1.528747

H -4.142669 -0.088086 -0.630150

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -703.268 | 35.4715 | 88.2631 |
| 106.679 | 126.4738 | 133.5541 |
| 209.2924 | 250.5034 | 327.1187 |
| 364.1513 | 393.9482 | 496.8172 |
| 573.2426 | 619.9492 | 676.1589 |
| 720.2208 | 813.6582 | 871.6969 |
| 946.6307 | 1020.373 | 1034.554 |
| 1044.897 | 1060.363 | 1071.638 |
| 1084.865 | 1154.227 | 1194.453 |
| 1218.344 | 1292.424 | 1331.272 |
| 1414.027 | 1419.397 | 1439.218 |
| 1451.751 | 1479.941 | 1483.01 |
| 1486.24 | 1500.174 | 1767.024 |
| 2097.779 | 3021.788 | 3047.892 |
| 3092.736 | 3104.366 | 3116.112 |
| 3125.572 | 3140.607 | 3152.747 |
| 3168.654 | 3174.921 | 3290.999 |

***i27 – i48***

C 0.188131 0.983126 0.744336

C -0.672128 1.254791 -0.464663

C 3.764288 -0.783541 -0.301171

C 2.501522 -0.157716 0.075109

C 1.462180 0.355576 0.388035

C -1.888002 0.746833 -0.651493

H 0.391292 1.925220 1.267664

H -0.357274 0.342054 1.444400

H -0.239456 1.902678 -1.222164

H 4.612184 -0.158266 -0.010187

H 3.814622 -0.939514 -1.381716

H 3.878234 -1.755412 0.185548

H -2.408112 1.007975 -1.577150

C -2.583437 -0.169709 0.265311

C -2.565550 -1.640262 0.021026

H -3.261970 0.240185 1.007567

H -3.029409 -2.193410 0.840175

H -1.539153 -2.003228 -0.109718

H -3.102980 -1.902869 -0.903357

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -178.231 | 19.6333 | 95.5224 |
| 114.3204 | 117.1237 | 162.6159 |
| 218.0703 | 236.3231 | 305.5602 |
| 334.9739 | 398.6332 | 449.2813 |
| 548.0481 | 612.5233 | 712.9579 |
| 810.107 | 887.413 | 937.3992 |
| 980.8119 | 1008.243 | 1040.166 |
| 1057.297 | 1062.654 | 1106.146 |
| 1127.348 | 1172.363 | 1214.488 |
| 1269.359 | 1322.057 | 1344.172 |
| 1406.389 | 1418.71 | 1432.908 |
| 1473.717 | 1474.838 | 1488.161 |
| 1491.984 | 1493.012 | 1735.152 |
| 2395.773 | 2988.417 | 3040.491 |
| 3048.51 | 3056.066 | 3085.645 |
| 3090.258 | 3118.955 | 3122.472 |
| 3123.943 | 3171.612 | 3180.493 |

***i50 – p76***

C -0.396773 1.911392 0.467377

C 0.033969 0.906122 -0.343566

C 3.795007 -0.679952 -0.029649

C 2.453780 -0.120148 -0.141578

C 1.350924 0.350503 -0.229911

C -1.061712 -0.964649 0.399058

C -2.355217 -1.128313 0.253582

C -3.316059 -0.176822 -0.401775

H -1.346464 2.399551 0.286266

H 0.161781 2.196071 1.350437

H -0.470527 0.732042 -1.289035

H 4.540647 0.013433 -0.427189

H 3.873788 -1.618467 -0.583778

H 4.043840 -0.880758 1.015428

H -0.301128 -1.575898 0.866635

H -2.799781 -2.048030 0.647501

H -2.808681 0.705408 -0.793492

H -4.075418 0.154397 0.313218

H -3.841577 -0.666547 -1.227226

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -435.523 | 40.8068 | 73.8013 |
| 106.6717 | 123.8037 | 137.493 |
| 158.9874 | 189.1514 | 240.3327 |
| 296.2094 | 340.3913 | 416.7892 |
| 484.242 | 547.0047 | 605.3779 |
| 629.6065 | 725.8221 | 852.0767 |
| 875.5443 | 897.7655 | 944.1122 |
| 969.2286 | 1044.901 | 1058.549 |
| 1061.841 | 1071.305 | 1131.869 |
| 1194.927 | 1277.434 | 1289.002 |
| 1418.663 | 1420.79 | 1439.361 |
| 1487.514 | 1489.333 | 1491.185 |
| 1495.449 | 1567.875 | 1710.149 |
| 2382.02 | 3045.145 | 3048.538 |
| 3068.455 | 3103.503 | 3118.789 |
| 3124.492 | 3151.501 | 3162.483 |
| 3177.985 | 3238.659 | 3262.911 |

***i47 – i52***

C 0.802681 1.957717 -0.194482

C -0.271317 0.921920 -0.383602

C 2.431695 -1.758704 0.099243

C 2.202500 -0.315071 0.029057

C 1.431376 0.658752 -0.101888

C -1.153455 0.533049 0.690524

C -2.198994 -0.308660 0.616356

C -2.683332 -1.035809 -0.599648

H 1.054310 2.562589 -1.062827

H 0.754441 2.536616 0.726663

H -0.516663 0.665370 -1.406177

H 3.103307 -2.089288 -0.697546

H 1.487763 -2.311376 0.006237

H 2.892810 -2.033548 1.051693

H -0.921385 0.962930 1.663326

H -2.756323 -0.494072 1.530734

H -2.604461 -2.119162 -0.456425

H -2.121119 -0.780105 -1.499049

H -3.739607 -0.819118 -0.789997

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -698.13 | 40.8029 | 84.9348 |
| 109.0757 | 120.8921 | 153.8513 |
| 204.1244 | 232.6301 | 357.231 |
| 378.3374 | 405.7441 | 486.8048 |
| 598.2084 | 703.8051 | 744.2799 |
| 823.0606 | 893.5626 | 950.0074 |
| 994.6094 | 1019.089 | 1031.912 |
| 1056.676 | 1058.896 | 1080.196 |
| 1102.575 | 1170.026 | 1191.348 |
| 1219.387 | 1290.591 | 1341.668 |
| 1407.264 | 1417.384 | 1465.429 |
| 1468.273 | 1475.232 | 1481.649 |
| 1490.101 | 1494.188 | 1670.85 |
| 2022.109 | 3014.863 | 3036.694 |
| 3089.267 | 3093.844 | 3094.514 |
| 3119.196 | 3133.6 | 3151.629 |
| 3169.839 | 3179.358 | 3210.94 |

***i52 – p81***

C 0.619656 1.865547 -0.108096

C -0.265461 0.638375 -0.327124

C 3.212461 -1.118334 0.042505

C 2.218281 -0.261294 -0.048329

C 1.209472 0.520136 -0.153080

C -1.148475 0.172546 0.764645

C -2.325512 -0.436018 0.635757

C -3.036093 -0.796822 -0.633205

H 0.784633 2.524129 -0.954274

H 0.561696 2.359511 0.857077

H -0.621144 0.501643 -1.342962

H 3.821666 -1.356406 -0.822680

H 2.321063 -2.986680 -0.218258

H 3.544764 -1.483819 1.008101

H -0.764604 0.350217 1.767052

H -2.842551 -0.712165 1.551728

H -3.208448 -1.876658 -0.681007

H -2.484488 -0.508703 -1.529111

H -4.018561 -0.315882 -0.674098

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -527.084 | 35.6093 | 89.4425 |
| 148.7663 | 162.2336 | 179.7435 |
| 230.4862 | 267.1034 | 310.7255 |
| 341.7289 | 388.4891 | 488.994 |
| 558.5112 | 605.5175 | 650.0217 |
| 685.0291 | 777.1066 | 857.8285 |
| 900.6434 | 935.4767 | 941.8521 |
| 979.5652 | 1015.181 | 1024.035 |
| 1038.203 | 1057.22 | 1068.477 |
| 1093.943 | 1103.12 | 1178.717 |
| 1294.888 | 1310.111 | 1368.662 |
| 1418.008 | 1454.007 | 1461.359 |
| 1485.067 | 1504.505 | 1529.546 |
| 1762.02 | 2102.979 | 3046.704 |
| 3102.728 | 3130.234 | 3137.357 |
| 3146.973 | 3153.87 | 3175.79 |
| 3183.339 | 3222.054 | 3232.851 |

***i48 – p69***

C 0.101425 -0.342535 -0.478297

C -0.599672 0.980112 -0.300409

C 4.136028 -0.061368 0.316843

C 2.709859 -0.164050 0.028223

C 1.535540 -0.254503 -0.203113

C -1.862021 1.176705 0.095230

C -2.879039 0.180712 0.426487

C -3.018004 -1.045196 -0.100387

H -0.351399 -1.099826 0.170918

H -0.040750 -0.700996 -1.506484

H 0.011435 1.855996 -0.498037

H 4.338733 -0.297685 1.364348

H 4.500215 0.950522 0.122540

H 4.711192 -0.751950 -0.304788

H -2.177921 2.209108 0.223369

H -3.611445 0.499436 1.164875

H -1.888246 -2.402204 1.274446

H -2.387827 -1.402999 -0.906021

H -3.848688 -1.678672 0.187376

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -442.084 | 37.2752 | 78.7389 |
| 99.5511 | 121.6807 | 173.9429 |
| 214.9618 | 241.8854 | 253.6381 |
| 292.2818 | 354.173 | 395.9515 |
| 434.6302 | 509.6933 | 607.5843 |
| 701.3497 | 779.1675 | 833.5016 |
| 900.1831 | 941.3982 | 956.8688 |
| 1024.66 | 1038.182 | 1054.821 |
| 1064.306 | 1067.729 | 1102.403 |
| 1175.695 | 1233.984 | 1274.034 |
| 1324.013 | 1342.264 | 1421.311 |
| 1430.113 | 1457.819 | 1470.493 |
| 1489.078 | 1490.822 | 1666.398 |
| 1721.492 | 2399.477 | 3026.04 |
| 3051.485 | 3068.031 | 3122.832 |
| 3125.291 | 3156.21 | 3165.646 |
| 3172.895 | 3190.043 | 3258.103 |

***i48 – p65***

C 0.146101 -0.134726 0.122826

C -0.600889 0.973347 -0.127605

C 4.230992 -0.128431 0.013028

C 2.774653 -0.123307 0.048030

C 1.571803 -0.121477 0.069127

C -2.036473 1.131770 0.014266

C -2.999383 0.198286 0.082907

C -2.850027 -1.288915 -0.001860

H -0.305790 -1.013143 0.568974

H -0.083752 -1.172511 -1.647688

H -0.063213 1.858422 -0.456375

H 4.634504 -0.779437 0.792535

H 4.629345 0.877043 0.169208

H 4.594749 -0.491394 -0.951947

H -2.364826 2.167329 0.049563

H -4.015572 0.564849 0.203997

H -3.779021 -1.750350 -0.342036

H -2.616151 -1.721343 0.978800

H -2.050932 -1.578742 -0.689347

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -682.275 | 51.8512 | 62.8686 |
| 82.4278 | 105.4068 | 172.2564 |
| 221.1933 | 248.5025 | 297.7449 |
| 342.8851 | 354.5955 | 376.0656 |
| 449.3436 | 505.6386 | 515.5368 |
| 689.2338 | 714.3873 | 859.6963 |
| 896.1324 | 916.4421 | 998.4454 |
| 1007.91 | 1051.595 | 1053.312 |
| 1058.522 | 1065.34 | 1102.143 |
| 1210.096 | 1280.238 | 1329.573 |
| 1337.829 | 1406.034 | 1417.958 |
| 1454.284 | 1482.131 | 1486.138 |
| 1489.466 | 1503.64 | 1613.941 |
| 1701.171 | 2375.193 | 3031.409 |
| 3049.202 | 3097.728 | 3119.208 |
| 3126.225 | 3131.181 | 3156.521 |
| 3175.034 | 3185.604 | 3208.01 |

***i48 – p64***

C 0.301889 -1.609811 0.329510

C 1.535988 -1.248621 -0.113522

C -3.151176 0.464094 -0.345568

C -1.919854 -0.272437 -0.095395

C -0.895181 -0.868312 0.107855

C 1.937667 0.009002 -0.725296

C 1.602432 1.256452 -0.369972

C 0.779196 1.690010 0.799089

H 0.165755 -2.631068 0.671820

H 0.477056 -1.275672 2.306712

H 2.314148 -2.003908 -0.035459

H -3.810451 -0.095055 -1.014360

H -2.937738 1.430401 -0.809551

H -3.691079 0.645616 0.587252

H 2.642796 -0.098644 -1.547157

H 2.014898 2.060304 -0.976095

H 1.257342 2.538106 1.297758

H 0.635577 0.888917 1.525139

H -0.214071 2.018740 0.473743

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -749.971 | 39.4935 | 78.0201 |
| 91.5068 | 178.5561 | 197.2304 |
| 248.3446 | 273.242 | 296.0652 |
| 338.9203 | 357.2981 | 399.6327 |
| 447.9223 | 545.3136 | 588.4502 |
| 691.8103 | 731.6247 | 815.25 |
| 856.2358 | 906.5394 | 999.3048 |
| 1005.343 | 1006.626 | 1054.411 |
| 1058.007 | 1069.904 | 1120.307 |
| 1165.675 | 1261.391 | 1291.113 |
| 1401.548 | 1417.777 | 1427.795 |
| 1464.241 | 1482.469 | 1482.968 |
| 1484.462 | 1505.764 | 1607.51 |
| 1714.349 | 2375.166 | 3037.416 |
| 3045.834 | 3097.681 | 3119.21 |
| 3119.795 | 3134.46 | 3143.809 |
| 3158.199 | 3166.793 | 3180.404 |

***i42 – i30***

C 2.517236 -1.093764 0.144940

C 1.336236 -0.395847 -0.069597

C -0.008977 -1.022528 -0.056863

C -1.184260 -0.311909 0.042604

C -1.182057 1.192880 0.031201

C 0.198271 1.790855 0.029072

C 1.322159 1.081223 -0.041816

C -2.517388 -0.987032 0.034272

H 2.525390 -2.171877 0.249762

H 3.466418 -0.575122 0.118267

H 0.728188 -0.785424 -1.214688

H -0.027268 -2.107640 -0.001638

H -1.752021 1.576601 0.891203

H -1.736204 1.559490 -0.849790

H 0.260812 2.874279 0.075611

H 2.286320 1.578567 -0.047012

H -2.423475 -2.074736 0.069027

H -3.123969 -0.671997 0.892286

H -3.091509 -0.725414 -0.865898

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1919.55 | 80.6795 | 126.0974 |
| 197.9696 | 280.912 | 322.2601 |
| 373.2019 | 415.1953 | 470.7905 |
| 517.3714 | 535.0952 | 586.2367 |
| 666.2859 | 696.2606 | 774.8879 |
| 868.3067 | 874.2448 | 924.2022 |
| 947.0274 | 951.8748 | 1003.129 |
| 1007.163 | 1039.597 | 1049.257 |
| 1096.625 | 1185.398 | 1206.768 |
| 1225.233 | 1305.986 | 1321.342 |
| 1378.83 | 1401.892 | 1421.155 |
| 1448.261 | 1473.2 | 1481.396 |
| 1488.412 | 1512.792 | 1567.199 |
| 1640.439 | 1745.725 | 2959.547 |
| 2993.392 | 3001.338 | 3052.967 |
| 3122.095 | 3168.38 | 3174.362 |
| 3177.892 | 3205.019 | 3268.068 |

***i42 – i45***

C 2.464681 -1.166654 0.129873

C 1.325179 -0.396407 -0.065356

C -0.012044 -1.022246 -0.070614

C -1.155838 -0.337594 -0.006136

C -1.201733 1.173970 0.004730

C 0.151411 1.814065 0.082996

C 1.312596 1.084719 -0.009815

C -2.489994 -1.019791 0.039229

H 2.404322 -2.245855 0.081954

H 3.440729 -0.711152 0.243799

H 1.447271 0.358089 -1.183582

H -0.034104 -2.107961 -0.091775

H -1.836653 1.507788 0.839103

H -1.738233 1.509033 -0.899149

H 0.210280 2.894691 0.130083

H 2.278039 1.570391 0.090556

H -2.394567 -2.105457 -0.018035

H -3.017555 -0.766688 0.965731

H -3.125069 -0.683260 -0.788133

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1892.67 | 83.7341 | 146.1719 |
| 209.0394 | 283.2629 | 330.9128 |
| 410.506 | 441.2843 | 477.9133 |
| 518.1904 | 526.5133 | 578.0278 |
| 649.6937 | 687.094 | 720.9781 |
| 858.5714 | 873.6787 | 896.3339 |
| 919.0303 | 954.2098 | 966.5895 |
| 1006.87 | 1043.912 | 1066.277 |
| 1113.295 | 1168.483 | 1190.388 |
| 1229.237 | 1311.755 | 1334.252 |
| 1361.506 | 1407.618 | 1424.411 |
| 1437.546 | 1479.849 | 1480.837 |
| 1493.952 | 1516.571 | 1559.684 |
| 1646.819 | 1760.263 | 2962.001 |
| 2999.349 | 3032.877 | 3089.855 |
| 3135.316 | 3164.351 | 3182.266 |
| 3184.609 | 3209.236 | 3265.412 |

***i45 – p48***

C -2.412783 -1.183165 -0.127685

C -1.309984 -0.447590 0.036482

C 0.018970 -1.056706 0.085895

C 1.149015 -0.340935 -0.026070

C 1.067961 1.116958 -0.225464

C -0.115860 1.760924 -0.199568

C -1.369257 1.054775 0.217140

C 2.514056 -0.959873 0.000521

H -2.360128 -2.264349 -0.198441

H -3.395180 -0.728108 -0.194164

H 0.070956 -2.138637 0.170237

H 1.961002 1.632058 -0.564904

H 1.779251 1.604616 1.606263

H -0.166919 2.825428 -0.400386

H -1.522855 1.264264 1.288032

H -2.240287 1.470299 -0.296017

H 2.461679 -2.039699 0.148072

H 3.047728 -0.765044 -0.935808

H 3.112044 -0.527155 0.809614

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -671.145 | 93.328 | 153.3833 |
| 203.1738 | 250.0975 | 297.9946 |
| 320.2681 | 382.8154 | 426.565 |
| 454.2759 | 527.4272 | 544.7807 |
| 595.4023 | 695.2897 | 709.1551 |
| 758.7911 | 870.1042 | 889.6824 |
| 907.6792 | 940.4672 | 958.4485 |
| 980.4469 | 1002.857 | 1024.015 |
| 1050.763 | 1072.115 | 1193.211 |
| 1197.555 | 1227.869 | 1316.347 |
| 1351.019 | 1367.213 | 1416.13 |
| 1440.897 | 1454.65 | 1462.538 |
| 1487.854 | 1495.774 | 1622.11 |
| 1700.831 | 1739.439 | 2990.76 |
| 3039.084 | 3098.728 | 3098.978 |
| 3141.171 | 3152.601 | 3176.101 |
| 3184.946 | 3207.348 | 3240.598 |

***i45 – p46***

C -2.380338 -1.238558 -0.085514

C -1.282565 -0.476057 -0.024614

C 0.065222 -1.046434 0.013050

C 1.178499 -0.307996 0.001888

C 1.123949 1.194538 -0.062808

C -0.257188 1.759794 -0.124199

C -1.363445 0.995526 -0.006969

C 2.550187 -0.912411 0.046242

H -2.312915 -2.320451 -0.112101

H -3.371427 -0.799315 -0.105115

H 0.140787 -2.130034 0.049079

H 1.705880 1.542191 -0.928768

H 1.650272 1.612783 0.809103

H -0.354188 2.837658 -0.203706

H -1.662434 1.183478 1.900604

H -2.344570 1.443844 -0.124786

H 2.508458 -2.001479 0.101822

H 3.126433 -0.634243 -0.843306

H 3.107778 -0.544847 0.914715

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -823.181 | 96.4694 | 136.514 |
| 197.3548 | 250.695 | 294.0311 |
| 349.8853 | 415.6681 | 431.1338 |
| 452.315 | 490.6196 | 537.9354 |
| 629.0765 | 701.4583 | 708.9316 |
| 789.05 | 879.6842 | 881.6547 |
| 907.5512 | 926.8194 | 955.6508 |
| 973.7252 | 1015.229 | 1027.357 |
| 1047.653 | 1066.556 | 1180.591 |
| 1199.204 | 1229.088 | 1323.091 |
| 1359.667 | 1402.181 | 1416.855 |
| 1439.804 | 1456.442 | 1466.441 |
| 1481.103 | 1493.702 | 1630.026 |
| 1701.428 | 1768.701 | 2999.962 |
| 3020.848 | 3032.255 | 3089.294 |
| 3137.117 | 3161.181 | 3172.312 |
| 3177.023 | 3196.597 | 3251.343 |

