**Supporting Information:**

**Interstellar Formation of Nitrogen Heteroaromatics [Indole, C8H7N; Pyrrole, C4H5N; Aniline, C6H5NH2] – Key Precursors to Amino Acids and Nucleobases**

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**Methods and Materials**

**Experimental**.The experiments were carried out in a contamination-free ultrahigh vacuum chamber operated at base pressures of a few 10−11 Torr using magnetically suspended turbomolecular pumps (Osaka, TG1300MUCWB and TG420MCAB) backed by an oil-free scroll pump (Edwards, GVSP30).[1](#_ENREF_1),[2](#_ENREF_2) A polished silver substrate was interfaced to a closed-cycle helium cryostat (Sumitomo Heavy Industries, RDK415E) that can be moved vertically via an adjustable bellows (McAllister, BLT86) and rotated horizontally via a rotatable flange (Thermionics Vacuum Products, RNN-600/FA/MCO). After cooling the substrate to 4.6 ± 0.1 K, acetylene (C2H2; 99.9%, Airgas) and ammonia (NH3; 99.999%, Matheson) were deposited onto the substrate surface through separate glass capillary arrays at partial pressures of 1.2 × 10−8 Torr for C2H2 and 0.8 × 10−8 Torr for NH3. A dry ice ethanol slush bath was used to remove the traces of acetone (CH3COCH3) in the acetylene.[3](#_ENREF_3) The formulae of interested ion signals were verified using isotopically substituted ice mixtures including 13C2H2−NH3 (13C2H2; >99 13C%, Cambridge Isotope), C2H2−15NH3 (15NH3; >98 15N%, Sigma Aldrich), and 13C2H2−15NH3. To measure the ice thickness, a photodiode recorded interference fringes between helium-neon laser (632.8 nm) reflections of the ice surface and silver substrate during the ice deposition.[4](#_ENREF_4) The ice thickness and the acetylene-to-ammonia ratio were determined to be 1,000 ± 100 nm and 1.0: (1.0 ± 0.2), respectively.[5](#_ENREF_5) After deposition, each ice was then processed with energetic electrons (5 keV; SPECS EQ 22/35) at a 70° angle of incidence at a current of 100 nA for 60 minutes, which correspond to doses of 5.0 ± 0.8 eV per C2H2 molecule and 3.5 ± 0.6 eV per NH3 molecule,[5](#_ENREF_5) simulating the irradiation of interstellar ices by secondary electrons generated in the track of GCRs in cold molecular clouds aged around 2 × 107 years.[6](#_ENREF_6) The average penetration depth (350 ± 30 nm) of the energetic electrons is significantly less than the ice thickness (1,000 ± 100 nm), preventing energetic electron-initiated interactions between the substrate and ice mixtures. A Fourier transform infrared (FTIR) spectrometer (Thermo Electron, Nicolet 6700) monitored the infrared spectra of ice mixtures before, during, and after irradiation with a spectral resolution of 4 cm−1.

After irradiation, the ice was heated from 5 K to 300 K at a rate of 1 K minute−1 (temperature-programmed desorption, TPD) to release molecules into the gas phase. A cryogenic silicon diode sensor (Lakeshore DT-670) was used to measure the temperature of the silver substrate, which was precisely regulated between 5 K and 300 K, with a precision of ± 0.1 K, by a programmable temperature controller (Lakeshore 336). During the TPD, subliming molecules were ionized by vacuum ultraviolet (VUV) single-photon ionization (SPI); individual isomers were selectively ionized by two-photon resonance-enhanced multiphoton ionization (REMPI). Tunable VUV photons were generated through the non-resonant (10.49 eV) or resonant (7.90 eV, and 8.10 – 8.27 eV) four-wave mixing method with the detailed parameters listed in Table S2. The synchronized laser beams were generated from two dye lasers (Sirah Lasertechnik GmbH, Cobra-Stretch) pumped by two pulsed (30 Hz) Nd: YAG lasers (Spectra-Physics, Quanta Ray Pro 250 and 270). Xenon (Specialty Gases, 99.999%) or krypton (Specialty Gases, 99.999%) gas was used as a nonlinear medium. The ultraviolet (UV) photons were generated via the frequency doubling process in a dye laser pumped by the third harmonic (355 nm) of a Nd:YAG laser. To determine the [1 + 1] REMPI wavelengths of aniline (**4**) and indole (**2**), separate experiments were performed with processed C2H2−NH3 ice under the same experimental conditions. During the TPD, the laser wavelengths were scanned over the relevant wavelength ranges; the wavelengths were calibrated with a wavelength meter (Coherent, Wavemaster). Wavelengths at 283.817 nm (4.369 eV) and 293.842 nm (4.219 eV) were found to produce the strongest signals for aniline (Figure S3) and indole (**2**) (Figure S4), respectively, and therefore they were used to detect aniline (**4**) and indole (**2**) molecules in separate irradiation experiments. The ionization laser beam was separated spatially by a biconvex lithium fluoride lens (Korth Kristalle, R1 = R2 = 131.2 mm) in an off-axis geometry and passed 2.0 ± 0.5 mm over the ice surface to ionize the subliming molecules. The resulting ions were then detected by a reflectron time-of-flight mass spectrometer (ReToF-MS; Jordan-TOF products) equipped with two microchannel plates in chevron geometry. The ion signals were amplified by a preamplifier (Ortec 9305), shaped in a discriminator (Advanced Research Instruments Corp., F100-TD), and finally recorded by a multichannel scaler (FAST ComTec, MCS6A). The ionization laser was synchronized with the multichannel scaler through a digital delay pulse generator (Quantum Composers, 9518). During TPD, each recorded spectrum was integrated over 3600 sweeps (2 minutes) in bins of 3.2 ns width. The resolving power (m/*∆*m) of this instrument was measured to be around 360 in the considered range. It is worth noting that a blank experiment was performed with C2H2−NH3 ice under identical conditions but without electron irradiation; no ion signals at the mass-to-charge ratios (*m/z*) of 67, 93, and 117 were observed (Figure S7). An additional experiment with C2H2−hydrogen cyanide (HCN, 5% seeded in helium) ice irradiated with a lower dose (20 nA, 15 minutes) was recorded at a photon energy of 10.49 eV (Figure S12).

**Computational**.Geometry optimization of various reactants, products, intermediates, and transition states involved in the variety of considered radical-molecule and radical-radical reactions leading to the formation of pyrrole, indole, and aniline were carried out using density functional theory with the *ω*B97X-D functional by Chai and Head-Gordon[7](#_ENREF_7) and 6-311G(d,p) basis set. Vibrational frequencies for each stationary structure were evaluated at the same *ω*B97X-D/6-311G(d,p) level of theory to verify whether the structure is a local minimum or a first-order saddle point (transition state) and to obtain the zero-point vibrational energy (ZPE) correction. Following the optimization, single-point energies were further improved using either explicitly correlated coupled cluster calculations with single and double excitations and perturbative treatment of triple excitations, CCSD(T)-F12,[8](#_ENREF_8),[9](#_ENREF_9) with Dunning’s cc-pVTZ-F12 basis set[10](#_ENREF_10) (for the pyrrole and aniline formation reactions), or employing the G3(MP2,CC) model chemistry scheme[11-13](#_ENREF_11) (for indole formation). Relative energies computed at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) + ZPE(*ω*B97X-D/6-311G(d,p)) and G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) + ZPE(*ω*B97X-D/6-311G(d,p)) levels of theory are anticipated to be accurate within 4 and 8 kJ mol−1, respectively[13](#_ENREF_13),[14](#_ENREF_14). All electronic structure calculations were performed using the Gaussian 09 and Molpro 2015 program packages[15](#_ENREF_15),[16](#_ENREF_16). Besides the potential energy surfaces presented in Figures 5–6, our electronic structure calculations reveal other reaction pathways leading to the formation of pyrrole (**3**) (Figures S13–S19) and indole (**2**) (Figures S20–S25). The computed Cartesian coordinates and vibrational frequencies of optimized structures (reactants, products, intermediates, and transition states) are listed in Table S3, which includes 88 reaction intermediates and 93 transition states. It is worth noting that gas-phase calculations may overestimate the reaction barrier because nearby molecules could participate in the reactions in the ice phase,[17-19](#_ENREF_17) in particular, to be directly involved in the H transfer processes (Figures S13, S14, S16, S18, and S19).

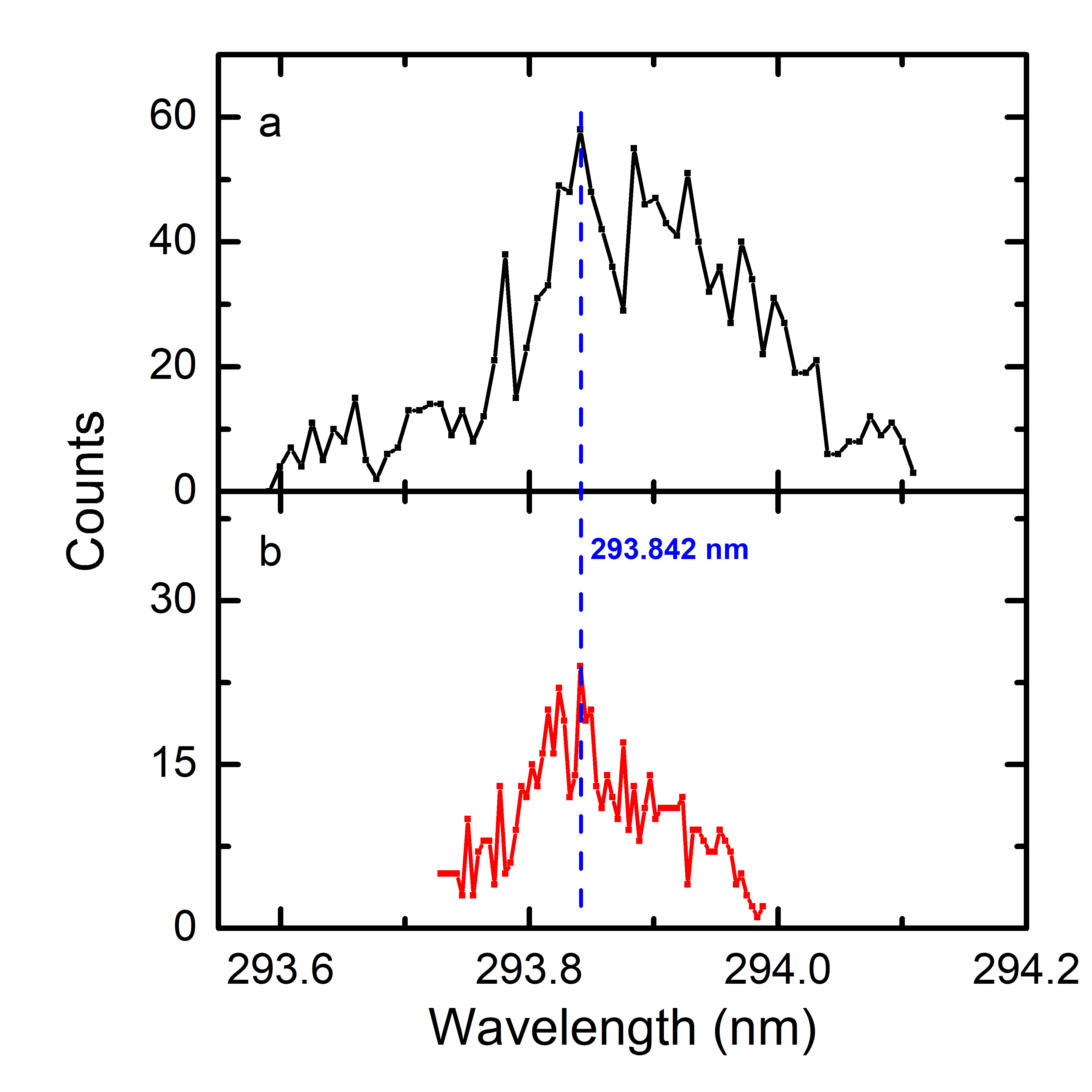
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**Figure S1.** Photoionization reflectron time-of-flight mass spectrometric data. PI-ReToF-MS data as a function of temperature and mass-to-charge (*m/z*) during the TPD of the irradiated acetylene–ammonia ices. Data were collected at a photon energy of 10.49 eV for C2H2–NH3 (a), 13C2H2–NH3 (b), C2H2–15NH3 (c), and 13C2H2–15NH3 ices (d).



**Figure S2.** TPD profiles of *m/z* = 67 measured at 10.49 eV and 7.90 eV in irradiated C2H2–NH3 ice.



**Figure S3.** Resonance-enhanced multiphoton ionization (REMPI) scan from 293.59–294.11 nm recorded in irradiated C2H2–NH3 ice during sublimation from 193–205 K (a). A precise scan was performed to determine the wavelength (λ = 293.842 nm) at the maximum signal (b), which corresponds to the S1 ← S0 transition origin (00) band of aniline.

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**Figure S4.** REMPI scan from 283.65–283.87 nm recorded in irradiated C2H2–NH3 ice during sublimation from 206–268 K. The arrow indicates the wavelength (λ = 283.817 nm) at the maximum signal, which corresponds to the S1 ← S0 transition origin (00) band of indole.

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**Figure S5.** TPD profiles of *m/z* = 93 measured at 10.49 eV and 7.90 eV, and the REMPI wavelength of 293.842 nm in irradiated C2H2–NH3 ice.

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**Figure S6.** TPD profiles of *m/z* = 117 measured at 10.49 eV and 7.90 eV, and the REMPI wavelength of 283.817 nm in irradiated C2H2–NH3 ice.

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**Figure S7**. TPD profiles measured as a function of temperature for the blank experiment in C2H2–NH3 ice recorded at a photon energy of 10.49 eV.

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**Figure S8.** Ion signals during TPD of acetylene−ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated C2H2–NH3 (*m/z* = 78), 13C2H2–NH3 (*m/z* = 84), C2H2–15NH3 (*m/z* = 78), and 13C2H2–15NH3 (*m/z* = 84) ices, confirming the formula C6H6. The shaded region indicates the range of sublimation temperature of benzene (**1**) in processed acetylene ices.[20](#_ENREF_20),[21](#_ENREF_21)

A graph of a chemical reaction

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**Figure S9.** Ion signals during TPD of acetylene−ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated C2H2–NH3 (*m/z* = 52), 13C2H2–NH3 (*m/z* = 56), C2H2–15NH3 (*m/z* = 52), and 13C2H2–15NH3 (*m/z* = 56) ices, confirming the formula C4H4. The shaded region indicates the range of sublimation temperature of vinylacetylene (**5**) in processed acetylene ices.[20](#_ENREF_20)



**Figure S10.** Ion signals during TPD of acetylene−ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated C2H2–NH3 (*m/z* = 41), 13C2H2–NH3 (*m/z* = 43), C2H2–15NH3 (*m/z* = 42), and 13C2H2–15NH3 (*m/z* = 44) ices, confirming the formula C2H3N. The shaded region indicates the sublimation event of ethynylamine (**6**) in processed acetylene−ammonia ices.[5](#_ENREF_5)

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**Figure S11.** Ion signals during TPD of acetylene−ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated C2H2–NH3 (*m/z* = 102), 13C2H2–NH3 (*m/z* = 110), C2H2–15NH3 (*m/z* = 102), and 13C2H2–15NH3 (*m/z* = 110) ices, confirming the formula C8H6. The shaded region indicates the range of sublimation temperature of phenylacetylene (**7**) in processed acetylene ices.[20](#_ENREF_20)



**Figure S12**. TPD profiles measured as a function of temperature for the irradiated (20 nA, 15 minutes) experiment in C2H2–HCN ice recorded at a photon energy of 10.49 eV.

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**Figure S13.** Potential energy surface for formation ofpyrrole (**3**) from **i2** calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory. Adding ammonia (NH3) molecules into the reaction results in a reduction of the barrier to form pyrrole (**3**). Relative energies (italics) are shown in kJ mol–1.

A diagram of a molecule

Description automatically generated

**Figure S14.** Potential energy surface for the bimolecular reaction of acetylene (C2H2) with ethynylamine (**6**) calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory. Adding ammonia molecules into the reaction results in a reduction of the barrier to form pyrrole (**3**). Relative energies (italics) are shown in kJ mol–1.

A diagram of a molecule

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**Figure S15.** Potential energy surface for the reaction of acetylene (C2H2) with the ethynylamidogen (**9**) radical, leading to the formation of 2-pyrrolyl (C4H4N, **16**) radical. Relative energies (italics) were calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory.

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**Figure S16.** Potential energy surface for the reaction of acetylene (C2H2) with the aminoethynyl (**15**) radical, leading to the formation of 3-pyrrolyl (C4H4N, **11**) radical. Relative energies (italics) were calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory. Adding ammonia molecules into the reaction results in a reduction of the barrier to form 3-pyrrolyl (**11**).

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**Figure S17.** Potential energy surface for the reaction of acetylene (C2H2) with the 2-aminoethenyl (**12**) radical calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory.

A diagram of a molecule

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**Figure S18.** Potential energy surface for the reaction of the vinyl (**8**) radical with ethynylamine (**6**) calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory. Adding ammonia (NH3) molecules into the reaction results in a reduction of the barrier from **i37** to **i39**. Relative energies (italics) are shown in kJ mol–1.

A close-up of a diagram

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**Figure S19.** Potential energy surface for the reaction of the ethynyl (**10**) plus 2-aminoethenyl (NH2CHĊH, **12**) calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level of theory. Direct participation of ammonia (NH3) molecules in the reaction creates a possibility for a hydrogen atom to be transferred from the nitrogen atom to the “bare” carbon atom. Relative energies (italics) are shown in kJ mol–1.

A diagram of a molecule

Description automatically generated

**Figure S20.** Potential energy surface for the reaction of ethynylamidogen (**9**) and phenyl (**14**) radicals calculated at the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level of theory.

A diagram of a molecule

Description automatically generated

**Figure S21.** Potential energy surface for the reaction of vinylacetylene (**5**) with the 2-pyrrolyl (**16**) radical calculated at the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level of theory.

A diagram of a molecule

Description automatically generated

**Figure S22.** Potential energy surface for the reaction of vinylacetylene (**5**) with the 2-pyrrolyl (**16**) radical calculated at the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level of theory.

A diagram of molecules and lines

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**Figure S23.** Potential energy surface for the reaction of vinylacetylene (**5**) with the 3-pyrrolyl (**11**) radical calculated at the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level of theory.

A diagram of a molecule

Description automatically generated

**Figure S24.** Potential energy surface for the bimolecular reaction of vinylacetylene (**5**) with the 3-pyrrolyl (**11**) radical calculated at the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level of theory.

A diagram of a molecule

Description automatically generated

**Figure S25.** Potential energy surface for the reaction of the vinylacetylene (**5**) with the 3-pyrrolyl (**11**) radical calculated at the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level of theory.

**Table S1.** Absorption peaks observed in C2H2–NH3 ice before and after electron irradiation (100 nA, 60 minutes) at 5 K. Assignment labels: stretching (*ν*) and bending (*δ*).

|  |  |
| --- | --- |
| Pristine ice, absorptions before irradiation (cm−1) |  |
| **C2H2** | Assignment[20-23](#_ENREF_20) |
| 3236 | ν3 |
| 1947 | ν2 |
| 1375 | ν4 + ν5 |
| 805, 753 | ν5 |
| **NH3** | Assignment[24](#_ENREF_24),[25](#_ENREF_25) |
| 3380 | ν3 |
| 3303 | 2ν4 |
| 3165 | ν1 |
| 1629 | ν4 |
| 1087 | ν2 |
| New absorptions after irradiation (cm−1) | Assignment[20](#_ENREF_20),[26-31](#_ENREF_26) |
| 2974 | ν6+ν7 (C4H4)/ν11 (C2H4)/ν10 (C2H6) |
| 2792 | ν(C−H) |
| 2109 | ν5 (C4H4) |
| 2054 | ν(C=C=N) |
| 1506 | ν(ring)/*δ*(NH2)/ṄH2 |
| 1435 | ν12 (C2H4) |
| 1304 | ν9 (C6H6)/ν4 (CH4) |
| 1274 | *δ*(NH) |
| 961 | *δ*(C=CH)aromatic |

**Table S2.** Parameters for the generation of vacuum ultraviolet (VUV; 3ω1 or 2ω1 – ω2) and ultraviolet (UV; ω2) lights. The uncertainty of photon wavelengths is less than 0.001 nm.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Photon energy (eV) | 10.49  (3ω1) | 8.10 – 8.27  (2ω1 – ω2) | 7.90  (2ω1 – ω2) | 4.219  (ω2) | 4.368  (ω2) |
| Nonlinear medium for four-wave mixing | Xenon | Krypton | Xenon | − | − |
| ω1 wavelength (nm) | 355 | 202.316 | 249.628 | − | − |
| Nd:YAG 1 output (nm) | 355 | 532 | 355 | − | − |
| Dye laser 1 output (nm) | − | 606.948 | 499.256 | − | − |
| ω2 wavelength (nm) | − | 298 – 311 a | 609.696 | 293.842 a | 283.817 a |
| Nd:YAG 2 output (nm) | − | 532 | 532 | 532 | 532 |
| Dye laser 2 output (nm) | − | 596 – 622 | 609.696 | 587.684 | 567.634 |

# a obtained through frequency doubling process.

**Table S3.** Cartesian coordinates and vibrational frequencies of optimized structures (reactants, products, intermediates, and transition states) calculated at the CCSD(T)-F12/cc-pVTZ-F12//*ω*B97X-D/6-311G(d,p) level and the G3(MP2,CC)//*ω*B97X-D/6-311G(d,p) level.

**Reactants and products**

***Acetylene***

**Cartesian coordinates**

C 0.000000 0.000000 0.598192

C 0.000000 0.000000 -0.598192

H 0.000000 0.000000 1.662187

H 0.000000 0.000000 -1.662187

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 675.1455 | 675.1455 | 768.9518 |
| 768.9518 | 2088.336 | 3423.093 |
| 3530.67 |  |  |

***Ammonia***

**Cartesian coordinates**

N 0.000000 0.000000 0.114745

H 0.000000 0.938582 -0.267738

H 0.812836 -0.469291 -0.267738

H -0.812836 -0.469291 -0.267738

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 1064.784 | 1682.874 | 1682.998 |
| 3507.326 | 3634.768 | 3635 |

***Benzene (1)***

**Cartesian coordinates**

C 1.379003 0.175768 -0.000001

C 0.841743 -1.106425 -0.000001

C -0.537179 -1.282193 0.000000

C -1.379003 -0.175768 0.000000

C -0.841743 1.106425 0.000000

C 0.537179 1.282193 0.000000

H 2.454596 0.312944 0.000005

H 1.498509 -1.969296 0.000001

H -0.957019 -2.281974 0.000002

H -2.454596 -0.312944 -0.000001

H -1.498509 1.969296 0.000001

H 0.957019 2.281974 0.000002

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 413.1913 | 414.2282 | 625.9993 |
| 627.3443 | 686.819 | 730.0167 |
| 862.6288 | 877.5347 | 991.8031 |
| 1004.368 | 1027.099 | 1028.037 |
| 1029.236 | 1070.853 | 1074.961 |
| 1178.398 | 1203.341 | 1210.547 |
| 1340.871 | 1384.089 | 1523.176 |
| 1528.737 | 1670.821 | 1672.722 |
| 3184.327 | 3191.905 | 3197.115 |
| 3208.994 | 3213.669 | 3222.537 |

***Indole (2)***

**Cartesian coordinates**

N 1.558908 -1.076624 -0.000036

C 2.378381 0.029070 -0.000025

C 1.621948 1.161607 0.000008

C 0.248178 0.745771 0.000035

C -0.978770 1.422864 0.000013

C -2.149074 0.690308 -0.000019

C -2.125626 -0.715717 -0.000014

C -0.932876 -1.412053 0.000012

C 0.247307 -0.666896 0.000028

H 1.871417 -2.030209 0.000156

H 3.451125 -0.087050 -0.000059

H 1.996585 2.172995 -0.000014

H -1.006300 2.507032 0.000014

H -3.104374 1.202587 -0.000048

H -3.061841 -1.262273 -0.000036

H -0.915768 -2.496435 0.000015

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 213.4478 | 246.5963 | 403.472 |
| 413.1689 | 431.2457 | 555.8567 |
| 590.8125 | 622.4174 | 623.2906 |
| 726.8646 | 755.6784 | 782.6987 |
| 788.8756 | 862.2803 | 879.8249 |
| 892.6123 | 916.9751 | 951.5005 |
| 990.926 | 1042.761 | 1092.459 |
| 1123.951 | 1152.724 | 1180.769 |
| 1233.504 | 1273.145 | 1317.391 |
| 1377.747 | 1391.005 | 1469.091 |
| 1501.149 | 1547.195 | 1581.2 |
| 1652.483 | 1696.432 | 3191.383 |
| 3198.7 | 3209.364 | 3221.297 |
| 3259.988 | 3280.178 | 3724.61 |

***Pyrrole (3)***

**Cartesian coordinates**

N -1.116972 -0.004172 -0.000235

C -0.334469 1.118024 -0.000025

C 0.976135 0.714387 -0.000020

C 0.981639 -0.707082 -0.000113

C -0.326101 -1.120471 -0.000137

H -2.120677 -0.007958 0.000731

H -0.771207 2.103680 0.000761

H 1.836312 1.365623 0.000243

H 1.846599 -1.351918 0.000611

H -0.755452 -2.109368 0.001067

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 501.1219 | 636.2196 | 647.7327 |
| 703.8612 | 740.4986 | 856.0911 |
| 885.0829 | 903.8719 | 905.6801 |
| 1038.571 | 1073.724 | 1103.861 |
| 1175.942 | 1192.966 | 1314.851 |
| 1440.203 | 1489.491 | 1527.269 |
| 1600.285 | 3250.215 | 3262.821 |
| 3283.781 | 3289.152 | 3720.48 |