***i45 – i43***

C -2.370600 -1.243386 0.173809

C -1.277109 -0.479242 -0.019476

C 0.041200 -1.043835 -0.119118

C 1.195104 -0.271490 -0.088248

C 1.061906 1.195258 0.104078

C -0.181867 1.791613 0.185933

C -1.412291 1.026683 -0.201287

C 2.561346 -0.887205 0.065477

H -2.294964 -2.322947 0.248179

H -3.358184 -0.805212 0.265453

H 0.141154 -2.123167 -0.170719

H 1.272246 0.658814 -1.095588

H 1.967619 1.738672 0.350666

H -0.259194 2.855312 0.372503

H -2.284153 1.393164 0.348221

H -1.632811 1.215335 -1.266216

H 2.624794 -1.841157 -0.461312

H 3.345579 -0.232005 -0.322570

H 2.771784 -1.067187 1.124366

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1954.5 | 97.9638 | 172.9498 |
| 210.5098 | 288.2917 | 332.5343 |
| 421.7754 | 448.4303 | 519.3976 |
| 532.9149 | 559.4028 | 656.668 |
| 669.7093 | 696.5729 | 780.5797 |
| 856.3222 | 865.0222 | 896.7521 |
| 934.7055 | 950.3112 | 975.5755 |
| 1019.783 | 1053.273 | 1076.271 |
| 1155.52 | 1176.45 | 1205.252 |
| 1233.788 | 1309.873 | 1337.611 |
| 1354.729 | 1401.874 | 1425.629 |
| 1443.294 | 1471.926 | 1492.877 |
| 1501.009 | 1530.893 | 1559.143 |
| 1627.804 | 1793.957 | 2955.012 |
| 3046.225 | 3081.017 | 3113.853 |
| 3137.878 | 3149.884 | 3186.472 |
| 3194.877 | 3218.949 | 3239.789 |

***i51 – p62***

C -0.408226 -0.298107 0.197059

C 0.421483 0.762270 0.031292

C -4.472132 -0.096129 -0.066085

C -3.020439 -0.163706 0.030044

C -1.819119 -0.213956 0.107801

C 1.881713 0.696982 0.176457

C 2.647578 -0.333967 -0.179601

C 4.129951 -0.401951 0.005442

H 0.014822 -1.279014 0.396412

H -0.022690 1.751465 -0.028399

H 0.325441 0.955193 -1.994762

H -4.828392 -0.647457 -0.940309

H -4.807851 0.939461 -0.158875

H -4.941446 -0.529408 0.820903

H 2.353977 1.582145 0.598412

H 2.180234 -1.192198 -0.659902

H 4.405539 -1.253847 0.635893

H 4.518778 0.506363 0.471069

H 4.636734 -0.541317 -0.954894

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -731.056 | 35.911 | 64.4184 |
| 75.127 | 123.5405 | 163.3917 |
| 206.9619 | 214.3693 | 291.601 |
| 305.7877 | 345.205 | 366.8354 |
| 397.6975 | 477.2384 | 501.8334 |
| 632.5642 | 799.9764 | 857.2839 |
| 877.6876 | 925.0698 | 997.7588 |
| 1009.884 | 1050.982 | 1056.465 |
| 1065.126 | 1080.08 | 1136.81 |
| 1216.311 | 1305.47 | 1318.572 |
| 1346.56 | 1357.13 | 1416.136 |
| 1426.328 | 1483.062 | 1484.156 |
| 1487.129 | 1497.394 | 1631.716 |
| 1746.197 | 2356.554 | 3037.571 |
| 3051.356 | 3095.836 | 3121.23 |
| 3128.226 | 3128.665 | 3153.862 |
| 3159.402 | 3172.53 | 3185.708 |

***i28 – p11b***

C -0.364582 -1.739754 -0.397369

C 3.118588 0.275576 0.273814

C 1.877260 -0.449649 0.041596

C 0.833535 -1.023373 -0.143989

H -0.229961 -2.726803 -0.830185

H 2.932477 1.351238 0.332762

H 3.832270 0.097585 -0.534453

H 3.584401 -0.040026 1.211223

C -1.629449 -1.319965 -0.173355

C -2.105314 -0.070677 0.380920

C -1.370456 0.905784 0.962755

C -0.517133 2.334257 -0.883268

H -2.410937 -2.015020 -0.467870

H -3.176095 0.091299 0.288175

H -0.323037 0.770377 1.194127

H -1.865132 1.768181 1.392959

H -1.458931 2.609246 -1.339090

H 0.069718 1.550045 -1.341910

H -0.009466 3.070691 -0.272373

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -305.423 | 35.5506 | 44.9286 |
| 68.6401 | 85.9689 | 107.9506 |
| 169.0137 | 236.2273 | 258.8583 |
| 337.5863 | 373.1292 | 404.1349 |
| 439.1992 | 468.0758 | 514.4129 |
| 671.8545 | 699.8346 | 704.9995 |
| 796.4899 | 817.4625 | 921.0227 |
| 953.9552 | 992.9498 | 1012.453 |
| 1052.17 | 1057.503 | 1108.624 |
| 1173.836 | 1276.311 | 1325.432 |
| 1409.66 | 1415.693 | 1419.112 |
| 1434.974 | 1472.821 | 1481.997 |
| 1483.997 | 1566.393 | 1666.094 |
| 2352.825 | 3043.804 | 3105.331 |
| 3115.529 | 3119.085 | 3154.032 |
| 3164.619 | 3174.716 | 3184.108 |
| 3272.64 | 3276.945 | 3290.882 |

***i29 – p11a***

C -0.619889 1.475262 0.413848

C -3.712029 -1.145039 -0.074035

C -2.604104 -0.214654 0.096854

C -1.686848 0.553641 0.236757

H -0.866498 2.408381 0.910623

H -3.879315 -1.360818 -1.132579

H -4.635097 -0.729751 0.337620

H -3.508525 -2.090674 0.435323

C 0.650684 1.263660 0.008868

C 1.124895 0.083003 -0.664064

C 2.420226 -0.103616 -1.011211

C 3.511339 -1.175653 0.910610

H 1.381146 2.045246 0.203391

H 0.398188 -0.700927 -0.858101

H 3.145131 0.696839 -0.907332

H 2.723797 -0.962364 -1.596169

H 2.928019 -2.086384 0.941633

H 3.287996 -0.410147 1.641939

H 4.519518 -1.229031 0.517887

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -343.028 | 31.4755 | 42.7458 |
| 73.0591 | 80.9945 | 86.3373 |
| 183.4631 | 227.1429 | 250.2167 |
| 340.5355 | 353.1999 | 422.49 |
| 438.3186 | 456.1166 | 507.8987 |
| 661.8639 | 726.035 | 729.0027 |
| 792.9487 | 810.4835 | 908.7641 |
| 944.9257 | 981.9877 | 1025.223 |
| 1052.931 | 1057.681 | 1136.376 |
| 1200.706 | 1257.414 | 1302.32 |
| 1387.22 | 1411.961 | 1418.013 |
| 1418.622 | 1475.395 | 1483.6 |
| 1483.93 | 1592.148 | 1628.189 |
| 2358.91 | 3044.86 | 3104.198 |
| 3115.652 | 3120.759 | 3155.164 |
| 3161.518 | 3177.549 | 3185.231 |
| 3252.47 | 3275.327 | 3283.02 |

***i8 – p1***

C 2.514641 -1.009682 -0.068819

C 1.227413 -0.234940 -0.047447

C 0.000000 -0.922647 -0.023528

C -1.227413 -0.234940 -0.047447

C -1.207883 1.152327 0.002142

C 0.000000 1.841750 0.034607

C 1.207883 1.152327 0.002142

C -2.514641 -1.009682 -0.068819

H 2.532029 -1.725835 -0.895077

H 2.631402 -1.577964 0.859921

H 3.377226 -0.349139 -0.172769

H 0.000000 -1.432869 1.820580

H 0.000000 -1.997229 -0.186404

H -2.143603 1.701704 0.007195

H 0.000000 2.925495 0.070311

H 2.143603 1.701704 0.007195

H -3.377226 -0.349139 -0.172770

H -2.631403 -1.577963 0.859922

H -2.532028 -1.725835 -0.895076

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -723.097 | 71.8511 | 78.1466 |
| 181.7583 | 224.6108 | 275.5878 |
| 300.1297 | 358.9788 | 416.8444 |
| 489.8595 | 527.2639 | 543.0044 |
| 548.3253 | 726.9405 | 744.2945 |
| 792.0956 | 920.5589 | 927.324 |
| 969.7551 | 996.8228 | 1003.57 |
| 1026.68 | 1042.196 | 1063.988 |
| 1068.398 | 1130.236 | 1186.081 |
| 1200.327 | 1288.249 | 1324.52 |
| 1345.546 | 1417.023 | 1419.373 |
| 1448.115 | 1488.994 | 1489.519 |
| 1495.05 | 1509.196 | 1545.477 |
| 1657.922 | 1658.373 | 3038.807 |
| 3039.447 | 3103.54 | 3103.714 |
| 3134.663 | 3134.888 | 3165.047 |
| 3180.126 | 3188.257 | 3206.962 |

***i8 – i32***

C -2.522478 -1.034962 -0.165265

C -1.278559 -0.256939 0.143038

C 0.052978 -0.987059 0.139285

C 1.274185 -0.232739 0.009871

C 1.236743 1.123392 -0.029999

C -0.032500 1.840949 -0.023103

C -1.210023 1.173461 0.023298

C 2.561043 -1.001382 -0.080927

H -2.532218 -1.997274 0.355777

H -2.597786 -1.248742 -1.240042

H -3.417760 -0.484971 0.135033

H 0.038673 -2.061508 0.002906

H -0.636474 -0.654347 1.188052

H 2.159822 1.686989 -0.105479

H -0.024076 2.922645 -0.085349

H -2.147977 1.718444 -0.030897

H 3.421778 -0.333352 -0.139627

H 2.562833 -1.643736 -0.967633

H 2.684855 -1.652480 0.790076

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -2570.45 | 126.8398 | 140.8083 |
| 180.8906 | 211.5815 | 265.3566 |
| 321.62 | 385.5976 | 485.5923 |
| 496.7639 | 516.1098 | 610.93 |
| 685.2722 | 716.9955 | 745.1167 |
| 830.8386 | 869.0689 | 940.5473 |
| 967.6035 | 981.0734 | 1021.812 |
| 1044.363 | 1061.603 | 1069.76 |
| 1152.375 | 1185.48 | 1221.558 |
| 1248.968 | 1298.453 | 1314.907 |
| 1390.063 | 1415.013 | 1425.467 |
| 1457.38 | 1482.751 | 1486.394 |
| 1497.16 | 1503.02 | 1601.065 |
| 1628.462 | 2206.181 | 3004.853 |
| 3036.822 | 3075.355 | 3098.188 |
| 3116.738 | 3136.318 | 3173.36 |
| 3190.34 | 3203.391 | 3210.394 |

***i32 – p42***

C 2.133354 -1.279218 0.889838

C 1.125594 -0.298720 -0.773935

C -0.175710 -0.852309 -0.671862

C -1.201506 -0.160924 -0.053226

C -0.957753 1.144936 0.397984

C 0.277336 1.754343 0.181980

C 1.302310 1.064332 -0.436078

C -2.562980 -0.780420 0.129223

H 2.022397 -2.333153 0.655094

H 1.529020 -0.910755 1.710877

H 3.144072 -0.887649 0.832446

H 1.838160 -0.769031 -1.442218

H -0.350043 -1.858689 -1.039371

H -1.754932 1.698774 0.883661

H 0.426728 2.784464 0.487183

H 2.258451 1.542389 -0.615656

H -2.777945 -0.941320 1.189968

H -2.632033 -1.745547 -0.376379

H -3.347750 -0.131607 -0.269142

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -577.333 | 37.9523 | 108.1316 |
| 138.741 | 145.4494 | 240.6212 |
| 349.5952 | 402.3133 | 477.2827 |
| 525.0235 | 571.6423 | 584.3113 |
| 644.5639 | 676.7589 | 766.104 |
| 807.6077 | 863.4974 | 885.9665 |
| 901.564 | 991.589 | 1000.768 |
| 1004.862 | 1008.644 | 1052.843 |
| 1066.2 | 1105.994 | 1180.941 |
| 1195.595 | 1234.774 | 1324.146 |
| 1352.261 | 1419.54 | 1425.971 |
| 1428.692 | 1463.105 | 1491.288 |
| 1504.086 | 1527.272 | 1612.018 |
| 1641.887 | 3043.443 | 3082.269 |
| 3108.559 | 3131.186 | 3174.399 |
| 3177.206 | 3188.245 | 3193.905 |
| 3208.863 | 3238.727 | 3251.007 |

***i32 – p1***

C -2.497876 -1.017345 -0.145293

C -1.205184 -0.264028 0.075813

C 0.028434 -0.947898 0.002204

C 1.239171 -0.274261 -0.017012

C 1.226243 1.124519 -0.022216

C 0.023460 1.822341 -0.036597

C -1.181358 1.143190 -0.015163

C 2.545908 -1.023742 -0.019648

H -2.460407 -2.010218 0.306243

H -2.675777 -1.137928 -1.218526

H -3.346707 -0.480275 0.281380

H -1.353055 -0.327253 1.882242

H 0.020095 -2.034128 0.001246

H 2.165840 1.667551 -0.038071

H 0.030607 2.906120 -0.072702

H -2.118959 1.688469 -0.029206

H 3.244405 -0.598490 -0.744626

H 2.399898 -2.077378 -0.265241

H 3.021274 -0.973120 0.964722

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -981.233 | 42.6135 | 171.0109 |
| 192.9587 | 215.6632 | 275.6231 |
| 388.4217 | 439.4285 | 461.4139 |
| 481.6591 | 529.8271 | 554.4428 |
| 580.9013 | 701.1786 | 741.8312 |
| 793.4969 | 892.1052 | 915.0551 |
| 931.4845 | 1002.029 | 1006.167 |
| 1014.591 | 1038.645 | 1067.446 |
| 1067.701 | 1133.134 | 1187.259 |
| 1199.125 | 1279.678 | 1316.693 |
| 1347.448 | 1419.041 | 1421.877 |
| 1453.325 | 1491.972 | 1493.895 |
| 1496.158 | 1512.236 | 1530.313 |
| 1635.469 | 1663.594 | 3045.144 |
| 3047.235 | 3111.76 | 3119.727 |
| 3133.633 | 3143.384 | 3174.271 |
| 3179.438 | 3189.453 | 3206.769 |

***i30 – p3***

C -2.536419 -0.883847 -0.015014

C -1.209866 -0.199816 0.051250

C -0.000543 -1.082243 0.199649

C 1.342630 -0.400258 0.025403

C 1.366333 1.057073 0.142046

C 0.239618 1.779048 0.110548

C -1.072836 1.144098 -0.029004

C 2.457537 -1.097723 -0.209664

H -2.666303 -1.569292 0.829979

H -2.609788 -1.487142 -0.927711

H -3.360318 -0.168455 -0.012799

H -0.079825 -1.931842 -0.488128

H -0.044952 -1.521829 1.207891

H 2.333777 1.544105 0.206116

H 0.280867 2.861368 0.157597

H -1.955217 1.774534 -0.006900

H -1.277784 1.381439 -1.995773

H 3.420006 -0.604854 -0.292812

H 2.440807 -2.176026 -0.328745

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -680.825 | 39.581 | 121.2738 |
| 182.0176 | 271.9952 | 296.7835 |
| 312.1466 | 362.6369 | 419.0748 |
| 491.4592 | 495.9954 | 526.1404 |
| 573.7447 | 702.6141 | 733.448 |
| 814.7247 | 872.8831 | 887.7767 |
| 921.7883 | 929.0248 | 966.0124 |
| 979.4523 | 1002.27 | 1010.437 |
| 1059.993 | 1076.073 | 1183.681 |
| 1205.979 | 1235.157 | 1317.734 |
| 1341.669 | 1378.287 | 1417.203 |
| 1431.024 | 1448.795 | 1469.069 |
| 1482.025 | 1486.861 | 1638.111 |
| 1686.336 | 1730.457 | 3001.464 |
| 3030.626 | 3064.271 | 3086.852 |
| 3142.143 | 3153.317 | 3183.119 |
| 3190.026 | 3213.307 | 3241.02 |

***i30 – i35***

C -2.511773 -0.957007 0.084021

C -1.214750 -0.251029 -0.144964

C 0.044434 -1.050954 -0.130621

C 1.344735 -0.424316 -0.004616

C 1.360585 1.045409 -0.070154

C 0.254846 1.788734 -0.027867

C -1.130116 1.222436 0.129640

C 2.490119 -1.121799 0.142911

H -2.696717 -1.092790 1.160727

H -2.515247 -1.951079 -0.372237

H -3.354166 -0.394361 -0.328326

H -0.516043 -0.708774 -1.212614

H -0.049049 -2.122287 0.012641

H 2.331574 1.524918 -0.146254

H 0.338180 2.870728 -0.065458

H -1.467195 1.412840 1.165379

H -1.836563 1.772346 -0.504521

H 3.445684 -0.616037 0.216972

H 2.491061 -2.204338 0.203600

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1935.45 | 106.6649 | 154.842 |
| 218.8728 | 276.5805 | 318.9613 |
| 350.4168 | 404.3864 | 456.9397 |
| 508.6659 | 576.3534 | 643.6226 |
| 696.8945 | 776.5033 | 804.2774 |
| 852.4817 | 870.1872 | 911.9176 |
| 926.8199 | 961.1164 | 1006.937 |
| 1016.835 | 1036.21 | 1056.128 |
| 1159.8 | 1211.576 | 1213.716 |
| 1268.118 | 1299.019 | 1329.235 |
| 1366.257 | 1397.78 | 1422.063 |
| 1455.169 | 1469.305 | 1480.464 |
| 1487.602 | 1502.444 | 1633.412 |
| 1740.305 | 2197.671 | 2933.594 |
| 2988.236 | 3040.45 | 3077.388 |
| 3119.543 | 3159.629 | 3173.264 |
| 3188.57 | 3196.122 | 3250.381 |

***i31 – i43***

C -2.578962 -0.849335 -0.101843

C -1.250206 -0.187746 0.124968

C -0.033901 -1.035692 0.170917

C 1.282745 -0.471896 0.025864

C 1.412609 1.031637 0.206917

C 0.160132 1.789246 -0.136548

C -1.060063 1.218560 -0.119053

C 2.362859 -1.233463 -0.234722

H -2.651147 -1.799606 0.434133

H -2.722966 -1.062634 -1.168047

H -3.400639 -0.210907 0.230479

H -0.174853 -2.108620 0.102530

H -0.691510 -0.585841 1.232890

H 2.258015 1.397853 -0.382783

H 1.673774 1.233674 1.257916

H 0.256692 2.851744 -0.332278

H -1.947067 1.818508 -0.297246

H 3.346050 -0.792489 -0.352503

H 2.282377 -2.309547 -0.344082

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -1888.36 | 83.5136 | 159.9186 |
| 219.6904 | 287.0987 | 309.8815 |
| 414.1763 | 442.3332 | 501.0148 |
| 528.33 | 554.5279 | 660.0897 |
| 696.5138 | 720.9859 | 796.5233 |
| 855.2651 | 863.2358 | 933.6855 |
| 945.3566 | 965.3899 | 974.0469 |
| 1022.986 | 1039.011 | 1057.474 |
| 1165.9 | 1188.178 | 1228.345 |
| 1257.135 | 1307.392 | 1339.048 |
| 1344.116 | 1404.071 | 1425.495 |
| 1450.463 | 1467.199 | 1477.624 |
| 1494.602 | 1508.317 | 1635.003 |
| 1641.316 | 2115.737 | 2980.217 |
| 3027.954 | 3081.237 | 3097.034 |
| 3129.837 | 3150.907 | 3181.181 |
| 3199.696 | 3203.572 | 3240.564 |

***i31 – p3***

C -2.604639 -0.770752 -0.072005

C -1.254328 -0.129032 -0.009456

C -0.093002 -1.024238 0.345774

C 1.265701 -0.464470 -0.003421

C 1.378195 0.996315 0.038383

C 0.274187 1.767138 -0.092390

C -1.052352 1.184631 -0.186455

C 2.302080 -1.241762 -0.322995

H -2.830111 -1.285694 0.869029

H -2.637939 -1.528060 -0.862824

H -3.391623 -0.038547 -0.260794

H -0.223511 -2.014841 -0.100785

H -0.130108 -1.177909 1.436408

H 2.367632 1.438188 -0.004454

H 1.584318 1.151415 2.197972

H 0.373624 2.845449 -0.148700

H -1.891123 1.840413 -0.397148

H 3.283035 -0.818596 -0.510862

H 2.200764 -2.318791 -0.402451

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -537.547 | 100.4084 | 147.3914 |
| 206.8674 | 236.4631 | 276.496 |
| 300.6162 | 353.6639 | 418.338 |
| 477.8869 | 488.332 | 518.4463 |
| 587.6054 | 701.6079 | 741.7143 |
| 801.3142 | 876.14 | 879.781 |
| 914.0303 | 934.4336 | 957.3403 |
| 985.2648 | 989.1289 | 1015.58 |
| 1067.159 | 1084.166 | 1181.979 |
| 1202.708 | 1231.679 | 1319.957 |
| 1343.9 | 1381.935 | 1421.702 |
| 1434.834 | 1457.083 | 1473.385 |
| 1482.526 | 1500.615 | 1596.324 |
| 1707.948 | 1738.296 | 2992.513 |
| 3033.553 | 3076.407 | 3090.623 |
| 3135.246 | 3152.184 | 3184.478 |
| 3195.6 | 3212.697 | 3240.611 |

***i30 – p43***

C -2.118465 -1.167348 -0.375152

C -1.182121 -0.394194 0.185291

C 0.111916 -0.941053 0.722093

C 1.300914 -0.277745 0.057996

C 1.150418 1.154087 -0.218832

C -0.016209 1.791394 -0.107275

C -1.304067 1.103385 0.263038

C 2.421211 -0.940599 -0.229237

H -2.019451 -2.247337 -0.392417

H -1.498928 -1.188958 -2.424298

H -3.053489 -0.750846 -0.734455

H 0.160227 -2.025416 0.606414

H 0.163733 -0.719202 1.797674

H 2.038289 1.697477 -0.528251

H -0.068948 2.857717 -0.304595

H -1.584556 1.397452 1.285466

H -2.111995 1.451837 -0.386965

H 3.272494 -0.438330 -0.676606

H 2.521042 -2.001962 -0.029510

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -460.676 | 92.3907 | 100.2039 |
| 189.6793 | 250.1643 | 305.3323 |
| 358.6606 | 411.7283 | 438.3215 |
| 470.5255 | 546.2872 | 571.1321 |
| 688.7834 | 726.1104 | 770.6119 |
| 813.825 | 860.5979 | 920.1302 |
| 933.3263 | 939.2083 | 947.2796 |
| 951.204 | 998.1782 | 1009.954 |
| 1015.483 | 1027.211 | 1173.992 |
| 1199.482 | 1231.239 | 1298.956 |
| 1316.861 | 1338.696 | 1353.294 |
| 1412.159 | 1450.352 | 1460.935 |
| 1470.329 | 1482.558 | 1697.29 |
| 1706.679 | 1751.249 | 3009.254 |
| 3019.245 | 3089.269 | 3117.068 |
| 3150.843 | 3155.354 | 3173.397 |
| 3196.94 | 3240.639 | 3242.786 |

***i31 – p43***

C -2.400567 -0.764634 -0.377843

C -1.228209 -0.201428 -0.057566

C -0.102112 -0.985289 0.578525

C 1.239204 -0.494452 0.099394

C 1.451918 0.984501 0.293890

C 0.225826 1.777580 -0.073682

C -0.977651 1.226617 -0.251151

C 2.139337 -1.287285 -0.468409

H -3.517508 -0.593509 1.684854

H -2.568198 -1.829345 -0.260604

H -3.202828 -0.181524 -0.817112

H -0.221898 -2.054440 0.393564

H -0.164991 -0.829532 1.665275

H 2.309105 1.327355 -0.292666

H 1.700647 1.185345 1.346547

H 0.352483 2.847449 -0.208291

H -1.819039 1.845326 -0.548846

H 3.092072 -0.902963 -0.818339

H 1.953689 -2.347816 -0.603322

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -284.447 | 98.2215 | 119.4481 |
| 140.3261 | 181.5556 | 314.5786 |
| 358.1265 | 406.5297 | 439.0338 |
| 470.2843 | 546.8477 | 574.4974 |
| 697.7707 | 724.8166 | 744.0813 |
| 819.3186 | 864.1913 | 917.3324 |
| 932.5242 | 939.2216 | 945.4289 |
| 953.0611 | 998.9313 | 1012.758 |
| 1019.493 | 1029.798 | 1176.561 |
| 1206.739 | 1237.139 | 1301.485 |
| 1320.897 | 1340.468 | 1357.384 |
| 1414.14 | 1456.852 | 1463.935 |
| 1472.835 | 1486.096 | 1678.2 |
| 1725.006 | 1760.007 | 3008.467 |
| 3017.725 | 3087.142 | 3117.252 |
| 3147.291 | 3157.924 | 3170.925 |
| 3194.139 | 3233.703 | 3248.26 |

***i8 – p3***

C 2.572074 -0.934663 -0.064833

C 1.276412 -0.187397 0.000944

C 0.029602 -1.019943 0.165348

C -1.277948 -0.297102 -0.079407

C -1.252989 1.157511 0.029543

C -0.093058 1.831130 0.057445

C 1.193070 1.147263 -0.020205

C -2.409792 -0.962176 -0.350838

H 2.601104 -1.585465 -0.945805

H 2.690277 -1.582654 0.811276

H 3.426188 -0.256628 -0.108632

H 0.026610 -1.392612 1.201832

H 0.089625 -1.914691 -0.463212

H -2.201878 1.683690 0.037232

H -0.097014 2.914727 0.107132

H 2.094394 1.747189 -0.096508

H -3.350978 -0.439144 -0.479615

H -3.083170 -1.543657 1.993049

H -2.419386 -2.038498 -0.484729

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -264.732 | 53.19 | 110.6568 |
| 132.4853 | 148.2568 | 203.7069 |
| 292.893 | 336.5894 | 416.73 |
| 465.7359 | 491.6159 | 513.2424 |
| 578.8419 | 706.5367 | 737.1182 |
| 814.2171 | 874.1593 | 876.3841 |
| 909.5433 | 927.9238 | 950.801 |
| 979.7606 | 1001.924 | 1009.057 |
| 1066.721 | 1081.442 | 1181.454 |
| 1204.687 | 1234.233 | 1320.16 |
| 1341.339 | 1379.188 | 1416.321 |
| 1433.361 | 1445.442 | 1469.216 |
| 1483.31 | 1487.837 | 1662.682 |
| 1682.121 | 1751.466 | 2997.047 |
| 3031.529 | 3070.577 | 3087.373 |
| 3136.632 | 3156.305 | 3182.459 |
| 3191.888 | 3211.494 | 3245.15 |

***i43 – p45***

C 2.371065 -1.041157 0.986328

C 1.002388 -0.381641 -0.848989

C -0.195207 -1.001998 -0.623196

C -1.302885 -0.320356 0.008675

C -1.034585 1.061124 0.579055

C 0.173222 1.745183 0.001214

C 1.126226 1.063928 -0.633843

C -2.515566 -0.892065 0.104653

H 2.371136 -2.118361 0.873941

H 1.756211 -0.621564 1.772186

H 3.281678 -0.511373 0.731826

H 1.746391 -0.874072 -1.462920

H -0.340955 -2.032327 -0.931378

H -0.876388 0.959013 1.663104

H -1.921940 1.691191 0.469882

H 0.270884 2.814184 0.158901

H 2.012898 1.565163 -1.006300

H -3.358302 -0.370627 0.545570

H -2.689554 -1.899328 -0.258195

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -438.287 | 63.7536 | 73.0236 |
| 91.5879 | 149.4269 | 280.8033 |
| 386.4981 | 447.441 | 456.2346 |
| 475.0298 | 490.9479 | 533.9588 |
| 600.5418 | 660.7498 | 729.5824 |
| 775.4801 | 781.4026 | 822.7327 |
| 880.266 | 927.5389 | 945.6481 |
| 950.8801 | 965.7803 | 993.026 |
| 1010.962 | 1033.763 | 1174.535 |
| 1201.548 | 1230.119 | 1321.105 |
| 1338.208 | 1401.366 | 1412.256 |
| 1415.566 | 1435.119 | 1461.71 |
| 1470.592 | 1521.912 | 1648.287 |
| 1722.518 | 3003.962 | 3087.41 |
| 3103.125 | 3154.639 | 3185.269 |
| 3190.535 | 3207.254 | 3221.035 |
| 3243.798 | 3269.235 | 3280 |

***i43 – p48***

C -2.549406 -0.847759 -0.080177

C -1.172402 -0.253376 0.046070

C -0.053626 -1.029039 0.070443

C 1.282595 -0.464829 0.011834

C 1.396964 1.028946 0.226940

C 0.158291 1.790642 -0.146409

C -1.031063 1.193252 -0.190636

C 2.359043 -1.236272 -0.193109

H -2.562255 -1.895649 0.223152

H -2.882581 -0.785930 -1.122194

H -3.272978 -0.302568 0.529956

H -1.262732 -0.113673 2.069325

H -0.149970 -2.110198 0.108175

H 2.273928 1.425081 -0.291340

H 1.574998 1.202155 1.300039

H 0.249270 2.857642 -0.319694

H -1.931397 1.759362 -0.406918

H 3.353873 -0.812396 -0.276303

H 2.267468 -2.313217 -0.283933

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -721.294 | 97.2153 | 150.2086 |
| 183.8703 | 288.6364 | 336.9192 |
| 362.1559 | 406.1769 | 437.9556 |
| 455.9379 | 532.319 | 545.4822 |
| 567.1099 | 686.7606 | 708.9024 |
| 753.3822 | 863.8459 | 873.4212 |
| 904.7625 | 939.9723 | 957.2309 |
| 984.1315 | 1011.704 | 1026.167 |
| 1047.886 | 1054.148 | 1190.19 |
| 1205.023 | 1235.502 | 1317.897 |
| 1350.387 | 1375.649 | 1409.741 |
| 1439.477 | 1454.071 | 1463.455 |
| 1482.114 | 1495.225 | 1594.297 |
| 1678.832 | 1730.976 | 2996.817 |
| 3043.092 | 3099.536 | 3114.053 |
| 3144.256 | 3152.41 | 3180.752 |
| 3181.525 | 3205.7 | 3242.025 |

***i35 – p44***

C -2.065222 -1.270090 1.045752

C -0.998447 -0.378634 -0.853794

C 0.244971 -0.917714 -0.736273

C 1.320035 -0.234570 -0.038468

C 1.006146 1.100337 0.488752

C -0.161183 1.701659 0.259649

C -1.249493 1.077953 -0.562187

C 2.533540 -0.790625 0.131759

H -1.533178 -0.677183 1.779821

H -1.813461 -2.321506 0.985968

H -3.092832 -0.997350 0.831754

H -1.738905 -0.889797 -1.459108

H 0.431972 -1.926498 -1.090801

H 1.771287 1.597890 1.076988

H -0.344819 2.695286 0.656864

H -2.219076 1.217438 -0.074013

H -1.327735 1.617147 -1.518350

H 3.324671 -0.268817 0.658561

H 2.759988 -1.776502 -0.258828

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -465.924 | 86.8318 | 94.7276 |
| 130.3904 | 207.3587 | 328.6946 |
| 367.3433 | 378.2031 | 477.9442 |
| 482.9017 | 520.2108 | 572.7417 |
| 609.2664 | 670.541 | 778.9565 |
| 794.2252 | 803.52 | 822.2718 |
| 891.2311 | 893.1538 | 940.0698 |
| 954.2695 | 969.0171 | 989.6774 |
| 1013.081 | 1032.204 | 1172.604 |
| 1209.375 | 1225.717 | 1334.155 |
| 1387.317 | 1388.379 | 1416.746 |
| 1422.435 | 1441.917 | 1468.847 |
| 1476.803 | 1566.192 | 1646.73 |
| 1741.845 | 3006.464 | 3071.132 |
| 3098.11 | 3155.658 | 3174.641 |
| 3183.154 | 3197.113 | 3205.009 |
| 3246.773 | 3262.001 | 3275.004 |

***i35 – p46***

C 2.488348 -0.940231 -0.075435

C 1.132176 -0.299943 0.032944

C -0.009287 -1.024512 -0.018333

C -1.334778 -0.419998 -0.019008

C -1.380844 1.045222 0.032916

C -0.276462 1.789091 -0.000439

C 1.096631 1.201249 -0.109029

C -2.451642 -1.164266 -0.051922

H 2.889644 -0.793305 -1.084706

H 2.441312 -2.012283 0.122341

H 3.195426 -0.490323 0.626051

H 1.095259 -0.269303 2.044490

H 0.047734 -2.109418 -0.001464

H -2.357234 1.514437 0.100982

H -0.350516 2.871531 0.034871

H 1.529206 1.462300 -1.087309

H 1.764712 1.659557 0.629123

H -3.434056 -0.705727 -0.048530

H -2.406334 -2.247138 -0.086016

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -718.547 | 112.7264 | 164.8934 |
| 219.5348 | 289.1501 | 337.3275 |
| 378.3345 | 410.987 | 470.0226 |
| 484.2458 | 497.817 | 546.7634 |
| 588.9342 | 684.1999 | 710.4336 |
| 793.4263 | 875.3562 | 882.9482 |
| 903.0589 | 928.5809 | 950.8266 |
| 977.9556 | 1010.293 | 1020.868 |
| 1045.345 | 1065.641 | 1177.748 |
| 1206.979 | 1228.821 | 1321.027 |
| 1366.818 | 1400.196 | 1418.526 |
| 1436.752 | 1464.999 | 1468.692 |
| 1489.868 | 1496.874 | 1650.384 |
| 1669.702 | 1751.146 | 3003.295 |
| 3039.244 | 3059.043 | 3105.321 |
| 3143.92 | 3162.234 | 3177.279 |
| 3178.308 | 3199.821 | 3253.284 |

***i30 – p46***

C -2.501241 -0.924960 -0.096575

C -1.150374 -0.284159 -0.056902

C -0.012006 -1.010635 0.024946

C 1.325769 -0.398132 -0.026469

C 1.364714 1.065831 0.007515

C 0.256878 1.804954 0.025268

C -1.119810 1.215038 -0.000286

C 2.438261 -1.136804 -0.108374

H -3.063433 -0.687481 0.814608

H -2.430761 -2.010652 -0.179829

H -3.088146 -0.548861 -0.941306

H -0.063715 -2.090161 -0.084095

H -0.087481 -1.354697 1.955300

H 2.340699 1.540805 0.015696

H 0.328390 2.887856 0.053936

H -1.681855 1.549240 0.885353

H -1.681298 1.621718 -0.853781

H 3.417764 -0.674311 -0.154553

H 2.396690 -2.220253 -0.126072

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -724.75 | 93.6802 | 114.2323 |
| 184.5505 | 267.2623 | 295.0597 |
| 321.6667 | 374.8245 | 420.039 |
| 485.7444 | 508.6162 | 542.6435 |
| 593.6542 | 708.4731 | 711.7194 |
| 795.3319 | 883.7707 | 904.4821 |
| 912.5915 | 931.3785 | 969.2915 |
| 973.2737 | 1008.826 | 1018.01 |
| 1045.246 | 1062.26 | 1182.593 |
| 1207.129 | 1228.726 | 1317.218 |
| 1361.647 | 1403.197 | 1417.292 |
| 1435.661 | 1455.99 | 1468.484 |
| 1481.718 | 1490.546 | 1653.113 |
| 1694.186 | 1762.391 | 2998.869 |
| 3023.621 | 3030.523 | 3089.687 |
| 3137.215 | 3161.13 | 3176.401 |
| 3179.363 | 3203.158 | 3250.894 |

***i31 – p48***

C -2.573575 -0.802882 -0.041143

C -1.185877 -0.237529 -0.047643

C -0.084635 -1.014556 0.086133

C 1.266608 -0.454138 -0.006176

C 1.388092 1.024584 0.279217

C 0.155029 1.804401 -0.076026

C -1.032529 1.207986 -0.207032

C 2.321233 -1.213946 -0.308445

H -3.154151 -0.382889 0.787168

H -2.564989 -1.888803 0.064255

H -3.100602 -0.547680 -0.966419

H -0.184408 -2.095765 0.099164

H -0.209297 -1.161031 2.272777

H 2.269460 1.440089 -0.216379

H 1.559395 1.152621 1.359655

H 0.246461 2.880758 -0.177676

H -1.920478 1.792958 -0.426597

H 3.313620 -0.789641 -0.416425

H 2.218918 -2.284152 -0.452827

***Frequencies***

|  |  |  |
| --- | --- | --- |
| -456.252 | 109.9989 | 137.4999 |
| 173.01 | 209.2957 | 250.6275 |
| 297.0099 | 337.3102 | 427.1846 |
| 453.0704 | 527.2979 | 552.0258 |
| 577.5938 | 701.6832 | 719.8991 |
| 760.7194 | 875.5035 | 885.4012 |
| 921.9987 | 944.4212 | 957.4426 |
| 984.5153 | 1008.891 | 1023.536 |
| 1047.393 | 1064.51 | 1197.475 |
| 1208.276 | 1229.032 | 1317.303 |
| 1352.807 | 1371.219 | 1413.681 |
| 1446.281 | 1454.073 | 1464.417 |
| 1484.621 | 1493.437 | 1619.398 |
| 1707.908 | 1737.704 | 2996.51 |
| 3040.409 | 3097.703 | 3100.359 |
| 3141.709 | 3151.307 | 3175.315 |
| 3184.019 | 3200.057 | 3239.761 |

***Products***

***p10a + CH3***

C 0.140396 0.714961 -0.000252

C 1.171285 -0.142974 -0.000266

C -3.792134 -0.380692 0.000509

C -2.388279 0.008281 -0.000648

C -1.225748 0.320450 -0.000679

C 2.563110 0.277710 0.000477

C 3.594658 -0.566652 0.000109

H 0.337088 1.784964 0.000273

H 0.973326 -1.211914 -0.000811

H -4.071598 -0.822013 0.960803

H -3.991138 -1.118909 -0.780598

H -4.435912 0.484214 -0.176444

H 2.746918 1.350197 0.001444

H 3.443404 -1.641872 -0.000897

H 4.618185 -0.211175 0.000732

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 55.8267 | 82.3862 | 85.9817 |
| 156.637 | 236.3778 | 280.6826 |
| 348.406 | 437.057 | 458.8177 |
| 550.4739 | 663.0101 | 821.8724 |
| 883.8556 | 938.9782 | 964.7419 |
| 974.012 | 1037.238 | 1049.56 |
| 1052.265 | 1198.578 | 1211.095 |
| 1294.075 | 1329.123 | 1348.404 |
| 1410.822 | 1456.841 | 1479.869 |
| 1487.136 | 1685.689 | 1740.487 |
| 2375.703 | 3050.852 | 3120.865 |
| 3127.385 | 3153.868 | 3162.033 |
| 3166.537 | 3179.805 | 3249.487 |

***p10b + CH3***

C 0.281635 -0.314982 -0.235168

C 1.156368 0.661154 0.044844

C 2.611403 0.524914 -0.055388

C 3.297710 -0.591617 0.182654

C -3.772668 0.023251 0.110051

C -2.325545 -0.093552 -0.010469

C -1.129045 -0.180493 -0.107999

H 0.647897 -1.272083 -0.599035

H 0.772133 1.631577 0.347521

H 3.154203 1.427580 -0.326682

H 2.806917 -1.501071 0.514680

H 4.374857 -0.624778 0.067891

H -4.169301 0.711513 -0.641018

H -4.051550 0.402544 1.096450

H -4.254304 -0.947333 -0.030966

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 77.8812 | 83.2641 | 97.0024 |
| 184.8089 | 224.4364 | 271.9406 |
| 325.0407 | 448.2182 | 508.5483 |
| 566.4162 | 661.7907 | 835.1539 |
| 888.9466 | 959.1356 | 983.9538 |
| 1002.529 | 1037.578 | 1054.809 |
| 1063.082 | 1081.062 | 1213.673 |
| 1316.36 | 1323.341 | 1353.711 |
| 1421.91 | 1455.53 | 1485.217 |
| 1486.44 | 1707.02 | 1718.368 |
| 2377.095 | 3048.525 | 3119.399 |
| 3124.894 | 3154.534 | 3160.05 |
| 3165.48 | 3183.567 | 3249.061 |