***Aniline (4)***

**Cartesian coordinates**

N 2.326736 0.000038 -0.074118

C 0.935255 -0.000002 -0.009595

C 0.220266 1.202364 -0.006262

C -1.166695 1.196673 0.003633

C -1.873485 0.000001 0.008999

C -1.166699 -1.196672 0.003655

C 0.220264 -1.202366 -0.006235

H 2.768317 -0.835174 0.276196

H 2.768304 0.834934 0.276968

H 0.759134 2.144805 -0.016063

H -1.699343 2.141484 0.007535

H -2.956773 0.000002 0.017456

H -1.699348 -2.141483 0.007576

H 0.759118 -2.144817 -0.016009

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 221.6451 | 286.2772 | 388.5944 |
| 419.5718 | 509.8614 | 541.8018 |
| 593.953 | 638.0537 | 708.7131 |
| 768.8114 | 834.9846 | 842.9233 |
| 892.2601 | 978.3354 | 994.9788 |
| 1016.042 | 1062.631 | 1080.285 |
| 1145.391 | 1184.894 | 1214.905 |
| 1325.84 | 1350.43 | 1375.493 |
| 1515.543 | 1552.463 | 1662.408 |
| 1667.595 | 1693.027 | 3182.513 |
| 3183.668 | 3199.841 | 3206.076 |
| 3223.716 | 3606.929 | 3707.891 |

***Vinylacetylene (5)***

**Cartesian coordinates**

C -1.899901 -0.173838 0.000001

C -0.734772 0.118044 -0.000001

C 0.642282 0.494146 -0.000004

C 1.648571 -0.378115 0.000004

H -2.929811 -0.438232 0.000002

H 0.844856 1.561434 0.000006

H 2.677071 -0.037282 -0.000004

H 1.470807 -1.447336 -0.000009

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 223.9837 | 308.3506 | 563.9499 |
| 676.5628 | 702.8568 | 706.388 |
| 894.6541 | 963.0477 | 1010.796 |
| 1117.303 | 1332.419 | 1445.456 |
| 1706.094 | 2243.637 | 3165.339 |
| 3181.842 | 3262.931 | 3487.017 |

***Ethynylamine (6)***

**Cartesian coordinates**

N 0.128010 -1.182754 0.000000

C -0.061211 1.360347 0.000000

C 0.000000 0.161386 0.000000

H -0.205880 -1.635867 -0.837650

H -0.205880 -1.635867 0.837650

H -0.117042 2.420609 0.000000

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 378.103 | 457.0034 | 520.4194 |
| 610.5933 | 714.7365 | 1097.72 |
| 1207.987 | 1649.646 | 2277.598 |
| 3495.49 | 3587.772 | 3679.068 |

***Phenylacetylene (7)***

**Cartesian coordinates**

C -0.119132 -1.207129 0.000149

C -1.506056 -1.203155 -0.000033

C -2.202394 -0.000058 -0.000037

C -1.506328 1.203124 -0.000004

C 0.586783 -0.000013 0.000051

C 2.019228 0.000048 -0.000004

C 3.219987 0.000088 -0.000046

C -0.119329 1.207103 0.000021

H 0.428652 -2.141832 -0.000257

H -2.045047 -2.143573 -0.000099

H -3.286444 -0.000185 -0.000104

H -2.045401 2.143499 -0.000018

H 4.283296 0.000145 -0.000094

H 0.428390 2.141893 -0.000008

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 137.2745 | 155.4812 | 366.7227 |
| 412.9701 | 474.7877 | 541.5413 |
| 555.6264 | 639.4061 | 663.8127 |
| 703.3922 | 711.5259 | 781.6306 |
| 782.0688 | 868.2194 | 948.2836 |
| 1002.296 | 1019.549 | 1023.236 |
| 1060.86 | 1112.24 | 1188.054 |
| 1211.568 | 1234.385 | 1320.032 |
| 1357.334 | 1488.024 | 1539.473 |
| 1648.272 | 1679.345 | 2244.399 |
| 3196.38 | 3205.343 | 3214.876 |
| 3222.268 | 3227.896 | 3483.02 |

***Vinyl (8)***

**Cartesian coordinates**

C 0.705695 -0.145126 0.000043

C -0.586139 0.030185 0.000008

H 1.596176 0.468312 -0.000193

H -1.031826 1.027826 0.000019

H -1.281689 -0.806492 -0.000133

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 714.0075 | 840.4995 | 933.957 |
| 1052.702 | 1393.892 | 1668.571 |
| 3080.482 | 3173.723 | 3244.261 |

***Ethynylamidogen (9)***

**Cartesian coordinates**

N 0.199650 -1.209956 0.000000

C -0.091959 1.273331 0.000000

C 0.000000 0.039543 0.000000

H -0.671255 -1.740382 0.000000

H -0.174542 2.332835 0.000000

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 391.4586 | 439.0174 | 482.5993 |
| 492.8083 | 1089.818 | 1234.455 |
| 1951.013 | 3473.279 | 3515.849 |

***Ethynyl (10)***

**Cartesian coordinates**

C 0.000000 0.000000 0.728771

C 0.000000 0.000000 -0.472490

H 0.000000 0.000000 -1.537681

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 479.621 | 479.621 | 2105.446 |
| 3467.291 |  |  |

***3-pyrrolyl (11)***

**Cartesian coordinates**

N -0.692252 0.807233 0.000165

C 0.672571 0.879890 0.000039

C 1.183526 -0.399846 -0.000164

C 0.053919 -1.241083 -0.000154

C -1.095874 -0.509447 0.000047

H -1.309487 1.599771 0.000317

H 1.180231 1.831633 0.000103

H 2.226314 -0.672027 -0.000303

H -2.136147 -0.787091 0.000116

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 472.9041 | 555.0542 | 644.482 |
| 669.2904 | 751.4329 | 848.2296 |
| 868.6323 | 893.6301 | 1044.395 |
| 1082.379 | 1169.544 | 1192.876 |
| 1247.526 | 1400.868 | 1465.722 |
| 1508.184 | 1558.444 | 3264.466 |
| 3282.734 | 3287.616 | 3710.187 |

***2-aminoethenyl (12)***

**Cartesian coordinates**

N -1.144817 -0.151780 -0.089763

C 1.278259 -0.300036 0.025044

C 0.146671 0.368942 -0.005115

H -1.840419 0.387918 0.401533

H -1.205423 -1.133662 0.135339

H 2.329501 -0.067096 0.000136

H 0.180477 1.461862 -0.028242

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 350.9439 | 473.396 | 546.6063 |
| 672.718 | 801.6183 | 830.63 |
| 1098.624 | 1232.48 | 1318.862 |
| 1652.527 | 1716.459 | 3088.343 |
| 3292.939 | 3590.155 | 3695.205 |

***Amino (13)***

**Cartesian coordinates**

N 0.000000 0.000000 0.143152

H 0.000000 0.801064 -0.501032

H 0.000000 -0.801064 -0.501032

**Vibrational frequencies**

1529.3416 3392.5823 3484.1199

***Phenyl (14)***

**Cartesian coordinates**

C 0.000000 1.318531 0.000008

C 1.208548 0.629476 0.000001

C 1.221224 -0.768106 0.000011

C 0.000000 -1.393561 0.000033

C -1.221224 -0.768106 0.000011

C -1.208548 0.629476 0.000001

H 0.000000 2.402524 0.000151

H 2.146711 1.174245 -0.000154

H 2.155250 -1.318632 -0.000115

H -2.155250 -1.318632 -0.000115

H -2.146711 1.174245 -0.000154

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 402.9057 | 428.6025 | 603.4573 |
| 623.5396 | 680.8597 | 726.6003 |
| 828.7893 | 903.511 | 984.5328 |
| 992.4926 | 1008.27 | 1030.581 |
| 1058.743 | 1083.794 | 1180.029 |
| 1186.905 | 1310.543 | 1328.027 |
| 1471.488 | 1486.828 | 1608.889 |
| 1662.023 | 3187.815 | 3193.394 |
| 3204.981 | 3208.334 | 3220.585 |

***Aminoethynyl (15)***

**Cartesian coordinates**

N -0.004320 -1.059142 0.000000

C 0.006831 1.520722 0.000000

C 0.000000 0.242827 0.000000

H -0.005374 -1.583651 0.862850

H -0.005374 -1.583651 -0.862850

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 285.9247 | 322.3054 | 514.9335 |
| 1129.881 | 1152.854 | 1646.472 |
| 2057.592 | 3567.927 | 3674.262 |

***2-pyrrolyl (16)***

**Cartesian coordinates**

N -1.064904 -0.445145 0.000032

C -0.687321 0.882032 0.000087

C 0.681667 0.925787 0.000017

C 1.177639 -0.417923 -0.000085

C 0.060537 -1.197019 -0.000073

H -2.006708 -0.792243 0.000052

H -1.423562 1.669346 0.000166

H 1.284010 1.821557 0.000037

H 2.205452 -0.739903 -0.000158

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 373.8766 | 503.5496 | 627.709 |
| 709.4518 | 761.0483 | 860.9699 |
| 879.454 | 893.6414 | 1027.084 |
| 1071.113 | 1126.558 | 1190.207 |
| 1259.544 | 1387.159 | 1438.875 |
| 1487.524 | 1580.363 | 3248.38 |
| 3281.974 | 3288.353 | 3721.472 |

***Phenylethynyl (17)***

**Cartesian coordinates**

C 0.045775 1.219540 0.013382

C 1.426126 1.212650 -0.006714

C 2.115813 -0.000010 -0.017253

C 1.426105 -1.212662 -0.006715

C 0.045755 -1.219531 0.013384

C -0.671544 0.000009 0.023596

C -2.068345 0.000016 0.040729

C -3.340546 -0.000008 -0.055969

H -0.510694 2.148691 0.019942

H 1.973361 2.147570 -0.015716

H 3.199878 -0.000024 -0.035097

H 1.973339 -2.147581 -0.015717

H -0.510719 -2.148680 0.019947

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 109.121 | 143.9347 | 246.8164 |
| 390.712 | 476.4153 | 484.9854 |
| 507.448 | 629.6306 | 687.8436 |
| 783.453 | 788.1472 | 862.7349 |
| 967.323 | 1013.887 | 1014 |
| 1029.06 | 1049.789 | 1112.732 |
| 1182.9 | 1188.033 | 1227.958 |
| 1322.98 | 1353.082 | 1478.244 |
| 1508.72 | 1612.226 | 1638.882 |
| 1988.97 | 3202.807 | 3213.566 |
| 3220.99 | 3230.08 | 3233.759 |

***2-ethynylphenyl (18)***

**Cartesian coordinates**

C 2.042478 -0.071590 -0.000012

C 3.242552 -0.077665 -0.000138

C 0.611950 -0.044191 0.000122

C -0.098674 1.168226 0.000066

C -1.486709 1.169338 0.000005

C -2.200959 -0.024898 -0.000080

C -1.522494 -1.246478 -0.000058

C -0.154485 -1.193515 0.000242

H 4.305832 -0.089762 -0.000159

H 0.455537 2.100040 0.000016

H -2.017623 2.113934 -0.000091

H -3.285416 -0.011930 -0.000228

H -2.060287 -2.187652 -0.000411

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 134.285 | 152.1005 | 362.984 |
| 419.6871 | 467.5995 | 524.2418 |
| 553.1206 | 635.1337 | 668.6079 |
| 707.7231 | 707.8756 | 755.1998 |
| 776.0236 | 870.1455 | 964.1584 |
| 997.0964 | 1005.034 | 1053.838 |
| 1131.872 | 1181.193 | 1230.858 |
| 1261.052 | 1322.018 | 1453.837 |
| 1491.351 | 1600.44 | 1667.172 |
| 2248.818 | 3195.473 | 3205.052 |
| 3212.683 | 3225.013 | 3483.441 |

**Intermediates**

***i1***

**Cartesian coordinates**

C 1.702481 -0.867979 -0.015081

C 1.341575 0.413456 0.034922

N -2.086606 -0.521561 -0.104387

C -0.025430 0.941968 -0.017985

C -1.104734 0.191484 -0.006517

H 0.974166 -1.667444 -0.112524

H 2.746098 -1.152002 0.036125

H 2.113003 1.173077 0.121069

H -2.532200 -0.790271 0.771394

H -0.178176 2.013995 -0.057385

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 63.6979 | 147.0411 | 421.9808 |
| 439.4693 | 537.8321 | 681.3255 |
| 715.5785 | 874.8834 | 924.676 |
| 942.9165 | 1011.969 | 1032.406 |
| 1067.822 | 1168.965 | 1351.021 |
| 1443.706 | 1457.27 | 1709.998 |
| 2138.447 | 3153.326 | 3177.39 |
| 3210.213 | 3249.516 | 3521.053 |

***i2***

**Cartesian coordinates**

C 0.662715 0.957050 0.000027

C -0.823468 0.848144 0.000030

N 1.030155 -0.456284 -0.000205

C -1.158629 -0.448515 -0.000031

C 0.042245 -1.335599 0.000168

H 1.050965 1.468114 0.887922

H 1.051069 1.468797 -0.887445

H -1.479017 1.709393 0.000011

H 1.996806 -0.740865 0.000094

H -2.168079 -0.837934 -0.000313

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 370.0682 | 459.2703 | 718.4605 |
| 745.2103 | 830.9494 | 862.4973 |
| 962.8502 | 970.0482 | 999.4173 |
| 1004.056 | 1018.624 | 1122.484 |
| 1167.717 | 1293.468 | 1333.188 |
| 1364.673 | 1463.279 | 1512.648 |
| 1622.933 | 3058.503 | 3101.29 |
| 3221.651 | 3246.753 | 3659.528 |

***i3***

**Cartesian coordinates**

N 0.981586 -0.581262 0.000037

C -1.224799 -0.206955 -0.000070

C -0.416202 -1.299351 -0.000057

H 1.480681 -0.924752 -0.819355

H 1.480595 -0.924794 0.819463

H -2.304336 -0.283406 -0.000129

C -0.521760 1.072569 0.000001

C 0.798616 0.869018 0.000065

H -0.986145 2.050514 0.000002

H 1.642980 1.539583 0.000126

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 330.7959 | 535.3667 | 637.9702 |
| 656.3801 | 755.4084 | 800.1407 |
| 855.6273 | 890.7059 | 960.0267 |
| 975.9631 | 1025.965 | 1124.811 |
| 1139.489 | 1147.325 | 1212.343 |
| 1352.889 | 1512.226 | 1601.184 |
| 1667.79 | 3225.079 | 3238.813 |
| 3277.805 | 3504.244 | 3568.934 |

***i4***

**Cartesian coordinates**

C 2.559979 -0.242879 -0.076285

C 1.405147 0.080807 0.009449

N -2.293483 -0.129583 -0.074159

C 0.052948 0.511012 0.100650

C -0.987152 -0.324886 0.127434

H 3.577856 -0.539604 -0.150231

H -2.963309 -0.775874 0.305709

H -2.624525 0.493076 -0.796746

H -0.121185 1.585159 0.192897

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 161.6514 | 194.0814 | 232.0806 |
| 370.3277 | 437.3246 | 537.5451 |
| 558.2615 | 630.5023 | 698.8906 |
| 782.1758 | 981.1996 | 1115.421 |
| 1221.662 | 1316.657 | 1642.967 |
| 1712.933 | 2234.083 | 3099.703 |
| 3487.543 | 3580.925 | 3715.84 |

***i5***

**Cartesian coordinates**

C 2.121698 -0.569416 -0.037771

C 1.168685 0.165547 0.001355

N -1.708311 -0.721229 0.046235

C 0.017573 1.003687 0.047618

C -1.216521 0.504591 -0.097858

H 2.972736 -1.205089 -0.076962

H -2.503032 -1.022712 -0.489932

H -1.219648 -1.420759 0.590467

H 0.159513 2.070712 0.172718

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 130.6581 | 277.4076 | 327.9636 |
| 357.5233 | 484.8107 | 523.0174 |
| 629.7223 | 656.892 | 697.0277 |
| 802.4514 | 971.7997 | 1102.076 |
| 1158.694 | 1373.948 | 1627.297 |
| 1683.072 | 2212.267 | 3197.75 |
| 3484.952 | 3551.612 | 3717.04 |

***i6***

**Cartesian coordinates**

C -1.000004 -0.694878 -0.000003

C 0.235091 -1.194960 -0.000024

N -0.801507 0.751396 0.000021

C 1.278947 -0.196122 -0.000016

C 0.754860 1.058220 0.000012

H -1.982291 -1.137137 -0.000001

H -1.180080 1.220537 -0.821515

H -1.180064 1.220507 0.821582

H 2.339629 -0.397239 -0.000030

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 336.9159 | 544.7477 | 623.3001 |
| 623.9609 | 730.3596 | 750.3533 |
| 829.2177 | 871.1613 | 998.2957 |
| 1055.348 | 1127.105 | 1145.846 |
| 1208.521 | 1258.856 | 1470.75 |
| 1593.095 | 1635.209 | 3256.964 |
| 3286.256 | 3498.561 | 3566.207 |

***i7***

**Cartesian coordinates**

C 2.153677 -0.487420 0.004119

C 1.175503 0.215633 0.001365

N -1.492258 -0.901978 -0.064778

C -0.007178 1.001179 0.005455

C -1.231547 0.437871 0.003121

H 3.031613 -1.086560 0.000128

H -2.383974 -1.227642 0.262551

H -0.716645 -1.527855 0.090365

H 0.082932 2.079006 0.003608

H -2.110845 1.073312 0.012427

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 146.3628 | 270.1539 | 375.2718 |
| 411.8161 | 488.5052 | 610.0686 |
| 620.9127 | 700.7592 | 710.3976 |
| 713.5904 | 969.4399 | 982.9693 |
| 1106.086 | 1189.001 | 1324.905 |
| 1435.746 | 1646.407 | 1722.18 |
| 2217.951 | 3194.827 | 3227.536 |
| 3485.095 | 3612.571 | 3742.589 |

***i8***

**Cartesian coordinates**

C -2.161289 -0.443208 0.000037

C -1.057800 0.237245 -0.000028

N 1.579162 -0.942865 -0.000056

C 0.055937 0.925024 -0.000064

C 1.398604 0.312671 0.000071

H -2.632122 -0.742860 -0.930434

H -2.632191 -0.742541 0.930578

H 2.575545 -1.154319 0.000072

H 0.000805 2.010185 -0.000200

H 2.221120 1.039202 0.000275

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 92.8515 | 152.3929 | 346.5927 |
| 418.7581 | 513.3616 | 737.2766 |
| 823.7469 | 876.7872 | 905.7569 |
| 934.7155 | 1008.648 | 1129.31 |
| 1136.04 | 1234.728 | 1379.417 |
| 1446.132 | 1484.785 | 1728.347 |
| 2071.558 | 3047.194 | 3153.56 |
| 3177.191 | 3237.308 | 3517.28 |

***i9***

**Cartesian coordinates**

C 1.058120 -0.536281 -0.000009

C -0.202154 -1.337469 0.000002

N 0.676415 0.888294 -0.000017

C -1.198002 -0.353166 0.000003

C -0.644890 0.934387 0.000008

H 1.661663 -0.760472 -0.885740

H 1.661455 -0.760458 0.885867

H 1.283299 1.690807 0.000022

H -2.266926 -0.526782 -0.000077

H -1.152847 1.894018 0.000032

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 273.6518 | 430.0321 | 562.3233 |
| 769.4489 | 797.6613 | 872.1557 |
| 878.0469 | 906.906 | 960.5088 |
| 1005.386 | 1092.311 | 1169.588 |
| 1181.116 | 1201.728 | 1250.214 |
| 1363.847 | 1403.935 | 1483.161 |
| 1589.304 | 3067.538 | 3115.818 |
| 3202.725 | 3221.038 | 3682.945 |

***i9b***

**Cartesian coordinates**

C 1.214768 0.130564 0.000000

C 0.815542 -1.135213 0.000000

N 0.000000 1.137397 0.000000

C -0.672598 -1.027359 0.000000

C -1.142155 0.224765 0.000000

H 2.162591 0.651022 0.000000

H 0.009545 1.735146 0.826695

H 0.009545 1.735146 -0.826695

H -1.338265 -1.884310 0.000000

H -2.136759 0.644666 0.000000

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 357.3871 | 468.6032 | 497.1051 |
| 656.7494 | 661.3871 | 786.0959 |
| 821.4932 | 839.3158 | 988.9299 |
| 990.9668 | 997.1436 | 1124.302 |
| 1141.557 | 1158.491 | 1264.295 |
| 1339.27 | 1540.769 | 1593.048 |
| 1619.971 | 3197.384 | 3245.841 |
| 3267.96 | 3465.386 | 3542.68 |

***i10***

**Cartesian coordinates**

C -0.204135 1.238204 -0.258137

C -1.002593 -0.026154 -0.423847

C -0.162597 -1.257128 -0.249682

C 1.161407 -1.206038 0.050654

C 1.834400 0.029421 0.209873

C 1.119036 1.239974 0.055642

N -2.172470 -0.113028 0.473779

H -0.741130 2.175145 -0.376641

H -1.423004 -0.045043 -1.442669

H -0.679184 -2.205464 -0.346507

H 1.715433 -2.130030 0.179846

H 2.888987 0.047623 0.455828

H 1.638176 2.183050 0.192794

H -1.855470 0.002988 1.431282

H -2.809621 0.653256 0.282596

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 93.3238 | 275.2226 | 318.0654 |
| 398.3086 | 445.2934 | 537.9635 |
| 588.0224 | 619.0193 | 703.7917 |
| 758.5601 | 810.0234 | 843.8518 |
| 888.1413 | 979.5542 | 988.6002 |
| 990.9675 | 998.5382 | 1038.878 |
| 1100.313 | 1117.52 | 1171.444 |
| 1179.106 | 1207.28 | 1311.867 |
| 1352.254 | 1380.198 | 1421.448 |
| 1465.64 | 1561.572 | 1623.598 |
| 1659.817 | 2969.87 | 3174.079 |
| 3188.069 | 3195.559 | 3208.563 |
| 3219.713 | 3515.198 | 3602.172 |

***i11***

**Cartesian coordinates**

C 1.412090 0.000011 -0.012756

C 2.616470 0.000007 -0.007844

C -0.016190 0.000006 -0.006271

C -0.729351 1.205180 -0.002952

C -2.116341 1.200677 0.004510

C -2.816648 -0.000008 0.008553

C -2.116329 -1.200686 0.004515

C -0.729339 -1.205175 -0.002944

N 3.963095 0.000004 -0.067892

H -0.185442 2.142465 -0.007218

H -2.653231 2.142766 0.006715

H -3.900591 -0.000013 0.014310

H -2.653210 -2.142780 0.006724

H -0.185422 -2.142455 -0.007202

H 4.405037 0.839094 0.276623

H 4.405021 -0.839176 0.276426

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 87.4094 | 88.0317 | 94.2774 |
| 275.3092 | 323.1305 | 408.513 |
| 413.6261 | 452.8027 | 535.4198 |
| 556.7081 | 579.0886 | 641.4173 |
| 712.0649 | 730.2958 | 774.7131 |
| 862.1199 | 932.6997 | 994.8059 |
| 1011.201 | 1020.443 | 1052.674 |
| 1085.314 | 1111.119 | 1185.794 |
| 1204.868 | 1213.322 | 1314.29 |
| 1357.79 | 1368.199 | 1486.655 |
| 1547.232 | 1643.714 | 1651.128 |
| 1680.626 | 2386.575 | 3192.117 |
| 3199.76 | 3211.281 | 3217.34 |
| 3224.523 | 3588.101 | 3681.32 |

***i12***

**Cartesian coordinates**

C -2.578877 -0.528340 -0.029517

C -2.309317 0.833713 -0.045685

C -0.997894 1.288693 -0.016340

C 0.070436 0.389705 0.030121

C -0.212291 -0.980379 0.050262

C -1.522444 -1.431944 0.019236

N 3.513930 -0.548958 0.049418

C 1.446110 0.907191 0.061598

C 2.522980 0.158876 -0.002369

H -3.602116 -0.884897 -0.052673

H -3.123005 1.549495 -0.080964

H -0.797532 2.355091 -0.030204

H 0.601031 -1.697548 0.097754

H -1.720442 -2.497903 0.037887

H 3.932324 -0.785239 -0.849149

H 1.600019 1.978613 0.127586

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 46.8709 | 115.5217 | 210.6329 |
| 342.2463 | 413.8508 | 428.5258 |
| 462.8184 | 477.6024 | 626.1019 |
| 636.9626 | 671.1904 | 712.6174 |
| 783.7837 | 845.6799 | 856.5009 |
| 883.0504 | 929.6544 | 992.8844 |
| 1012.787 | 1021.628 | 1024.829 |
| 1063.569 | 1113.199 | 1148.345 |
| 1186.573 | 1217.02 | 1224.519 |
| 1325.892 | 1364.962 | 1435.069 |
| 1504.812 | 1550.634 | 1654.347 |
| 1682.057 | 2142.686 | 3186.079 |
| 3188.941 | 3199.218 | 3200.688 |
| 3208.896 | 3221.058 | 3517.56 |

***i13***

**Cartesian coordinates**

C 1.981491 -0.811687 -0.264584

C 2.120490 0.625256 -0.031669

C 1.046262 1.408462 0.185320

C -0.262699 0.789593 0.172718

C -0.350236 -0.675660 0.448103

C 0.811138 -1.442753 -0.106095

N -1.725275 -0.945175 0.021674

C -1.477525 1.223143 -0.223377

C -2.459773 0.114837 -0.289046

H 2.857949 -1.365400 -0.582199

H 3.109163 1.064230 -0.103977

H 1.137225 2.486110 0.255744

H -0.336606 -0.829701 1.541791

H 0.714588 -2.511191 -0.265064

H -2.136906 -1.856854 0.147444

H -1.723384 2.241877 -0.493672

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 164.4852 | 185.889 | 338.6885 |
| 394.4453 | 491.4295 | 519.2063 |
| 534.83 | 591.9683 | 697.4991 |
| 706.3675 | 726.2358 | 795.2073 |
| 864.5025 | 883.076 | 897.2849 |
| 916.4682 | 979.2635 | 1001.54 |
| 1012.32 | 1020.359 | 1072.097 |
| 1114.978 | 1157.777 | 1186.444 |
| 1206.288 | 1239.107 | 1280.902 |
| 1331.053 | 1377.854 | 1408.158 |
| 1449.545 | 1490.955 | 1623.374 |
| 1636.101 | 1717.048 | 2978.278 |
| 3188.557 | 3197.957 | 3210.649 |
| 3218.951 | 3227.46 | 3650.88 |