***p11a*** ***+ CH3***

C 0.204006 1.377239 0.000018

C -0.997706 0.613543 -0.001826

C -2.026904 -0.011051 -0.002309

C -3.270612 -0.769826 0.001240

C 1.441354 0.855479 0.001068

C 2.987802 -1.052748 0.000065

C 1.746685 -0.566081 -0.000338

H 0.085770 2.456518 0.001250

H -3.081934 -1.828417 -0.192652

H -3.772069 -0.686095 0.968966

H -3.954606 -0.399746 -0.766705

H 2.285741 1.539695 0.003093

H 3.853132 -0.396273 0.001535

H 3.177877 -2.119543 -0.001192

H 0.898345 -1.245470 -0.001800

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 82.5915 | 119.2763 | 135.8382 |
| 176.2681 | 238.1967 | 344.1311 |
| 344.5192 | 450.0967 | 477.2245 |
| 661.2365 | 696.7473 | 790.8751 |
| 812.9387 | 945.6015 | 955.4388 |
| 1004.075 | 1058.221 | 1061.406 |
| 1065.908 | 1135.481 | 1199.5 |
| 1275.813 | 1321.121 | 1403.469 |
| 1426.216 | 1476.674 | 1488.591 |
| 1491.367 | 1671.261 | 1734.951 |
| 2372.411 | 3049.636 | 3120.37 |
| 3125.276 | 3150.35 | 3171.221 |
| 3181.579 | 3192.738 | 3246.307 |

***p11b + CH3***

C 0.551239 -1.396577 0.032344

C -0.696571 -0.718237 0.009289

C -1.779890 -0.191980 -0.008553

C 1.374857 1.638889 0.066016

C 2.158777 0.566666 -0.067838

C 1.775775 -0.842866 -0.002517

C -3.076980 0.469977 -0.028227

H 0.486236 -2.480068 0.077006

H 0.311531 1.559751 0.251381

H 1.799136 2.634178 -0.004362

H 3.219966 0.733335 -0.237027

H 2.608692 -1.540114 0.007191

H -3.598709 0.325358 0.921374

H -2.962407 1.544235 -0.193458

H -3.707679 0.068094 -0.825184

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 74.4117 | 89.1857 | 105.909 |
| 171.1998 | 245.6838 | 335.167 |
| 355.7856 | 462.4921 | 478.7354 |
| 675.1284 | 690.6601 | 800.6214 |
| 810.0662 | 947.7782 | 974.3942 |
| 1012.18 | 1055.404 | 1057.849 |
| 1063.449 | 1108.655 | 1175.238 |
| 1279.206 | 1363.342 | 1420.404 |
| 1441.962 | 1472.601 | 1485.857 |
| 1488.756 | 1684.517 | 1718.672 |
| 2369.19 | 3051.141 | 3123.278 |
| 3126.001 | 3156.463 | 3167.357 |
| 3174.185 | 3192.216 | 3268.188 |

***p12a + H***

C 0.007721 2.482101 -0.000025

C 0.214547 0.989762 0.000040

C -0.974672 0.193778 -0.000261

C -1.999061 -0.438433 -0.000507

C -3.231111 -1.216322 0.000049

C 1.439731 0.434171 0.000338

C 2.948454 -1.505461 -0.000343

C 1.717699 -0.992306 0.000399

H -0.563799 2.790178 0.880309

H -0.562879 2.790264 -0.880927

H 0.962808 3.010345 0.000472

H -3.198805 -1.995209 -0.765900

H -3.383998 -1.699882 0.968382

H -4.094662 -0.577724 -0.200804

H 2.300699 1.099000 0.000521

H 3.828162 -0.868300 -0.001120

H 3.115382 -2.576103 -0.000239

H 0.857255 -1.656311 0.001165

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 79.2953 | 110.8606 | 118.3584 |
| 138.418 | 186.5459 | 203.8324 |
| 231.8406 | 302.409 | 368.8867 |
| 394.5467 | 460.7388 | 584.5067 |
| 619.8072 | 677.5559 | 698.4517 |
| 915.0286 | 950.3893 | 951.4787 |
| 1046.81 | 1050.745 | 1056.89 |
| 1061.221 | 1062.943 | 1072.977 |
| 1182.401 | 1252.885 | 1322.479 |
| 1379.121 | 1418.49 | 1422.233 |
| 1459.673 | 1478.567 | 1486.141 |
| 1491.156 | 1498.588 | 1681.833 |
| 1737.437 | 2370.741 | 3044.334 |
| 3050.008 | 3107.991 | 3120.579 |
| 3126.129 | 3142.809 | 3147.864 |
| 3163.57 | 3177.972 | 3244.541 |

***p12b + H***

C -0.746664 2.418720 -0.086596

C -0.651694 0.914730 -0.004045

C 0.679062 0.395720 0.016199

C 1.826501 0.031739 0.036019

C -0.974035 -2.229033 -0.213270

C -1.864988 -1.310010 0.161583

C -1.753822 0.145233 0.065413

C 3.202573 -0.444792 0.060107

H -0.269228 2.783914 -1.000355

H -0.227277 2.881823 0.757389

H -1.787161 2.748395 -0.081043

H -0.024425 -1.965361 -0.661253

H -1.189525 -3.283929 -0.085691

H -2.810595 -1.658534 0.571740

H -2.703875 0.673882 0.082923

H 3.810101 0.083638 -0.678828

H 3.651665 -0.283390 1.043519

H 3.248721 -1.514288 -0.160854

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 67.0218 | 73.8174 | 82.4834 |
| 152.3594 | 172.1845 | 223.8716 |
| 239.5117 | 312.4424 | 337.251 |
| 368.0144 | 528.1377 | 582.3303 |
| 632.8436 | 666.7151 | 708.3183 |
| 901.9226 | 961.2398 | 968.823 |
| 1019.006 | 1047.519 | 1054.643 |
| 1057.872 | 1070.853 | 1073.143 |
| 1138.338 | 1242.669 | 1347.768 |
| 1412.331 | 1415.722 | 1425.564 |
| 1459.875 | 1478.818 | 1481.551 |
| 1488.013 | 1501.432 | 1699.053 |
| 1718.761 | 2369.126 | 3046.702 |
| 3049.115 | 3113.23 | 3118.497 |
| 3126.072 | 3138.847 | 3147.655 |
| 3169.106 | 3176.192 | 3265.242 |

***p13a + H***

C -0.276141 1.985094 0.000153

C -0.106778 0.487159 -0.000218

C 1.250510 0.031336 -0.000665

C 2.405293 -0.308251 -0.000859

C 3.799051 -0.733337 0.000332

C -1.106906 -0.414364 -0.000042

C -3.465893 -1.087194 0.000055

C -2.533506 -0.133191 0.000294

H 0.208489 2.416171 -0.880240

H 0.210101 2.415792 0.879839

H -1.321387 2.291396 0.001167

H 4.246527 -0.596778 0.988395

H 3.884594 -1.789465 -0.266497

H 4.383818 -0.152396 -0.717343

H -0.832698 -1.466113 -0.000202

H -3.198404 -2.139671 -0.000409

H -4.522566 -0.847308 0.000286

H -2.852258 0.904864 0.000708

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 35.9513 | 85.4177 | 95.6391 |
| 117.7575 | 122.4787 | 227.2111 |
| 241.6528 | 313.2606 | 382.3446 |
| 390.7779 | 434.7124 | 558.3648 |
| 582.6458 | 675.8017 | 750.3193 |
| 918.1554 | 920.9346 | 946.4789 |
| 1011.146 | 1024.338 | 1055.248 |
| 1061.225 | 1066.017 | 1068.38 |
| 1199.456 | 1275.634 | 1326.524 |
| 1368.42 | 1422.45 | 1427.275 |
| 1457.869 | 1482.815 | 1483.78 |
| 1487.04 | 1498.437 | 1681.33 |
| 1737.444 | 2373.089 | 3049.043 |
| 3057.821 | 3117.634 | 3119.02 |
| 3126.968 | 3149.529 | 3159.179 |
| 3168.35 | 3183.904 | 3244.61 |

***p13b + H***

C 0.622467 1.643910 -0.203168

C 0.175969 0.206902 -0.110296

C -1.239526 0.004058 -0.025284

C -2.434185 -0.123288 0.046691

C 3.292968 -0.040036 0.417372

C 2.453424 -0.879644 -0.188885

C 0.991541 -0.864354 -0.122883

C -3.878468 -0.295021 0.135942

H 0.642717 2.108780 0.787687

H -0.080354 2.213648 -0.814388

H 1.620335 1.723095 -0.636979

H 2.943441 0.759819 1.060362

H 4.365701 -0.152474 0.308990

H 2.876977 -1.700334 -0.765015

H 0.516468 -1.841562 -0.117321

H -4.392836 0.660138 0.005746

H -4.236086 -0.982096 -0.635307

H -4.161514 -0.704178 1.109282

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 68.0776 | 83.9259 | 95.5925 |
| 131.0123 | 187.277 | 253.403 |
| 265.2271 | 312.5115 | 337.9692 |
| 397.6439 | 550.0705 | 555.1689 |
| 570.3177 | 650.577 | 785.4403 |
| 903.8613 | 926.3536 | 966.2119 |
| 1024.877 | 1046.682 | 1053.101 |
| 1064.695 | 1066.992 | 1071.163 |
| 1112.914 | 1291.791 | 1338.302 |
| 1386.627 | 1421.391 | 1427.232 |
| 1461.982 | 1485.904 | 1487.306 |
| 1493.03 | 1501.492 | 1708.359 |
| 1715.25 | 2374.187 | 3050.411 |
| 3051.378 | 3118.992 | 3121.448 |
| 3125.894 | 3148.61 | 3151.817 |
| 3166.132 | 3183.22 | 3252.701 |

***p39 + C2H3***

C 1.132268 0.116939 0.000006

C 1.796695 1.274582 -0.000002

C 1.821464 -1.223775 -0.000002

C -2.958892 -0.044793 -0.000003

C -1.503105 0.019257 0.000003

C -0.302028 0.087385 0.000004

H 2.881162 1.292559 -0.000003

H 1.275929 2.224319 -0.000006

H 1.530025 -1.803090 0.880591

H 2.906399 -1.105518 0.000068

H 1.530131 -1.803018 -0.880677

H -3.303658 -1.081675 0.001438

H -3.369142 0.448185 -0.885041

H -3.369253 0.450666 0.883595

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 40.6061 | 114.1576 | 134.1695 |
| 169.315 | 310.0292 | 360.8824 |
| 383.2361 | 548.8619 | 579.0869 |
| 664.7475 | 742.5326 | 933.451 |
| 938.2265 | 1035.907 | 1056.124 |
| 1056.163 | 1072.148 | 1097.043 |
| 1331.673 | 1414.291 | 1420.324 |
| 1441.78 | 1477.039 | 1483.222 |
| 1486.848 | 1498.116 | 1717.304 |
| 2378.255 | 3045.836 | 3052.882 |
| 3112.028 | 3125.709 | 3125.819 |
| 3143.108 | 3165.867 | 3260.304 |

***p49 + H***

C -0.565046 2.397133 -0.266931

C -0.396549 1.124690 0.099045

C 0.886835 0.490308 0.042379

C 1.940522 -0.089111 0.017661

C 3.219089 -0.786404 -0.017930

C -1.543456 0.257055 0.584000

C -1.721098 -2.151228 -0.093073

C -1.848829 -0.861916 -0.373279

H -1.542297 2.864955 -0.217050

H 0.264938 2.997676 -0.618900

H 3.750224 -0.669659 0.930329

H 3.071116 -1.854496 -0.194770

H 3.856256 -0.393363 -0.813901

H -2.428634 0.889304 0.707242

H -1.291775 -0.158671 1.564760

H -1.379591 -2.486625 0.882012

H -1.949568 -2.916027 -0.826830

H -2.179480 -0.556265 -1.364124

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 47.7174 | 55.1025 | 106.6987 |
| 118.5204 | 142.5331 | 237.5877 |
| 314.0665 | 347.5501 | 386.9941 |
| 439.7847 | 565.591 | 591.7442 |
| 637.658 | 729.8568 | 750.5923 |
| 917.9276 | 942.8178 | 949.2925 |
| 958.9372 | 976.8782 | 1034.023 |
| 1058.567 | 1063.013 | 1085.213 |
| 1129.717 | 1242.566 | 1304.926 |
| 1329.084 | 1338.197 | 1421.735 |
| 1447.102 | 1455.005 | 1481.335 |
| 1487.226 | 1490.128 | 1712.763 |
| 1739.63 | 2379.606 | 3052.573 |
| 3054.953 | 3104.893 | 3123.793 |
| 3128.458 | 3147.304 | 3163.401 |
| 3164.053 | 3240.559 | 3258.015 |

***p50 + H***

C -0.021017 2.531991 -0.130472

C 0.098171 1.038726 0.014205

C -0.957753 0.254950 -0.002612

C -1.974508 -0.499282 -0.017039

C -3.025495 -1.283112 -0.032045

C 1.502574 0.496723 0.171942

C 2.261224 -1.825696 -0.355468

C 1.592118 -0.979312 0.414240

H -1.057651 2.839182 -0.264619

H 0.562173 2.877846 -0.990880

H 0.383381 3.033062 0.755677

H -4.025316 -0.878803 -0.150338

H -2.922538 -2.358022 0.072540

H 1.972750 1.034819 1.007511

H 2.080432 0.767874 -0.720709

H 2.790916 -1.488966 -1.242164

H 2.302243 -2.885602 -0.131285

H 1.061729 -1.351317 1.287760

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 51.0117 | 76.8526 | 104.5138 |
| 142.0657 | 176.113 | 228.1947 |
| 305.8039 | 374.7523 | 408.6384 |
| 424.3486 | 552.6636 | 562.0396 |
| 574.8347 | 632.9756 | 737.3653 |
| 886.6414 | 903.8324 | 933.448 |
| 964.1834 | 994.917 | 1033.887 |
| 1038.891 | 1047.956 | 1129.181 |
| 1160.049 | 1210.295 | 1261.003 |
| 1324.969 | 1355.652 | 1409.256 |
| 1445.345 | 1453.128 | 1473.301 |
| 1488.463 | 1489.849 | 1739.504 |
| 1744.917 | 2242.25 | 3013.304 |
| 3038.685 | 3054.398 | 3096.781 |
| 3144.921 | 3148.332 | 3160.142 |
| 3173.01 | 3230.085 | 3239.926 |

***p51 + H***

C -0.172374 2.180949 -0.002382

C -0.213531 0.675948 -0.315340

C 1.121468 0.077753 -0.197925

C 2.217270 -0.400189 -0.084679

C 3.545648 -0.987508 0.049839

C -1.192266 -0.035705 0.602093

C -3.364560 -1.199296 -0.236739

C -2.281455 -0.616027 0.189563

H 0.532978 2.690393 -0.662233

H 0.145267 2.347624 1.030089

H -1.163769 2.619534 -0.136412

H -0.560111 0.542306 -1.344985

H 3.773434 -1.194283 1.098452

H 3.614165 -1.927545 -0.503120

H 4.311697 -0.309992 -0.335437

H -0.952480 -0.038613 1.663169

H -3.361174 -2.247580 -0.517753

H -4.301209 -0.657385 -0.318348

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 38.5386 | 105.2215 | 110.0576 |
| 131.6338 | 178.334 | 255.9747 |
| 285.3965 | 302.4958 | 341.7172 |
| 353.6566 | 493.6793 | 519.1511 |
| 538.5121 | 637.9437 | 770.0315 |
| 889.0632 | 899.2516 | 906.4374 |
| 1020.631 | 1023.023 | 1058.607 |
| 1064.949 | 1094.751 | 1100.852 |
| 1155.645 | 1195.922 | 1270.294 |
| 1338.741 | 1383.799 | 1413.537 |
| 1421.665 | 1483.023 | 1488.823 |
| 1490.904 | 1498.522 | 1503.023 |
| 2089.698 | 2393.084 | 3050.322 |
| 3052.438 | 3072.881 | 3121.677 |
| 3124.563 | 3134.519 | 3141.377 |
| 3143.428 | 3158.382 | 3225.793 |

***p52 + H***

C -0.522656 2.472459 0.054189

C -1.216841 1.161831 -0.113807

C 0.793292 -0.201323 -0.049629

C 1.982146 -0.374714 0.016277

C 3.422518 -0.580393 0.099071

C -0.630424 -0.045654 -0.137041

C -2.581621 -1.533516 0.300375

C -1.407142 -1.299173 -0.276308

H -0.717869 3.125954 -0.802350

H 0.555777 2.346861 0.159747

H -0.899834 2.992108 0.941486

H -2.295900 1.193410 -0.241255

H 3.922319 -0.207842 -0.798753

H 3.840774 -0.056343 0.962165

H 3.655824 -1.642784 0.202934

H -3.046416 -0.807678 0.960059

H -3.107225 -2.467741 0.139958

H -0.943082 -2.073046 -0.882755

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 41.663 | 79.8786 | 97.0884 |
| 127.9587 | 177.6211 | 192.0066 |
| 235.4168 | 292.2054 | 356.7278 |
| 397.6749 | 481.3827 | 565.7029 |
| 598.9224 | 687.7802 | 739.2482 |
| 879.3286 | 935.6188 | 959.1429 |
| 1016.766 | 1029.205 | 1057.808 |
| 1059.318 | 1067.268 | 1110.315 |
| 1151.178 | 1243.831 | 1322.357 |
| 1375.388 | 1417.755 | 1423.17 |
| 1458.882 | 1484.439 | 1486.972 |
| 1488.56 | 1489.327 | 1712.999 |
| 1724.217 | 2376.829 | 3040.785 |
| 3053.101 | 3097.134 | 3124.654 |
| 3127.887 | 3143.019 | 3155.249 |
| 3174.284 | 3178.385 | 3247.943 |

***p53 + H***

C 2.512688 -1.399444 -0.055474

C 1.032753 -1.213453 0.050108

C -1.094102 -0.091519 -0.024551

C -2.296195 -0.070971 0.017894

C -3.752376 -0.059277 0.076908

C 0.340811 -0.069046 -0.085370

C 1.989398 1.772133 0.294851

C 0.933412 1.265052 -0.333754

H 2.966757 -1.512509 0.935709

H 2.999514 -0.557715 -0.550354

H 2.736833 -2.314601 -0.610491

H 0.451580 -2.113190 0.233100

H -4.171500 -0.925772 -0.440751

H -4.100108 -0.083338 1.113063

H -4.152526 0.842778 -0.392430

H 2.506158 1.226073 1.076651

H 2.355303 2.765350 0.060431

H 0.409648 1.872069 -1.068597

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 32.4937 | 80.9077 | 100.6098 |
| 136.1829 | 197.3919 | 259.0988 |
| 282.8118 | 304.3612 | 337.93 |
| 424.9978 | 451.128 | 516.4342 |
| 569.6493 | 737.5833 | 760.038 |
| 874.66 | 935.6769 | 965.6173 |
| 998.9225 | 1034.341 | 1051.889 |
| 1059.613 | 1072.92 | 1113.992 |
| 1149.487 | 1267.153 | 1334.346 |
| 1366.733 | 1417.69 | 1431.265 |
| 1462.071 | 1483.771 | 1486.867 |
| 1498.691 | 1513.041 | 1713.631 |
| 1725.673 | 2377.979 | 3035.433 |
| 3051.416 | 3095.146 | 3121.193 |
| 3127.006 | 3138.914 | 3156.982 |
| 3172.81 | 3179.594 | 3249.095 |

***p54 + C2H3***

C -2.058797 1.147399 0.000394

C -1.990793 -0.344973 -0.001081

C 0.449857 -0.541397 0.001963

C 1.575634 -0.115635 0.001853

C 2.938469 0.400633 -0.001217

C -0.872913 -1.077397 0.000033

H -2.589248 1.509476 -0.886342

H -1.063377 1.593910 0.015416

H -2.614927 1.506535 0.872356

H -2.939362 -0.875718 -0.003895

H 3.321924 0.498659 1.017837

H 3.605278 -0.268545 -0.550688

H 2.981373 1.384596 -0.474755

H -0.950405 -2.160700 -0.001597

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 63.8301 | 85.4994 | 100.4738 |
| 171.3948 | 263.665 | 349.2574 |
| 413.9261 | 506.395 | 606.5902 |
| 748.1925 | 792.5268 | 939.8037 |
| 994.9002 | 1051.892 | 1059.062 |
| 1068.72 | 1104.323 | 1179.564 |
| 1276.746 | 1398.777 | 1417.868 |
| 1444.087 | 1481.953 | 1483.231 |
| 1487.156 | 1490.532 | 1727.104 |
| 2375.566 | 3043.156 | 3050.881 |
| 3100.227 | 3121.307 | 3125.261 |
| 3143.982 | 3168.883 | 3189.861 |