***i14***

**Cartesian coordinates**

C 2.140830 -0.700417 -0.000006

C 0.934008 -1.398310 0.000001

C -0.221394 -0.647991 0.000003

C -0.255182 0.742622 -0.000002

C 0.959675 1.425103 -0.000009

C 2.143343 0.693558 -0.000011

H 3.077845 -1.243778 -0.000008

H 0.913814 -2.482750 0.000005

H 0.982534 2.508677 -0.000013

H 3.092258 1.218410 -0.000016

N -1.609202 -1.096020 0.000011

C -1.653598 1.169971 0.000002

C -2.573028 0.174424 0.000008

H -1.852932 -1.647666 0.820137

H -1.852938 -1.647680 -0.820104

H -1.944094 2.213164 -0.000002

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 184.4761 | 218.8045 | 377.4195 |
| 379.287 | 424.6881 | 538.553 |
| 570.6976 | 597.7453 | 636.6408 |
| 734.9038 | 743.3243 | 754.3159 |
| 790.6197 | 857.1382 | 873.8052 |
| 894.5343 | 904.4661 | 954.1488 |
| 1006.68 | 1048.148 | 1122.409 |
| 1155.53 | 1168.426 | 1172.291 |
| 1186.39 | 1207.929 | 1262.735 |
| 1309.853 | 1365.674 | 1494.791 |
| 1515.029 | 1566.858 | 1614.321 |
| 1661.725 | 1689.032 | 3196.687 |
| 3203.041 | 3215.458 | 3216.259 |
| 3226.113 | 3507.335 | 3572.813 |

***i15***

**Cartesian coordinates**

C -2.525514 0.552967 0.000086

C -2.266599 -0.812566 0.000151

C -0.962457 -1.283030 0.000049

C 0.104725 -0.383220 -0.000102

C -0.148038 0.987615 -0.000149

C -1.459051 1.443338 -0.000070

C 3.500276 0.563095 0.000371

N 1.414140 -0.882842 -0.000082

C 2.516774 -0.126160 -0.000281

H -3.545320 0.918358 0.000157

H -3.085695 -1.522830 0.000281

H -0.769233 -2.351348 0.000141

H 0.680113 1.686078 -0.000277

H -1.644778 2.511564 -0.000141

H 4.372978 1.167999 0.000558

H 1.532265 -1.882167 -0.000473

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 62.3602 | 133.1268 | 220.5619 |
| 262.9631 | 350.7191 | 419.4927 |
| 453.8979 | 466.7019 | 511.9297 |
| 531.5486 | 634.3429 | 656.5879 |
| 709.1232 | 739.1392 | 768.0778 |
| 836.6225 | 846.0732 | 908.5133 |
| 986.6969 | 1004.566 | 1017.847 |
| 1061.479 | 1108.759 | 1145.111 |
| 1186.222 | 1215.382 | 1292.394 |
| 1342.579 | 1365.035 | 1470.021 |
| 1539.165 | 1557.197 | 1669.768 |
| 1684.77 | 2272.529 | 3184.106 |
| 3197.687 | 3208.328 | 3220.846 |
| 3227.262 | 3495.969 | 3665.543 |

***i16***

**Cartesian coordinates**

C -2.091734 0.724387 -0.154058

C -2.086774 -0.711475 -0.038423

C -0.936459 -1.425016 0.107410

C 0.281677 -0.698648 0.117349

C 0.318620 0.762072 0.250874

C -0.953222 1.443235 -0.054322

C 1.769861 1.079491 -0.066269

N 1.524046 -1.089011 -0.094944

C 2.518824 -0.059184 -0.176462

H -3.038097 1.224310 -0.323524

H -3.033083 -1.236543 -0.105834

H -0.938659 -2.508764 0.120660

H 0.444420 0.907185 1.353945

H -0.965376 2.525615 -0.112076

H 2.164244 2.082194 0.029741

H 1.773468 -2.060093 -0.214898

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 173.09 | 202.6425 | 352.7139 |
| 405.4604 | 531.2087 | 534.9688 |
| 554.4575 | 596.5501 | 642.1932 |
| 713.6317 | 723.9636 | 790.4399 |
| 803.7371 | 823.8555 | 875.7259 |
| 882.7324 | 927.5244 | 982.0401 |
| 990.6691 | 1005.533 | 1013.863 |
| 1056.288 | 1116.433 | 1175.801 |
| 1190.909 | 1208 | 1243.52 |
| 1331.128 | 1397.299 | 1425.684 |
| 1456.708 | 1476.078 | 1550.795 |
| 1604.791 | 1693.195 | 2870.886 |
| 3196.514 | 3205.212 | 3217.368 |
| 3224.24 | 3232.975 | 3640.027 |

***i17***

**Cartesian coordinates**

C 2.143259 0.695873 -0.000003

C 2.135815 -0.696220 0.000006

C 0.936633 -1.406097 0.000000

C -0.230752 -0.665879 -0.000007

C -0.247821 0.723347 0.000001

C 0.949252 1.417094 -0.000003

C -1.697470 1.131981 0.000002

N -1.586690 -1.096206 -0.000008

C -2.515267 -0.151164 0.000031

H 3.089810 1.223901 0.000008

H 3.075439 -1.236536 0.000022

H 0.926451 -2.490201 0.000012

H -1.981011 1.728762 -0.874095

H 0.963828 2.501583 -0.000004

H -1.981017 1.728964 0.873983

H -1.828560 -2.076645 -0.000030

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 193.439 | 207.868 | 353.6283 |
| 388.0755 | 425.6009 | 542.3043 |
| 578.9726 | 623.6437 | 705.5948 |
| 760.0154 | 764.2434 | 782.2174 |
| 868.0982 | 870.221 | 900.3262 |
| 906.2973 | 937.0438 | 961.6194 |
| 1005.025 | 1048.633 | 1132.008 |
| 1145.323 | 1184.198 | 1201.567 |
| 1227.302 | 1248.253 | 1316.7 |
| 1334.187 | 1372.421 | 1409.725 |
| 1461.749 | 1508.652 | 1539.49 |
| 1675.933 | 1692.598 | 3059.329 |
| 3095.375 | 3195.606 | 3202.917 |
| 3212.7 | 3224.069 | 3631.61 |

***i18***

**Cartesian coordinates**

C -1.990446 1.225387 0.089274

C -2.980573 0.277457 0.071146

C -2.372534 -1.003866 -0.120307

C -1.036290 -0.743615 -0.209276

N -0.785976 0.579871 -0.083240

H -2.037396 2.295723 0.209355

H -4.037643 0.466202 0.182979

H -2.862544 -1.961125 -0.183774

H 0.125947 1.008313 -0.115248

C 2.707701 1.703854 0.084046

C 2.564114 0.523834 -0.098799

C 2.370032 -0.869018 -0.341736

C 1.707326 -1.669713 0.494712

H 2.860098 2.742683 0.254888

H 2.774321 -1.256430 -1.271685

H 1.565538 -2.718187 0.263835

H 1.297531 -1.302193 1.427971

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 38.5702 | 47.0104 | 62.1243 |
| 76.1559 | 96.7392 | 148.2271 |
| 234.0167 | 349.9845 | 459.4281 |
| 554.0833 | 571.0984 | 633.6425 |
| 702.6567 | 717.1909 | 720.09 |
| 733.2061 | 769.4812 | 863.6231 |
| 880.8245 | 895.8899 | 897.6606 |
| 1003.662 | 1023.171 | 1038.637 |
| 1082.618 | 1118.135 | 1131.806 |
| 1194.334 | 1277.055 | 1326.582 |
| 1394.526 | 1447.519 | 1451.354 |
| 1488.563 | 1580.758 | 1691.397 |
| 2231.933 | 3170.964 | 3184.37 |
| 3252.314 | 3269.799 | 3278.676 |
| 3285.037 | 3479.18 | 3653.751 |

***i19***

**Cartesian coordinates**

C 2.125431 1.263015 0.055215

C 2.856330 0.107872 0.153634

C 1.951170 -0.978018 0.001234

C 0.697926 -0.451201 -0.190936

N 0.818751 0.913427 -0.155818

H 2.422965 2.297098 0.120879

H 3.920708 0.045391 0.318010

H 2.188689 -2.030867 0.024815

H 0.047985 1.554257 -0.236049

C -3.713060 0.774728 -0.140773

C -2.754174 0.105814 0.204025

C -1.663774 -0.644891 0.569409

C -0.629596 -1.113655 -0.414955

H -4.562391 1.342987 -0.434562

H -1.502660 -0.856710 1.621386

H -0.481854 -2.193464 -0.310703

H -0.986219 -0.934671 -1.434165

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 19.8364 | 50.6303 | 161.2995 |
| 191.1323 | 308.0973 | 362.0236 |
| 401.7322 | 490.2271 | 514.5583 |
| 542.2933 | 625.2343 | 638.5207 |
| 665.2371 | 680.2963 | 729.6567 |
| 746.6146 | 807.8142 | 877.96 |
| 894.1547 | 905.8724 | 984.1814 |
| 1029.022 | 1053.082 | 1123.709 |
| 1144.61 | 1148.676 | 1203.079 |
| 1264.436 | 1298.889 | 1318.516 |
| 1415.602 | 1462.907 | 1475.722 |
| 1498.896 | 1524.119 | 1638.795 |
| 2026.27 | 3051.356 | 3097.702 |
| 3190.96 | 3251.199 | 3265.052 |
| 3285.183 | 3472.997 | 3696.943 |

***i20***

**Cartesian coordinates**

C -1.968316 -1.205846 0.003013

C -2.737687 -0.106208 0.311747

C -1.866881 0.991874 0.168456

C -0.620578 0.588460 -0.218840

N -0.708905 -0.784659 -0.320992

C 2.781881 -1.432886 0.017231

C 2.347735 -0.331685 0.217072

C 1.808711 1.010593 0.429285

C 0.629909 1.350903 -0.506943

H -2.224587 -2.253607 -0.009189

H -3.777517 -0.109554 0.594915

H 1.485699 1.108632 1.469879

H 0.075223 -1.384766 -0.519863

H 3.192197 -2.400760 -0.143939

H 2.615209 1.733333 0.271679

H 0.400817 2.412618 -0.398769

H 0.946655 1.195491 -1.543897

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 43.273 | 99.7961 | 132.3979 |
| 194.1259 | 312.3045 | 364.163 |
| 365.2601 | 506.9607 | 549.4173 |
| 609.2557 | 638.1629 | 674.3734 |
| 693.9304 | 709.0446 | 718.9438 |
| 836.8256 | 844.9505 | 889.6745 |
| 915.913 | 974.9392 | 1010.652 |
| 1045.049 | 1096.364 | 1147.258 |
| 1190.512 | 1216.159 | 1248.764 |
| 1299.891 | 1356.952 | 1371.264 |
| 1422.02 | 1464.507 | 1474.334 |
| 1490.682 | 1510.021 | 1617.175 |
| 2243.917 | 3058.285 | 3062.317 |
| 3108.48 | 3128.514 | 3259.557 |
| 3279.564 | 3482.83 | 3675.012 |

***i21***

**Cartesian coordinates**

C -1.720469 1.080805 0.054947

C -2.401158 -0.109528 0.090635

N -1.482457 -1.128647 0.017521

C -0.224251 -0.606632 -0.053497

C -0.336157 0.765226 -0.039508

C 0.881753 1.586580 -0.138135

C 2.028267 0.945633 -0.005328

C 2.235413 -0.496801 0.299338

C 1.061135 -1.344184 -0.257571

H -2.163974 2.063471 0.102316

H -3.455541 -0.315464 0.178040

H -1.705305 -2.107936 0.026087

H 0.812474 2.655100 -0.314702

H 3.179345 -0.866849 -0.108622

H 2.289600 -0.614264 1.389716

H 1.216579 -1.516478 -1.330843

H 1.056819 -2.323640 0.230080

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 132.7684 | 221.7734 | 255.2135 |
| 379.7357 | 391.0401 | 463.0701 |
| 495.192 | 581.6789 | 638.1408 |
| 664.7575 | 705.9731 | 725.0007 |
| 762.0697 | 838.2333 | 866.2207 |
| 877.1145 | 920.3071 | 932.5229 |
| 993.004 | 1027.167 | 1091.025 |
| 1115.351 | 1186.827 | 1190.551 |
| 1204.803 | 1220.894 | 1292.087 |
| 1327.902 | 1343.367 | 1391.017 |
| 1458.069 | 1471.704 | 1492.509 |
| 1522.446 | 1543.145 | 1627.518 |
| 1705.364 | 3021.31 | 3028.69 |
| 3089.621 | 3096.947 | 3188.456 |
| 3260.12 | 3285.908 | 3713.41 |

***i22***

**Cartesian coordinates**

N -1.563830 -1.066109 -0.000068

C -2.419313 0.013757 -0.000120

C -1.670642 1.156016 0.000001

C -0.294561 0.760007 0.000130

C -0.273145 -0.626730 0.000067

C 0.929103 1.491879 0.000122

C 2.135366 0.767296 -0.000118

C 0.953918 -1.469138 0.000202

C 2.182423 -0.601008 -0.000177

H -1.850219 -2.028772 -0.000219

H -3.488051 -0.127624 -0.000247

H -2.053953 2.164591 0.000002

H 0.968476 -2.140370 -0.874156

H 0.930266 2.574523 0.000216

H 3.072018 1.315659 -0.000333

H 0.968627 -2.139729 0.875081

H 3.140764 -1.107987 -0.000510

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 133.1089 | 220.7678 | 274.7435 |
| 385.3056 | 467.6087 | 503.3496 |
| 503.3654 | 598.5214 | 626.2908 |
| 653.5806 | 673.4051 | 724.912 |
| 744.8995 | 765.2524 | 869.8615 |
| 885.3511 | 924.5399 | 944.7 |
| 947.177 | 966.4468 | 1071.283 |
| 1096.256 | 1117.647 | 1183.611 |
| 1189.637 | 1200.757 | 1245.383 |
| 1279.093 | 1365.481 | 1382.633 |
| 1438.067 | 1461.318 | 1472.626 |
| 1497.247 | 1538.258 | 1588.521 |
| 1622.734 | 2960.179 | 2968.578 |
| 3177.374 | 3198.437 | 3216.113 |
| 3255.503 | 3279.941 | 3712.998 |

***i23***

**Cartesian coordinates**

C -1.867357 -0.594154 0.002918

C -3.063190 -0.721031 -0.010409

C -0.451870 -0.400594 0.008187

C 0.069853 0.910963 0.010340

C 1.460824 1.073843 0.000190

C 2.303284 -0.023531 -0.008688

C 1.789476 -1.318267 -0.005549

C 0.417631 -1.495685 0.002813

N -0.770758 2.002195 0.068961

H -4.117585 -0.858165 -0.013581

H 1.874792 2.076919 0.006812

H 3.376267 0.133435 -0.016850

H 2.452627 -2.174303 -0.010853

H -0.009926 -2.491488 0.001273

H -1.733759 1.835791 -0.178440

H -0.399020 2.873183 -0.269900

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 122.6125 | 152.2703 | 226.7346 |
| 364.2214 | 381.9108 | 387.1482 |
| 468.3434 | 484.4109 | 515.5498 |
| 564.2917 | 580.2357 | 602.0317 |
| 624.4936 | 739.6834 | 748.8255 |
| 757.968 | 767.3743 | 864.919 |
| 870.4828 | 960.882 | 992.759 |
| 1063.145 | 1090.991 | 1169.114 |
| 1192.624 | 1227.381 | 1301.158 |
| 1352.517 | 1355.569 | 1504.299 |
| 1544.799 | 1643.161 | 1665.261 |
| 1690.712 | 2229.787 | 3189.149 |
| 3203.12 | 3213.1 | 3226.639 |
| 3481.019 | 3614.922 | 3728.71 |

***i24***

**Cartesian coordinates**

C 1.834088 -0.369233 -0.000002

C 3.124777 -0.460306 0.000029

C 0.516632 -0.293798 -0.000019

C -0.172483 1.034562 -0.000008

C -1.639869 0.979229 0.000023

C -2.311753 -0.183084 0.000021

C -1.626795 -1.463114 -0.000008

C -0.286315 -1.515120 -0.000023

N 0.520161 2.109552 -0.000027

H 3.682952 -0.487523 -0.930930

H -2.169305 1.927128 0.000048

H -3.396738 -0.177735 0.000040

H -2.212796 -2.374272 -0.000008

H 0.240792 -2.462009 -0.000041

H 3.682904 -0.487545 0.931016

H -0.098623 2.920280 -0.000015

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 43.8786 | 140.3165 | 178.2156 |
| 324.5079 | 390.0804 | 445.0254 |
| 459.9607 | 478.4293 | 570.8295 |
| 591.6271 | 594.8652 | 697.4922 |
| 743.0804 | 774.1092 | 846.0584 |
| 867.246 | 884.9701 | 906.1996 |
| 992.8769 | 999.775 | 1003.485 |
| 1012.784 | 1089.677 | 1174.614 |
| 1208.47 | 1251.162 | 1264.024 |
| 1383.98 | 1413.639 | 1460.603 |
| 1482.829 | 1642.23 | 1673.172 |
| 1733.925 | 2051.401 | 3140.976 |
| 3184.853 | 3199.238 | 3209.671 |
| 3223.823 | 3223.988 | 3497.744 |

***i25***

**Cartesian coordinates**

C -2.180489 -0.665976 0.000018

C -2.097710 0.748347 0.000121

C -0.902994 1.429084 0.000036

C 0.275670 0.656671 -0.000143

C 0.226592 -0.773467 -0.000085

C -1.033501 -1.416856 -0.000077

C 2.401488 -0.152180 0.000170

N 1.557163 1.047981 -0.000344

C 1.516361 -1.355410 -0.000005

H -3.154838 -1.138755 0.000027

H -3.020900 1.319404 0.000269

H -0.874496 2.512486 0.000119

H -1.058256 -2.500712 -0.000131

H 3.052969 -0.175787 -0.881699

H 3.051419 -0.175852 0.883242

H 1.871457 2.002067 0.000375

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 132.6969 | 214.3821 | 269.8982 |
| 355.5716 | 412.3745 | 452.4197 |
| 547.8742 | 551.9225 | 609.3625 |
| 762.686 | 765.8848 | 771.1062 |
| 790.2553 | 859.3434 | 863.1028 |
| 900.1066 | 963.2748 | 996.0798 |
| 1012.231 | 1018.881 | 1031.265 |
| 1147.735 | 1165.207 | 1184.864 |
| 1205.017 | 1253.17 | 1312.803 |
| 1333.395 | 1380.334 | 1393.945 |
| 1446.898 | 1492.202 | 1559.738 |
| 1620.942 | 1697.277 | 3050.001 |
| 3091.219 | 3187.395 | 3209.842 |
| 3213.125 | 3229.457 | 3703.119 |

***i26***

**Cartesian coordinates**

N -0.916243 -1.294915 0.052375

C -2.019475 1.003332 0.040995

C -1.498209 -0.079740 0.027581

H 0.071024 -1.270833 0.275563

H -1.109326 -1.866475 -0.756947

H -2.514495 1.941780 0.085385

C 1.731222 0.669600 -0.124173

C 2.708635 0.004536 0.068429

H 0.844023 1.241797 -0.285803

H 3.589432 -0.568229 0.238190

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 56.9391 | 62.8232 | 91.4994 |
| 123.5705 | 153.4879 | 390.9734 |
| 466.8054 | 523.5801 | 648.4025 |
| 699.0631 | 708.0244 | 731.0722 |
| 798.2959 | 810.554 | 1101.568 |
| 1222.283 | 1652.222 | 2081.604 |
| 2271.017 | 3396.273 | 3492.82 |
| 3513.784 | 3561.441 | 3661.171 |

***i27***

**Cartesian coordinates**

N -0.911355 1.330572 0.000008

C -2.095497 -0.872550 -0.000034

C -1.482371 0.203794 -0.000007

H 0.107280 1.238048 0.000240

H -2.698178 -1.747995 -0.000079

C 2.614985 0.063079 -0.000071

C 1.733875 -0.747917 0.000067

H 3.406765 0.774452 -0.000123

H 0.937666 -1.456948 0.000174

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 55.5285 | 75.4991 | 84.7167 |
| 144.6458 | 265.2216 | 388.2124 |
| 463.2919 | 495.2643 | 499.1427 |
| 704.7186 | 722.0106 | 800.755 |
| 825.0053 | 1108.135 | 1236.741 |
| 1938.032 | 2083.525 | 3411.213 |
| 3469.247 | 3477.831 | 3520.947 |

***i28***

**Cartesian coordinates**

N -0.045064 0.504200 0.000092

C 2.397156 -0.194403 -0.000061

C 1.244695 0.143335 0.000005

H -0.266603 1.485947 -0.000015

H 3.417643 -0.488013 -0.000115

C -1.097694 -0.423692 0.000055

C -2.380862 -0.150938 -0.000083

H -0.749002 -1.453688 0.000169

H -3.066358 0.680546 -0.000181

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 51.7159 | 179.9626 | 357.6055 |
| 401.7932 | 456.7266 | 505.3531 |
| 576.322 | 610.1542 | 744.5962 |
| 776.6292 | 873.5463 | 1078.52 |
| 1224.365 | 1290.474 | 1470.289 |
| 1698.262 | 2275.091 | 3168.301 |
| 3293.376 | 3498.252 | 3666.819 |

***i29***

**Cartesian coordinates**

N -0.035331 0.868742 -0.000020

C 2.099148 -0.508358 0.000005

C 1.095066 0.149190 -0.000003

C -1.310148 0.296232 0.000004

C -1.584325 -0.987419 0.000001

H 0.037600 1.870661 0.000071

H 2.988889 -1.087838 0.000011

H -2.108976 1.038823 0.000017

H -2.468635 -1.600710 0.000002

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 128.0328 | 152.2298 | 229.3893 |
| 394.1578 | 474.1729 | 536.1078 |
| 609.1225 | 637.5218 | 739.0143 |
| 818.075 | 866.0022 | 977.8898 |
| 1222.97 | 1313.292 | 1516.498 |
| 1712.056 | 2276.253 | 3124.426 |
| 3300.311 | 3496.061 | 3691.56 |

***i30***

**Cartesian coordinates**

N -0.929914 -1.158547 0.000158

C -2.015209 1.177467 -0.000332

C -1.509994 0.004359 0.000053

C 2.488505 -0.129879 -0.000276

C 1.659742 0.735925 0.000347

H -1.463087 -2.015684 -0.000082

H 0.084155 -1.214772 0.000229

H 3.253682 -0.869964 -0.000847

H 0.896383 1.483019 0.000845

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 68.9301 | 78.5561 | 105.5091 |
| 185.9156 | 214.2595 | 314.7817 |
| 352.3513 | 556.6144 | 704.7189 |
| 722.4234 | 809.8845 | 836.6045 |
| 1136.927 | 1170.488 | 1631.624 |
| 2059.401 | 2075.022 | 3397.351 |
| 3508.371 | 3512.575 | 3655.456 |

***i31***

**Cartesian coordinates**

N -2.399706 0.163144 -0.075067

C 0.119557 -0.228970 -0.004799

C -1.071524 -0.046425 -0.007897

H -2.711465 1.062055 0.260262

H -2.973403 -0.597908 0.255539

C 2.452331 0.468990 0.004853

C 1.526392 -0.467135 0.007410

H 2.490816 1.549015 -0.006859

H 1.831459 -1.513926 0.019125

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 110.1905 | 148.9875 | 195.5874 |
| 340.5402 | 453.9977 | 523.5649 |
| 566.1844 | 686.8802 | 754.988 |
| 866.3746 | 925.2816 | 1203.049 |
| 1262.473 | 1306.883 | 1648.996 |
| 1658.695 | 2375.985 | 3120.289 |
| 3253.05 | 3592.267 | 3686.281 |

***i32***

**Cartesian coordinates**

N -0.795880 0.746296 0.000035

C 0.084390 -1.269168 -0.000019

C -1.149334 -0.794430 0.000027

C 0.664458 0.909764 -0.000009

C 1.184317 -0.324905 -0.000042

H -1.241383 1.152733 0.821466

H -1.241434 1.152753 -0.821360

H 1.108932 1.893036 -0.000011

H 2.242055 -0.550160 -0.000078

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 305.9141 | 493.7638 | 567.6765 |
| 655.9753 | 728.7904 | 766.2387 |
| 835.3373 | 949.4413 | 962.0774 |
| 1051.764 | 1112.919 | 1134.615 |
| 1148.675 | 1329.929 | 1497.944 |
| 1592.441 | 1626.281 | 3235.28 |
| 3267.561 | 3500.332 | 3569.381 |

***i33***

**Cartesian coordinates**

N 0.973493 1.215571 -0.188095

C 1.586593 -1.135691 -0.258317

C 1.690984 0.094336 0.205077

H 0.813068 1.888687 0.544619

H 0.130334 1.018285 -0.707990

H 2.139782 -2.054820 -0.158836

H 2.449687 0.300884 0.965521

C -2.786095 0.066991 -0.043326

C -1.788439 -0.554631 0.186740

H -3.679195 0.609474 -0.243876

H -0.886393 -1.097538 0.376183

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 51.7619 | 69.7204 | 83.2574 |
| 112.1023 | 162.9276 | 370.1169 |
| 481.7732 | 544.8754 | 682.591 |
| 702.5647 | 712.6341 | 804.8798 |
| 810.4602 | 826.7557 | 845.2793 |
| 1108.035 | 1244.757 | 1324.985 |
| 1658.651 | 1710.789 | 2076.3 |
| 3081.272 | 3288.021 | 3371.895 |
| 3506.651 | 3590.472 | 3696.563 |

***i34***

**Cartesian coordinates**

N 1.387963 -0.876445 -0.054250

C -0.026154 1.083482 -0.005140

C 1.176327 0.472545 -0.004978

C -1.522699 -0.917174 -0.015127

C -1.300954 0.384066 0.016752

H 0.589131 -1.472253 0.124535

H 2.275235 -1.226162 0.262319

H -0.046748 2.164948 -0.010144

H 2.080947 1.072583 -0.000822

H -2.385754 -1.566513 -0.024889

H -2.187673 1.025002 0.079711

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 188.2946 | 236.6384 | 326.9767 |
| 416.9851 | 433.8797 | 544.0562 |
| 622.937 | 700.8968 | 730.4724 |
| 845.4477 | 897.8074 | 966.6436 |
| 978.9733 | 1124.332 | 1189.417 |
| 1268.43 | 1330.946 | 1451.218 |
| 1624.896 | 1649.248 | 1725.072 |
| 3054.697 | 3184.633 | 3230.722 |
| 3255.274 | 3542.761 | 3720.814 |

***i35***

**Cartesian coordinates**

N -1.163437 -0.000126 0.030522

C 1.035098 0.699128 0.018541

C -0.265264 1.182285 -0.091244

C -0.264990 -1.182371 -0.091606

C 1.035200 -0.698920 0.018497

H -1.878114 -0.000141 -0.695583

H -1.664610 -0.000362 0.932738

H 1.911753 1.328753 0.051104

H -0.689015 2.141452 0.160311

H -0.688312 -2.141361 0.161483

H 1.912093 -1.328194 0.051168

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 268.6474 | 313.0924 | 427.4146 |
| 546.7707 | 720.4059 | 778.023 |
| 805.5896 | 846.4239 | 890.1828 |
| 968.874 | 969.6083 | 1079.563 |
| 1094.022 | 1130.867 | 1157.365 |
| 1218.089 | 1310.656 | 1421.464 |
| 1501.059 | 1512.711 | 1637.677 |
| 3190.258 | 3237.246 | 3251.926 |
| 3268.637 | 3275.291 | 3463.79 |

***i36***

**Cartesian coordinates**

C 1.500603 -0.948105 -0.082388

C 1.305667 0.366086 0.064054

H 0.690495 -1.635063 -0.299963

H 2.497783 -1.367595 -0.020411

H 2.179547 0.990225 0.240166

N -1.658420 -0.658578 0.064056

C 0.039500 1.103207 0.003739

C -1.178260 0.574256 -0.140731

H -2.541201 -0.928504 -0.334383

H -1.332539 -1.207160 0.849923

H 0.109796 2.185484 0.048225

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 111.2143 | 191.9516 | 287.8191 |
| 366.482 | 395.7531 | 468.4369 |
| 650.1394 | 705.7208 | 834.1038 |
| 926.695 | 927.9004 | 1036.211 |
| 1054.136 | 1135.067 | 1154.296 |
| 1334.966 | 1385.285 | 1445.422 |
| 1632.39 | 1660.784 | 1709.261 |
| 3153.076 | 3166.879 | 3182.027 |
| 3252.06 | 3550.773 | 3705.261 |

***i37***

**Cartesian coordinates**

C 0.908077 0.803360 0.000039

C -0.559346 1.084019 -0.000033

N 0.922456 -0.705042 -0.000035

C -1.268791 -0.111855 0.000004

C -0.548101 -1.306407 0.000040

H 1.438517 1.174015 -0.883879

H 1.438387 1.173903 0.884084

H -0.961295 2.087227 -0.000055

H 1.394527 -1.087484 -0.813838

H 1.394682 -1.087575 0.813633

H -2.353047 -0.139483 0.000004

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 59.0037 | 422.1573 | 515.2199 |
| 602.7373 | 733.4272 | 766.3 |
| 831.3209 | 918.3782 | 930.838 |
| 966.4717 | 993.2997 | 1073.57 |
| 1135.87 | 1143.544 | 1215.776 |
| 1283.824 | 1320.289 | 1387.994 |
| 1411.292 | 1505.147 | 1646.926 |
| 3036.761 | 3071.851 | 3206.901 |
| 3247.188 | 3532.362 | 3593.569 |

***i38***

**Cartesian coordinates**

N 1.430666 -0.912760 -0.000010

C 0.020300 1.037751 0.000001

C 1.291230 0.367370 0.000005

C -1.571931 -0.866074 0.000006

C -1.267782 0.462418 -0.000006

H -0.790887 -1.614177 0.000026

H 2.419747 -1.155425 -0.000001

H 0.070380 2.122436 0.000002

H 2.156516 1.042007 0.000026

H -2.608118 -1.185100 0.000001

H -2.093199 1.170792 -0.000020

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 160.4934 | 284.3844 | 322.0995 |
| 414.2569 | 565.6806 | 678.8743 |
| 766.2175 | 842.9517 | 923.5301 |
| 934.5526 | 1020.713 | 1070.6 |
| 1096.027 | 1172.817 | 1252.148 |
| 1284.388 | 1395.184 | 1431.384 |
| 1490.364 | 1559.825 | 1620.511 |
| 3046.476 | 3159.051 | 3171.149 |
| 3193.275 | 3288.793 | 3516.858 |

***i39***

**Cartesian coordinates**

C 1.148625 0.389149 0.020070

C -0.101958 1.220690 -0.008415

N 0.626535 -0.972778 -0.105018

C -1.194384 0.376722 0.014820

C -0.754264 -0.940911 0.013560

H 1.844409 0.621994 -0.798167

H 1.710629 0.517399 0.961670

H -0.107295 2.299911 -0.028284

H 1.138786 -1.725635 0.323439

H -2.232437 0.676805 0.012654

H -1.327951 -1.854932 0.023599

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 268.9579 | 459.5879 | 525.2713 |
| 561.3912 | 628.887 | 798.1764 |
| 851.3241 | 885.0427 | 945.3073 |
| 973.294 | 1000.594 | 1065.298 |
| 1119.178 | 1165.123 | 1183.645 |
| 1302.115 | 1335.832 | 1404.406 |
| 1467.587 | 1501.287 | 1526.71 |
| 2938.978 | 3003.014 | 3237.111 |
| 3256.089 | 3269.113 | 3665.591 |

***i40***

**Cartesian coordinates**

C 2.012464 1.044162 0.006503

C 2.327695 -0.311756 0.040360

C 1.348285 -1.319618 0.024470

C 0.056971 -0.853381 -0.019960

C -0.272412 0.502571 -0.028321

C 0.681676 1.490924 -0.032028

C -2.898164 0.658405 0.064757

N -1.300367 -1.293094 -0.141356

C -1.702808 0.099715 -0.028341

H 2.816250 1.770941 0.015980

H 3.372290 -0.601264 0.076119

H 1.612467 -2.369432 0.044929

H -2.992972 1.733114 0.144666

H 0.445635 2.548276 -0.046711

H -3.800505 0.059065 0.062239

H -1.672842 -1.955177 0.527624

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 127.8078 | 245.5763 | 260.3149 |
| 389.3408 | 457.0766 | 516.0753 |
| 530.4303 | 567.7945 | 644.1039 |
| 665.7486 | 741.7787 | 765.6528 |
| 784.1695 | 814.8924 | 846.9182 |
| 878.7476 | 885.7543 | 947.8219 |
| 950.3303 | 996.9736 | 1023.166 |
| 1070.751 | 1136.47 | 1174.929 |
| 1197.029 | 1251.942 | 1275.072 |
| 1331.091 | 1402.874 | 1436.954 |
| 1492.282 | 1510.362 | 1683.979 |
| 1696.59 | 1802.694 | 3172.851 |
| 3191.256 | 3206.129 | 3217.365 |
| 3223.752 | 3268.552 | 3590.598 |

***i41***

**Cartesian coordinates**

N 0.753058 0.921891 -0.416442

C 1.426237 -0.027184 -1.155968

C 2.429799 -0.536717 -0.374125

C 2.373105 0.105607 0.904945

C 1.314381 0.960005 0.813932

C -2.663771 1.484254 0.051239

C -2.436568 0.303585 0.014687

C -2.201779 -1.104173 -0.054115

C -1.118242 -1.703596 0.437476

H -0.135687 1.330731 -0.658082

H 1.121148 -0.263669 -2.162333

H 3.148889 -1.283146 -0.675868

H 3.034513 -0.037972 1.743073

H -2.878626 2.524465 0.109750

H -2.974816 -1.685559 -0.548302

H -0.999478 -2.776630 0.345518

H -0.326327 -1.152141 0.932916

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 24.235 | 53.9048 | 64.7416 |
| 100.5582 | 116.5974 | 151.9275 |
| 247.547 | 335.2023 | 458.3587 |
| 569.5039 | 608.7695 | 637.1357 |
| 675.3729 | 708.863 | 712.9731 |
| 718.5992 | 768.1419 | 863.0633 |
| 882.6733 | 893.9833 | 899.3538 |
| 1012.827 | 1023.546 | 1030.05 |
| 1079.081 | 1116.974 | 1129.925 |
| 1192.447 | 1266.714 | 1324.491 |
| 1390.518 | 1439.473 | 1451.869 |
| 1484.508 | 1578.796 | 1701.569 |
| 2231.029 | 3160.991 | 3180.628 |
| 3256.818 | 3259.983 | 3282.916 |
| 3289.137 | 3478.808 | 3670.719 |

***i42***

**Cartesian coordinates**

N 0.925713 -0.884051 -0.148475

C 2.245283 -1.224779 -0.055352

C 2.965647 -0.073577 0.146440

C 2.040934 1.000496 0.175965

C 0.781803 0.471135 -0.009406

C -0.511785 1.140277 -0.063964

C -1.664826 0.556638 -0.252691

C -2.843609 -0.068837 -0.445877

C -3.659023 -0.566887 0.565764

H 0.161394 -1.521567 -0.292303

H 2.563891 -2.251221 -0.140348

H 4.036256 -0.009967 0.261170

H 2.262026 2.047509 0.317202

H -0.477817 2.221678 0.068748

H -3.178353 -0.183161 -1.476583

H -4.596520 -1.053138 0.329240

H -3.377410 -0.468563 1.606926

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 54.9773 | 64.1247 | 149.7049 |
| 185.1435 | 265.8835 | 347.7045 |
| 431.9738 | 529.981 | 541.5088 |
| 567.4392 | 636.1602 | 673.7792 |
| 731.6801 | 736.8292 | 760.9461 |
| 808.9925 | 852.3149 | 901.1264 |
| 905.1176 | 921.2643 | 953.8122 |
| 991.5361 | 1056.985 | 1083.305 |
| 1125.118 | 1146.457 | 1192.049 |
| 1243.315 | 1311.101 | 1318.401 |
| 1398.868 | 1467.689 | 1493.139 |
| 1495.285 | 1518.434 | 1633.445 |
| 1919.623 | 3128.215 | 3139.141 |
| 3171.285 | 3255.567 | 3267.928 |
| 3277.147 | 3286.436 | 3697.131 |

***i43***

**Cartesian coordinates**

N 1.651358 1.051058 -0.157110

C 2.921949 0.572574 -0.029477

C 2.860936 -0.788622 0.194058

C 1.493319 -1.094958 0.187222

C 0.729662 0.027981 -0.025775

C -0.694731 0.261227 -0.120317

C -1.629203 -0.697577 -0.162914

C -3.070309 -0.449658 -0.212441

C -3.700183 0.578778 0.355375

H 1.413795 2.010506 -0.342486

H 3.775676 1.227306 -0.106416

H 3.698409 -1.451344 0.339340

H -1.307955 -1.736354 -0.186436

H -1.009743 1.302119 -0.173275

H -3.659828 -1.188409 -0.751271

H -4.770319 0.711706 0.248122

H -3.168175 1.308594 0.957807

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 46.5045 | 96.0549 | 118.4941 |
| 196.2427 | 235.5878 | 314.2166 |
| 425.5364 | 466.8339 | 536.6213 |
| 606.8324 | 642.9136 | 673.7582 |
| 696.6059 | 793.6381 | 850.307 |
| 879.3602 | 885.7371 | 950.6723 |
| 977.5256 | 985.3523 | 997.9903 |
| 1035.108 | 1087.798 | 1114.861 |
| 1135.678 | 1197.454 | 1248.819 |
| 1315.94 | 1343.683 | 1355.703 |
| 1421.943 | 1459.72 | 1463.741 |
| 1496.015 | 1593.863 | 1705.918 |
| 1727.619 | 3152.276 | 3154.198 |
| 3160.856 | 3172.349 | 3248.18 |
| 3266.371 | 3285.884 | 3697.524 |

***i44***

**Cartesian coordinates**

N 1.808396 0.894007 -0.270557

C 2.757875 -0.085744 -0.294859

C 2.168989 -1.250988 0.128742

C 0.811214 -0.960342 0.407191

C 0.600384 0.380416 0.141455

C -0.559689 1.246422 0.274413

C -1.852818 0.907890 0.154043

C -2.360182 -0.402456 -0.242411

C -3.623450 -0.764466 -0.193014

H 1.947188 1.841029 -0.576706

H 3.769172 0.121812 -0.605269

H 2.661937 -2.203759 0.241194

H 0.077826 -1.639891 0.811343

H -0.339110 2.286160 0.507535

H -1.628178 -1.115678 -0.633341

H -4.200043 -1.643076 -0.444751

H -2.601512 1.670961 0.340533

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 56.6284 | 100.1811 | 185.0822 |
| 209.5747 | 274.676 | 361.8998 |
| 457.3799 | 501.0313 | 603.1715 |
| 634.5957 | 644.5528 | 698.3308 |
| 732.616 | 761.2537 | 792.1029 |
| 817.3178 | 839.2007 | 890.4335 |
| 905.2202 | 906.9773 | 989.5727 |
| 1005.616 | 1070.673 | 1100.833 |
| 1139.6 | 1153.461 | 1249.485 |
| 1260.909 | 1279.625 | 1311.272 |
| 1434.057 | 1479.737 | 1480.283 |
| 1517.783 | 1622.515 | 1660.725 |
| 1718.176 | 3076.163 | 3148.397 |
| 3190.019 | 3251.017 | 3256.407 |
| 3269.475 | 3286.866 | 3704.956 |

***i45***

**Cartesian coordinates**

C 1.478060 -1.327374 0.048927

C 2.461852 -0.438339 -0.378600

N 1.982275 0.864906 -0.348423

C 0.690475 0.798509 0.092225

C 0.365113 -0.529761 0.341500

C -0.547492 1.321899 0.483201

C -1.049473 -0.109565 0.808891

C -2.204077 -0.663340 0.029673

C -2.922753 0.013102 -0.855852

H 1.607505 -2.396487 0.119197

H 3.470334 -0.638379 -0.705233

H 2.507862 1.677724 -0.613365

H -0.991383 2.301120 0.578971

H -1.208099 -0.284268 1.879865

H -2.441148 -1.707170 0.228900

H -3.744895 -0.450737 -1.389341

H -2.706322 1.053068 -1.079826

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 71.9488 | 151.9094 | 158.3791 |
| 262.519 | 337.9995 | 434.3287 |
| 464.7447 | 475.0683 | 582.9858 |
| 617.1491 | 620.1849 | 675.0355 |
| 699.1274 | 759.2406 | 837.5982 |
| 859.9038 | 882.7912 | 933.9011 |
| 961.6447 | 997.0286 | 1038.85 |
| 1051.212 | 1080.937 | 1099.516 |
| 1130.767 | 1195.522 | 1206.913 |
| 1273.048 | 1314.587 | 1332.449 |
| 1350.904 | 1419.604 | 1451.134 |
| 1485.833 | 1521.275 | 1602.997 |
| 1736.494 | 3046.956 | 3142.306 |
| 3156.801 | 3238.254 | 3253.218 |
| 3256.729 | 3279.274 | 3723.012 |

***i46***

**Cartesian coordinates**

N 1.731017 -0.962485 -0.107952

C 2.684728 0.007575 -0.123476

C 2.058093 1.217329 0.056143

C 0.673402 0.960894 0.176651

C 0.478638 -0.406688 0.065219

C -0.666834 -1.283864 0.116639

C -1.989846 -1.037689 0.058777

C -2.719586 0.214600 -0.104203

C -2.287523 1.458494 -0.084969

H 1.902756 -1.943100 -0.244587

H 3.727063 -0.232497 -0.259816

H 2.543097 2.179531 0.103589

H -0.105985 1.685437 0.351710

H -0.401766 -2.336662 0.203077

H -2.630462 -1.912534 0.111348

H -3.794490 0.082138 -0.271412

H -2.743753 2.431175 -0.202930

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 31.0765 | 107.8494 | 175.5827 |
| 227.379 | 236.6488 | 418.5995 |
| 464.0056 | 492.2024 | 615.3287 |
| 629.4395 | 634.4309 | 697.652 |
| 743.1205 | 754.3234 | 773.2464 |
| 830.3624 | 885.9378 | 893.6624 |
| 899.0955 | 908.7621 | 979.7074 |
| 993.8684 | 1017.245 | 1075.013 |
| 1138.132 | 1156.519 | 1249.576 |
| 1272.255 | 1304.145 | 1328.439 |
| 1440.654 | 1480.519 | 1492.977 |
| 1516.437 | 1620.737 | 1651.839 |
| 1709.121 | 3054.822 | 3143.974 |
| 3183.514 | 3246.911 | 3253.722 |
| 3267.131 | 3286.127 | 3705.19 |

***i47***

**Cartesian coordinates**

C 2.009415 1.271511 -0.050882

C 2.678660 0.065485 -0.092677

N 1.766951 -0.943739 -0.015135

C 0.480845 -0.433261 0.071751

C 0.650712 0.931548 0.036192

C -0.654212 -1.323322 0.148059

C -1.963466 -1.054705 -0.006200

C -2.609540 0.227131 -0.261462

C -2.231662 1.425406 0.189394

H 2.455720 2.251558 -0.094566

H 3.733562 -0.140587 -0.185975

H 1.989891 -1.923694 -0.051056

H -0.392304 -2.367899 0.305023

H -2.632357 -1.911170 0.009093

H -3.511515 0.169744 -0.868254

H -2.782242 2.319596 -0.080366

H -1.393926 1.549867 0.866989

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 64.3746 | 77.2176 | 155.3492 |
| 208.4553 | 239.3554 | 401.5464 |
| 442.5794 | 468.9271 | 583.5847 |
| 618.2632 | 637.4383 | 690.4986 |
| 715.9476 | 800.4508 | 809.0554 |
| 856.6153 | 884.8858 | 937.8154 |
| 947.7632 | 993.0247 | 1004.644 |
| 1027.309 | 1096.593 | 1114.617 |
| 1147.408 | 1200.146 | 1250.104 |
| 1279.603 | 1341.123 | 1401.68 |
| 1444.25 | 1463.882 | 1486.517 |
| 1506.905 | 1594.911 | 1687.364 |
| 1716.755 | 3143.169 | 3151.708 |
| 3157.64 | 3177.914 | 3244.792 |
| 3264.841 | 3284.667 | 3695.529 |

***i48***

**Cartesian coordinates**

N 1.549301 -1.123657 0.011660

C 0.237492 -0.719585 0.184005

C 0.257936 0.766490 0.427440

C -0.991036 1.427304 -0.074037

C -2.127978 0.691270 -0.200374

C -2.135433 -0.721350 -0.042294

C -0.921540 -1.431757 0.064695

C 1.638996 1.141691 -0.062631

C 2.331443 0.014592 -0.244141

H 1.762192 -2.005592 -0.424526

H 0.270537 0.913427 1.532698

H -0.990471 2.500594 -0.226641

H -3.056070 1.186001 -0.467612

H -3.067895 -1.264158 -0.134878

H -0.904739 -2.511339 -0.043131

H 2.031687 2.145222 -0.119834

H 3.370375 -0.110492 -0.513670

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 149.1073 | 202.5236 | 358.4694 |
| 393.9104 | 478.765 | 522.7119 |
| 537.8631 | 551.067 | 581.7882 |
| 666.9839 | 695.1791 | 716.9755 |
| 749.1358 | 841.309 | 855.7258 |
| 866.7443 | 878.3549 | 920.0336 |
| 961.1457 | 1000.974 | 1047.198 |
| 1059.865 | 1114.731 | 1128.017 |
| 1138.799 | 1169.273 | 1230.028 |
| 1260.039 | 1271.012 | 1326.545 |
| 1360.317 | 1397.667 | 1440.526 |
| 1460.077 | 1565.141 | 1649.076 |
| 1674.377 | 2806.154 | 3185.804 |
| 3188.739 | 3207.489 | 3221.95 |
| 3247.975 | 3271.995 | 3667.708 |

***i49***

**Cartesian coordinates**

N 1.614089 -1.064737 0.000003

C 0.295741 -0.675122 0.000026

C 0.274849 0.719346 0.000017

C -1.016494 1.473145 0.000045

C -2.207730 0.556073 -0.000047

C -2.107243 -0.803929 -0.000032

C -0.863709 -1.478354 0.000042

C 1.616530 1.162547 -0.000018

C 2.417936 0.043064 -0.000033

H 1.935809 -2.015657 -0.000025

H -1.069281 2.145076 0.870761

H -1.069230 2.145265 -0.870524

H -3.188160 1.019963 -0.000129

H -3.016588 -1.396175 -0.000084

H -0.809829 -2.559996 0.000063

H 1.967177 2.183577 -0.000025

H 3.492198 -0.049512 -0.000064

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 126.8114 | 233.7246 | 269.9953 |
| 387.4216 | 454.9212 | 494.1314 |
| 506.7614 | 597.6794 | 620.9932 |
| 639.131 | 673.9448 | 711.3409 |
| 746.2854 | 748.5178 | 852.6095 |
| 884.7926 | 920.2892 | 941.2937 |
| 943.2587 | 967.1412 | 1061.949 |
| 1079.423 | 1128.671 | 1190.324 |
| 1199.865 | 1216.424 | 1242.68 |
| 1263.033 | 1356.597 | 1389.277 |
| 1422.858 | 1442.558 | 1458.823 |
| 1504.245 | 1538.336 | 1570.113 |
| 1625.194 | 2982.488 | 2992.571 |
| 3179.387 | 3203.995 | 3218.158 |
| 3252.784 | 3280.588 | 3719.026 |

***i50***

**Cartesian coordinates**

C -2.720388 0.944946 -0.002202

C -2.967881 -0.406499 0.030259

N -1.765184 -1.049273 0.018341

C -0.736203 -0.137418 -0.016582

C -1.317341 1.117030 -0.032403

C 4.177382 0.448723 0.038326

C 3.084960 -0.282233 -0.016508

C 1.720045 0.224010 0.022166

C 0.644144 -0.573769 -0.035796

H -3.468064 1.722401 -0.007743

H -3.896139 -0.953735 0.059502

H -1.642839 -2.046165 0.048156

H -0.784738 2.054537 -0.071357

H 5.243911 0.278520 0.023649

H 1.596807 1.299728 0.103495

H 0.804090 -1.649249 -0.107447

H 3.194961 -1.369870 -0.100195

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 40.9138 | 109.6171 | 115.3905 |
| 177.9536 | 297.9553 | 356.0742 |
| 369.3199 | 496.8737 | 513.5866 |
| 622.8497 | 635.8373 | 686.8425 |
| 732.9345 | 771.1476 | 812.0804 |
| 821.6552 | 839.4104 | 891.6456 |
| 899.0878 | 906.0077 | 989.673 |
| 1002.759 | 1069.592 | 1138.049 |
| 1142.027 | 1154.803 | 1232.842 |
| 1267.797 | 1306.151 | 1332.618 |
| 1366.261 | 1473.028 | 1488.226 |
| 1510.401 | 1621.385 | 1664.567 |
| 1722.909 | 3050.223 | 3144.483 |
| 3186.965 | 3260.211 | 3264.568 |
| 3271.369 | 3288.379 | 3706.261 |

***i51***

**Cartesian coordinates**

C 2.796129 0.718981 0.074945

C 2.841744 -0.650938 -0.031199

N 1.557517 -1.107269 -0.069918

C 0.673725 -0.056162 0.003592

C 1.433694 1.095410 0.098753

C -3.746823 -0.715162 0.204979

C -3.139089 0.410064 -0.102438

C -1.696325 0.666359 -0.107843

C -0.754802 -0.283900 -0.025075

H 3.649841 1.375675 0.134812

H 3.678159 -1.329379 -0.077896

H 1.288161 -2.071358 -0.158666

H 1.042964 2.097022 0.190076

H -4.764363 -1.072261 0.263104

H -3.770760 1.259488 -0.383426

H -1.396315 1.706318 -0.196342

H -1.079829 -1.322539 0.023482

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 31.4607 | 88.2551 | 121.8618 |
| 164.9471 | 239.9427 | 331.674 |
| 427.6699 | 499.9289 | 522.2595 |
| 615.4547 | 634.5335 | 683.2239 |
| 735.4901 | 762.8069 | 813.3744 |
| 831.1851 | 877.1276 | 894.7655 |
| 900.2383 | 905.8378 | 989.3139 |
| 995.1053 | 1033.561 | 1058.831 |
| 1133.669 | 1146.023 | 1238.112 |
| 1269.426 | 1299.18 | 1342.079 |
| 1358.259 | 1469.728 | 1486.263 |
| 1506.998 | 1624.688 | 1649.017 |
| 1720.373 | 3062.289 | 3147.013 |
| 3187.697 | 3254.926 | 3264.723 |
| 3267.505 | 3285.574 | 3705.971 |

***i52***

**Cartesian coordinates**

C 2.597594 0.911825 -0.000023

C 2.837978 -0.445648 0.000080

N 1.632684 -1.087480 0.000075

C 0.591945 -0.170601 -0.000031

C 1.204404 1.098336 -0.000092

C -0.750724 -0.555006 -0.000042

C -1.876439 0.388682 -0.000224

C -3.198691 0.010909 -0.643621

C -3.198501 0.011398 0.643866

H 3.353287 1.681839 -0.000061

H 3.766064 -0.994359 0.000150

H 1.506650 -2.083526 0.000140

H 0.682053 2.041834 -0.000164

H -0.991854 -1.615199 0.000045

H -1.595357 1.441634 -0.000651

H -3.697745 -0.180238 -1.578488

H -3.697287 -0.179004 1.579028

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 57.1894 | 101.704 | 141.9126 |
| 247.8954 | 337.0983 | 411.2969 |
| 422.6834 | 443.7423 | 610.4776 |
| 624.3701 | 626.8742 | 688.189 |
| 713.8881 | 763.4066 | 768.3574 |
| 783.337 | 886.3362 | 887.8065 |
| 894.9868 | 928.2491 | 983.0562 |
| 1025.778 | 1051.252 | 1058.582 |
| 1092.519 | 1134.878 | 1148.462 |
| 1178.795 | 1230.674 | 1300.622 |
| 1352.054 | 1406.714 | 1437.346 |
| 1506.685 | 1509.698 | 1573.229 |
| 1740.05 | 3105.585 | 3164.021 |
| 3260.751 | 3262.826 | 3272.112 |
| 3286.54 | 3312.196 | 3713.278 |