***p55 + C2H3***

C 3.138140 -0.113108 0.000019

C 1.670921 -0.399744 -0.000041

C -0.679530 0.257845 0.000013

C -1.865306 0.053267 0.000072

C -3.300453 -0.200228 0.000028

C 0.719408 0.536157 -0.000055

H 3.620275 -0.552087 0.879492

H 3.337130 0.960932 -0.000461

H 3.620519 -0.552892 -0.878914

H 1.372354 -1.445362 0.000003

H -3.620360 -0.633524 -0.951267

H -3.573753 -0.896764 0.796798

H -3.857073 0.727428 0.154238

H 1.001821 1.587137 -0.000106

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 55.8911 | 107.6327 | 114.6984 |
| 189.7898 | 275.8967 | 295.3903 |
| 394.9763 | 468.0742 | 517.1082 |
| 813.137 | 819.8098 | 953.36 |
| 988.7593 | 1052.353 | 1059.193 |
| 1073.354 | 1136.137 | 1206.699 |
| 1317.093 | 1333.851 | 1417.577 |
| 1425.695 | 1479.078 | 1483.64 |
| 1487.88 | 1498.798 | 1740.859 |
| 2378.269 | 3041.25 | 3051.205 |
| 3100.826 | 3120.79 | 3126.96 |
| 3130.028 | 3148.483 | 3167.943 |

***p56 + H***

C 1.895287 2.127907 -0.189177

C 1.126004 1.244354 0.428760

C -0.902799 -0.001796 -0.155628

C -2.101052 -0.002367 -0.080304

C -3.557121 -0.001495 -0.000384

C 0.564770 -0.000225 -0.227592

C 1.901998 -2.124085 -0.189323

C 1.129196 -1.243494 0.428454

H 2.281944 2.999723 0.326027

H 2.164357 2.011343 -1.234866

H 0.862494 1.381472 1.475168

H -3.910323 0.801128 0.651698

H -3.999951 0.145754 -0.988537

H -3.926610 -0.949530 0.398307

H 0.862470 0.000304 -1.282146

H 2.171730 -2.005895 -1.234660

H 2.291074 -2.994954 0.325661

H 0.865118 -1.382131 1.474518

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 64.1218 | 72.6807 | 77.6859 |
| 116.7028 | 130.06 | 273.5159 |
| 285.7509 | 289.2586 | 398.3834 |
| 435.5257 | 499.4591 | 500.2281 |
| 669.6413 | 683.9092 | 838.2402 |
| 926.7499 | 961.6875 | 965.2451 |
| 980.4386 | 1037.583 | 1042.795 |
| 1060.139 | 1063.305 | 1123.375 |
| 1161.939 | 1187.913 | 1273.136 |
| 1305.647 | 1323.386 | 1337.731 |
| 1423.704 | 1455.077 | 1457.01 |
| 1486.224 | 1489.963 | 1732.17 |
| 1742.374 | 2393.728 | 3048.891 |
| 3054.645 | 3119.502 | 3124.118 |
| 3153.164 | 3153.865 | 3171.989 |
| 3175.16 | 3245.918 | 3246.405 |

***p57 + H***

C -0.377420 2.507647 -0.158838

C -0.030602 1.185147 0.482179

C -0.689924 -0.053144 0.043358

C -1.734649 -0.797051 -0.016491

C -2.794865 -1.554827 -0.080699

C 0.744098 0.125384 -0.309405

C 2.866077 -1.162595 -0.228352

C 1.767863 -0.704012 0.359924

H -1.262993 2.944034 0.309896

H -0.591882 2.376003 -1.222256

H 0.448960 3.216473 -0.058236

H 0.216036 1.232475 1.541161

H -3.500392 -1.464516 -0.899973

H -2.999869 -2.297199 0.683382

H 0.947417 0.373577 -1.349027

H 3.080317 -0.952524 -1.271866

H 3.584572 -1.767352 0.312258

H 1.574365 -0.940265 1.404607

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 73.0693 | 110.2322 | 154.5482 |
| 209.5305 | 215.8254 | 256.2686 |
| 330.8523 | 375.4157 | 423.1113 |
| 485.1394 | 588.1631 | 603.5082 |
| 651.2663 | 759.3774 | 856.5526 |
| 872.8673 | 891.4819 | 953.1264 |
| 1006.991 | 1024.079 | 1024.948 |
| 1048.343 | 1055.938 | 1101.553 |
| 1129.364 | 1152.222 | 1209.084 |
| 1299.655 | 1320.441 | 1343.296 |
| 1414.551 | 1426.233 | 1466.427 |
| 1496.43 | 1506.523 | 1556.802 |
| 1735.869 | 2138.681 | 3050.334 |
| 3125.281 | 3127.043 | 3137.534 |
| 3144.314 | 3147.773 | 3150.288 |
| 3160.614 | 3230.19 | 3246.562 |

***p42 + CH3***

C 1.195538 1.199818 0.002023

C -0.193735 1.196971 -0.009046

C -0.908973 0.000002 -0.012244

C -0.193737 -1.196970 -0.009045

C 1.195536 -1.199819 0.002023

C 1.895986 -0.000001 0.008429

C -2.415550 0.000000 0.009653

H 1.731705 2.142463 0.002303

H -0.732363 2.139656 -0.017490

H -0.732367 -2.139654 -0.017490

H 1.731700 -2.142466 0.002302

H 2.980100 -0.000002 0.014617

H -2.820424 -0.884482 -0.487029

H -2.820427 0.884525 -0.486952

H -2.788313 -0.000044 1.038980

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 34.8642 | 207.7988 | 350.0785 |
| 417.0356 | 478.6255 | 533.5122 |
| 639.4238 | 717.9088 | 748.6522 |
| 808.5812 | 866.281 | 920.6975 |
| 995.496 | 1010.276 | 1013.52 |
| 1024.216 | 1064.215 | 1067.412 |
| 1121.635 | 1186.055 | 1217.239 |
| 1245.97 | 1332.672 | 1363.76 |
| 1419.204 | 1477.626 | 1499.92 |
| 1511.653 | 1547.483 | 1660.972 |
| 1684.996 | 3050.519 | 3116.919 |
| 3140.232 | 3183.009 | 3184.436 |
| 3198.008 | 3207.204 | 3220.419 |

***p1 + H***

C 2.514963 -1.033952 0.006534

C 1.218549 -0.265606 -0.006499

C 0.000002 -0.941214 -0.011637

C -1.218547 -0.265611 -0.006540

C -1.204417 1.127834 -0.000270

C -0.000003 1.818600 0.002619

C 1.204416 1.127837 -0.000223

C -2.514961 -1.033956 0.006561

H 2.510011 -1.829121 -0.743379

H 2.680066 -1.502609 0.981512

H 3.365844 -0.381223 -0.198287

H 0.000005 -2.028761 -0.022633

H -2.142370 1.673914 -0.001767

H -0.000004 2.903220 0.002943

H 2.142366 1.673921 -0.001681

H -3.365733 -0.381447 -0.199415

H -2.680609 -1.501586 0.981945

H -2.509586 -1.829902 -0.742511

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 101.1151 | 101.8826 | 197.0954 |
| 229.1919 | 276.9222 | 409.5253 |
| 442.0371 | 525.766 | 539.3609 |
| 549.2396 | 717.6343 | 744.0453 |
| 787.8462 | 902.4466 | 918.2242 |
| 927.3635 | 996.9835 | 1003.002 |
| 1027.264 | 1040.423 | 1072.154 |
| 1074.803 | 1136.274 | 1182.911 |
| 1203.896 | 1291.103 | 1321.434 |
| 1349.55 | 1420.062 | 1422.737 |
| 1467.381 | 1494.587 | 1495.267 |
| 1500.325 | 1519.841 | 1541.364 |
| 1666.199 | 1686.82 | 3047.079 |
| 3047.695 | 3113.249 | 3113.402 |
| 3136.376 | 3136.643 | 3169.041 |
| 3183.593 | 3191.635 | 3211.684 |

***p44 + CH3***

C -1.042990 1.251076 -0.000004

C 0.289724 1.243525 -0.000006

C 1.068751 0.000000 -0.000001

C 0.289724 -1.243525 -0.000006

C -1.042991 -1.251076 -0.000003

C -1.868365 0.000000 0.000006

C 2.407902 0.000000 0.000006

H -1.577451 2.196253 -0.000006

H 0.840985 2.179018 -0.000009

H 0.840984 -2.179020 -0.000011

H -1.577451 -2.196253 -0.000006

H -2.540333 0.000000 -0.869782

H -2.540289 0.000001 0.869833

H 2.971511 -0.926496 0.000008

H 2.971511 0.926496 0.000010

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 116.4393 | 305.867 | 372.729 |
| 384.6247 | 510.2396 | 558.1417 |
| 601.2898 | 686.549 | 789.3702 |
| 802.7072 | 803.9673 | 896.1845 |
| 914.7541 | 960.7094 | 964.237 |
| 975.8652 | 1013.785 | 1023.656 |
| 1027.59 | 1185.131 | 1229.457 |
| 1230.296 | 1338.353 | 1395.328 |
| 1399.501 | 1449.145 | 1458.141 |
| 1475.877 | 1686.516 | 1711.33 |
| 1778.503 | 3014.857 | 3032.297 |
| 3156.411 | 3175.788 | 3176.547 |
| 3197.461 | 3200.398 | 3246.299 |

***p45 + CH3***

C 1.831094 0.043797 -0.133275

C 1.227349 -1.144539 -0.085295

C -0.243150 -1.272168 0.199734

C -1.029444 0.013410 0.027950

C -0.271722 1.262990 0.113557

C 1.066810 1.278335 0.038837

C -2.350322 0.014089 -0.173146

H 2.899677 0.114201 -0.303620

H 1.796011 -2.060911 -0.204866

H -0.683634 -2.067411 -0.408592

H -0.350096 -1.605861 1.243053

H -0.831321 2.190100 0.187448

H 1.602697 2.220656 0.071158

H -2.906347 0.943072 -0.240169

H -2.910672 -0.909329 -0.274580

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 63.8772 | 260.4228 | 383.5535 |
| 437.1575 | 482.1043 | 552.5186 |
| 596.8266 | 674.3314 | 760.124 |
| 775.535 | 826.3803 | 906.1617 |
| 937.4333 | 954.0288 | 966.3779 |
| 985.6579 | 1006.255 | 1017.25 |
| 1036.084 | 1190.576 | 1209.371 |
| 1229.833 | 1322.024 | 1350.695 |
| 1403.023 | 1440.465 | 1448.149 |
| 1474.563 | 1664.696 | 1705.32 |
| 1747.358 | 3004.996 | 3087.622 |
| 3154.335 | 3183.136 | 3189.162 |
| 3205.166 | 3216.2 | 3242.72 |

***p46 + H***

C -2.502470 -0.950538 0.000011

C -1.144409 -0.314249 0.000013

C -0.014848 -1.027508 0.000090

C 1.319293 -0.421252 0.000019

C 1.362279 1.044575 0.000080

C 0.254372 1.783769 0.000040

C -1.120699 1.190281 -0.000108

C 2.436827 -1.160190 -0.000093

H -3.077106 -0.639834 0.879705

H -2.436399 -2.039938 0.000790

H -3.076526 -0.641052 -0.880491

H -0.064925 -2.113388 0.000191

H 2.338819 1.518849 0.000155

H 0.325327 2.867304 0.000088

H -1.682848 1.560380 0.869818

H -1.682589 1.560248 -0.870270

H 3.417683 -0.697938 -0.000158

H 2.396497 -2.243956 -0.000141

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 98.0283 | 127.8892 | 194.6462 |
| 292.8185 | 335.9744 | 420.4396 |
| 440.1147 | 487.3031 | 538.7111 |
| 584.0904 | 694.3638 | 711.4303 |
| 793.4194 | 878.2767 | 883.3785 |
| 903.435 | 930.4697 | 953.1698 |
| 974.4961 | 1006.749 | 1017.487 |
| 1048.384 | 1066.788 | 1179.861 |
| 1207.216 | 1230.381 | 1320.846 |
| 1363.617 | 1403.028 | 1418.134 |
| 1440.274 | 1461.012 | 1468.752 |
| 1478.865 | 1493.691 | 1686.984 |
| 1721.792 | 1782.071 | 3006.279 |
| 3024.211 | 3030.212 | 3086.216 |
| 3136.578 | 3161.257 | 3172.764 |
| 3177.463 | 3201.525 | 3250.752 |

***p3 + H***

C 2.564604 -0.812764 -0.108497

C 1.231008 -0.140155 -0.005522

C 0.048116 -1.028167 0.294126

C -1.307938 -0.407521 0.031775

C -1.371903 1.052817 0.084945

C -0.256682 1.794766 0.024932

C 1.063596 1.183393 -0.097202

C -2.390865 -1.149356 -0.216954

H 2.578131 -1.526363 -0.939572

H 2.780795 -1.383484 0.802267

H 3.369022 -0.090732 -0.259857

H 0.108286 -1.287484 1.363040

H 0.140318 -1.977270 -0.243421

H -2.350311 1.520954 0.115929

H -0.324608 2.877414 0.027976

H 1.918811 1.830187 -0.266337

H -3.365427 -0.691494 -0.348355

H -2.334628 -2.229809 -0.297297

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 82.2211 | 162.4214 | 205.9829 |
| 295.7255 | 340.1813 | 419.2479 |
| 466.0654 | 490.25 | 513.3584 |
| 581.8149 | 691.4093 | 737.8093 |
| 804.0696 | 873.9876 | 876.123 |
| 911.138 | 931.8734 | 955.9367 |
| 983.1314 | 997.4677 | 1013.343 |
| 1068.066 | 1082.527 | 1182.964 |
| 1205.094 | 1235.625 | 1319.217 |
| 1343.136 | 1380.113 | 1420.412 |
| 1434.82 | 1455.162 | 1472.642 |
| 1483.017 | 1496.219 | 1669.455 |
| 1710.937 | 1755.922 | 2993.247 |
| 3031.747 | 3079.574 | 3088.759 |
| 3134.631 | 3148.666 | 3183.174 |
| 3192.637 | 3210.643 | 3236.482 |

***p48 + H***

C -2.572178 -0.845121 0.039428

C -1.186035 -0.270945 0.008721

C -0.082253 -1.031035 0.100009

C 1.265214 -0.465512 0.028874

C 1.382334 1.030102 0.237160

C 0.128732 1.790525 -0.088491

C -1.054072 1.181689 -0.168467

C 2.336822 -1.234813 -0.183789

H -2.555456 -1.928554 0.169087

H -3.105913 -0.617399 -0.889469

H -3.153612 -0.409490 0.858807

H -0.170551 -2.111415 0.174058

H 2.232621 1.426812 -0.324408

H 1.613517 1.214566 1.297481

H 0.207078 2.865956 -0.210291

H -1.955397 1.753608 -0.367828

H 3.332094 -0.811914 -0.270105

H 2.244236 -2.311510 -0.278004

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 86.1886 | 149.7816 | 197.4024 |
| 293.3714 | 310.4419 | 425.0958 |
| 452.6088 | 524.9006 | 547.7813 |
| 564.2832 | 697.2429 | 710.6875 |
| 762.4669 | 869.77 | 885.5038 |
| 907.9335 | 941.9996 | 958.3021 |
| 979.7316 | 1011.462 | 1024.802 |
| 1050.874 | 1070.723 | 1194.574 |
| 1206.929 | 1233.519 | 1318.658 |
| 1353.367 | 1371.354 | 1415.437 |
| 1444.778 | 1453.045 | 1461.583 |
| 1487.503 | 1495.332 | 1679.042 |
| 1708.67 | 1757.524 | 3000.718 |
| 3039.048 | 3091.619 | 3098.039 |
| 3139.132 | 3150.206 | 3173.828 |
| 3175.524 | 3199.843 | 3238.053 |

***p43 + H***

C -2.097858 -1.232195 -0.516646

C -1.199512 -0.459379 0.081025

C 0.096804 -0.986202 0.639622

C 1.282905 -0.260390 0.040895

C 1.093620 1.176108 -0.185046

C -0.095395 1.772278 -0.078891

C -1.368433 1.030408 0.233720

C 2.433906 -0.873739 -0.235999

H -1.943747 -2.301257 -0.620366

H -3.016747 -0.822498 -0.923711

H 0.184823 -2.063313 0.485259

H 0.106811 -0.804887 1.723843

H 1.971424 1.758776 -0.448936

H -0.176061 2.843715 -0.235638

H -1.671245 1.262902 1.265410

H -2.176772 1.389534 -0.409805

H 3.281020 -0.326351 -0.636064

H 2.564274 -1.937956 -0.072071

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 102.8299 | 121.9869 | 306.5873 |
| 354.9817 | 406.641 | 439.2356 |
| 469.0592 | 542.7892 | 572.2869 |
| 688.4891 | 717.5625 | 744.8351 |
| 813.2412 | 862.5536 | 917.9593 |
| 933.2465 | 940.0491 | 947.2836 |
| 955.1106 | 1000.079 | 1013.496 |
| 1019.165 | 1030.357 | 1174 |
| 1203.474 | 1235.402 | 1299.382 |
| 1319.737 | 1339.006 | 1355.851 |
| 1413.596 | 1455.653 | 1463.359 |
| 1473.28 | 1486.64 | 1699.911 |
| 1750.795 | 1760.651 | 3009.778 |
| 3022.523 | 3089.852 | 3116.202 |
| 3147.358 | 3155.64 | 3167.103 |
| 3192.603 | 3233.452 | 3242.854 |

***p58 + H***

C 0.685685 1.627587 0.000153

C -0.641896 1.422664 -0.000499

C 3.534155 -1.300103 -0.000422

C 2.510549 -0.263244 0.000968

C 1.664489 0.593504 0.000802

C -1.288446 0.122593 -0.000325

C -2.613749 -0.040812 -0.000187

C -3.314838 -1.361038 0.000270

H 1.063512 2.645355 0.000044

H -1.292409 2.293591 -0.001127

H 3.562070 -1.818318 -0.962623

H 3.338972 -2.042359 0.777855

H 4.521928 -0.869316 0.180628

H -0.636886 -0.748820 -0.000251

H -3.248601 0.844743 -0.000293

H -3.960061 -1.460503 0.879422

H -2.604053 -2.190151 0.000521

H -3.960165 -1.461135 -0.878731

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 63.0926 | 81.4329 | 90.8099 |
| 138.9581 | 182.1175 | 191.7206 |
| 229.3643 | 286.4884 | 374.5905 |
| 428.6395 | 471.0771 | 544.6058 |
| 647.8424 | 768.2988 | 793.0095 |
| 860.3915 | 951.2481 | 993.9411 |
| 1036.206 | 1057.768 | 1059.063 |
| 1070.339 | 1090.043 | 1141.937 |
| 1190.808 | 1255.781 | 1302.629 |
| 1335.298 | 1415.186 | 1419.721 |
| 1437.931 | 1483.752 | 1484.594 |
| 1488.528 | 1489.736 | 1683.183 |
| 1752.439 | 2373.538 | 3039.481 |
| 3047.949 | 3097.115 | 3119.769 |
| 3122.388 | 3128.473 | 3144.653 |
| 3160.36 | 3167.768 | 3191.067 |

***p59 + H***

C 0.588584 0.734144 0.001374

C -0.452830 -0.111659 0.003391

C 4.507564 -0.411645 -0.002810

C 3.108168 -0.006056 0.000586

C 1.949694 0.321363 0.001781

C -1.840584 0.316564 0.000703

C -2.877270 -0.524936 0.000781

C -4.315680 -0.117412 -0.002934

H 0.405486 1.806458 -0.001880

H -0.262747 -1.182277 0.006660

H 4.629610 -1.382019 -0.490561

H 4.893001 -0.495628 1.016898

H 5.122384 0.316464 -0.537837

H -2.023765 1.390345 -0.002204

H -2.677052 -1.595581 0.003559

H -4.831831 -0.516381 -0.882352

H -4.425435 0.969338 -0.005375

H -4.835520 -0.512905 0.875866

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 53.1973 | 64.5161 | 72.6551 |
| 127.8905 | 185.2636 | 192.7955 |
| 243.2009 | 305.3295 | 320.7334 |
| 396.3822 | 447.859 | 488.3711 |
| 587.8938 | 793.9654 | 816.2744 |
| 889.5093 | 954.0316 | 959.9027 |
| 1017.02 | 1052.799 | 1059.5 |
| 1068.385 | 1109.627 | 1189.845 |
| 1213.148 | 1264.223 | 1334.476 |
| 1349.987 | 1366.689 | 1419.63 |
| 1422.3 | 1478.043 | 1482.708 |
| 1488.717 | 1498.133 | 1702.302 |
| 1757.095 | 2374.968 | 3040.793 |
| 3049.209 | 3099.546 | 3118.51 |
| 3125.018 | 3128.849 | 3150.763 |
| 3155.212 | 3162.672 | 3176.883 |