***i53***

**Cartesian coordinates**

C 2.097181 -1.189539 -0.000003

C 2.696866 0.050839 0.000223

N 1.711227 0.994076 0.000158

C 0.457756 0.396595 -0.000115

C 0.704829 -0.991575 -0.000208

C -0.711440 1.168369 -0.000306

C -2.102477 0.682031 -0.000503

C -2.525600 -0.627217 -0.643215

C -2.526083 -0.626271 0.643907

H 2.613944 -2.136706 -0.000014

H 3.738835 0.327863 0.000433

H 1.860256 1.987068 0.000260

H -0.051330 -1.757859 -0.000347

H -0.587309 2.247935 -0.000190

H -2.831150 1.493047 -0.001346

H -2.633424 -1.150826 -1.577992

H -2.634602 -1.148439 1.579408

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 55.7366 | 108.2337 | 159.6206 |
| 251.5189 | 291.9974 | 404.0192 |
| 445.3727 | 539.8416 | 590.7933 |
| 614.2211 | 645.2902 | 689.6248 |
| 708.2345 | 755.5933 | 783.7983 |
| 788.5521 | 882.9466 | 884.3654 |
| 890.0895 | 912.3986 | 963.9429 |
| 1025.581 | 1031.047 | 1068.925 |
| 1071.302 | 1130.499 | 1151.306 |
| 1193.28 | 1237.284 | 1304.639 |
| 1393.773 | 1413.327 | 1435.054 |
| 1502.587 | 1509.497 | 1572.717 |
| 1739.383 | 3101.633 | 3172.617 |
| 3259.286 | 3263.292 | 3279.484 |
| 3304.742 | 3312.741 | 3711.337 |

***i54***

**Cartesian coordinates**

C -2.310275 0.964084 0.211702

C -2.612195 -0.362120 0.038708

N -1.435626 -1.030857 -0.169280

C -0.380797 -0.156292 -0.132334

C -0.900356 1.095301 0.104403

C 1.028035 -0.615628 -0.296659

C 1.958786 -0.501072 0.921158

C 2.792484 0.385765 0.246098

C 2.018743 0.375782 -0.910811

H -3.022995 1.753977 0.391190

H -3.557901 -0.879521 0.040617

H -1.351868 -2.019440 -0.327424

H -0.321240 2.001987 0.191198

H 1.057112 -1.604359 -0.770796

H 1.920782 -0.923926 1.915125

H 3.709116 0.894069 0.518705

H 2.049834 0.878296 -1.867246

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 31.0513 | 128.1936 | 149.5768 |
| 317.5221 | 381.8443 | 429.8453 |
| 494.7457 | 552.0131 | 570.7659 |
| 638.0742 | 689.9981 | 721.724 |
| 791.0998 | 816.461 | 887.6107 |
| 899.5437 | 919.0639 | 930.8568 |
| 935.4245 | 962.7713 | 964.3526 |
| 1007.874 | 1051.142 | 1129.701 |
| 1149.163 | 1150.797 | 1189.795 |
| 1208.006 | 1230.553 | 1287.173 |
| 1328.681 | 1371.785 | 1464.986 |
| 1469.404 | 1501.196 | 1522.374 |
| 1635.798 | 3048.627 | 3217.728 |
| 3245.137 | 3253.465 | 3260.504 |
| 3267.311 | 3285.841 | 3708.658 |

***i55***

**Cartesian coordinates**

N -2.073247 -1.218196 0.01219

C -3.051953 -0.263662 -0.01067

C -2.456514 0.978620 0.01298

C -1.071259 0.718540 0.05037

C -0.832620 -0.623463 0.05075

H -2.237202 -2.209168 0.00278

H -4.095814 -0.534143 -0.04250

H -2.963286 1.929930 0.00328

H 0.081940 -1.193370 0.07276

C 3.106448 -1.576433 -0.16568

C 2.758903 -0.455654 0.09550

C 2.342026 0.865978 0.43363

C 1.688747 1.669254 -0.40735

H 3.424412 -2.562639 -0.40423

H 2.566729 1.196255 1.44325

H 1.384280 2.662304 -0.10068

H 1.448998 1.359124 -1.41724

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 24.814 | 42.326 | 49.2582 |
| 60.0943 | 95.9461 | 113.8933 |
| 226.8519 | 331.2929 | 474.3211 |
| 564.7978 | 566.1047 | 644.6955 |
| 661.6997 | 678.4108 | 702.4978 |
| 706.3738 | 779.8225 | 847.7506 |
| 865.4646 | 894.2177 | 897.0746 |
| 969.9936 | 1009.548 | 1057.537 |
| 1086.723 | 1113.198 | 1170.783 |
| 1189.908 | 1260.074 | 1319.506 |
| 1403.2 | 1440.773 | 1467.933 |
| 1507.911 | 1561.98 | 1689.486 |
| 2235.181 | 3173.289 | 3188.804 |
| 3260.828 | 3271.605 | 3280.712 |
| 3283.222 | 3484.167 | 3706.891 |

***i56***

**Cartesian coordinates**

N -2.246657 -1.157742 0.020894

C -2.892902 0.041383 -0.088546

C -1.940220 1.025856 -0.141348

C -0.665471 0.397035 -0.062246

C -0.893279 -0.953830 0.039289

H -2.695450 -2.052667 0.091715

H -3.969160 0.098640 -0.115707

H -2.128328 2.085424 -0.229176

H -0.197308 -1.774037 0.117438

C 3.900658 -0.583713 -0.402958

C 2.882330 -0.145724 0.103632

C 1.730365 0.349173 0.663565

C 0.677651 1.077112 -0.116659

H 4.790365 -0.966119 -0.841373

H 1.556094 0.183686 1.722304

H 0.568665 2.089854 0.293346

H 1.006934 1.195663 -1.153174

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 33.5497 | 39.8668 | 172.1474 |
| 199.8989 | 279.3432 | 370.2768 |
| 401.8505 | 495.5014 | 496.8532 |
| 536.9895 | 617.734 | 646.3446 |
| 649.3488 | 684.8617 | 710.6961 |
| 730.3652 | 794.6988 | 863.8831 |
| 886.2624 | 915.7202 | 985.9844 |
| 1043 | 1094.948 | 1099.942 |
| 1156.953 | 1174.483 | 1207.232 |
| 1249.117 | 1307.211 | 1333.836 |
| 1423.861 | 1443.583 | 1481.951 |
| 1500.236 | 1543.031 | 1633.43 |
| 2029.794 | 3025.421 | 3088.907 |
| 3183.84 | 3253.803 | 3274.639 |
| 3282.167 | 3475.092 | 3723.586 |

***i57***

**Cartesian coordinates**

N -1.847112 -1.287129 0.150229

C -2.691338 -0.206004 0.025164

C -1.913429 0.908922 -0.143203

C -0.534379 0.516227 -0.123777

C -0.571860 -0.834642 0.071832

C 2.807052 -1.430756 -0.292485

C 2.395428 -0.363947 0.071351

C 1.890084 0.939257 0.497286

C 0.661073 1.401037 -0.302539

H -2.123536 -2.237106 0.318846

H -3.761435 -0.323290 0.083324

H -2.276608 1.918761 -0.269638

H 1.633311 0.888111 1.560055

H 3.171821 -2.375775 -0.614721

H 2.691352 1.677323 0.392434

H 0.406767 2.415556 0.018254

H 0.932317 1.465764 -1.361927

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 20.0889 | 75.9607 | 150.8868 |
| 189.0993 | 260.2513 | 355.7903 |
| 365.2829 | 414.6963 | 527.137 |
| 566.2038 | 630.078 | 668.5909 |
| 681.3296 | 697.5302 | 707.9197 |
| 837.3303 | 855.4576 | 901.4578 |
| 907.7343 | 992.2605 | 1018.307 |
| 1056.73 | 1083.033 | 1127.825 |
| 1184.946 | 1220.058 | 1266.572 |
| 1290.709 | 1364.527 | 1376.395 |
| 1407.523 | 1442.442 | 1474.173 |
| 1488.391 | 1524.914 | 1612.691 |
| 2246.11 | 3050.07 | 3055.986 |
| 3095.233 | 3102.375 | 3243.993 |
| 3279.651 | 3487.578 | 3724.042 |

***i58***

**Cartesian coordinates**

N 1.658821 0.991994 0.044960

C 2.397961 -0.161167 0.100052

C 1.532312 -1.227076 0.026198

C 0.219737 -0.698949 -0.065773

C 0.332310 0.673767 -0.053719

C -0.819019 1.571424 -0.146142

C -1.992270 0.980531 0.001248

C -2.254850 -0.449910 0.310427

C -1.122995 -1.345088 -0.261331

H 2.030548 1.922255 0.114356

H 3.471238 -0.129732 0.195193

H 1.815862 -2.268672 0.037846

H -0.698631 2.634424 -0.330770

H -2.299131 -0.558014 1.402550

H -3.221387 -0.776948 -0.081571

H -1.170807 -2.327436 0.215415

H -1.298550 -1.501027 -1.333498

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 136.0472 | 211.1695 | 272.9133 |
| 379.3066 | 389.7347 | 463.4436 |
| 482.2429 | 583.2536 | 637.2812 |
| 664.0422 | 703.8921 | 725.5798 |
| 762.8313 | 820.4949 | 855.788 |
| 876.8456 | 917.6077 | 929.493 |
| 989.1394 | 1026.581 | 1077.435 |
| 1113.959 | 1178.793 | 1190.851 |
| 1216.097 | 1225.518 | 1284.576 |
| 1324.006 | 1341.11 | 1389.492 |
| 1460.677 | 1467.478 | 1495.047 |
| 1503.687 | 1544.516 | 1625.286 |
| 1697.964 | 3024.326 | 3031.042 |
| 3096.231 | 3101.736 | 3182.251 |
| 3250.197 | 3281.633 | 3714.921 |

***i59***

**Cartesian coordinates**

N -1.091306 0.931768 -0.463112

C -1.554146 -0.176903 -1.112560

C -2.283281 -0.939099 -0.224532

C -2.213144 -0.238246 0.995737

C -1.480386 0.904169 0.856684

C 2.417700 1.690088 -0.161870

C 2.045143 0.566988 0.053321

C 1.575203 -0.756873 0.315577

C 2.298979 -1.848584 0.076089

H -0.423272 1.580870 -0.843723

H -1.329538 -0.346222 -2.153652

H -2.792914 -1.863489 -0.441801

H -1.200278 1.679981 1.548481

H 2.777869 2.674305 -0.342401

H 0.572794 -0.835822 0.729129

H 1.898521 -2.831749 0.291959

H 3.299555 -1.789488 -0.336885

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 16.2646 | 32.1827 | 67.5802 |
| 87.0093 | 95.8846 | 155.3431 |
| 230.1745 | 338.9688 | 508.1175 |
| 559.1593 | 570.4965 | 644.16 |
| 678.6751 | 687.0203 | 701.476 |
| 716.2367 | 766.7735 | 859.1781 |
| 871.3519 | 892.9112 | 895.7802 |
| 978.9492 | 1040.431 | 1048.64 |
| 1083.421 | 1119.604 | 1176.126 |
| 1193.398 | 1250.868 | 1337.356 |
| 1401.188 | 1446.639 | 1465.817 |
| 1506.112 | 1556.956 | 1703.543 |
| 2232.394 | 3159.645 | 3172.527 |
| 3256.959 | 3261.885 | 3280.456 |
| 3290.163 | 3484.064 | 3693.169 |

***i60***

**Cartesian coordinates**

N -2.318860 -1.147962 0.044281

C -2.955277 0.046659 -0.156802

C -2.000735 1.028631 -0.172861

C -0.735199 0.403664 0.026632

C -0.973592 -0.946746 0.157245

C 0.559370 1.091818 0.079140

C 1.723409 0.530743 0.258268

C 2.913059 -0.075154 0.443906

C 3.734766 -0.553488 -0.571919

H -2.772524 -2.041737 0.101060

H -4.025590 0.099684 -0.272165

H -2.177527 2.084260 -0.312811

H -0.287347 -1.762633 0.318140

H 0.521725 2.175272 -0.047138

H 3.250787 -0.191352 1.473388

H 4.679691 -1.027729 -0.340291

H 3.448001 -0.456789 -1.611807

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 42.2695 | 64.974 | 142.7924 |
| 194.7071 | 267.4636 | 353.4262 |
| 425.1142 | 509.456 | 541.835 |
| 569.8352 | 645.8181 | 652.0839 |
| 721.02 | 722.0831 | 750.411 |
| 791.3059 | 841.9673 | 882.9471 |
| 913.6533 | 922.9242 | 951.0981 |
| 996.2197 | 1081.252 | 1099.448 |
| 1105.325 | 1173.481 | 1191.98 |
| 1225.481 | 1309.875 | 1342.323 |
| 1404.472 | 1453.286 | 1493.428 |
| 1497.261 | 1546.444 | 1625.009 |
| 1925.374 | 3109.167 | 3138.975 |
| 3170.605 | 3256.269 | 3275.481 |
| 3279.433 | 3285.052 | 3719.652 |

***i61***

**Cartesian coordinates**

N 2.649224 -0.815759 0.000164

C 2.911054 0.568146 0.000077

C 1.721087 1.214548 -0.000107

C 0.715238 0.190269 -0.000122

C 1.352017 -1.153091 0.000020

C -0.670530 0.381155 -0.000161

C -1.572175 -0.662856 -0.000155

C -3.006735 -0.542206 -0.000044

C -3.721258 0.597857 0.000235

H 3.384869 -1.503682 0.000279

H 3.921206 0.951933 0.000143

H 1.572309 2.283864 -0.000206

H -1.145091 -1.660581 -0.000207

H -1.036807 1.405778 -0.000156

H -3.553018 -1.481568 -0.000187

H -4.804206 0.573908 0.000300

H -3.256017 1.577729 0.000425

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 46.5126 | 110.2585 | 136.6532 |
| 227.0077 | 259.5334 | 259.6438 |
| 438.7327 | 511.2901 | 551.0699 |
| 600.414 | 632.343 | 731.7808 |
| 740.5529 | 788.4084 | 879.9521 |
| 884.174 | 916.7159 | 919.3147 |
| 930.6425 | 982.5223 | 1001.987 |
| 1034.817 | 1036.374 | 1073.494 |
| 1093.404 | 1177.655 | 1242.38 |
| 1277.256 | 1318.751 | 1339.968 |
| 1362.387 | 1419.906 | 1449.952 |
| 1491.636 | 1498.267 | 1596.789 |
| 1649.593 | 3155.449 | 3160.606 |
| 3171.757 | 3197.81 | 3240.687 |
| 3250.592 | 3263.042 | 3666.121 |

***i62***

**Cartesian coordinates**

C -1.870258 0.961219 0.337997

C -2.750119 -0.085791 0.317464

N -2.080921 -1.182804 -0.154347

C -0.785467 -0.854309 -0.430487

C -0.607577 0.481206 -0.127627

C 0.594119 1.295346 -0.284976

C 1.875092 0.916932 -0.160099

C 2.339329 -0.402824 0.262581

C 3.582900 -0.825650 0.202157

H -2.086567 1.966816 0.665051

H -3.788910 -0.143676 0.599281

H -2.487808 -2.088724 -0.301297

H -0.106034 -1.568837 -0.865799

H 0.408978 2.338656 -0.528366

H 1.585744 -1.071581 0.691392

H 4.123137 -1.721291 0.473873

H 2.649790 1.651489 -0.355765

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 56.6883 | 94.4838 | 190.7428 |
| 213.7479 | 272.8608 | 365.8085 |
| 458.489 | 514.9675 | 595.5045 |
| 633.056 | 646.1859 | 688.8737 |
| 714.1667 | 759.583 | 780.5225 |
| 814.4709 | 832.6325 | 868.0056 |
| 888.0475 | 914.7404 | 983.2895 |
| 1013.316 | 1087.833 | 1100.845 |
| 1116.701 | 1180.672 | 1244.818 |
| 1264.212 | 1275.923 | 1330.724 |
| 1419.37 | 1454.003 | 1499.478 |
| 1543.744 | 1620.966 | 1659.196 |
| 1720.196 | 3072.711 | 3161.727 |
| 3190.77 | 3253.171 | 3259.557 |
| 3277.913 | 3285.436 | 3723.014 |

***i63***

**Cartesian coordinates**

N 1.429442 -1.235804 0.076618

C 2.469602 -0.426496 -0.364989

C 2.078704 0.893023 -0.390824

C 0.717596 0.886638 0.049772

C 0.374732 -0.418560 0.315881

C -0.572370 1.364884 0.451024

C -1.039965 -0.070936 0.800994

C -2.191014 -0.671424 0.047634

C -2.923121 -0.029208 -0.851981

H 1.477208 -2.234943 0.164782

H 3.416243 -0.868600 -0.634254

H 2.704530 1.718056 -0.692660

H -1.037582 2.328695 0.592950

H -1.173466 -0.238010 1.877268

H -2.416231 -1.711140 0.280785

H -3.743740 -0.517321 -1.365891

H -2.718044 1.006370 -1.104374

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 51.7997 | 123.393 | 159.5004 |
| 254.9667 | 329.4605 | 337.9864 |
| 450.757 | 465.9278 | 604.2005 |
| 614.771 | 621.7669 | 684.1878 |
| 722.643 | 758.2316 | 841.4433 |
| 861.1196 | 884.0262 | 939.2899 |
| 969.738 | 996.6583 | 1041.236 |
| 1060.236 | 1071.322 | 1095.757 |
| 1135.868 | 1194.865 | 1197.334 |
| 1278.97 | 1316.616 | 1334.376 |
| 1358.803 | 1452.089 | 1458.883 |
| 1498.482 | 1534.752 | 1583.03 |
| 1737.14 | 3038.581 | 3137.901 |
| 3154.928 | 3239.101 | 3250.711 |
| 3258.815 | 3280.946 | 3715.025 |

***i64***

**Cartesian coordinates**

N 1.979223 1.143625 -0.063005

C 2.688084 -0.013290 0.136906

C 1.796817 -1.047060 0.134267

C 0.486205 -0.502783 -0.065059

C 0.652355 0.865353 -0.188170

C -0.706263 -1.324945 -0.125232

C -2.018790 -1.030613 -0.060561

C -2.247223 1.480758 0.084246

C -2.703626 0.245871 0.118238

H 2.378270 2.062887 -0.124077

H 3.758186 0.001337 0.265222

H 2.033238 -2.091429 0.271902

H -0.072985 1.639686 -0.378410

H -0.481375 -2.385636 -0.215047

H -2.693913 -1.879430 -0.112181

H -2.683547 2.461715 0.211932

H -3.777799 0.145755 0.313886

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 34.1658 | 108.2032 | 169.2403 |
| 228.8747 | 238.6702 | 411.8795 |
| 466.4908 | 517.6432 | 606.8924 |
| 628.5858 | 644.1176 | 682.6579 |
| 726.566 | 754.3506 | 765.4044 |
| 822.9749 | 879.5348 | 888.9571 |
| 898.5057 | 912.5286 | 975.626 |
| 1009.564 | 1014.576 | 1095.836 |
| 1104.611 | 1176.315 | 1247.157 |
| 1280.328 | 1299.374 | 1339.997 |
| 1425.663 | 1469.362 | 1498.224 |
| 1547.057 | 1615.1 | 1654.234 |
| 1708.758 | 3050.987 | 3155.741 |
| 3185.483 | 3241.195 | 3256.32 |
| 3259.685 | 3284.569 | 3719.779 |

***i65***

**Cartesian coordinates**

N -1.890364 -1.190500 -0.069607

C -2.671385 -0.050180 -0.039066

C -1.832364 1.024905 0.029045

C -0.476473 0.545027 0.043268

C -0.589951 -0.823583 -0.075629

C 0.703914 1.380001 0.124202

C 1.997054 1.040021 -0.032121

C 2.541208 -0.289502 -0.272369

C 2.126677 -1.431044 0.287247

H -2.230133 -2.125500 -0.207777

H -3.745660 -0.109644 -0.109540

H -2.131922 2.061800 0.074469

H 0.491650 2.436728 0.266127

H 2.719456 1.851848 -0.051563

H 3.379166 -0.332349 -0.966499

H 2.579927 -2.379937 0.023392

H 1.377982 -1.443319 1.071183

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 70.4274 | 108.5128 | 146.443 |
| 218.7613 | 244.4311 | 391.3159 |
| 424.2911 | 486.8383 | 563.7417 |
| 603.9249 | 621.2425 | 680.4117 |
| 722.4432 | 804.2601 | 811.8232 |
| 860.4684 | 896.0855 | 929.6381 |
| 953.848 | 979.3788 | 1016.637 |
| 1034.12 | 1081.421 | 1099.251 |
| 1112.579 | 1195.682 | 1259.286 |
| 1291.046 | 1335.594 | 1377.319 |
| 1433.561 | 1441.285 | 1469.177 |
| 1525.519 | 1586.924 | 1677.938 |
| 1709.006 | 3145.814 | 3160.97 |
| 3165.036 | 3184.755 | 3246.49 |
| 3251.98 | 3278.622 | 3712.544 |

***i66***

**Cartesian coordinates**

N 1.586430 -1.078308 -0.114776

C 2.333951 0.081156 -0.204213

C 1.569699 1.201035 -0.070386

C 0.227874 0.785989 0.161941

C 0.273489 -0.699358 0.419375

C -0.990896 1.438002 0.073307

C -2.160028 0.690658 -0.027501

C -0.939369 -1.418766 -0.078261

C -2.099493 -0.731431 -0.192338

H 2.029370 -1.897379 0.271500

H 3.389990 0.020459 -0.429397

H 1.909437 2.213449 -0.229718

H 0.315546 -0.834212 1.524944

H -1.024669 2.519143 -0.011026

H -3.117045 1.190732 -0.114635

H -0.889211 -2.489597 -0.240302

H -3.009793 -1.258140 -0.459476

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 156.9335 | 191.1313 | 362.84 |
| 408.4019 | 502.8262 | 528.2811 |
| 538.6616 | 551.9228 | 595.8246 |
| 679.1964 | 707.3175 | 767.0203 |
| 784.8008 | 852.7908 | 861.1276 |
| 877.7528 | 908.8191 | 916.2119 |
| 977.1707 | 1000.494 | 1058.781 |
| 1069.515 | 1105.656 | 1129.655 |
| 1159.698 | 1179.323 | 1233.084 |
| 1269.626 | 1295.636 | 1330.238 |
| 1381.003 | 1389.511 | 1435.964 |
| 1468.922 | 1543.939 | 1579.458 |
| 1634.911 | 2804.764 | 3184.205 |
| 3189.93 | 3206.568 | 3217.417 |
| 3238.589 | 3263.826 | 3645.249 |

***i67***

**Cartesian coordinates**

N 2.625250 -0.920699 -0.000010

C 2.984582 0.400347 0.000185

C 1.834433 1.141706 0.000125

C 0.729767 0.236865 -0.000101

C 1.266737 -1.035404 -0.000193

C -0.673112 0.623076 -0.000214

C -1.730401 -0.199974 0.000112

C -3.108160 0.275773 -0.000080

C -4.184256 -0.480574 0.000221

H 3.266487 -1.693313 -0.000058

H 4.020188 0.698640 0.000351

H 1.773967 2.219480 0.000252

H 0.788707 -2.001617 -0.000419

H -0.858496 1.695912 -0.000589

H -3.240643 1.364139 -0.000512

H -5.254107 -0.331777 0.000160

H -1.590388 -1.277464 0.000557

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 30.0648 | 110.8253 | 116.6086 |
| 181.5966 | 293.7786 | 367.5032 |
| 369.843 | 506.8411 | 515.355 |
| 631.1421 | 646.6176 | 676.1074 |
| 715.5695 | 766.4167 | 798.1089 |
| 818.1201 | 844.1146 | 871.9696 |
| 901.763 | 913.1569 | 998.0872 |
| 1003.016 | 1094.319 | 1107.553 |
| 1143.123 | 1176.515 | 1226.394 |
| 1259.398 | 1316.603 | 1336.547 |
| 1359.018 | 1437.69 | 1494.664 |
| 1541.297 | 1618.454 | 1664.177 |
| 1723.358 | 3049.494 | 3149.903 |
| 3172.673 | 3252.543 | 3258.488 |
| 3274.296 | 3281.894 | 3720.165 |

***i68***

**Cartesian coordinates**

N -2.692810 -0.721555 0.110908

C -2.869120 0.625913 -0.057242

C -1.629525 1.201437 -0.122319

C -0.657802 0.162793 0.005637

C -1.361879 -1.015344 0.155494

C 0.785702 0.346150 -0.018695

C 1.701788 -0.615285 -0.193736

C 3.152734 -0.399470 -0.169352

C 3.792238 0.638391 0.323041

H -3.432657 -1.392444 0.213302

H -3.854281 1.058820 -0.117954

H -1.424037 2.252280 -0.258690

H -1.016398 -2.024630 0.311671

H 1.136169 1.368504 0.109175

H 1.377945 -1.634817 -0.386584

H 3.758415 -1.200602 -0.607078

H 4.819701 0.956258 0.422831

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 33.2454 | 90.6101 | 126.1579 |
| 174.8854 | 233.6582 | 347.8573 |
| 419.0084 | 512.5137 | 520.1042 |
| 621.5944 | 646.4256 | 669.1218 |
| 719.378 | 758.7051 | 801.2333 |
| 830.826 | 877.1273 | 878.9477 |
| 911.5732 | 913.6512 | 997.3534 |
| 1010.795 | 1031.199 | 1101.374 |
| 1107.144 | 1174.485 | 1233.46 |
| 1267.463 | 1312.928 | 1342.214 |
| 1360.628 | 1436.724 | 1496.96 |
| 1544.038 | 1621.863 | 1655.908 |
| 1720.836 | 3062.244 | 3163.526 |
| 3174.619 | 3257.702 | 3264.459 |
| 3279.004 | 3285.794 | 3719.643 |

***i69***

**Cartesian coordinates**

N 2.522318 -0.874083 -0.000044

C 2.847715 0.458675 0.000053

C 1.689962 1.178048 0.000085

C 0.586203 0.251139 -0.000001

C 1.162712 -1.021739 -0.000070

C -0.785734 0.592408 -0.000001

C -1.887283 -0.375582 -0.000170

C -3.219847 -0.028100 0.643645

C -3.219986 -0.027706 -0.643493

H 3.183063 -1.629237 -0.000049

H 3.877071 0.779813 0.000078

H 1.608966 2.254306 0.000106

H 0.709173 -1.999061 -0.000098

H -1.051488 1.645742 0.000049

H -1.588581 -1.424503 -0.000447

H -3.718279 0.163818 1.578703

H -3.718601 0.164852 -1.578318

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 54.9202 | 89.0832 | 143.6989 |
| 267.0443 | 333.3497 | 410.5084 |
| 417.1327 | 441.544 | 604.9065 |
| 619.7267 | 623.5295 | 653.1073 |
| 686.8177 | 752.6321 | 764.1946 |
| 774.2692 | 859.2435 | 882.6953 |
| 901.6734 | 928.6923 | 986.6033 |
| 1022.932 | 1047.535 | 1074.486 |
| 1095.037 | 1109.896 | 1173.125 |
| 1176.087 | 1227.242 | 1303.394 |
| 1345.037 | 1405.162 | 1470.17 |
| 1494.192 | 1543.27 | 1578.627 |
| 1740.167 | 3095.055 | 3173.021 |
| 3255.113 | 3262.056 | 3278.56 |
| 3289.288 | 3311.554 | 3722.397 |

***i70***

**Cartesian coordinates**

N 2.033851 -1.117697 -0.000003

C 2.698636 0.081947 0.000009

C 1.769746 1.078556 0.000004

C 0.459394 0.476333 -0.000010

C 0.682550 -0.904474 -0.000014

C -0.754506 1.207946 -0.000010

C -2.125337 0.676387 0.000003

C -2.505461 -0.648999 -0.643654

C -2.505439 -0.649001 0.643672

H 2.471437 -2.020685 -0.000001

H 3.776141 0.122742 0.000021

H 1.973585 2.138535 0.000010

H -0.009151 -1.728445 -0.000028

H -0.663496 2.289650 -0.000012

H -2.885358 1.458199 0.000012

H -2.608834 -1.174149 -1.578327

H -2.608778 -1.174144 1.578353

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 62.1344 | 101.2413 | 151.94 |
| 271.7853 | 285.034 | 410.435 |
| 441.672 | 525.307 | 572.2291 |
| 622.0273 | 637.8005 | 668.2676 |
| 696.052 | 758.3417 | 763.2135 |
| 772.1543 | 857.9914 | 882.8417 |
| 896.2189 | 908.103 | 964.2089 |
| 1021.219 | 1027.132 | 1070.204 |
| 1096.625 | 1103.334 | 1170.379 |
| 1188.299 | 1231.419 | 1302.677 |
| 1386.494 | 1424.302 | 1459.621 |
| 1496.13 | 1535.454 | 1581.237 |
| 1737.781 | 3101.239 | 3185.314 |
| 3255.114 | 3259.241 | 3282.126 |
| 3304.597 | 3308.736 | 3722.888 |

***i71***

**Cartesian coordinates**

N 2.202653 -0.961004 0.069279

C 2.630886 0.336187 0.012238

C 1.519681 1.136893 -0.061791

C 0.374368 0.292195 -0.049608

C 0.836758 -1.001317 0.032162

H 2.801436 -1.764751 0.123915

H 3.680862 0.579938 0.027552

H 1.517743 2.215035 -0.121212

H 0.297251 -1.934494 0.066333

C -1.059240 0.716710 -0.104087

C -1.993544 0.213616 1.005186

C -2.786786 -0.466721 0.084754

C -2.005424 -0.087219 -1.003598

H -1.125650 1.797916 -0.264744

H -1.987509 0.335453 2.079480

H -3.687060 -1.062163 0.179348

H -2.015828 -0.281969 -2.067161

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 14.7147 | 123.1724 | 148.4713 |
| 315.9667 | 385.3922 | 426.4752 |
| 500.9378 | 549.8318 | 564.6196 |
| 647.9099 | 676.8849 | 705.7978 |
| 790.1262 | 800.7926 | 860.6769 |
| 909.083 | 913.9378 | 919.6277 |
| 935.5356 | 949.7793 | 958.1085 |
| 1001.641 | 1082.382 | 1098.838 |
| 1157.127 | 1171.874 | 1187.345 |
| 1206.639 | 1226.595 | 1308.982 |
| 1326.901 | 1364.776 | 1444.949 |
| 1465.496 | 1494.75 | 1542.234 |
| 1625.244 | 3068.934 | 3210.528 |
| 3237.576 | 3252.279 | 3253.648 |
| 3275.375 | 3279.991 | 3721.674 |

**Transition states**

***i1 – i2***

**Cartesian coordinates**

C -0.912904 1.023991 0.060564

C -1.126812 -0.359077 -0.009601

N 1.145373 0.698725 -0.227313

C -0.037590 -1.219626 0.026093

C 1.165837 -0.507289 0.121175

H -0.473406 1.464102 0.949621

H -1.600473 1.686638 -0.459260

H -2.106614 -0.753824 -0.259618

H 1.743111 1.377677 0.234163

H -0.111416 -2.293661 -0.063106

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -606.872 | 402.5393 | 558.2762 |
| 596.3095 | 669.0316 | 721.2089 |
| 798.6082 | 841.4211 | 934.7428 |
| 958.1409 | 1022.486 | 1087.15 |
| 1112.471 | 1140.933 | 1207.226 |
| 1395.057 | 1449.035 | 1532.267 |
| 1685.724 | 3142.519 | 3199.449 |
| 3218.945 | 3251.759 | 3565.75 |

***i2 – i3***

**Cartesian coordinates**

C 0.666767 0.969907 -0.029017

C -0.710791 0.949352 -0.005639

N 1.005767 -0.496748 -0.013686

C -1.159621 -0.384142 -0.012844

C -0.121740 -1.328746 -0.020045

H 1.103602 0.171153 0.980623

H 1.406140 1.711969 -0.284642

H -1.321674 1.840193 0.044779

H 1.929613 -0.825934 -0.258041

H -2.205745 -0.658376 0.018353

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1612.78 | 577.9274 | 587.0062 |
| 648.8493 | 784.022 | 843.18 |
| 859.7155 | 869.9743 | 895.8858 |
| 959.4134 | 1024.806 | 1081.375 |
| 1123.121 | 1205.781 | 1262.722 |
| 1341.288 | 1382.801 | 1430.72 |
| 1542.748 | 2261.045 | 3224.978 |
| 3243.008 | 3284.843 | 3637.587 |

***i3 – pyrrole (3)***

**Cartesian coordinates**

N 1.034419 -0.426938 0.000822

C -1.175996 -0.321456 0.000872

C -0.211665 -1.306738 -0.095894

C -0.644647 1.002134 -0.007110

C 0.712608 0.928765 -0.007619

H 1.906805 -0.787891 -0.359846

H 0.742767 -1.105088 0.906725

H -2.231417 -0.550916 0.056820

H -1.212247 1.922097 0.018343

H 1.471358 1.694135 0.030712

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1299.91 | 538.9385 | 597.0165 |
| 670.8703 | 738.2924 | 777.6936 |
| 856.3227 | 879.2623 | 882.9838 |
| 953.2961 | 1052.498 | 1102.766 |
| 1136.305 | 1183.333 | 1215.434 |
| 1383.831 | 1440.253 | 1471.793 |
| 1604.058 | 2313.662 | 3232.786 |
| 3246.417 | 3279.799 | 3642.406 |

***i4 – i5***

**Cartesian coordinates**

C -2.429152 -0.480796 -0.027583

C -1.370673 0.090118 0.005331

C -0.121473 0.790844 0.030145

H -3.363095 -0.987042 -0.054965

H -0.179033 1.881328 0.058743

N 2.208486 -0.427581 -0.002945

C 1.045763 0.180354 0.013394

H 3.026980 0.003007 -0.408102

H 2.308964 -1.387346 0.297214

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -402.565 | 169.4052 | 173.5646 |
| 268.4313 | 413.0704 | 444.826 |
| 521.4801 | 604.1645 | 715.8553 |
| 723.3933 | 892.2387 | 1091.131 |
| 1106.393 | 1321.645 | 1641.693 |
| 1880.755 | 2221.711 | 3076.175 |
| 3485.666 | 3536.661 | 3626.807 |

***i5 – i6***

**Cartesian coordinates**

C -0.395539 1.173223 0.000025

C 0.893646 0.991688 -0.000015

N -1.158189 -0.423303 0.000008

C 1.190015 -0.466782 0.000005

C 0.067765 -1.176226 -0.000024

H -1.170465 1.919734 -0.000050

H -1.720000 -0.595867 0.830210

H -1.719991 -0.595771 -0.830219

H 2.182458 -0.896397 0.000053

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -739.458 | 271.1856 | 375.3746 |
| 596.0392 | 658.0922 | 659.72 |
| 754.8777 | 889.54 | 965.2704 |
| 973.0457 | 1021.611 | 1128.738 |
| 1158.345 | 1258.408 | 1580.128 |
| 1586.553 | 1608.382 | 3240.719 |
| 3316.404 | 3504.668 | 3592.189 |

***i6 – 3-pyrrolyl (11)***

**Cartesian coordinates**

C -1.014668 -0.656009 -0.007552

C 0.229132 -1.197240 -0.003633

N -0.793306 0.718169 0.001345

C 1.246218 -0.222668 0.000236

C 0.695137 1.047843 -0.100376

H -1.999002 -1.092142 0.033594

H -1.453196 1.397381 -0.353137

H -0.238652 1.235643 0.911057

H 2.309085 -0.399629 0.067029

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1388.48 | 554.1844 | 585.5934 |
| 666.7726 | 728.3598 | 773.1 |
| 837.3829 | 842.117 | 863.7101 |
| 1096.975 | 1105.162 | 1167.831 |
| 1209.938 | 1312.917 | 1381.4 |
| 1452.797 | 1551.401 | 2256.591 |
| 3260.608 | 3283.047 | 3630.91 |

***i7 – i8***

**Cartesian coordinates**

C 1.583014 0.590485 0.092352

C 1.067670 -0.565989 -0.010870

N -0.943357 1.049725 -0.051021

C -0.125814 -1.201755 -0.053453

C -1.177720 -0.228927 -0.048841

H 2.308379 1.157055 -0.467973

H 0.469507 1.141161 0.402155

H -1.749674 1.618628 0.175424

H -0.321724 -2.216351 0.258833

H -2.185894 -0.611454 0.113582

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1458.84 | 341.6874 | 384.9475 |
| 522.6393 | 592.7844 | 614.5794 |
| 736.2002 | 770.1798 | 776.8306 |
| 858.0609 | 1015.079 | 1050.519 |
| 1150.542 | 1191.016 | 1330.728 |
| 1368.372 | 1426.455 | 1535.225 |
| 1699.205 | 1931.745 | 3134.074 |
| 3250.811 | 3293.796 | 3602.219 |

***i8 – i9***

**Cartesian coordinates**

C -1.153690 -0.708483 -0.000120

C -1.139773 0.668695 0.000130

N 0.752619 -1.004104 0.000275

C 0.088640 1.229688 -0.000064

C 1.137532 0.220467 -0.000052

H -1.420432 -1.234465 -0.914980

H -1.420921 -1.234780 0.914427

H 1.454175 -1.734453 -0.000573

H 0.328758 2.285834 0.000073

H 2.193832 0.484392 -0.000241

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -484.895 | 302.297 | 488.9303 |
| 685.3483 | 694.8688 | 727.1114 |
| 792.6171 | 893.6858 | 995.3835 |
| 1016.996 | 1035.659 | 1040.206 |
| 1125.583 | 1147.455 | 1302.73 |
| 1378.554 | 1418.951 | 1562.417 |
| 1667.738 | 3133.397 | 3159.335 |
| 3208.325 | 3212.469 | 3600.615 |

***i9 – pyrrole (3)***

**Cartesian coordinates**

C 1.095370 -0.347331 -0.021628

C 0.039891 -1.328726 -0.104309

N 0.577194 0.951398 -0.018292

C -1.126907 -0.480185 0.003267

C -0.777574 0.843262 0.000918

H 2.143659 -0.498733 -0.247800

H 0.873044 -0.986234 0.999185

H 1.097161 1.810079 0.039385

H -2.145960 -0.839654 0.029923

H -1.392942 1.732635 0.037865

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -893.764 | 435.3519 | 585.4728 |
| 616.5848 | 806.8557 | 835.0183 |
| 900.3948 | 910.9479 | 956.2193 |
| 1051.671 | 1063.683 | 1126.207 |
| 1135.55 | 1179.321 | 1247.293 |
| 1345.396 | 1398.916 | 1505.233 |
| 1544.401 | 2272.969 | 3226.464 |
| 3227.865 | 3247.404 | 3690.305 |

***i7 – i9b***

**Cartesian coordinates**

C -1.100888 -0.688440 -0.000001

C -1.263873 0.596926 0.000001

N 0.637929 -1.011002 0.000000

C 0.076676 1.219491 0.000000

C 1.102717 0.358721 0.000000

H -1.613707 -1.635107 -0.000001

H 0.926864 -1.526646 0.828167

H 0.926870 -1.526649 -0.828163

H 0.241100 2.291885 0.000000

H 2.165575 0.553343 -0.000001

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -387.047 | 287.4508 | 470.9893 |
| 590.7168 | 638.5279 | 726.3111 |
| 734.6217 | 785.7766 | 968.473 |
| 987.5805 | 1021.485 | 1052.462 |
| 1146.376 | 1163.513 | 1180.585 |
| 1362.125 | 1593.615 | 1628.963 |
| 1635.096 | 3201.828 | 3253.472 |
| 3309.169 | 3497.774 | 3584.209 |

***Benzene (1) + amino (13) – i10***

**Cartesian coordinates**

C 0.228809 1.177128 0.523906

C 0.864174 -0.079018 0.717013

C 0.094994 -1.253474 0.475043

C -1.145883 -1.163348 -0.114406

C -1.705970 0.087090 -0.408184

C -1.018168 1.251351 -0.072766

N 2.155390 -0.121787 -0.827781

H 0.747251 2.082997 0.818708

H 1.697711 -0.142895 1.404453

H 0.528948 -2.218995 0.704693

H -1.703377 -2.066671 -0.336396

H -2.684459 0.148057 -0.870175

H -1.471569 2.218877 -0.257201

H 1.454079 -0.151868 -1.574470

H 2.435949 0.864628 -0.818789

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -585.253 | 136.3242 | 163.2273 |
| 190.0394 | 396.0845 | 420.532 |
| 609.801 | 616.5975 | 678.3798 |
| 728.5064 | 778.3953 | 844.5637 |
| 857.0946 | 901.4735 | 961.5977 |
| 996.0042 | 1007.757 | 1019.226 |
| 1039.272 | 1052.633 | 1063.124 |
| 1177.717 | 1187.678 | 1205.04 |
| 1329.781 | 1379.919 | 1494.191 |
| 1510.692 | 1549.051 | 1602.012 |
| 1629.482 | 3185.932 | 3193.34 |
| 3201.525 | 3213.778 | 3215.723 |
| 3226.733 | 3413.96 | 3513.154 |

***i10 – aniline (4) + H***

**Cartesian coordinates**

C 0.198501 1.216726 -0.019704

C 0.928092 0.000008 0.100555

C 0.198516 -1.216718 -0.019658

C -1.180646 -1.203347 -0.040859

C -1.885426 -0.000006 -0.027488

C -1.180663 1.203341 -0.040875

N 2.321072 -0.000047 -0.045373

H 0.741902 2.155616 -0.028994

H 0.807948 0.000080 1.799279

H 0.741929 -2.155601 -0.028884

H -1.718594 -2.143971 -0.082257

H -2.968406 -0.000015 -0.045993

H -1.718618 2.143960 -0.082285

H 2.697959 -0.835104 -0.462955

H 2.698123 0.835348 -0.462126

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1219.6 | 120.4088 | 200.4818 |
| 365.879 | 418.4749 | 494.1412 |
| 516.1561 | 528.1903 | 559.7245 |
| 629.594 | 674.1649 | 685.306 |
| 770.1666 | 814.771 | 836.0693 |
| 907.6397 | 976.8084 | 991.9922 |
| 1005.66 | 1050.248 | 1076.843 |
| 1147.491 | 1179.434 | 1208.886 |
| 1305.371 | 1332.597 | 1372.59 |
| 1509.126 | 1523.387 | 1612.63 |
| 1657.773 | 1671.558 | 3188.642 |
| 3190.731 | 3204.345 | 3208.999 |
| 3225.593 | 3616.047 | 3718.046 |

***i11 – i12***

**Cartesian coordinates**

C -1.424572 0.022075 -0.180515

C -2.659177 0.026561 -0.068473

C -0.006988 0.012729 -0.090985

C 0.693672 -1.202724 -0.052404

C 2.076673 -1.209943 0.034002

C 2.783564 -0.013025 0.079174

C 2.098808 1.196737 0.036139

C 0.715775 1.214863 -0.048436

N -3.990211 -0.137131 0.056465

H 0.139836 -2.133101 -0.093055

H 2.606381 -2.155160 0.064660

H 3.865276 -0.023110 0.147037

H 2.645749 2.132077 0.068331

H 0.179383 2.155615 -0.085363

H -2.748427 -0.079129 1.081938

H -4.423256 0.779082 0.170182

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1379.49 | 82.0757 | 88.268 |
| 206.5947 | 253.4214 | 304.9239 |
| 356.4886 | 407.3446 | 416.5765 |
| 478.3479 | 517.966 | 522.2995 |
| 637.9407 | 710.2887 | 729.8801 |
| 779.2767 | 863.587 | 944.869 |
| 1001.099 | 1020.609 | 1021.264 |
| 1040.834 | 1068.451 | 1111.732 |
| 1162.711 | 1187.713 | 1212.549 |
| 1315.551 | 1350.754 | 1356.826 |
| 1486.098 | 1538.91 | 1639.537 |
| 1672.637 | 2196.414 | 2734.638 |
| 3195.327 | 3203.92 | 3213.241 |
| 3220.478 | 3226.559 | 3505.26 |

***i12 – i13***

**Cartesian coordinates**

C 2.105475 -0.725763 -0.241073

C 2.113966 0.699161 -0.152833

C 0.978287 1.388642 0.147409

C -0.252298 0.681586 0.283395

C -0.227816 -0.762170 0.428920

C 0.987954 -1.438063 0.065627

N -1.955842 -0.967173 -0.325915

C -1.498513 1.211186 -0.048592

C -2.458338 0.197535 -0.188221

H 3.023805 -1.242527 -0.496323

H 3.033607 1.234949 -0.358507

H 0.968804 2.472976 0.153786

H -0.715040 -1.174320 1.314153

H 1.021851 -2.520627 0.114553

H -2.460083 -1.772203 0.033992

H -1.674347 2.259280 -0.248052

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -547.942 | 177.6952 | 216.3503 |
| 357.0414 | 439.6254 | 518.6792 |
| 557.0323 | 565.8172 | 600.1755 |
| 652.0934 | 736.3319 | 752.7208 |
| 817.2044 | 834.8485 | 860.7355 |
| 894.3145 | 921.5001 | 977.3209 |
| 1004.585 | 1014.115 | 1032.436 |
| 1131.703 | 1148.056 | 1173.11 |
| 1193.301 | 1204.676 | 1264.639 |
| 1319.073 | 1384.18 | 1418.685 |
| 1473.759 | 1497.483 | 1574.948 |
| 1594.014 | 1679.155 | 3109.682 |
| 3192.08 | 3199.937 | 3211.596 |
| 3221.168 | 3238.017 | 3559.921 |

***i13 – i14***

**Cartesian coordinates**

C 2.116148 -0.717288 -0.077467

C 2.120984 0.701694 0.005559

C 0.961994 1.430394 0.067876

C -0.283237 0.753843 0.041553

C -0.243100 -0.660778 0.085176

C 0.942045 -1.420062 -0.062578

N -1.692278 -1.023919 0.018373

C -1.631692 1.157825 -0.086953

C -2.530816 0.087657 -0.098428

H 3.057930 -1.246558 -0.158426

H 3.075267 1.216233 -0.005873

H 0.989234 2.513719 0.086431

H -0.972438 -1.027234 1.087350

H 0.920513 -2.502013 -0.119098

H -1.996162 -1.978463 -0.110848

H -1.942357 2.192048 -0.156570

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1596.86 | 201.7258 | 236.8812 |
| 368.4437 | 428.5849 | 532.3453 |
| 560.8529 | 585.3464 | 614.2125 |
| 704.591 | 745.7504 | 751.1044 |
| 761.6924 | 845.0591 | 857.7571 |
| 878.799 | 909.5312 | 968.3676 |
| 1008.205 | 1026.707 | 1040.712 |
| 1099.097 | 1165.332 | 1180.015 |
| 1195.042 | 1210.388 | 1275.549 |
| 1326.91 | 1347.353 | 1400.684 |
| 1426.185 | 1492.461 | 1518.977 |
| 1618.638 | 1667.175 | 2138.982 |
| 3198.798 | 3207.411 | 3217.915 |
| 3226.578 | 3229.068 | 3645.479 |

***i14 – indole (2)***

**Cartesian coordinates**

C 2.127673 -0.713032 0.005367

C 0.934706 -1.410515 0.009724

C -0.238467 -0.660912 -0.006141

C -0.255740 0.739193 -0.015346

C 0.969395 1.423805 -0.006999

C 2.140363 0.692822 0.001340

N -1.574356 -1.079914 -0.001059

C -1.632108 1.163463 0.003617

C -2.521942 0.127047 -0.080251

H 3.066388 -1.254368 0.008445

H 0.915142 -2.494422 0.020184

H 0.992779 2.507487 -0.005780

H 3.093796 1.208892 0.007367

H -2.366410 -0.832131 0.862090

H -1.876319 -1.942583 -0.432448

H -1.948157 2.195288 0.079689

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1555.81 | 205.1332 | 240.2522 |
| 390.7853 | 431.5996 | 504.3466 |
| 547.5729 | 586.3633 | 614.5045 |
| 652.3738 | 729.5202 | 765.2198 |
| 768.7836 | 786.3635 | 854.5208 |
| 880.6555 | 900.2822 | 910.2779 |
| 964.8833 | 1007.034 | 1043.604 |
| 1129.11 | 1151.441 | 1159.943 |
| 1186.484 | 1254.047 | 1273.428 |
| 1317.267 | 1372.86 | 1416.834 |
| 1467.375 | 1517.965 | 1546.268 |
| 1653.896 | 1685.917 | 2266.945 |
| 3197.38 | 3205.521 | 3215.856 |
| 3225.341 | 3235.82 | 3638.962 |

***i15 – i16***

**Cartesian coordinates**

C 2.174157 0.683171 0.157711

C 2.109952 -0.725111 0.115026

C 0.917190 -1.383351 -0.083015

C -0.255452 -0.622488 -0.185860

C -0.207087 0.795195 -0.260561

C 1.045440 1.432080 -0.062047

C -2.035057 1.065825 0.260722

N -1.526603 -1.097096 -0.030013

C -2.496505 -0.154965 0.169241

H 3.127504 1.169340 0.326366

H 3.015647 -1.301621 0.265910

H 0.867883 -2.466648 -0.070048

H -0.847548 1.240185 -1.047340

H 1.106327 2.512309 -0.127465

H -2.400306 2.062267 0.078129

H -1.699106 -2.078302 0.117232

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -529.909 | 167.691 | 224.0751 |
| 377.9881 | 431.2813 | 493.701 |
| 557.5927 | 570.8754 | 602.7161 |
| 623.2823 | 630.6653 | 707.3407 |
| 761.2539 | 765.8647 | 786.9729 |
| 861.7135 | 874.6986 | 963.637 |
| 1004.621 | 1014.242 | 1031.908 |
| 1056.156 | 1094.08 | 1172.196 |
| 1180.666 | 1193.174 | 1291.498 |
| 1312.015 | 1396.117 | 1430.946 |
| 1506.384 | 1511.431 | 1582.408 |
| 1625.782 | 1670.393 | 2934.039 |
| 3194.751 | 3200.923 | 3212.466 |
| 3223.44 | 3311.085 | 3660.84 |

***i16 – i17***

**Cartesian coordinates**

C -2.119176 0.702452 -0.090843

C -2.096444 -0.722145 -0.022052

C -0.922434 -1.421860 0.064138

C 0.277541 -0.687065 0.071432

C 0.288696 0.752705 0.127591

C -0.974748 1.436095 -0.037118

C 1.764491 1.093443 -0.075126

N 1.558274 -1.075803 -0.054086

C 2.520873 -0.065699 -0.112165

H -3.075130 1.203277 -0.189515

H -3.036483 -1.260255 -0.061721

H -0.910448 -2.505766 0.069834

H 0.725517 0.989000 1.171181

H -0.999030 2.519020 -0.067474

H 2.133211 2.105899 0.011649

H 1.821647 -2.048112 -0.110497

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -617.009 | 204.8155 | 248.6284 |
| 373.5829 | 439.4946 | 535.7299 |
| 557.1762 | 595.6097 | 612.6828 |
| 722.8818 | 741.252 | 766.9787 |
| 788.1136 | 798.7996 | 869.7971 |
| 873.0237 | 906.5823 | 972.4321 |
| 1007.807 | 1020.591 | 1063.593 |
| 1079.952 | 1102.962 | 1174.286 |
| 1198.573 | 1203.844 | 1268.59 |
| 1335.009 | 1347.359 | 1415.573 |
| 1442.596 | 1489.2 | 1527.256 |
| 1608.663 | 1684.021 | 2596.831 |
| 3197.54 | 3206.384 | 3218.191 |
| 3225.407 | 3249.663 | 3648.851 |