***p60 + H***

C 0.505972 -0.948109 -0.001430

C -0.630390 -0.233699 -0.000641

C 4.258094 0.661303 0.001886

C 2.918125 0.089464 -0.001689

C 1.807217 -0.374652 -0.002169

C -1.948744 -0.844872 0.001377

C -3.123865 -0.205290 0.001568

C -3.359139 1.273134 -0.000736

H 0.453159 -2.034798 -0.000901

H -0.555908 0.849246 -0.001203

H 4.363701 1.409962 -0.787540

H 5.012262 -0.112684 -0.160082

H 4.470123 1.146890 0.958147

H -1.961873 -1.932663 0.003116

H -4.023375 -0.816532 0.003513

H -2.436638 1.854213 -0.003111

H -3.941319 1.567959 0.878396

H -3.943752 1.564733 -0.879332

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 71.0633 | 85.297 | 97.7501 |
| 112.1492 | 120.7265 | 185.3702 |
| 249.5173 | 315.4408 | 355.0123 |
| 396.4029 | 497.706 | 510.6392 |
| 627.5712 | 747.0897 | 816.6887 |
| 884.9354 | 941.3308 | 971.9514 |
| 1024.225 | 1045.195 | 1055.623 |
| 1065.129 | 1066.134 | 1170.867 |
| 1208.402 | 1264.615 | 1293.034 |
| 1334.899 | 1406.718 | 1423.181 |
| 1444.772 | 1483.471 | 1486.179 |
| 1489.854 | 1492.838 | 1690.999 |
| 1747.566 | 2373.539 | 3038.958 |
| 3046.826 | 3093.108 | 3118.416 |
| 3120.975 | 3139.44 | 3153.896 |
| 3161.142 | 3174.651 | 3194.204 |

***p61 + H***

C 0.458062 1.417502 -0.000083

C -0.799635 0.943301 -0.001030

C 3.853480 -0.852839 0.000453

C 2.638606 -0.048564 0.000653

C 1.631650 0.611458 0.000299

C -1.149211 -0.467032 -0.001652

C -2.387180 -0.975005 -0.000617

C -3.685125 -0.228725 0.001428

H 0.616149 2.491671 0.000533

H -1.603105 1.672335 -0.000983

H 4.000897 -1.334174 -0.969954

H 3.801862 -1.635360 0.761772

H 4.729771 -0.234129 0.208753

H -0.311100 -1.158417 -0.002764

H -2.479860 -2.058690 -0.000568

H -4.284778 -0.505346 -0.871882

H -3.559058 0.854219 -0.007180

H -4.274659 -0.492685 0.885564

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 49.1572 | 52.4023 | 73.1946 |
| 115.9931 | 178.9772 | 205.499 |
| 254.6138 | 314.987 | 398.622 |
| 402.5766 | 554.7639 | 559.772 |
| 679.5642 | 745.7116 | 784.8115 |
| 813.8496 | 943.6554 | 995.5354 |
| 1028.139 | 1034.785 | 1056.945 |
| 1062.416 | 1062.523 | 1146.431 |
| 1185.353 | 1265.115 | 1306.148 |
| 1385.602 | 1419.84 | 1424.56 |
| 1477.868 | 1481.384 | 1486.589 |
| 1491.33 | 1493.516 | 1676.699 |
| 1747.78 | 2370.738 | 3039.043 |
| 3047.982 | 3092.629 | 3118.179 |
| 3123.528 | 3143.086 | 3163.357 |
| 3180.204 | 3189.714 | 3209.219 |

***p62 + H***

C 0.396078 -0.232559 -0.257859

C -0.429136 0.782537 0.036029

C -1.888520 0.730476 -0.060085

C -2.637776 -0.349875 0.167207

C -4.127510 -0.398440 0.042801

C 4.459572 -0.110399 0.129741

C 3.009716 -0.148718 -0.009593

C 1.811153 -0.172401 -0.118666

H -0.015362 -1.164017 -0.639336

H 0.007267 1.725387 0.355526

H -2.384595 1.666434 -0.312102

H -2.148063 -1.269405 0.483271

H -4.431856 -1.147879 -0.695240

H -4.536923 0.566682 -0.263961

H -4.591537 -0.683286 0.992626

H 4.878910 0.747018 -0.403022

H 4.913727 -1.017464 -0.276425

H 4.746966 -0.027196 1.181216

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 43.3159 | 65.6979 | 77.7781 |
| 129.6249 | 166.0664 | 203.5178 |
| 226.6554 | 308.0745 | 329.8958 |
| 356.3313 | 484.6116 | 501.4075 |
| 627.6418 | 788.1359 | 859.2142 |
| 886.4911 | 931.5093 | 987.7603 |
| 1003.524 | 1052.666 | 1060.961 |
| 1073.493 | 1075.153 | 1136.682 |
| 1214.493 | 1320.412 | 1325.367 |
| 1345.966 | 1362.716 | 1419.47 |
| 1424.259 | 1480.659 | 1484.519 |
| 1485.638 | 1498.457 | 1711.303 |
| 1745.918 | 2374.56 | 3040.445 |
| 3050.8 | 3099.586 | 3121.201 |
| 3125.905 | 3128.414 | 3151.797 |
| 3160.002 | 3163.013 | 3178.195 |

***p63 + H***

C 0.424847 1.810526 0.039143

C -0.918046 1.752136 -0.006999

C -1.805177 0.594845 -0.081645

C -1.492024 -0.693293 0.092217

C -2.479056 -1.812600 -0.000719

C 3.113270 -1.259920 -0.037506

C 2.145734 -0.171272 -0.005955

C 1.332536 0.717308 0.015290

H 0.887105 2.791979 0.092306

H -1.428707 2.711165 -0.000032

H -2.846310 0.836163 -0.290531

H -0.467017 -0.966537 0.321202

H -2.180751 -2.530726 -0.771774

H -3.481577 -1.449416 -0.238859

H -2.529358 -2.366334 0.942870

H 3.225907 -1.710758 0.952153

H 4.093765 -0.900040 -0.358828

H 2.794435 -2.041870 -0.731471

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 57.037 | 59.6619 | 74.485 |
| 146.8731 | 187.289 | 201.243 |
| 229.4105 | 286.9953 | 376.9955 |
| 395.2003 | 505.5142 | 557.3356 |
| 678.2906 | 747.0934 | 842.7331 |
| 864.1253 | 907.1959 | 1002.225 |
| 1025.434 | 1044.87 | 1055.37 |
| 1059.245 | 1076.959 | 1138.248 |
| 1180.165 | 1285.148 | 1354.952 |
| 1366.007 | 1418.248 | 1421.069 |
| 1463.776 | 1482.827 | 1484.176 |
| 1486.19 | 1495.919 | 1692.016 |
| 1739.662 | 2367.107 | 3037.704 |
| 3047.509 | 3095.825 | 3117.16 |
| 3125.088 | 3128.82 | 3140.374 |
| 3168.949 | 3190.457 | 3200.498 |

***p64 + H***

C 0.288141 -1.621614 0.406028

C 1.527711 -1.276885 0.023208

C -3.147176 0.460319 -0.323800

C -1.919274 -0.277014 -0.057600

C -0.897608 -0.878011 0.151196

C 1.934212 -0.064373 -0.690269

C 1.626450 1.200689 -0.389858

C 0.833121 1.688609 0.779724

H 0.150552 -2.569217 0.919342

H 2.317278 -2.000672 0.213182

H -3.813669 -0.115748 -0.970892

H -2.931382 1.410592 -0.818775

H -3.680941 0.674209 0.605811

H 2.601744 -0.233545 -1.532913

H 2.022932 1.971964 -1.046655

H 1.311489 2.567832 1.220778

H 0.724358 0.922047 1.548295

H -0.175822 1.982221 0.470050

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 78.6989 | 89.3834 | 129.6144 |
| 189.2154 | 209.7103 | 259.0353 |
| 319.9515 | 330.9655 | 382.4903 |
| 431.6498 | 525.349 | 593.8044 |
| 694.8148 | 731.7899 | 799.6599 |
| 862.3418 | 910.6633 | 1000.126 |
| 1003.236 | 1017.456 | 1056.597 |
| 1060.245 | 1073.643 | 1128.307 |
| 1170.681 | 1271.358 | 1284.484 |
| 1401.269 | 1419.195 | 1429.182 |
| 1467.133 | 1487.049 | 1490.236 |
| 1494.813 | 1524.252 | 1701.321 |
| 1735.033 | 2374.17 | 3044.811 |
| 3049.356 | 3104.97 | 3120.537 |
| 3123.521 | 3138.174 | 3148.396 |
| 3156.795 | 3173.189 | 3180.817 |

***p65* + *H***

C -0.145229 0.016205 -0.358438

C 0.635440 0.977883 0.156680

C -4.191590 -0.215529 0.144265

C -2.748132 -0.124430 -0.031200

C -1.555324 -0.045309 -0.171783

C 2.085287 1.084423 -0.007653

C 2.983804 0.093793 -0.020276

C 2.731170 -1.370282 0.171203

H 0.291755 -0.759465 -0.980620

H 0.155830 1.777055 0.717033

H -4.658682 -0.694775 -0.719688

H -4.633083 0.777205 0.262169

H -4.439305 -0.802691 1.032663

H 2.463236 2.100652 -0.093270

H 4.024579 0.376219 -0.160112

H 3.533362 -1.820365 0.761784

H 2.710261 -1.896955 -0.789686

H 1.779497 -1.557398 0.672929

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 71.824 | 77.5225 | 93.9907 |
| 123.4177 | 174.7135 | 237.3138 |
| 279.581 | 319.7619 | 371.8724 |
| 440.8061 | 504.3222 | 515.006 |
| 687.4783 | 728.4117 | 861.6314 |
| 890.2585 | 920.3735 | 998.7109 |
| 1018.944 | 1045.249 | 1057.686 |
| 1063.983 | 1074.841 | 1123.367 |
| 1211.48 | 1278.416 | 1329.073 |
| 1342.243 | 1415.046 | 1424.648 |
| 1449.177 | 1484.667 | 1489.347 |
| 1496.449 | 1529.167 | 1710.282 |
| 1731.838 | 2376.637 | 3042.514 |
| 3046.231 | 3102.945 | 3115.823 |
| 3122.828 | 3139.273 | 3152.941 |
| 3166.152 | 3180.273 | 3186.958 |

***p66 + H***

C -0.648300 1.733156 0.000414

C 0.805508 1.336053 -0.000479

C -3.323007 -1.400425 -0.000436

C -2.373809 -0.292766 0.000305

C -1.597104 0.622464 0.000401

C 1.278371 0.090973 0.000310

C 2.700451 -0.231829 -0.000530

C 3.184815 -1.472717 0.000336

H -0.840291 2.369337 0.873460

H -0.841175 2.370006 -0.871941

H 1.504850 2.170117 -0.001752

H -3.340906 -1.899403 0.971541

H -3.055961 -2.141294 -0.757892

H -4.333381 -1.044652 -0.216615

H 0.578692 -0.742297 0.001799

H 3.390903 0.609639 -0.001936

H 2.524665 -2.334977 0.001775

H 4.251062 -1.665925 -0.000365

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 62.5932 | 68.0123 | 101.7721 |
| 160.263 | 179.2664 | 202.9892 |
| 254.3136 | 286.4714 | 396.6162 |
| 424.7499 | 472.3517 | 621.5597 |
| 644.6462 | 768.3163 | 835.1381 |
| 946.6429 | 958.6147 | 975.2431 |
| 1006.297 | 1011.148 | 1052.461 |
| 1060.925 | 1064.722 | 1174.836 |
| 1192.609 | 1240.371 | 1283.563 |
| 1325.713 | 1346.441 | 1374.726 |
| 1417.823 | 1456.633 | 1460.79 |
| 1485.969 | 1490.836 | 1701.044 |
| 1766.605 | 2399.594 | 3032.366 |
| 3054.755 | 3059.002 | 3127.648 |
| 3128.009 | 3149.197 | 3160.147 |
| 3162.672 | 3172.317 | 3245.782 |

***p67 + H***

C -0.311354 0.735442 -0.798081

C 0.577594 0.989054 0.393494

C 1.793314 0.483577 0.613618

C 2.533828 -0.438591 -0.241633

C 3.760331 -0.873905 0.043844

C -3.993401 -0.709254 0.368253

C -2.695597 -0.193851 -0.053486

C -1.624572 0.222543 -0.400329

H -0.451968 1.678280 -1.340932

H 0.150404 0.040497 -1.503115

H 0.155560 1.658513 1.137917

H 2.303553 0.779646 1.527680

H 2.055556 -0.787734 -1.152295

H 4.277160 -0.553955 0.943895

H 4.285969 -1.560891 -0.608731

H -3.921014 -1.184267 1.349704

H -4.363955 -1.453616 -0.340968

H -4.732118 0.093437 0.432764

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 22.6559 | 99.6604 | 118.8349 |
| 122.0496 | 179.4105 | 222.0025 |
| 271.4566 | 374.8978 | 377.9704 |
| 400.1575 | 514.6486 | 615.5969 |
| 651.6305 | 782.6419 | 833.101 |
| 915.4823 | 943.4925 | 956.4739 |
| 1011.343 | 1029.358 | 1047.902 |
| 1061.029 | 1068.168 | 1170.69 |
| 1174.052 | 1240.994 | 1300.309 |
| 1323.366 | 1342.081 | 1406.236 |
| 1424.471 | 1474.824 | 1476.009 |
| 1489.597 | 1493.386 | 1692.029 |
| 1760.597 | 2398.524 | 3043.361 |
| 3049.629 | 3105.18 | 3121.099 |
| 3123.798 | 3154.779 | 3158.393 |
| 3182.106 | 3186.166 | 3250.414 |

***p68 + H***

C 0.456677 1.576493 -0.037832

C -0.907983 0.943154 -0.136835

C 3.622097 -1.056682 0.101331

C 2.498161 -0.128063 0.052129

C 1.578103 0.641957 0.012669

C -1.161219 -0.362761 -0.166223

C -2.505630 -0.949738 -0.236951

C -3.594085 -0.459081 0.351688

H 0.593978 2.257452 -0.886862

H 0.481797 2.215524 0.853967

H -1.733332 1.649235 -0.197996

H 3.285743 -2.083441 -0.062408

H 4.119405 -1.014644 1.073427

H 4.359717 -0.815901 -0.668089

H -0.323547 -1.056696 -0.160733

H -2.590344 -1.873503 -0.805611

H -4.559882 -0.937910 0.238623

H -3.550266 0.428211 0.975824

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 55.9729 | 75.795 | 100.1683 |
| 170.8728 | 189.7929 | 218.442 |
| 221.6092 | 264.8177 | 391.9325 |
| 400.2293 | 529.6692 | 615.1144 |
| 686.7543 | 762.8369 | 824.2879 |
| 953.0179 | 972.2027 | 983.0466 |
| 1004.931 | 1020.455 | 1044.014 |
| 1051.384 | 1064.611 | 1101.534 |
| 1177.185 | 1244.028 | 1301.046 |
| 1319.227 | 1352.884 | 1378.017 |
| 1415.989 | 1459.418 | 1462.058 |
| 1486.797 | 1491.508 | 1718.571 |
| 1751.106 | 2398.989 | 3031.804 |
| 3053.617 | 3060.296 | 3126.318 |
| 3126.645 | 3147.331 | 3159.358 |
| 3168.418 | 3174.46 | 3240.485 |

***p69 + H***

C 0.065866 -0.428004 -0.494164

C -0.654155 0.896186 -0.439427

C 4.077079 -0.022183 0.367822

C 2.659302 -0.170559 0.058045

C 1.492022 -0.296288 -0.192198

C -1.887968 1.116049 0.019839

C -2.836041 0.128602 0.549974

C -3.058856 -1.090355 0.061547

H -0.396069 -1.135994 0.201314

H -0.043720 -0.867833 -1.493791

H -0.078899 1.748316 -0.790101

H 4.272860 -0.254707 1.417525

H 4.409690 1.002026 0.181524

H 4.683869 -0.691186 -0.247402

H -2.232283 2.147457 0.043612

H -3.423906 0.459167 1.404263

H -2.550762 -1.454576 -0.824848

H -3.784274 -1.753352 0.519275

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 47.3813 | 82.2429 | 116.7054 |
| 144.4019 | 188.8016 | 224.9966 |
| 280.9361 | 344.1863 | 401.328 |
| 422.9728 | 509.404 | 585.6847 |
| 706.1596 | 770.0486 | 831.5919 |
| 904.1684 | 946.2337 | 971.7772 |
| 1020.385 | 1035.851 | 1056.49 |
| 1064.518 | 1069.895 | 1096.02 |
| 1178.115 | 1249.559 | 1276.655 |
| 1331.557 | 1343.714 | 1422.965 |
| 1429.729 | 1462.571 | 1475.65 |
| 1490.504 | 1492.371 | 1716.931 |
| 1734.69 | 2397.817 | 3028.713 |
| 3050.122 | 3083.196 | 3121.454 |
| 3123.873 | 3146.312 | 3157.898 |
| 3166.312 | 3186.326 | 3250.045 |

***p70 + H***

C -0.445116 1.010921 -0.207956

C 0.522217 0.250579 0.677237

C 1.648067 -0.251804 0.257053

C 2.776591 -0.745758 -0.168406

C 4.088097 -0.007565 -0.163757

C -4.230977 -0.612088 -0.035803

C -2.894951 -0.031311 -0.109160

C -1.794243 0.444159 -0.167802

H -0.490701 2.055962 0.120485

H -0.071817 1.017143 -1.235436

H 0.234741 0.124716 1.718330

H 2.779092 -1.764799 -0.550928

H 4.829404 -0.544797 0.435497

H 3.972931 0.995819 0.248453

H 4.489512 0.077490 -1.178076

H -4.198808 -1.597338 0.435933

H -4.661903 -0.729109 -1.033237

H -4.900555 0.022123 0.550543

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 36.9293 | 71.5131 | 120.1423 |
| 132.5536 | 163.7373 | 194.7237 |
| 223.2194 | 257.2421 | 339.9 |
| 399.355 | 498.1442 | 539.7644 |
| 578.0613 | 715.9504 | 786.7426 |
| 865.3909 | 919.4272 | 950.8657 |
| 1041.914 | 1060.634 | 1062.086 |
| 1066.551 | 1107.314 | 1163.341 |
| 1173.915 | 1219.803 | 1293.649 |
| 1337.884 | 1411.53 | 1423.515 |
| 1465.64 | 1466.475 | 1489.29 |
| 1489.777 | 1493.301 | 1514.275 |
| 2100.575 | 2398.174 | 3043.144 |
| 3045.56 | 3049.844 | 3101.685 |
| 3108.422 | 3120.222 | 3124.195 |
| 3138.521 | 3156.838 | 3168.554 |

***p71 + H***

C -0.596043 1.898709 -0.195656

C 0.889123 1.678736 0.014632

C -2.849459 -1.536153 0.081581

C -2.060437 -0.313758 -0.018494

C -1.407320 0.689321 -0.100513

C 1.447306 0.535390 0.292434

C 1.995046 -0.614813 0.561805

C 2.484817 -1.591777 -0.472052

H -0.949991 2.633352 0.537366

H -0.746139 2.361121 -1.178385

H 1.513772 2.564648 -0.076243

H -2.734020 -1.993368 1.067469

H -2.533014 -2.265328 -0.668322

H -3.911376 -1.330141 -0.074001

H 2.105942 -0.896786 1.607147

H 3.554023 -1.786732 -0.344622

H 2.318470 -1.211857 -1.480801

H 1.964136 -2.548845 -0.372033

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 53.1186 | 79.9296 | 128.5912 |
| 135.5153 | 178.5096 | 211.4251 |
| 215.2594 | 282.2861 | 328.5864 |
| 401.5577 | 465.8781 | 564.7888 |
| 646.1371 | 707.203 | 763.8782 |
| 885.9648 | 903.2699 | 968.4615 |
| 975.3547 | 1065.918 | 1068.202 |
| 1071.481 | 1104.36 | 1151.311 |
| 1188.604 | 1249.927 | 1292.707 |
| 1364.515 | 1416.273 | 1429.014 |
| 1465.794 | 1485.884 | 1491.017 |
| 1492.572 | 1494.84 | 1517.206 |
| 2104.613 | 2404.647 | 3034.977 |
| 3045.613 | 3049.913 | 3063.959 |
| 3107.181 | 3119.993 | 3124.222 |
| 3142.11 | 3158.662 | 3159.204 |