***i17 – indole (2)***

**Cartesian coordinates**

C 2.142071 0.703652 0.005650

C 2.121536 -0.700913 0.007906

C 0.934978 -1.409878 -0.001365

C -0.251771 -0.673258 -0.008310

C -0.246138 0.729959 -0.009718

C 0.963922 1.426491 -0.001920

C -1.645941 1.111678 -0.037216

N -1.569009 -1.083280 -0.004464

C -2.480797 -0.051552 -0.094482

H 3.094573 1.220154 0.009179

H 3.061499 -1.241362 0.018145

H 0.928169 -2.493773 0.000719

H 0.977763 2.510702 -0.006500

H -2.035431 2.113524 -0.165561

H -2.415657 0.702262 0.967273

H -1.855012 -2.045625 0.044724

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1204.47 | 207.1687 | 245.3289 |
| 397.9885 | 431.2648 | 549.17 |
| 569.1956 | 588.5446 | 626.5997 |
| 668.6708 | 755.2237 | 778.7689 |
| 780.6503 | 842.0045 | 872.1547 |
| 902.0687 | 934.7201 | 966.2479 |
| 1004.168 | 1044.08 | 1084.881 |
| 1146.961 | 1169.445 | 1194.551 |
| 1239.451 | 1264.484 | 1289.894 |
| 1320.874 | 1372.716 | 1377.104 |
| 1446.566 | 1514.509 | 1539.685 |
| 1657.167 | 1692.204 | 2154.094 |
| 3196.287 | 3204.629 | 3214.941 |
| 3225.245 | 3232.519 | 3697.656 |

***i18 – i19***

**Cartesian coordinates**

C -1.992105 -1.275514 0.046534

C -2.943513 -0.289151 0.004865

C -2.275754 0.975798 -0.019340

C -0.945004 0.672145 0.006789

N -0.757040 -0.667609 0.048766

H -2.085531 -2.349178 0.072937

H -4.011988 -0.443302 -0.007488

H -2.725518 1.954358 -0.051431

H 0.138660 -1.128108 0.069589

C 2.909732 -1.555944 -0.197177

C 2.587371 -0.432521 0.088678

C 2.169803 0.880448 0.449745

C 1.478087 1.678413 -0.375346

H 3.219029 -2.539519 -0.458598

H 2.396143 1.200073 1.461894

H 1.169689 2.666784 -0.058889

H 1.267091 1.390115 -1.397865

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -92.5269 | 41.942 | 50.0534 |
| 75.1151 | 105.3299 | 166.5461 |
| 228.0585 | 360.7032 | 480.3921 |
| 559.7829 | 567.0592 | 634.8388 |
| 684.6569 | 709.0247 | 713.5088 |
| 721.7072 | 772.67 | 853.3869 |
| 876.6526 | 891.8045 | 898.5745 |
| 968.9828 | 1002.79 | 1034.669 |
| 1076.768 | 1114.854 | 1134.243 |
| 1193.64 | 1271.202 | 1316.305 |
| 1391.572 | 1440.683 | 1449.806 |
| 1485.132 | 1578.206 | 1653.005 |
| 2221.922 | 3170.419 | 3186.713 |
| 3247.355 | 3269.709 | 3273.613 |
| 3279.854 | 3481.508 | 3670.496 |

***i19 – i20***

**Cartesian coordinates**

C -2.785790 -0.196903 -0.288764

C -2.058144 -1.309821 0.065380

C -0.733352 -0.841656 0.258257

C -0.693946 0.499767 0.031129

N -1.954287 0.901298 -0.307592

C 3.703487 -0.495629 -0.645835

C 2.713690 -0.226587 -0.016826

C 1.517993 0.065558 0.710995

C 0.616355 1.201574 0.180476

H -3.832758 -0.098908 -0.531145

H -2.445364 -2.311252 0.162627

H 0.676184 -0.908075 0.584411

H -2.240761 1.834761 -0.543570

H 4.581977 -0.730547 -1.196569

H 1.678771 0.105239 1.788648

H 0.581857 2.035156 0.888978

H 0.998342 1.586715 -0.769111

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1880.95 | 51.9388 | 133.1444 |
| 183.9122 | 240.2215 | 363.7052 |
| 404.9119 | 467.1954 | 487.2949 |
| 566.5507 | 615.713 | 644.6212 |
| 658.8887 | 703.1555 | 708.1311 |
| 721.9347 | 859.4073 | 864.4731 |
| 889.6055 | 927.64 | 993.1058 |
| 1028.483 | 1081.152 | 1094.714 |
| 1138.855 | 1188.858 | 1208.398 |
| 1248.375 | 1262.591 | 1323.55 |
| 1356.926 | 1431.108 | 1488.218 |
| 1504.563 | 1515.484 | 1614.405 |
| 1668.225 | 2207.775 | 3055.914 |
| 3095.295 | 3132.686 | 3259.502 |
| 3278.742 | 3482.717 | 3708.157 |

***i20 – i21***

**Cartesian coordinates**

C -1.822281 1.200255 0.070470

C -2.510997 0.010480 0.131162

N -1.610798 -1.015063 0.011744

C -0.336821 -0.511428 -0.126467

C -0.463063 0.850178 -0.099725

C 1.693241 1.722172 -0.143528

C 2.202353 0.640793 0.089307

C 2.125994 -0.794081 0.361216

C 0.870498 -1.375360 -0.329737

H -2.253838 2.185949 0.144229

H -3.564196 -0.184933 0.259559

H -1.848665 -1.991611 0.019599

H 1.543564 2.757837 -0.345101

H 3.019924 -1.322047 0.019475

H 2.055510 -0.935797 1.444510

H 1.079075 -1.479229 -1.400588

H 0.690675 -2.382785 0.059920

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -402.784 | 86.8034 | 133.2894 |
| 231.413 | 293.3263 | 342.7147 |
| 395.6026 | 465.9677 | 534.7017 |
| 612.9805 | 637.9454 | 690.1643 |
| 692.4941 | 709.8038 | 739.0448 |
| 847.7134 | 853.8995 | 879.0224 |
| 924.0963 | 988.1056 | 1017.652 |
| 1028.91 | 1108.659 | 1139.569 |
| 1189.31 | 1218.353 | 1227.131 |
| 1286.787 | 1349.219 | 1377.016 |
| 1440.165 | 1468.808 | 1476.366 |
| 1491.695 | 1509.31 | 1606.578 |
| 2094.459 | 3042.061 | 3060.511 |
| 3086.378 | 3109.24 | 3255.99 |
| 3275.668 | 3447.99 | 3700.725 |

***i21 – i22***

**Cartesian coordinates**

C -1.693211 1.124177 -0.049957

C -2.410878 -0.037268 -0.064994

N -1.527220 -1.093937 -0.003996

C -0.251728 -0.620317 0.040524

C -0.308754 0.766872 0.018707

C 0.907229 1.521072 0.138871

C 2.105123 0.891038 -0.203443

C 2.183936 -0.518653 -0.163490

C 0.996989 -1.430035 0.149096

H -2.102098 2.121758 -0.090082

H -3.473625 -0.209155 -0.121422

H -1.788001 -2.064087 -0.006250

H 0.884914 2.555959 0.462599

H 3.041699 -0.994914 -0.635688

H 1.002618 -2.251255 -0.578363

H 1.090880 -1.900347 1.137885

H 2.861917 0.218283 0.667412

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1595.93 | 108.164 | 219.2578 |
| 262.6788 | 382.593 | 477.1701 |
| 493.5499 | 525.2504 | 570.1071 |
| 629.7542 | 654.8736 | 680.8351 |
| 709.4016 | 738.0973 | 760.9685 |
| 836.7586 | 871.0673 | 911.7994 |
| 925.8838 | 973.0952 | 1077.076 |
| 1095.804 | 1111.397 | 1180.999 |
| 1200.534 | 1237.658 | 1241.352 |
| 1287.22 | 1335.271 | 1365.867 |
| 1385.087 | 1449.365 | 1463.926 |
| 1473.299 | 1526.455 | 1535.649 |
| 1611.684 | 2164.575 | 3005.741 |
| 3047.907 | 3141.267 | 3186.42 |
| 3262.675 | 3286.187 | 3713.038 |

***i22 – indole (2)***

**Cartesian coordinates**

N -1.553096 1.072717 -0.070324

C -2.396227 -0.014898 -0.010823

C -1.660742 -1.160037 0.037348

C -0.280074 -0.769556 0.011749

C -0.255422 0.637433 -0.056835

C 0.934694 -1.470075 0.035024

C 2.123002 -0.761180 -0.023105

C 0.945353 1.372838 -0.053060

C 2.132798 0.635443 -0.093155

H -1.844295 2.033256 -0.075955

H -3.466194 0.122851 -0.013735

H -2.052983 -2.163556 0.084170

H 0.941684 -2.553061 0.087616

H 3.066256 -1.295116 -0.023855

H 0.939979 1.926452 1.754802

H 0.949347 2.437445 -0.255648

H 3.077591 1.162900 -0.147986

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -819.968 | 202.218 | 232.7716 |
| 298.7785 | 373.31 | 409.5088 |
| 436.0032 | 495.318 | 552.279 |
| 590.214 | 619.4892 | 628.7945 |
| 730.3406 | 759.2546 | 779.5671 |
| 802.6613 | 880.1217 | 889.1619 |
| 899.3364 | 919.1978 | 975.4413 |
| 1007.404 | 1038.32 | 1095.089 |
| 1122.113 | 1143.067 | 1180.311 |
| 1232.673 | 1265.989 | 1313.056 |
| 1374.566 | 1390.477 | 1469.176 |
| 1497.872 | 1534.31 | 1574.421 |
| 1631.291 | 1672.252 | 3194.948 |
| 3201.119 | 3211.39 | 3223.453 |
| 3262.101 | 3282.303 | 3724.476 |

***i23 – i24***

**Cartesian coordinates**

C 1.621971 -1.047301 -0.065211

C 2.772119 -0.551910 0.150704

C 0.315858 -0.666145 -0.140700

C 0.211200 0.806051 -0.098456

C -1.137673 1.314722 -0.017284

C -2.215164 0.488826 0.032150

C -2.080868 -0.929058 0.062777

C -0.840965 -1.481670 0.002761

N 1.292892 1.541659 -0.034166

H 3.743547 -0.621765 -0.309727

H -1.273933 2.390692 -0.039358

H -3.209147 0.922982 0.060323

H -2.963033 -1.552905 0.131712

H -0.706522 -2.556650 0.020500

H 2.388475 0.525845 0.580941

H 1.091493 2.499098 0.234332

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1295.17 | 147.7519 | 185.9516 |
| 285.3147 | 391.8924 | 442.1419 |
| 500.2995 | 539.5257 | 542.8887 |
| 569.8365 | 580.6024 | 700.3796 |
| 737.4251 | 745.2156 | 761.863 |
| 798.5263 | 840.7412 | 856.8418 |
| 888.5561 | 978.1008 | 1002.697 |
| 1030.448 | 1103.291 | 1154.467 |
| 1212.607 | 1246.649 | 1320.698 |
| 1343.398 | 1371.969 | 1420.714 |
| 1514.442 | 1526.739 | 1579.033 |
| 1697.069 | 1852.793 | 1947.899 |
| 3188.098 | 3204.516 | 3211.308 |
| 3228.002 | 3294.373 | 3573.349 |

***i24 – i25***

**Cartesian coordinates**

C 1.543955 -1.240272 -0.000005

C 2.586887 -0.374798 -0.000015

C 0.286008 -0.739235 0.000006

C 0.270668 0.747460 0.000008

C -1.023851 1.391913 -0.000005

C -2.151780 0.642355 -0.000011

C -2.137135 -0.797306 0.000001

C -0.958359 -1.459305 0.000008

N 1.426641 1.323454 0.000015

H 3.134825 -0.185734 -0.920383

H 3.134861 -0.185747 0.920334

H -1.078557 2.475150 -0.000022

H -3.114223 1.144800 -0.000025

H -3.079038 -1.331914 0.000004

H -0.914877 -2.542203 0.000024

H 1.432153 2.336598 0.000036

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -460.411 | 142.1193 | 196.6137 |
| 330.88 | 420.4945 | 480.4621 |
| 515.4339 | 550.7167 | 557.0368 |
| 644.8018 | 651.2545 | 715.2959 |
| 762.1879 | 764.703 | 781.6345 |
| 855.2971 | 890.9487 | 971.2532 |
| 977.0436 | 998.5799 | 1006.475 |
| 1014.75 | 1092.592 | 1148.054 |
| 1201.179 | 1228.35 | 1272.815 |
| 1368.067 | 1400.683 | 1427.984 |
| 1491.886 | 1562.943 | 1613.292 |
| 1668.734 | 1728.658 | 3140.576 |
| 3186.131 | 3204.093 | 3210.809 |
| 3223.509 | 3228.07 | 3590.338 |

***i25 – indole (2)***

**Cartesian coordinates**

C 2.162022 -0.678077 0.008619

C 2.110901 0.727686 0.015394

C 0.915364 1.419574 0.002792

C -0.257915 0.658271 -0.023132

C -0.236584 -0.754830 -0.015311

C 0.997490 -1.418234 -0.004881

C -2.361409 -0.105985 0.003285

N -1.566134 1.056913 -0.043889

C -1.580633 -1.313261 -0.095090

H 3.125590 -1.173392 0.017187

H 3.040852 1.286172 0.028178

H 0.894239 2.503366 0.004460

H 1.013667 -2.502179 -0.009677

H -2.300381 -0.706084 1.047759

H -3.417633 -0.015767 -0.224257

H -1.888799 1.998636 0.093514

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -777.739 | 198.3117 | 235.9162 |
| 368.2086 | 412.2526 | 435.0824 |
| 552.678 | 568.7592 | 603.1456 |
| 620.5982 | 765.0315 | 773.6087 |
| 781.7804 | 861.5182 | 877.8885 |
| 898.9868 | 953.804 | 981.8424 |
| 1010.55 | 1040.63 | 1068.291 |
| 1119.187 | 1150.087 | 1177.115 |
| 1232.689 | 1253.198 | 1293.112 |
| 1312.425 | 1368.585 | 1387.505 |
| 1439.021 | 1492.044 | 1542.845 |
| 1638.663 | 1692.954 | 2329.333 |
| 3191.62 | 3207.433 | 3213.225 |
| 3215.567 | 3226.339 | 3696.714 |

***i26 – i3***

**Cartesian coordinates**

N 1.176626 -0.842883 -0.000042

C 0.221101 1.333128 0.000064

C 1.169426 0.508067 0.000188

H 1.544980 -1.276882 0.836604

H 1.543578 -1.276380 -0.837568

H 0.036418 2.391443 -0.000755

C -1.416152 0.276815 0.000033

C -1.275652 -0.950784 0.000023

H -2.145748 1.065035 0.000025

H -1.407950 -2.006389 0.000144

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -564.203 | 187.8549 | 208.1918 |
| 262.365 | 447.976 | 488.5769 |
| 539.2022 | 606.8452 | 700.7887 |
| 714.2379 | 742.0725 | 763.5871 |
| 890.0457 | 973.0256 | 1167.238 |
| 1180.712 | 1640.409 | 1843.592 |
| 1953.208 | 3318.671 | 3344.515 |
| 3464.248 | 3565.031 | 3655.059 |

***i27 – i28***

**Cartesian coordinates**

N 0.159147 -0.929177 -0.147343

C 2.194526 0.558149 0.054728

C 1.220066 -0.147325 -0.097355

H -0.141053 -1.093826 -1.105940

H 3.063775 1.157647 0.169891

C -1.400145 -0.020589 0.574809

C -2.067983 0.566978 -0.275830

H -1.249616 -0.292317 1.598984

H -2.465918 0.989457 -1.169641

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -741.204 | 77.7697 | 156.1272 |
| 311.701 | 441.6802 | 483.0281 |
| 509.6919 | 517.7982 | 638.1043 |
| 702.8756 | 746.3373 | 791.1369 |
| 949.897 | 1092.051 | 1198.207 |
| 1835.634 | 2097.614 | 3365.625 |
| 3458.858 | 3487.207 | 3530.495 |

***i28 – i29***

**Cartesian coordinates**

N -0.052775 0.789559 -0.227630

C 2.148106 -0.438567 0.126500

C 1.105856 0.130386 -0.055555

H -0.165226 1.243647 -1.121499

H 3.073482 -0.932571 0.290096

C -1.274079 0.271729 0.356937

C -1.846997 -0.817571 -0.081289

H -1.677570 0.855961 1.179413

H -1.658571 -1.569820 -0.834158

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -182.497 | 164.9651 | 310.1004 |
| 402.6628 | 481.2011 | 540.8217 |
| 567.5611 | 744.9217 | 762.7226 |
| 859.9582 | 913.6553 | 1016.494 |
| 1180.113 | 1303.284 | 1440.948 |
| 1663.411 | 2266.124 | 3172.879 |
| 3260.266 | 3495.185 | 3626.445 |

***i29 – 2-pyrrolyl (16)***

**Cartesian coordinates**

N 0.258294 -1.080200 -0.052401

C -1.541406 0.511484 0.017257

C -0.998270 -0.595951 0.000434

C 1.204355 -0.042072 0.001246

C 0.759014 1.200785 0.011610

H 0.487040 -2.017557 0.224556

H -2.275946 1.280980 -0.036255

H 2.249627 -0.334886 0.008344

H 1.189066 2.187390 -0.013109

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -461.379 | 261.2755 | 358.1603 |
| 450.4221 | 509.0293 | 533.7082 |
| 646.527 | 704.1429 | 746.3784 |
| 840.0155 | 877.3599 | 1064.069 |
| 1164.104 | 1256.666 | 1447.245 |
| 1658.161 | 1991.789 | 3183.863 |
| 3301.775 | 3454.21 | 3710.607 |

***i30 – i31***

**Cartesian coordinates**

N -2.156463 0.401067 0.00000

C -0.076050 -1.106783 0.00000

C -1.049621 -0.304401 0.00000

C 1.874568 0.915152 0.00000

C 1.968694 -0.295946 0.00000

H -2.626042 0.629457 0.86143

H -2.626042 0.629458 -0.86143

H 1.634150 1.951718 0.00000

H 2.407632 -1.266236 0.00000

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -458.348 | 15.0382 | 93.3235 |
| 233.9455 | 263.6186 | 337.0115 |
| 374.4529 | 496.2829 | 586.2826 |
| 676.8248 | 768.1702 | 829.0835 |
| 1139.062 | 1148.154 | 1643.248 |
| 1952.592 | 2034.337 | 3417.996 |
| 3503.043 | 3594.797 | 3704.211 |

***i31 – i32***

**Cartesian coordinates**

N -1.185029 0.645115 -0.000034

C 0.097824 -1.240050 -0.000042

C -1.064074 -0.729895 0.000091

C 0.982988 0.975512 0.000069

C 1.257728 -0.309898 -0.000010

H -1.585726 1.055292 0.837132

H -1.585366 1.055149 -0.837447

H 1.546804 1.895728 -0.000015

H 2.272701 -0.695991 -0.000082

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -503.778 | 168.5684 | 355.9837 |
| 489.0846 | 507.1543 | 585.7536 |
| 646.8546 | 737.7657 | 840.7373 |
| 845.4931 | 989.992 | 1116.241 |
| 1133.123 | 1191.879 | 1575.991 |
| 1614.529 | 1738.396 | 3172.916 |
| 3271.274 | 3530.276 | 3624.938 |

***i32 – 3-pyrrolyl (11)***

**Cartesian coordinates**

N 0.754795 0.759179 -0.000781

C -0.104373 -1.241669 0.006746

C 1.145361 -0.742017 -0.089744

C -0.629835 0.920047 -0.011095

C -1.184442 -0.326451 -0.003700

H 1.395062 1.452847 -0.363457

H 1.287020 0.217918 0.898977

H -1.083776 1.898721 0.029406

H -2.242132 -0.543192 0.027305

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1357.31 | 529.0305 | 545.2846 |
| 619.2897 | 693.7299 | 751.3529 |
| 825.8286 | 865.6192 | 910.2099 |
| 1058.397 | 1119.566 | 1149.887 |
| 1175.952 | 1356.844 | 1404.071 |
| 1446.391 | 1559.644 | 2280.436 |
| 3249.288 | 3270.41 | 3629.959 |

***i33 – i34***

**Cartesian coordinates**

N -1.385237 -1.026961 0.079650

C -0.383402 1.176779 -0.146066

C -1.412265 0.349673 -0.127895

H -2.186875 -1.391811 0.569665

H -0.512592 -1.361826 0.462390

H -0.303456 2.217312 -0.419560

H -2.410016 0.738937 -0.345489

C 2.028427 -0.562371 -0.349296

C 1.644898 0.259840 0.457102

H 2.210377 -1.234501 -1.154556

H 1.633277 0.877083 1.326941

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -439.832 | 67.4141 | 125.3156 |
| 148.6041 | 260.2879 | 393.7617 |
| 517.6273 | 565.3414 | 588.5465 |
| 685.3875 | 707.2392 | 752.5524 |
| 784.7148 | 870.6993 | 881.0653 |
| 1105.255 | 1244.665 | 1325.019 |
| 1646.016 | 1713.433 | 1949.655 |
| 3090.632 | 3265.797 | 3400.122 |
| 3490.172 | 3586.706 | 3695.5 |

***i34 – i35***

**Cartesian coordinates**

N -1.014730 -0.791457 0.033442

C 0.215476 1.186264 -0.059445

C -1.027231 0.645618 -0.003948

C 0.869546 -1.064013 -0.122294

C 1.271645 0.227986 0.026711

H -1.229938 -1.232143 -0.851599

H -1.625505 -1.186411 0.751437

H 0.378225 2.256365 -0.033078

H -1.956648 1.171106 0.165350

H 1.294114 -1.956139 0.333276

H 2.266252 0.512292 0.354374

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -695.84 | 277.9548 | 527.0034 |
| 554.4973 | 602.6066 | 637.9898 |
| 725.3617 | 774.7135 | 819.9692 |
| 906.91 | 962.3691 | 1007.969 |
| 1029.701 | 1060.238 | 1139.317 |
| 1207.656 | 1222.417 | 1401.786 |
| 1479.791 | 1588.032 | 1650.628 |
| 3156.823 | 3189.977 | 3219.668 |
| 3240.818 | 3421.963 | 3596.452 |

***i35 – pyrrole (3) + H***

**Cartesian coordinates**

N -1.117199 -0.000011 -0.013482

C 1.028603 0.710225 -0.025230

C -0.267699 1.137934 0.088213

C -0.267687 -1.137924 0.088244

C 1.028605 -0.710208 -0.025230

H -1.769427 -0.000034 -1.162418

H -1.927268 -0.000027 0.592772

H 1.894144 1.350960 -0.094296

H -0.701113 2.122833 0.048360

H -0.701006 -2.122858 0.048276

H 1.894135 -1.350958 -0.094302

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1745.05 | 383.7555 | 565.9351 |
| 592.5174 | 641.3082 | 783.6832 |
| 821.3563 | 835.8139 | 856.0707 |
| 877.8617 | 915.9655 | 1020.652 |
| 1046.22 | 1078.349 | 1146.616 |
| 1156.771 | 1289.836 | 1316.436 |
| 1340.439 | 1451.681 | 1519.06 |
| 1579.576 | 3253.571 | 3266.867 |
| 3291.048 | 3295.709 | 3597.61 |

***ethynylamine (6) + vinyl (8) – i37***

**Cartesian coordinates**

C 1.824604 -0.918962 -0.077042

C 1.772523 0.380271 0.085132

H 0.920846 -1.499033 -0.255684

H 2.764622 -1.471990 -0.044737

H 2.552800 1.113291 0.261931

N -1.898248 -0.765887 0.020585

C -0.396369 1.289766 -0.061271

C -1.221073 0.395554 -0.021857

H -2.723409 -0.815735 -0.557972

H -2.040216 -1.147243 0.944064

H -0.065015 2.302141 -0.041470

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -400.268 | 42.0892 | 90.7558 |
| 133.0716 | 209.0613 | 261.1168 |
| 365.1445 | 438.4221 | 544.8049 |
| 623.6251 | 723.4873 | 807.0467 |
| 899.3219 | 951.5486 | 1095.221 |
| 1101.629 | 1197.183 | 1397.538 |
| 1646.342 | 1663.452 | 2171.434 |
| 3087.962 | 3172.069 | 3196.552 |
| 3438 | 3587.372 | 3681.462 |

***i36 – i37***

**Cartesian coordinates**

C 0.835811 1.056712 -0.127897

C 1.199556 -0.292431 0.077905

N -1.084555 0.676972 0.134689

C 0.140142 -1.236207 -0.067348

C -1.132119 -0.733197 -0.101408

H 1.313498 1.837028 0.465265

H 0.588843 1.389333 -1.134959

H 2.129851 -0.567770 0.560689

H -1.428913 0.912800 1.066922

H -1.599359 1.224599 -0.545559

H 0.327623 -2.304065 -0.042689

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -739.75 | 228.1859 | 467.4355 |
| 513.2401 | 631.8362 | 715.3788 |
| 781.9037 | 866.4838 | 880.243 |
| 927.215 | 985.2992 | 1018.996 |
| 1032.253 | 1072.7 | 1109.694 |
| 1187.501 | 1284.256 | 1360.891 |
| 1456.359 | 1513.152 | 1610.836 |
| 3095.882 | 3163.367 | 3201.981 |
| 3217.112 | 3470.767 | 3602.408 |

***i36 – i38***

**Cartesian coordinates**

C 1.528367 -0.940091 -0.052955

C 1.341733 0.374879 0.060574

N -1.688351 -0.779166 -0.050184

C 0.054374 1.078498 -0.029010

C -1.129028 0.484801 0.028667

H 0.705155 -1.620020 -0.245016

H 2.520263 -1.368032 0.033913

H 2.204063 1.014684 0.232637

H -2.299816 0.267817 -0.431996

H -2.159390 -0.987905 0.834336

H 0.075506 2.159100 -0.116238

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -2069.19 | 102.2196 | 181.5725 |
| 277.4673 | 400.001 | 426.3186 |
| 659.4128 | 734.1204 | 844.3997 |
| 917.3809 | 956.2785 | 1031.894 |
| 1049.507 | 1083.969 | 1116.994 |
| 1125.611 | 1331.874 | 1364.976 |
| 1449.55 | 1690.756 | 1720.964 |
| 2392.009 | 3156.114 | 3169.252 |
| 3198.249 | 3251.185 | 3463.802 |