***p72 + H***

C -0.713410 -0.980062 -0.000042

C 0.547035 -0.252438 -0.000009

C -4.212028 0.734059 0.000030

C -3.033812 0.156387 0.000001

C -1.900841 -0.403965 -0.000024

C 1.736377 -0.860954 0.000013

C 3.079154 -0.194172 0.000063

C 3.062888 1.329941 -0.000043

H -0.661555 -2.067771 -0.000084

H 0.477369 0.831337 0.000007

H -4.307055 1.814772 0.000082

H -5.124344 0.146873 0.000009

H 1.756074 -1.950366 0.000003

H 3.639857 -0.557462 -0.870612

H 3.639730 -0.557344 0.870870

H 2.553109 1.721717 0.884267

H 2.553223 1.721589 -0.884476

H 4.081408 1.723869 -0.000003

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 67.3481 | 70.8119 | 131.687 |
| 195.9472 | 202.6748 | 253.4614 |
| 302.0015 | 319.3964 | 342.1523 |
| 491.8876 | 514.3469 | 571.8892 |
| 608.6653 | 750.1099 | 860.2545 |
| 879.4083 | 888.017 | 900.1741 |
| 956.0192 | 1008.7 | 1031.622 |
| 1036.01 | 1107.811 | 1112.484 |
| 1182.312 | 1263.46 | 1294.705 |
| 1345.693 | 1352.75 | 1383.241 |
| 1424.963 | 1453.41 | 1478.268 |
| 1504.7 | 1517.254 | 1701.225 |
| 1745.792 | 2232.173 | 3030.471 |
| 3055.313 | 3055.552 | 3128.995 |
| 3134.871 | 3146.643 | 3148.704 |
| 3150.766 | 3192.37 | 3231.631 |

***p73 + H***

C 0.495842 -0.248734 -0.259435

C -0.370615 0.880943 0.047332

C -1.702684 0.907024 -0.079686

C -2.607379 -0.197323 -0.535992

C -3.571147 -0.637565 0.571687

C 4.364303 -0.144683 0.193779

C 3.061585 -0.180694 0.040506

C 1.807053 -0.217941 -0.108132

H 0.047028 -1.166422 -0.630414

H 0.134213 1.771065 0.410702

H -2.209747 1.829033 0.199213

H -2.036517 -1.059022 -0.889399

H -3.188961 0.160318 -1.393831

H -4.171277 0.205157 0.926704

H -3.021099 -1.038770 1.426438

H -4.256267 -1.408905 0.211609

H 4.980442 -1.005611 -0.043486

H 4.860432 0.746994 0.562115

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 32.1209 | 68.5148 | 86.1916 |
| 199.4205 | 223.3875 | 249.9794 |
| 266.1653 | 307.3864 | 425.3394 |
| 493.5502 | 550.348 | 579.1076 |
| 609.8645 | 785.0231 | 808.7732 |
| 883.1672 | 886.6094 | 897.33 |
| 951.0385 | 1023.342 | 1031.982 |
| 1035.839 | 1078.842 | 1097.805 |
| 1175.652 | 1281.815 | 1293.645 |
| 1313.916 | 1344.086 | 1416.339 |
| 1429.896 | 1468.782 | 1490.695 |
| 1502.7 | 1511.732 | 1694.431 |
| 1740.288 | 2232.577 | 3046.722 |
| 3048.878 | 3102.343 | 3126.186 |
| 3132.845 | 3147.901 | 3156.519 |
| 3173.298 | 3192.98 | 3234.046 |

***p74 + H***

C -0.364156 -0.965303 0.754369

C 0.742896 -0.908420 0.053822

C -3.925203 0.671714 -0.406501

C -2.653244 0.093890 0.007700

C -1.598529 -0.382393 0.334264

C 1.845649 -0.846559 -0.632041

C 2.877860 0.249444 -0.519177

C 2.552319 1.318296 0.516044

H -0.358265 -1.486131 1.709384

H -4.092028 0.514071 -1.475037

H -3.947085 1.747798 -0.215445

H -4.755507 0.214105 0.137005

H 2.045468 -1.638701 -1.351841

H 2.994832 0.708022 -1.508067

H 3.844535 -0.214530 -0.291181

H 2.466801 0.882274 1.514689

H 1.602166 1.808031 0.288060

H 3.333526 2.081045 0.541550

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 49.9925 | 72.8182 | 95.2156 |
| 135.9368 | 152.1714 | 240.7514 |
| 263.4731 | 304.429 | 370.2804 |
| 399.9337 | 465.819 | 535.8745 |
| 655.7898 | 741.8485 | 806.6145 |
| 829.0632 | 865.7776 | 917.9524 |
| 1011.998 | 1055.69 | 1063.966 |
| 1096.867 | 1114.712 | 1134.33 |
| 1206.065 | 1299.566 | 1303.481 |
| 1377.612 | 1419.976 | 1427.961 |
| 1470.153 | 1485.984 | 1491.503 |
| 1495.52 | 1507.33 | 1510.936 |
| 2082.169 | 2385.028 | 3039.154 |
| 3050.459 | 3054.561 | 3069.828 |
| 3122.225 | 3123.914 | 3129.134 |
| 3136.868 | 3146.48 | 3156.303 |

***p75 + H***

C -0.577757 1.099763 -0.202672

C 0.535497 0.578787 0.254442

C 1.645910 0.062529 0.690116

C 2.575008 -0.790894 -0.137818

C 3.957602 -0.153985 -0.291525

C -4.243897 -0.696515 -0.001845

C -2.934807 -0.060631 -0.076184

C -1.849208 0.453995 -0.125282

H -0.545076 2.082415 -0.668127

H 1.941393 0.264332 1.719365

H 2.126505 -0.963972 -1.118886

H 2.675658 -1.769102 0.345493

H 4.426790 0.009360 0.683068

H 3.883957 0.813556 -0.794266

H 4.618775 -0.795453 -0.879299

H -4.166017 -1.686574 0.453889

H -4.679485 -0.814099 -0.997415

H -4.932589 -0.098766 0.600786

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 62.9624 | 80.3483 | 115.7544 |
| 126.5356 | 177.6451 | 239.7009 |
| 257.7531 | 297.3411 | 380.6915 |
| 400.9765 | 494.5501 | 523.2876 |
| 594.2206 | 774.4237 | 808.2518 |
| 817.0601 | 896.2972 | 919.0529 |
| 1021.205 | 1059.96 | 1064.182 |
| 1094.729 | 1112.472 | 1153.933 |
| 1206.423 | 1279.425 | 1315.245 |
| 1361.911 | 1422.143 | 1423.622 |
| 1476.916 | 1489.706 | 1490.223 |
| 1498.908 | 1507.905 | 1517.469 |
| 2083.78 | 2385.695 | 3044.863 |
| 3047.58 | 3048.089 | 3098.973 |
| 3118.104 | 3122.486 | 3123.02 |
| 3129.573 | 3140.639 | 3155.89 |

***p76 + C3H5\_b***

C -2.399426 0.473677 0.000001

C -1.471392 -0.482327 -0.000012

C 2.564241 0.161451 0.000016

C 1.124440 -0.061610 0.000040

C -0.065584 -0.237953 -0.000009

H -2.129897 1.523631 -0.000017

H -3.453698 0.223627 0.000029

H -1.774515 -1.526164 0.000006

H 2.792614 1.229603 0.025236

H 3.022491 -0.263392 -0.896744

H 3.029335 -0.306731 0.871280

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 24.4431 | 140.0762 | 188.5809 |
| 332.0014 | 390.8488 | 545.7793 |
| 709.4461 | 726.7034 | 964.8887 |
| 1023.757 | 1054.747 | 1055.003 |
| 1058.66 | 1201.186 | 1328.813 |
| 1418.595 | 1451.104 | 1483.735 |
| 1484.151 | 1707.08 | 2378.718 |
| 3046.618 | 3118.232 | 3122.656 |
| 3157.391 | 3168.863 | 3255.855 |

***p76’ + C3H5\_a***

C -2.399426 0.473677 0.000001

C -1.471392 -0.482327 -0.000012

C 2.564241 0.161451 0.000016

C 1.124440 -0.061610 0.000040

C -0.065584 -0.237953 -0.000009

H -2.129897 1.523631 -0.000017

H -3.453698 0.223627 0.000029

H -1.774515 -1.526164 0.000006

H 2.792614 1.229603 0.025236

H 3.022491 -0.263392 -0.896744

H 3.029335 -0.306731 0.871280

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 24.4431 | 140.0762 | 188.5809 |
| 332.0014 | 390.8488 | 545.7793 |
| 709.4461 | 726.7034 | 964.8887 |
| 1023.757 | 1054.747 | 1055.003 |
| 1058.66 | 1201.186 | 1328.813 |
| 1418.595 | 1451.104 | 1483.735 |
| 1484.151 | 1707.08 | 2378.718 |
| 3046.618 | 3118.232 | 3122.656 |
| 3157.391 | 3168.863 | 3255.855 |

***p77 + H***

C 0.698924 1.541603 -0.458266

C 0.024389 0.630243 0.535960

C -3.803798 -0.674066 -0.131234

C -2.442767 -0.205953 0.103849

C -1.321536 0.176088 0.305720

C 1.151496 0.109345 -0.351224

C 2.456014 -0.208085 0.260259

C 3.234651 -1.221467 -0.099979

H 1.356871 2.307623 -0.064260

H 0.131642 1.827012 -1.334844

H 0.285312 0.783071 1.578295

H -4.372012 0.048293 -0.722714

H -4.328120 -0.821866 0.816196

H -3.802860 -1.626444 -0.667519

H 0.833675 -0.553866 -1.148323

H 2.779715 0.456535 1.060710

H 2.945299 -1.903659 -0.893560

H 4.186242 -1.402944 0.385511

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 67.2689 | 92.5346 | 116.1937 |
| 120.4699 | 242.4494 | 258.6953 |
| 319.4635 | 345.6374 | 437.4217 |
| 508.1655 | 527.8839 | 662.2775 |
| 744.8828 | 838.1725 | 889.3791 |
| 937.5238 | 950.4079 | 964.6729 |
| 1012.364 | 1032.834 | 1055.998 |
| 1062.637 | 1072.851 | 1107.62 |
| 1113.352 | 1199.803 | 1230.132 |
| 1238.469 | 1316.609 | 1344.906 |
| 1414.509 | 1425.333 | 1474.794 |
| 1488.035 | 1489.566 | 1505.584 |
| 1737.588 | 2393.455 | 3052.096 |
| 3123.718 | 3124.932 | 3143.37 |
| 3148.054 | 3158.996 | 3170.826 |
| 3186.57 | 3243.005 | 3245.072 |

***p78 + H***

C -0.890077 1.648887 -0.089181

C 0.608870 1.695524 0.076099

C -3.027915 -1.598812 -0.006278

C -2.309618 -0.503239 -0.035311

C -1.616453 0.556476 -0.064378

C 1.236662 0.376321 0.409580

C 2.169401 -0.221987 -0.320558

C 2.805366 -1.537494 0.007336

H -1.390592 2.603412 -0.240955

H 0.833971 2.426654 0.864517

H 1.049577 2.103866 -0.841551

H -2.564361 -2.568378 0.143160

H -4.105164 -1.567187 -0.132847

H 0.876616 -0.107421 1.316414

H 2.511785 0.264460 -1.233636

H 2.648587 -2.260053 -0.799855

H 2.394689 -1.960024 0.927272

H 3.887478 -1.429384 0.133630

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 47.9241 | 98.904 | 116.9778 |
| 180.4462 | 216.2079 | 225.3755 |
| 282.5876 | 297.2478 | 391.2214 |
| 484.8013 | 498.7873 | 574.6453 |
| 629.6155 | 789.0545 | 831.6924 |
| 862.9862 | 900.6647 | 938.7772 |
| 976.3481 | 1016.379 | 1033.567 |
| 1036.912 | 1077.843 | 1115.261 |
| 1140.114 | 1229.007 | 1299.229 |
| 1332.69 | 1345.547 | 1380.9 |
| 1424.784 | 1454.232 | 1475.577 |
| 1491.168 | 1501.275 | 1728.957 |
| 1779.322 | 2245.341 | 3023.377 |
| 3038.217 | 3062.149 | 3098.635 |
| 3123.814 | 3143.29 | 3147.045 |
| 3150.364 | 3156.188 | 3228.362 |

***p79 + H***

C 0.871801 1.885463 -0.314635

C 0.174150 0.907495 0.663360

C -3.475270 -0.715221 -0.269173

C -2.180616 -0.130670 0.060575

C -1.112269 0.346990 0.332682

C 1.372821 0.530903 -0.114776

C 2.209247 -0.438171 -0.418426

C 2.141817 -1.815698 0.168193

H 1.400138 2.721122 0.133482

H 0.345980 2.112390 -1.236327

H 0.324971 1.126008 1.717368

H -4.058247 -0.045720 -0.906716

H -4.054161 -0.905298 0.638206

H -3.352652 -1.664987 -0.795965

H 2.995726 -0.238556 -1.143304

H 1.310392 -1.901808 0.870060

H 3.069601 -2.063547 0.693826

H 2.008171 -2.566150 -0.617424

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.1757 | 111.8581 | 114.9141 |
| 168.3769 | 174.8853 | 214.3262 |
| 269.5821 | 322.1599 | 378.5646 |
| 472.3485 | 518.4221 | 566.7156 |
| 699.3215 | 739.7736 | 834.8127 |
| 930.3506 | 957.7737 | 982.0024 |
| 1044.942 | 1056.888 | 1062.564 |
| 1065.016 | 1073.309 | 1103.539 |
| 1127.647 | 1138.116 | 1211.975 |
| 1334.811 | 1385.609 | 1420.124 |
| 1422.748 | 1466.932 | 1487.409 |
| 1488.444 | 1492.159 | 1499.762 |
| 1892.545 | 2394.159 | 3040.635 |
| 3049.754 | 3099.4 | 3120.854 |
| 3122.934 | 3129.227 | 3136.874 |
| 3149.099 | 3158.808 | 3218.79 |

***p80 + H***

C -0.903293 1.743719 -0.362071

C -0.011968 0.797113 0.446128

C -3.216239 -1.416092 -0.004559

C -2.296682 -0.490714 0.011796

C -1.388109 0.416038 0.038926

C 1.144087 0.139515 -0.200655

C 2.279683 -0.164805 0.418656

C 3.452874 -0.836222 -0.225869

H -1.306361 2.612456 0.147875

H -0.653480 1.899108 -1.407416

H 0.120498 1.053070 1.494200

H -3.968739 -1.472561 0.774958

H -3.253441 -2.155265 -0.797854

H 1.020478 -0.106376 -1.254960

H 2.381963 0.079341 1.475214

H 4.352741 -0.217529 -0.148030

H 3.266817 -1.035200 -1.283836

H 3.677413 -1.788365 0.265742

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 58.6233 | 116.4886 | 176.0509 |
| 188.8268 | 209.9529 | 219.9969 |
| 341.5814 | 396.011 | 435.3816 |
| 463.4109 | 579.9786 | 621.0697 |
| 670.0416 | 828.302 | 880.8872 |
| 881.6427 | 952.4417 | 959.6089 |
| 991.871 | 1005.857 | 1027.156 |
| 1040.433 | 1062.98 | 1074.755 |
| 1109.085 | 1126.129 | 1201.118 |
| 1277.445 | 1340.793 | 1352.661 |
| 1407.176 | 1426.269 | 1468.872 |
| 1490.882 | 1500.012 | 1554.882 |
| 1772.305 | 2140.864 | 3038.886 |
| 3098.364 | 3124.757 | 3129.623 |
| 3148.109 | 3149.678 | 3152.786 |
| 3160.169 | 3220.04 | 3232.544 |

***p81 + H***

C 0.722063 1.779940 -0.067818

C -0.206491 0.587413 -0.317620

C 3.247227 -1.234395 0.005790

C 2.248569 -0.398317 -0.069783

C 1.259952 0.416537 -0.152961

C -1.103617 0.127010 0.765519

C -2.307272 -0.424966 0.627883

C -3.040718 -0.714344 -0.646692

H 0.903170 2.456779 -0.896253

H 0.680702 2.250267 0.910031

H -0.574272 0.494910 -1.334345

H 3.815814 -1.509691 -0.876342

H 3.535520 -1.678758 0.952668

H -0.705711 0.257023 1.769904

H -2.829895 -0.707734 1.538715

H -3.239199 -1.786889 -0.739773

H -2.492488 -0.399608 -1.535693

H -4.011919 -0.209570 -0.654815

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 42.8326 | 94.1345 | 141.3965 |
| 175.9962 | 201.2369 | 279.5261 |
| 318.5867 | 389.5484 | 487.6775 |
| 548.3369 | 587.2281 | 618.9209 |
| 659.226 | 777.2761 | 857.2757 |
| 872.2178 | 940.1642 | 954.5991 |
| 984.2854 | 1017.453 | 1021.368 |
| 1035.83 | 1054.504 | 1068.844 |
| 1085.241 | 1103.402 | 1177.66 |
| 1293.588 | 1305.306 | 1377.446 |
| 1412.466 | 1454.499 | 1465.147 |
| 1485.337 | 1499.94 | 1551.58 |
| 1761.257 | 2141.691 | 3046.377 |
| 3102.413 | 3129.43 | 3136.292 |
| 3145.594 | 3150.652 | 3172.459 |
| 3177.588 | 3219.599 | 3229.253 |

***p82 + H***

C 0.076255 2.485399 0.000709

C -0.064552 1.152348 -0.000409

C 3.227653 -1.283545 0.000873

C 2.051302 -0.423407 -0.001560

C 1.091502 0.300798 -0.001411

C -1.396717 0.526711 -0.000065

C -1.631483 -0.783956 -0.000244

C -2.992487 -1.403635 0.000357

H 1.053714 2.950427 0.000760

H -0.793545 3.133228 0.001691

H 3.728697 -1.250489 0.971687

H 3.943309 -0.963365 -0.760412

H 2.954304 -2.321276 -0.204581

H -2.233154 1.222860 0.000600

H -0.782799 -1.464896 -0.000692

H -3.130363 -2.040828 -0.879268

H -3.780345 -0.647078 0.001958

H -3.128655 -2.042864 0.878760

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 75.8223 | 79.8335 | 103.3179 |
| 141.157 | 190.046 | 204.0626 |
| 209.0405 | 313.1813 | 384.2392 |
| 396.3173 | 454.3461 | 616.4362 |
| 646.1392 | 675.406 | 734.728 |
| 855.3075 | 925.2936 | 932.9498 |
| 1011.688 | 1012.239 | 1056.461 |
| 1063.916 | 1072.067 | 1086.04 |
| 1134.28 | 1302.498 | 1337.26 |
| 1364.455 | 1417.583 | 1421.105 |
| 1444.799 | 1483.301 | 1487.141 |
| 1489.829 | 1490.788 | 1683.354 |
| 1758.789 | 2382.758 | 3041.582 |
| 3051.811 | 3100.724 | 3124.627 |
| 3125.356 | 3130.257 | 3162.591 |
| 3165.409 | 3169.278 | 3265.685 |

***p83 + H***

C 0.200998 2.079424 -0.013950

C -0.000187 0.759427 -0.112150

C -3.736862 -0.902749 0.098867

C -2.411571 -0.302223 0.019489

C -1.321503 0.203123 -0.035247

C 1.096928 -0.213044 -0.315816

C 2.295395 -0.128911 0.256914

C 3.411468 -1.102113 0.041489

H -0.621969 2.760583 0.163644

H 1.194297 2.498470 -0.124977

H -4.494146 -0.232494 -0.315094

H -4.002284 -1.114755 1.137853

H -3.771664 -1.842587 -0.457517

H 0.865838 -1.060297 -0.958130

H 2.489078 0.690510 0.946882

H 4.295371 -0.598040 -0.362787

H 3.123257 -1.893786 -0.653472

H 3.714223 -1.565218 0.986021

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 67.05 | 84.6413 | 89.7886 |
| 159.3052 | 185.6795 | 210.9873 |
| 225.4249 | 313.3562 | 379.7932 |
| 392.9749 | 431.868 | 583.5121 |
| 610.7154 | 743.3203 | 758.6871 |
| 844.7305 | 923.0083 | 943.1659 |
| 996.2113 | 1013.45 | 1054.576 |
| 1060.901 | 1074.614 | 1083.681 |
| 1134.357 | 1277.524 | 1336.361 |
| 1364.201 | 1418.575 | 1420.786 |
| 1442.259 | 1484.291 | 1486.533 |
| 1487.686 | 1496.464 | 1692.761 |
| 1752.611 | 2381.161 | 3042.691 |
| 3049.724 | 3102.27 | 3120.358 |
| 3126.181 | 3131.988 | 3158.669 |
| 3163.224 | 3167.06 | 3263.348 |

***p84 + H***

C -0.733542 2.416035 0.086120

C -0.597970 1.083011 0.006092

C 3.199342 -0.448657 -0.041854

C 1.849581 0.098800 -0.019345

C 0.724777 0.523423 -0.000639

C -1.801060 0.236823 -0.103929

C -1.946169 -1.090623 -0.068063

C -0.926054 -2.171592 0.117334

H -1.715601 2.875863 0.078836

H 0.128914 3.066361 0.159274

H 3.713893 -0.253756 0.902448

H 3.787148 -0.001475 -0.847329

H 3.174981 -1.530196 -0.199053

H -2.709874 0.819566 -0.232750

H -2.965302 -1.452107 -0.191578

H -1.287506 -2.898046 0.851305

H 0.038494 -1.793556 0.446559

H -0.778582 -2.715974 -0.822012

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 44.3646 | 73.7145 | 79.7085 |
| 117.6012 | 151.3934 | 250.5158 |
| 306.8164 | 324.9928 | 352.5683 |
| 405.989 | 533.2493 | 614.8005 |
| 639.7361 | 714.838 | 720.5568 |
| 802.7828 | 902.4671 | 934.3368 |
| 979.6291 | 1021.307 | 1051.887 |
| 1058.739 | 1077.152 | 1081.02 |
| 1121.383 | 1294.048 | 1363.103 |
| 1409.819 | 1415.135 | 1430.891 |
| 1463.277 | 1482.113 | 1487.466 |
| 1491.8 | 1498.446 | 1668.769 |
| 1752.255 | 2381.062 | 3044.738 |
| 3051.01 | 3097.541 | 3123.785 |
| 3124.943 | 3147.54 | 3168.962 |
| 3176.203 | 3186.802 | 3266.027 |

***p85 + H***

C 0.616124 1.746498 -0.218939

C 0.161663 0.491224 -0.322893

C -3.770123 -0.449591 0.330167

C -2.373425 -0.107894 0.094413

C -1.222076 0.186218 -0.091455

C 1.014429 -0.656093 -0.710494

C 2.227124 -0.944774 -0.236138

C 2.997263 -0.211522 0.819140

H 1.650694 1.981756 -0.437189

H -0.043138 2.557819 0.064782

H -4.429572 0.146440 -0.305666

H -4.042114 -0.260975 1.371882

H -3.953342 -1.505629 0.117992

H 0.566645 -1.336193 -1.430293

H 2.711832 -1.830525 -0.640492

H 2.364551 0.473002 1.386452

H 3.812640 0.371607 0.376956

H 3.455933 -0.921700 1.512774

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 40.9345 | 99.0548 | 134.1789 |
| 139.8908 | 175.768 | 263.8655 |
| 270.3995 | 331.462 | 366.2481 |
| 431.1129 | 535.5172 | 564.8916 |
| 616.3166 | 749.0003 | 784.4281 |
| 800.062 | 909.2014 | 956.0361 |
| 972.1489 | 1019.395 | 1059.748 |
| 1068.697 | 1072.702 | 1083.835 |
| 1120.792 | 1281.287 | 1299.085 |
| 1408.163 | 1424.362 | 1440.241 |
| 1451.075 | 1489.903 | 1491.045 |
| 1491.418 | 1502.94 | 1693.262 |
| 1743.397 | 2380.285 | 3042.008 |
| 3049.571 | 3099.537 | 3121.162 |
| 3125.451 | 3141.802 | 3158.77 |
| 3168.424 | 3180.821 | 3264.916 |

***p86 + H***

C 0.327317 2.459880 0.000091

C 0.118214 0.966311 -0.000033

C 3.153440 -1.481151 -0.000028

C 2.130807 -0.656532 -0.000019

C 1.150040 0.139376 -0.000012

C -1.275598 0.496252 -0.000177

C -1.669134 -0.778385 0.000145

C -3.093152 -1.230120 0.000000

H 1.386682 2.713829 0.000210

H -0.141932 2.907680 0.882252

H -0.141755 2.907792 -0.882107

H 3.007027 -2.555952 -0.000183

H 4.172567 -1.109331 0.000105

H -2.030616 1.280802 -0.000546

H -0.907638 -1.556307 0.000554

H -3.304806 -1.848752 -0.878443

H -3.785905 -0.385571 -0.000539

H -3.305222 -1.847971 0.878894

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 41.5727 | 75.9387 | 131.079 |
| 159.5209 | 173.6486 | 197.5654 |
| 222.9281 | 303.6169 | 376.6893 |
| 435.4777 | 466.2639 | 521.2823 |
| 599.5731 | 622.8023 | 737.2856 |
| 831.0735 | 855.466 | 933.689 |
| 1011.566 | 1020.056 | 1032.312 |
| 1055.054 | 1073.243 | 1102.474 |
| 1174.809 | 1242.149 | 1337.659 |
| 1362.963 | 1413.34 | 1416.193 |
| 1448.267 | 1484.289 | 1485.594 |
| 1489.761 | 1494.893 | 1713.607 |
| 1742.34 | 2225.024 | 3036.435 |
| 3042.033 | 3094.224 | 3103.757 |
| 3128.246 | 3150.037 | 3154.899 |
| 3157.999 | 3166.116 | 3235.274 |

***p87 + H***

C 0.724452 2.404327 0.256561

C 0.479343 0.944134 -0.038540

C -3.163677 -0.443613 -0.108607

C -1.939659 0.029980 -0.073517

C -0.751305 0.458421 -0.042076

C 1.664876 0.134122 -0.344720

C 1.823093 -1.184756 -0.185760

C 0.827340 -2.157086 0.364035

H 1.217131 2.882339 -0.596681

H 1.389249 2.511320 1.119414

H -0.207294 2.930510 0.461221

H -3.354780 -1.480204 -0.366263

H -4.017423 0.185758 0.119216

H 2.514301 0.702956 -0.716851

H 2.784468 -1.599340 -0.478876

H 0.191574 -2.557878 -0.433415

H 0.162231 -1.687018 1.091360

H 1.333769 -3.001614 0.836616

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 59.2578 | 78.7365 | 129.8182 |
| 149.1037 | 163.9917 | 263.0031 |
| 300.2524 | 313.8846 | 369.2284 |
| 495.1235 | 517.7791 | 545.4281 |
| 590.0499 | 653.6445 | 732.8365 |
| 752.0774 | 873.9628 | 935.3862 |
| 996.5717 | 1006.354 | 1032.632 |
| 1052.336 | 1063.87 | 1091.214 |
| 1164.192 | 1223.65 | 1294.179 |
| 1404.043 | 1410.5 | 1447.519 |
| 1451.262 | 1484.507 | 1486.12 |
| 1493.048 | 1505.303 | 1709.858 |
| 1728.732 | 2227.913 | 3042.436 |
| 3045.158 | 3104.952 | 3107.396 |
| 3138.352 | 3144.656 | 3155.32 |
| 3159.437 | 3180.331 | 3229.179 |

***p88 + H***

C 0.084623 2.263230 0.187337

C 0.085063 0.772230 -0.074373

C -3.574131 -1.057599 0.057518

C -2.267327 -0.414228 0.009806

C -1.180815 0.099605 -0.034765

C 1.188639 0.108755 -0.329074

C 2.293052 -0.535361 -0.569660

C 3.162576 -1.168280 0.484175

H -0.545117 2.774785 -0.545634

H 1.095712 2.667214 0.128922

H -0.325686 2.471086 1.179244

H -4.103182 -0.934854 -0.891155

H -4.192645 -0.626684 0.848805

H -3.470634 -2.127980 0.251655

H 2.617121 -0.633026 -1.604900

H 3.273727 -2.240467 0.297761

H 2.736350 -1.031843 1.478756

H 4.164278 -0.728343 0.470763

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 66.3666 | 93.6556 | 100.2556 |
| 142.5663 | 159.8071 | 182.5443 |
| 189.6929 | 257.4974 | 299.7643 |
| 352.6606 | 486.8338 | 487.8224 |
| 559.6722 | 613.2403 | 671.21 |
| 813.7854 | 876.5916 | 995.8838 |
| 1056.236 | 1058.538 | 1059.299 |
| 1062.666 | 1068.249 | 1107.122 |
| 1223.254 | 1288.098 | 1407.058 |
| 1413.366 | 1419.098 | 1447.869 |
| 1481.845 | 1486.891 | 1488.602 |
| 1491.345 | 1497.879 | 1518.627 |
| 2087.623 | 2381.522 | 3046.744 |
| 3051.708 | 3052.665 | 3111.211 |
| 3121.416 | 3122.67 | 3126.802 |
| 3136.305 | 3150.881 | 3153.829 |

***p89 + H***

C 1.952357 -0.693339 0.000072

C 1.952360 0.693334 -0.000055

C 0.743540 1.378304 -0.000126

C -0.473624 0.702229 -0.000074

C -1.770304 1.468066 0.000157

C -1.770303 -1.468065 -0.000140

C -0.473627 -0.702221 0.000035

C 0.743533 -1.378304 0.000106

H 2.887458 -1.242047 0.000136

H 2.887465 1.242036 -0.000089

H 0.743486 2.464057 -0.000206

H -2.374792 1.227939 0.880783

H -2.376432 1.226199 -0.878872

H -1.591519 2.544553 -0.001201

H -2.376218 -1.226444 0.879102

H -1.591511 -2.544552 0.000859

H -2.375007 -1.227708 -0.880553

H 0.743472 -2.464056 0.000185

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 73.9748 | 161.4469 | 175.5241 |
| 266.2542 | 326.9478 | 418.6681 |
| 446.6175 | 516.3771 | 526.1988 |
| 595.4907 | 735.4075 | 757.8958 |
| 760.0258 | 843.1808 | 880.8254 |
| 954.9303 | 1006.778 | 1019.243 |
| 1023.904 | 1050.379 | 1075.708 |
| 1085.499 | 1152.092 | 1192.156 |
| 1217.129 | 1260.204 | 1319.008 |
| 1331.72 | 1420.375 | 1430.508 |
| 1474.972 | 1482.184 | 1501.75 |
| 1502.198 | 1514.269 | 1541.2 |
| 1655.823 | 1686.359 | 3038.089 |
| 3038.573 | 3093.765 | 3097.064 |
| 3136.834 | 3138.288 | 3182.447 |
| 3187.226 | 3201.507 | 3217.117 |

***p90 + H***

C -1.937986 0.597729 -0.000025

C -1.855141 -0.895101 0.000041

C -0.449751 -1.409298 0.000010

C 0.642961 -0.638529 -0.000003

C 2.020549 -1.238970 -0.000033

C 1.565266 1.662880 0.000045

C 0.511124 0.834674 0.000006

C -0.855168 1.372377 -0.000045

H -2.926896 1.045637 -0.000059

H -2.393673 -1.296429 0.870225

H -2.393750 -1.296519 -0.870051

H -0.331515 -2.490005 -0.000007

H 2.587156 -0.922753 0.881439

H 2.587118 -0.922735 -0.881524

H 1.969160 -2.328906 -0.000048

H 1.422641 2.738024 0.000052

H 2.587383 1.305716 0.000085

H -0.958753 2.453391 -0.000086

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 85.5407 | 212.6982 | 260.5215 |
| 311.6728 | 352.8072 | 402.9461 |
| 422.658 | 490.1881 | 569.9931 |
| 601.1285 | 717.6419 | 721.5123 |
| 793.6231 | 835.4378 | 837.2834 |
| 903.0597 | 918.0553 | 971.6949 |
| 973.226 | 1009.128 | 1015.819 |
| 1067.99 | 1089.617 | 1177.399 |
| 1203.528 | 1218.737 | 1311.924 |
| 1384.226 | 1400.324 | 1416.339 |
| 1449.167 | 1463.669 | 1472.264 |
| 1484.283 | 1509.23 | 1683.678 |
| 1721.005 | 1776.983 | 3015.051 |
| 3032.32 | 3040.972 | 3101.666 |
| 3139.425 | 3167.365 | 3169.429 |
| 3176.147 | 3200.38 | 3255.782 |

***p91 + H***

C -2.048039 0.248789 -0.050343

C -1.722583 -1.039426 -0.159209

C -0.335882 -1.474118 -0.020938

C 0.692919 -0.610228 0.050249

C 2.115660 -1.086717 0.107919

C 1.378544 1.740526 -0.239592

C 0.420387 0.839771 -0.001244

C -1.005491 1.279326 0.268602

H -3.079062 0.575228 -0.136531

H -2.482697 -1.789201 -0.349384

H -0.135818 -2.541362 -0.013808

H 2.650066 -0.631445 0.947316

H 2.657247 -0.818559 -0.805185

H 2.158843 -2.171546 0.217363

H 1.147003 2.798308 -0.307973

H 2.416647 1.461137 -0.371814

H -1.092799 1.512625 1.341328

H -1.212513 2.217273 -0.253983

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 80.1349 | 180.5634 | 235.6187 |
| 317.4718 | 347.4911 | 427.7778 |
| 478.0148 | 496.9244 | 523.543 |
| 599.6542 | 699.9832 | 721.3854 |
| 765.5393 | 832.2531 | 892.0069 |
| 915.6713 | 941.3085 | 962.2621 |
| 988.4637 | 1004.511 | 1023.716 |
| 1071.869 | 1089.562 | 1170.7 |
| 1198.035 | 1228.861 | 1306.582 |
| 1349.062 | 1402.979 | 1421.45 |
| 1441.151 | 1454.894 | 1465.165 |
| 1488.522 | 1505.111 | 1680.512 |
| 1703.544 | 1746.757 | 2996.976 |
| 3041.409 | 3090.63 | 3101.799 |
| 3137.318 | 3165.586 | 3178.989 |
| 3189.55 | 3208.759 | 3253.867 |

***p92 + H***

C -1.510052 -1.115264 0.345482

C -1.925832 0.165263 -0.221271

C -1.020368 1.071184 -0.596324

C 0.455567 0.863230 -0.376907

C 0.896511 1.699672 0.843438

C 2.055106 -1.050102 -0.413098

C 0.823438 -0.595634 -0.163038

C -0.217774 -1.472609 0.371367

H -2.271440 -1.793365 0.715129

H -2.985756 0.362407 -0.338577

H -1.330701 2.025842 -1.010273

H 1.001918 1.235841 -1.249574

H 1.974095 1.601096 0.997146

H 0.385055 1.350984 1.744307

H 0.656435 2.756610 0.698277

H 2.331298 -2.076509 -0.196122

H 2.818760 -0.410801 -0.844361

H 0.080764 -2.446540 0.746153

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 77.9368 | 193.0692 | 258.9895 |
| 279.0033 | 375.4522 | 398.5227 |
| 481.5418 | 532.9296 | 592.7384 |
| 686.2387 | 699.9271 | 749.4104 |
| 777.8238 | 837.349 | 876.9512 |
| 923.7747 | 946.4181 | 962.7763 |
| 1006.786 | 1008.701 | 1018.512 |
| 1034.652 | 1089.704 | 1120.152 |
| 1190.21 | 1210.997 | 1310.134 |
| 1322.817 | 1349.347 | 1396.154 |
| 1416.178 | 1439.742 | 1472.576 |
| 1496.378 | 1504.189 | 1660.406 |
| 1701.033 | 1744.64 | 3045.465 |
| 3062.886 | 3127.537 | 3133.913 |
| 3150.533 | 3179.349 | 3185.278 |
| 3201.641 | 3212.879 | 3238.801 |

***p93 + H***

C 1.604746 -1.029465 -0.236247

C 1.915734 0.436687 -0.126331

C 0.794952 1.193458 0.597581

C -0.551946 0.802096 0.044494

C -1.405544 1.684226 -0.470313

C -2.030386 -1.183758 0.244556

C -0.813708 -0.660949 0.059985

C 0.366672 -1.516329 -0.131466

H 2.433213 -1.710097 -0.408539

H 2.864883 0.577570 0.399734

H 2.057080 0.854478 -1.131585

H 0.942865 2.272686 0.517493

H 0.830962 0.930598 1.661689

H -2.342738 1.373911 -0.918762

H -1.182452 2.746176 -0.468115

H -2.185717 -2.257292 0.225349

H -2.895110 -0.557587 0.430881

H 0.193889 -2.586241 -0.201699

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 102.0691 | 180.7724 | 288.4418 |
| 338.6294 | 374.0542 | 430.5281 |
| 476.1036 | 556.863 | 631.746 |
| 688.9755 | 732.6397 | 768.4871 |
| 770.5723 | 816.659 | 879.6195 |
| 898.7484 | 927.3136 | 944.2461 |
| 973.3199 | 986.7463 | 1008.187 |
| 1049.712 | 1058.238 | 1188.155 |
| 1197.426 | 1235.617 | 1279.405 |
| 1342.51 | 1352.769 | 1372.404 |
| 1421.437 | 1448.577 | 1466.879 |
| 1486.413 | 1496.577 | 1687.995 |
| 1729.498 | 1747.437 | 3030.365 |
| 3041.543 | 3086.91 | 3112.014 |
| 3154.762 | 3160.772 | 3174.049 |
| 3196.863 | 3243.714 | 3251.629 |

***p94 + H***

C 1.826254 0.628569 0.213239

C 1.826154 -0.628782 -0.213353

C 0.573581 -1.420388 -0.475575

C -0.667477 -0.739697 0.054934

C -1.680946 -1.411951 0.595055

C -1.680592 1.412236 -0.595178

C -0.667334 0.739790 -0.054899

C 0.573779 1.420227 0.475783

H 2.770874 1.133841 0.392499

H 2.770708 -1.134086 -0.392879

H 0.666228 -2.420784 -0.041668

H 0.466298 -1.565518 -1.559597

H -1.662962 -2.494614 0.671724

H -2.551333 -0.896886 0.985856

H -1.662361 2.494894 -0.671848

H -2.551008 0.897340 -0.986137

H 0.666482 2.420743 0.042164

H 0.466550 1.565040 1.559852

***Frequencies***

|  |  |  |
| --- | --- | --- |
| 105.098 | 111.3272 | 265.0585 |
| 319.9615 | 393.4076 | 429.0506 |
| 470.2685 | 557.8958 | 614.8211 |
| 667.4989 | 725.3501 | 725.9052 |
| 788.575 | 843.993 | 921.6108 |
| 936.8191 | 938.8146 | 945.8685 |
| 982.6226 | 987.4221 | 993.1301 |
| 1030.14 | 1037.452 | 1195.317 |
| 1209.943 | 1230.678 | 1248.259 |
| 1338.072 | 1350.531 | 1359.909 |
| 1426.669 | 1443.821 | 1458.551 |
| 1478.416 | 1480.461 | 1727.671 |
| 1734.595 | 1760.703 | 3018.391 |
| 3019.012 | 3078.817 | 3078.843 |
| 3153.171 | 3153.935 | 3167.193 |
| 3191.298 | 3244.544 | 3245.166 |

***Fragments***

***CH3***

C -0.000134 -0.000001 0.000023

H -1.080503 0.038158 -0.000046

H 0.507588 -0.954443 -0.000046

H 0.573721 0.916289 -0.000046

***Frequencies***

470.9451 1399.8856 1409.5749

3117.6199 3301.0861 3304.8947

***C2H3***

C 0.705692 -0.145170 0.000001

C -0.586151 0.030184 0.000004

H 1.596113 0.468363 -0.000011

H -1.031552 1.027946 -0.000006

H -1.281806 -0.806397 -0.000015

***Frequencies***

714.0578 840.5185 933.8993

1052.7836 1393.8374 1668.5191

3080.5313 3173.8401 3244.2107

***C3H5\_a***

C 1.360710 -0.154448 -0.000002

C 0.212046 0.468550 0.000003

C -1.144382 -0.198036 -0.000001

H 1.712354 -1.177916 0.000006

H 0.205954 1.559708 0.000001

H -1.716533 0.103752 0.882327

H -1.055489 -1.285695 0.000001

H -1.716526 0.103757 -0.882332

***Frequencies***

168.9855 385.3664 647.3666

840.5820 851.0793 933.7929

1054.3478 1100.1094 1271.3097

1401.6285 1481.6880 1487.2425

1697.5024 3041.1762 3107.3980

3119.5989 3142.8723 3240.2883

***C3H5\_b***

C -1.309507 -0.319898 -0.000002

C -0.212496 0.389802 0.000004

C 1.190894 -0.152769 -0.000003

H -2.374484 -0.136085 0.000000

H -0.304052 1.482050 -0.000004

H 1.192372 -1.243371 -0.000111

H 1.736365 0.197200 0.881404

H 1.736452 0.197396 -0.881279

***Frequencies***

179.5659 408.1387 600.9251

805.6738 822.0556 937.9675

1062.3207 1115.0819 1277.4664

1403.5440 1483.2804 1487.1065

1707.6747 3046.7708 3056.3888

3110.6582 3150.5075 3256.8466