***i37 – i39***

**Cartesian coordinates**

C 0.928705 0.790587 0.009925

C -0.540590 1.082488 -0.007488

N 0.926486 -0.685623 0.020388

C -1.260677 -0.084898 -0.007768

C -0.493538 -1.269255 -0.081226

H 1.467414 1.163547 -0.872598

H 1.443823 1.182616 0.895938

H -0.938481 2.087653 0.009569

H 1.621042 -1.188541 -0.514885

H 0.459994 -1.438161 0.831648

H -2.342588 -0.121286 0.026951

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1753.89 | 242.3731 | 489.2452 |
| 581.6574 | 638.3219 | 723.0461 |
| 787.9117 | 836.1551 | 922.8577 |
| 942.116 | 977.4516 | 1019.799 |
| 1086.119 | 1112.236 | 1125.903 |
| 1204.787 | 1325.269 | 1351.403 |
| 1425.519 | 1451.814 | 1500.237 |
| 2320.057 | 3001.502 | 3035.327 |
| 3220.085 | 3246.29 | 3618.503 |

***i38 – i39***

**Cartesian coordinates**

N 0.930156 -0.934813 0.086465

C 0.049009 1.197430 -0.101047

C 1.172678 0.347950 -0.014865

C -1.073202 -0.893116 -0.089001

C -1.144045 0.510074 0.067392

H 1.700269 -1.577468 0.223022

H 0.144276 2.273965 -0.062335

H 2.182608 0.746934 0.061417

H -1.691106 -1.533218 0.539923

H -0.862697 -1.321223 -1.062955

H -2.011079 0.980669 0.520800

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -647.519 | 203.4579 | 454.3633 |
| 557.2841 | 624.0565 | 668.4908 |
| 787.8175 | 826.59 | 898.1934 |
| 945.9783 | 1007.454 | 1047.007 |
| 1072.106 | 1101.907 | 1137.509 |
| 1205.835 | 1320.478 | 1429.517 |
| 1465.447 | 1518.94 | 1555.561 |
| 3115.651 | 3152.195 | 3175.933 |
| 3196.371 | 3236.045 | 3591.376 |

***i39 – pyrrole (3) + H***

**Cartesian coordinates**

C 1.121277 0.087116 0.112288

C 0.249658 1.169156 0.089270

N 0.350994 -1.050776 0.094884

C -1.058428 0.656937 -0.036725

C -0.963797 -0.716291 -0.040923

H 1.727308 0.155944 -1.721687

H 2.164553 0.045561 0.379185

H 0.542743 2.206215 0.129607

H 0.715283 -1.985166 0.051513

H -1.972369 1.224132 -0.116167

H -1.726733 -1.472761 -0.130103

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -643.676 | 319.2177 | 353.8252 |
| 524.534 | 625.3526 | 653.093 |
| 737.8363 | 782.1736 | 878.9623 |
| 890.9369 | 902.5578 | 918.9818 |
| 1046.931 | 1066.677 | 1100.916 |
| 1177.364 | 1186.025 | 1315.882 |
| 1425.891 | 1472.326 | 1520.999 |
| 1573.489 | 3258.317 | 3268.261 |
| 3279.272 | 3287.295 | 3719.882 |

***i15 – i40***

**Cartesian coordinates**

C -2.049484 0.990621 -0.062225

C -2.289339 -0.386074 -0.110223

C -1.270211 -1.339471 -0.038911

C 0.011299 -0.832645 0.080102

C 0.237529 0.544496 0.130661

C -0.755924 1.499359 0.064844

C 2.929404 0.853658 -0.238926

N 1.333538 -1.248490 0.160808

C 1.865699 0.110306 0.033144

H -2.884780 1.676747 -0.130188

H -3.312564 -0.729082 -0.215485

H -1.480941 -2.399541 -0.097608

H 1.284473 0.734485 0.939627

H -0.551839 2.561175 0.105921

H 3.812160 0.247126 -0.485145

H 1.724884 -1.992984 -0.393584

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -875.842 | 133.7217 | 206.5644 |
| 272.6982 | 314.2598 | 381.0701 |
| 407.1435 | 507.4261 | 538.7402 |
| 604.2559 | 648.4878 | 683.0718 |
| 761.4941 | 768.7475 | 812.0086 |
| 865.8378 | 871.3388 | 903.725 |
| 957.4424 | 995.5597 | 1001.172 |
| 1006.142 | 1030.408 | 1142.002 |
| 1156.671 | 1186.247 | 1242.66 |
| 1274.367 | 1334.268 | 1401.046 |
| 1480.733 | 1512.561 | 1581.373 |
| 1668.655 | 1691.868 | 2225.537 |
| 3074.766 | 3201.67 | 3218.128 |
| 3229.704 | 3238.425 | 3671.218 |

***i25 – i40***

**Cartesian coordinates**

C -2.119634 -0.764569 0.086490

C -2.167647 0.629508 0.178560

C -1.013526 1.414292 0.091389

C 0.149425 0.705367 -0.124306

C 0.212810 -0.677488 -0.243728

C -0.924036 -1.456694 -0.125030

C 2.470883 -0.429655 0.608530

N 1.545994 0.962879 -0.202172

C 1.668252 -0.632939 -0.510673

H -3.045067 -1.322598 0.177574

H -3.126446 1.114693 0.320915

H -1.050065 2.494502 0.168501

H -0.908982 -2.537166 -0.207594

H 3.465210 -0.009745 0.475480

H 2.241402 -0.773618 1.623978

H 1.942824 1.566842 -0.911036

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -761.675 | 164.3229 | 242.6667 |
| 371.583 | 412.951 | 445.972 |
| 541.4354 | 567.4435 | 584.4178 |
| 663.0818 | 730.0593 | 765.069 |
| 789.6172 | 834.988 | 850.1083 |
| 879.4233 | 913.6005 | 950.7015 |
| 999.1873 | 1025.407 | 1090.972 |
| 1102.675 | 1124.082 | 1146.877 |
| 1175.911 | 1189.601 | 1244.922 |
| 1304.913 | 1355.5 | 1418.765 |
| 1481.92 | 1511.691 | 1548.98 |
| 1658.844 | 1690.193 | 3055.005 |
| 3176.129 | 3189.286 | 3201.675 |
| 3212.328 | 3219.059 | 3592.495 |

***i41 – i42***

**Cartesian coordinates**

N -0.781105 0.671921 -0.165180

C -2.005658 1.300759 -0.135316

C -2.962143 0.338198 0.056750

C -2.306149 -0.930002 0.148544

C -0.975832 -0.656996 0.002414

C 1.211707 -1.825507 0.075256

C 1.994292 -0.926804 -0.132629

C 2.781190 0.225820 -0.396845

C 2.964079 1.209272 0.490378

H 0.114516 1.111056 -0.292939

H -2.090321 2.368849 -0.255019

H -4.025560 0.510898 0.127801

H -2.765482 -1.893321 0.298751

H 0.698205 -2.733996 0.284536

H 3.236970 0.286709 -1.381076

H 3.567842 2.074167 0.243254

H 2.522657 1.163749 1.479642

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -207.232 | 37.1267 | 56.0677 |
| 65.877 | 106.6338 | 129.8858 |
| 229.2564 | 342.8397 | 484.3625 |
| 564.6191 | 567.8634 | 636.7564 |
| 687.607 | 697.4436 | 712.6702 |
| 715.1799 | 782.1959 | 860.1733 |
| 876.8599 | 898.0944 | 903.0535 |
| 971.4742 | 1025.944 | 1042.341 |
| 1080.572 | 1115.696 | 1133.593 |
| 1194.123 | 1276.05 | 1322.996 |
| 1398.214 | 1442.643 | 1451.462 |
| 1485.889 | 1582.397 | 1672.578 |
| 2158.998 | 3162.25 | 3180.62 |
| 3250.871 | 3261.825 | 3270.203 |
| 3281.862 | 3465.042 | 3696.761 |

***i42 – i43***

**Cartesian coordinates**

N 1.964616 1.044450 0.006089

C 2.913009 0.072022 0.226755

C 2.303367 -1.168227 0.193586

C 0.947075 -0.917656 -0.100670

C 0.759112 0.436447 -0.176093

C -0.634950 0.853312 -0.306145

C -1.418646 -0.225519 -0.280215

C -2.830527 -0.485522 -0.258365

C -3.693115 0.138324 0.553763

H 2.146378 2.032385 -0.011027

H 3.953942 0.331842 0.341627

H 2.805935 -2.114404 0.317937

H -0.442897 -1.189389 -0.224293

H -0.982625 1.871653 -0.444700

H -3.196834 -1.259460 -0.929748

H -4.753767 -0.084703 0.524565

H -3.354380 0.881838 1.267319

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -2120.28 | 66.2408 | 91.4527 |
| 158.4636 | 225.7571 | 327.6476 |
| 381.8446 | 440.2905 | 487.011 |
| 570.5022 | 586.9074 | 671.0322 |
| 685.8209 | 700.7161 | 761.9393 |
| 866.2009 | 868.1137 | 891.5067 |
| 954.0567 | 982.0018 | 1012.181 |
| 1022.896 | 1043.062 | 1096.875 |
| 1102.712 | 1133.102 | 1194.913 |
| 1231.937 | 1324.865 | 1341.271 |
| 1432.611 | 1440.636 | 1479.089 |
| 1521.898 | 1578.372 | 1646.232 |
| 1682.915 | 1751.069 | 3151.114 |
| 3161.611 | 3199.62 | 3250.655 |
| 3258.718 | 3277.801 | 3705 |

***i42 – i44***

**Cartesian coordinates**

N 1.839382 -0.981374 0.137367

C 2.863050 -0.077073 0.185926

C 2.331535 1.167539 -0.041782

C 0.936909 1.004333 -0.230131

C 0.649057 -0.340645 -0.108271

C -0.599694 -1.085923 -0.200004

C -1.810199 -0.551798 -0.070332

C -2.501968 0.693879 0.188067

C -3.746587 0.225553 0.090876

H 1.930711 -1.968185 0.302526

H 3.877854 -0.389626 0.371542

H 2.885065 2.092644 -0.080961

H 0.222770 1.777778 -0.465159

H -0.523082 -2.153823 -0.388260

H -2.116990 1.684095 0.400220

H -4.755425 0.618386 0.175171

H -3.129198 -1.006835 -0.162746

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -2294.89 | 38.8006 | 96.8544 |
| 127.4551 | 220.6602 | 291.7623 |
| 403.65 | 419.0098 | 492.057 |
| 633.7138 | 663.4549 | 697.2261 |
| 710.8196 | 732.0346 | 774.0274 |
| 803.2018 | 843.4324 | 891.0365 |
| 899.2539 | 913.7915 | 932.0316 |
| 986.2957 | 1027.929 | 1062.251 |
| 1070.446 | 1134.626 | 1144.718 |
| 1203.867 | 1248.498 | 1299.574 |
| 1378.823 | 1471.65 | 1483.655 |
| 1510.886 | 1602.12 | 1627.531 |
| 1733.626 | 1936.841 | 3167.25 |
| 3186.659 | 3229.97 | 3257.973 |
| 3273.817 | 3287.886 | 3708.433 |

***i43 – i45***

**Cartesian coordinates**

C -1.932249 -1.287719 0.169671

C -2.745169 -0.169046 0.218442

N -1.996917 0.976460 0.078832

C -0.686122 0.589910 -0.072886

C -0.615859 -0.796023 -0.004818

C 0.606711 1.064069 -0.315012

C 1.296622 -0.118574 -0.749944

C 2.646307 -0.444549 -0.301181

C 3.161277 -0.007957 0.851200

H -2.275145 -2.306095 0.265889

H -3.814852 -0.104654 0.355618

H -2.371156 1.906464 0.024713

H 1.076489 1.996330 -0.025820

H 0.985248 -0.562378 -1.686663

H 3.243140 -1.088925 -0.941688

H 4.178601 -0.241345 1.143466

H 2.566985 0.584713 1.539832

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -496.121 | 88.6822 | 134.7879 |
| 200.6109 | 278.215 | 340.9922 |
| 422.7637 | 470.1688 | 577.029 |
| 619.5899 | 656.2818 | 681.9804 |
| 713.4272 | 735.608 | 753.7853 |
| 798.3499 | 878.3913 | 881.13 |
| 967.754 | 975.5071 | 1005.402 |
| 1044.049 | 1059.365 | 1093.604 |
| 1126.362 | 1161.536 | 1183.462 |
| 1256.602 | 1321.436 | 1338.525 |
| 1400.914 | 1441.233 | 1452.574 |
| 1479.944 | 1501.317 | 1595.564 |
| 1690.597 | 3152.72 | 3167.01 |
| 3211.955 | 3215.55 | 3248.681 |
| 3248.77 | 3269.921 | 3714.262 |

***i44 – i46***

**Cartesian coordinates**

N -1.795616 0.903543 0.153493

C -2.716335 -0.097950 0.079709

C -2.037433 -1.274663 -0.124957

C -0.658019 -0.965724 -0.174177

C -0.522656 0.399906 0.000360

C 0.607763 1.312007 0.025169

C 1.909210 1.049449 -0.119560

C 2.527731 -0.281784 -0.342094

C 2.834912 -1.138862 0.596410

H -2.009647 1.874788 0.296970

H -3.770902 0.101147 0.181737

H -2.484641 -2.251209 -0.225258

H 0.153115 -1.660278 -0.312050

H 0.340434 2.357561 0.170027

H 2.601865 1.886814 -0.101572

H 2.775711 -0.531109 -1.382182

H 3.292336 -2.116786 0.652723

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -113.077 | 43.6151 | 147.1634 |
| 173.2752 | 263.9121 | 340.0395 |
| 488.2869 | 504.7519 | 540.383 |
| 634.7728 | 665.1472 | 681.8917 |
| 737.5173 | 749.4234 | 765.3116 |
| 828.6844 | 835.0633 | 891.7969 |
| 905.1277 | 905.6938 | 980.5874 |
| 999.846 | 1025.277 | 1076.664 |
| 1136.007 | 1156.549 | 1237.574 |
| 1254.135 | 1255.803 | 1317.402 |
| 1428.02 | 1480.326 | 1485.377 |
| 1513.827 | 1625.597 | 1689.288 |
| 1742.957 | 3026.483 | 3147.906 |
| 3176.589 | 3252.295 | 3256.406 |
| 3283.419 | 3296.945 | 3705.685 |

***i45 – i47***

**Cartesian coordinates**

C -1.701352 -1.145928 -0.595442

C -2.395833 -0.429553 0.363433

N -1.700752 0.705072 0.712174

C -0.533644 0.707764 -0.010793

C -0.515884 -0.412145 -0.831997

C 0.639952 1.441766 -0.235871

C 1.512032 0.492415 -0.850653

C 2.153088 -0.626333 -0.146534

C 2.351002 -0.697649 1.169507

H -2.037850 -2.066488 -1.045680

H -3.349436 -0.644512 0.823008

H -1.972748 1.348726 1.433294

H 0.753031 2.518607 -0.285760

H 2.062689 0.806755 -1.741453

H 2.533589 -1.418192 -0.786769

H 2.844677 -1.553612 1.613918

H 2.015140 0.091187 1.834319

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -554.932 | 79.0662 | 140.9596 |
| 189.3654 | 265.3956 | 321.8073 |
| 430.8152 | 454.4359 | 597.5703 |
| 612.4613 | 650.8569 | 668.2928 |
| 686.3339 | 748.7308 | 794.5322 |
| 863.3614 | 877.3667 | 907.4859 |
| 930.6741 | 938.6486 | 981.6474 |
| 1040.339 | 1068.512 | 1095.31 |
| 1128.791 | 1140.025 | 1160.203 |
| 1274.164 | 1323.008 | 1343.23 |
| 1399.808 | 1432.375 | 1451.013 |
| 1476.948 | 1498.104 | 1594.625 |
| 1693.784 | 3097.989 | 3156.911 |
| 3175.744 | 3198.663 | 3250.932 |
| 3251.95 | 3272.758 | 3710.363 |

***i46 – i47***

**Cartesian coordinates**

N 1.745010 -0.969863 -0.000002

C 2.614748 0.080742 0.000005

C 1.892159 1.253389 0.000003

C 0.534866 0.871989 -0.000007

C 0.444637 -0.505120 -0.000007

C -0.693895 -1.379952 -0.000004

C -1.996100 -1.024103 0.000004

C -2.571039 0.311868 0.000006

C -1.936417 1.484780 -0.000003

H 2.011389 -1.939109 -0.000001

H 3.681581 -0.080831 0.000013

H 2.302546 2.250367 0.000008

H -0.679427 1.478422 -0.000005

H -0.472267 -2.444844 -0.000005

H -2.719312 -1.833146 0.000008

H -3.660930 0.337240 0.000011

H -2.412396 2.459388 -0.000009

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1392.32 | 86.0853 | 177.6506 |
| 282.0555 | 288.5188 | 399.5006 |
| 460.3963 | 480.8267 | 484.9741 |
| 613.6189 | 629.7878 | 676.8703 |
| 704.4739 | 724.6345 | 788.2351 |
| 820.2789 | 858.9426 | 907.6866 |
| 926.1002 | 946.6334 | 965.7831 |
| 988.0554 | 1012.854 | 1101.911 |
| 1118.619 | 1152.708 | 1214.081 |
| 1267.343 | 1270.383 | 1321.477 |
| 1420.25 | 1453.099 | 1484.791 |
| 1491.067 | 1514.896 | 1620.07 |
| 1652.313 | 1708.056 | 3130.945 |
| 3158.774 | 3197.747 | 3212.08 |
| 3262.347 | 3282.115 | 3704.617 |

***i46 – i48***

**Cartesian coordinates**

N 1.466366 -1.046274 -0.355770

C 2.381121 -0.023534 -0.389896

C 1.851343 1.060822 0.244944

C 0.520806 0.710462 0.658148

C 0.316821 -0.624575 0.267659

C -0.902345 -1.375081 0.307168

C -2.099584 -0.778418 0.093265

C -2.257265 0.597771 -0.358051

C -1.332491 1.547852 -0.275406

H 1.542503 -1.900009 -0.880268

H 3.343290 -0.160064 -0.858073

H 2.353598 1.998104 0.423860

H 0.011208 1.163789 1.494182

H -0.854011 -2.453791 0.429989

H -2.994122 -1.392481 0.117437

H -3.198664 0.814492 -0.867711

H -1.338790 2.562079 -0.656012

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -447.082 | 126.4905 | 168.7558 |
| 277.144 | 328.0692 | 436.9335 |
| 469.3177 | 487.5509 | 612.6553 |
| 623.3026 | 640.8112 | 680.8413 |
| 750.3669 | 764.1927 | 799.7735 |
| 835.3192 | 886.7423 | 888.1446 |
| 917.6877 | 922.0664 | 975.3956 |
| 992.9909 | 1022.86 | 1063.435 |
| 1132.926 | 1150.719 | 1199.95 |
| 1243.789 | 1273.193 | 1283.911 |
| 1410.002 | 1444.22 | 1463.99 |
| 1537.529 | 1559.081 | 1606.382 |
| 1656.051 | 3100.037 | 3164.37 |
| 3189.763 | 3222.273 | 3244.091 |
| 3258.64 | 3279.315 | 3704.266 |

***i47 – i49***

**Cartesian coordinates**

C -1.854103 1.241480 0.084306

C -2.570527 0.062035 0.110958

N -1.701506 -0.982593 -0.006994

C -0.405185 -0.508740 -0.103223

C -0.502654 0.865050 -0.024098

C 0.739301 -1.379350 -0.168011

C 2.018192 -0.995695 0.053684

C 1.829004 1.440695 -0.284825

C 2.401441 0.372162 0.316993

H -2.268266 2.234347 0.158203

H -3.630638 -0.106899 0.222077

H -1.961086 -1.953231 0.028090

H 0.537441 -2.438530 -0.308073

H 2.776957 -1.767312 0.143596

H 2.068330 2.451295 0.025366

H 1.311028 1.336731 -1.230112

H 3.143960 0.535918 1.095111

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -289.581 | 117.5194 | 168.1769 |
| 259.982 | 274.1103 | 407.1065 |
| 464.7247 | 471.4319 | 612.2138 |
| 617.3986 | 626.3628 | 685.6024 |
| 730.8882 | 793.0086 | 816.607 |
| 847.4471 | 864.7416 | 911.5199 |
| 955.3033 | 979.4629 | 987.6101 |
| 1012.826 | 1090.57 | 1112.539 |
| 1143.364 | 1194.664 | 1242.45 |
| 1256.2 | 1299.492 | 1393.38 |
| 1437.194 | 1449.827 | 1482.394 |
| 1507.759 | 1574.355 | 1610.346 |
| 1658.723 | 3148.788 | 3162.628 |
| 3166.275 | 3185.442 | 3253.949 |
| 3257.282 | 3275.852 | 3699.83 |

***i48 – indole (2) + H***

**Cartesian coordinates**

N 1.547950 -1.095916 -0.019259

C 0.239852 -0.691466 0.045517

C 0.246047 0.739435 0.135158

C -0.988196 1.418011 -0.068737

C -2.149820 0.685017 -0.096697

C -2.131241 -0.722568 -0.018577

C -0.938640 -1.425860 0.022073

C 1.631395 1.144885 -0.060218

C 2.369370 0.011686 -0.112495

H 1.854838 -2.048315 -0.097459

H 0.295289 0.806811 1.805312

H -1.005448 2.499359 -0.136339

H -3.102231 1.192198 -0.200152

H -3.068637 -1.266113 -0.039541

H -0.926894 -2.510040 0.009717

H 2.007438 2.154873 -0.079686

H 3.437391 -0.112205 -0.203183

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1145.95 | 206.3557 | 240.4718 |
| 381.5225 | 404.1403 | 433.1101 |
| 498.9729 | 548.0191 | 559.7067 |
| 592.0794 | 621.4488 | 640.7632 |
| 731.1935 | 754.3705 | 765.6839 |
| 805.9191 | 869.1573 | 886.1951 |
| 898.4199 | 907.5993 | 942.9902 |
| 991.0245 | 1037.074 | 1092.21 |
| 1121.499 | 1151.185 | 1176.874 |
| 1222.608 | 1272.286 | 1307.498 |
| 1357.745 | 1385.068 | 1451.673 |
| 1489.827 | 1537.153 | 1596.849 |
| 1623.71 | 1677.416 | 3192.54 |
| 3200.754 | 3212.778 | 3221.825 |
| 3263.312 | 3284.741 | 3719.287 |

***i49 – indole (2) + H***

**Cartesian coordinates**

N -1.599853 -1.072251 0.037422

C -2.396489 0.046774 -0.016766

C -1.615036 1.163444 -0.070722

C -0.255967 0.719368 -0.052696

C -0.280811 -0.688479 0.015775

C 0.883535 -1.459249 0.036166

C 2.095362 -0.791308 -0.031017

C 2.154651 0.604097 -0.100169

C 0.993378 1.380442 -0.053943

H -1.930705 -2.018998 0.073433

H -3.471325 -0.046977 -0.012640

H -1.967405 2.181791 -0.112667

H 0.842611 -2.541505 0.088308

H 3.118818 1.094986 -0.157054

H 1.074374 1.899888 1.771957

H 1.043782 2.447727 -0.235547

H 3.017085 -1.361685 -0.037509

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -836.245 | 204.5972 | 235.2252 |
| 290.5279 | 375.3909 | 410.275 |
| 420.8296 | 490.096 | 552.554 |
| 595.5268 | 620.643 | 626.6073 |
| 730.395 | 759.9687 | 779.6862 |
| 800.4358 | 876.9727 | 881.5099 |
| 894.0686 | 918.1284 | 972.9434 |
| 1018.337 | 1039.94 | 1088.356 |
| 1122.881 | 1144.661 | 1181.796 |
| 1232.043 | 1268.564 | 1306.377 |
| 1376.494 | 1389.801 | 1471.055 |
| 1493.478 | 1529.807 | 1572.153 |
| 1632.477 | 1672.693 | 3192.082 |
| 3201.712 | 3209.669 | 3221.709 |
| 3261.342 | 3281.242 | 3722.671 |

***i19 – i50***

**Cartesian coordinates**

C 2.595261 0.968005 -0.171769

C 2.885744 -0.376918 -0.152884

N 1.714602 -1.059050 -0.018887

C 0.659871 -0.177605 0.056617

C 1.194070 1.095793 -0.049968

C -4.033600 0.219349 -0.468106

C -2.878800 -0.032904 -0.021008

C -1.728550 0.255277 0.722629

C -0.711453 -0.603715 0.202433

H 3.314614 1.765017 -0.274939

H 3.829383 -0.892971 -0.228851

H 1.630133 -2.058410 0.043210

H 0.617780 2.008159 -0.062842

H -4.878475 -0.027577 -1.075652

H -1.607607 1.028263 1.475095

H -0.861044 -1.676132 0.325805

H -1.942246 -0.816693 -0.777290

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -2155.79 | 74.191 | 88.2182 |
| 176.7397 | 223.0023 | 310.6253 |
| 394.3225 | 409.7879 | 487.6432 |
| 511.1807 | 523.6193 | 578.7749 |
| 633.4212 | 668.4734 | 730.4361 |
| 743.8391 | 762.9049 | 820.9312 |
| 839.9458 | 903.394 | 904.5211 |
| 997.3265 | 1012.298 | 1059.606 |
| 1095.252 | 1135.558 | 1150.952 |
| 1164.503 | 1242.505 | 1299.857 |
| 1325.888 | 1438.638 | 1466.493 |
| 1480.799 | 1511.274 | 1521.506 |
| 1621.902 | 1810.342 | 3121.472 |
| 3181.546 | 3255.373 | 3267.362 |
| 3284.504 | 3386.033 | 3710.015 |

***i50 – i51***

**Cartesian coordinates**

C -2.766275 0.824316 -0.119770

C -2.908131 -0.542094 -0.122227

N -1.663407 -1.088389 -0.001843

C -0.712895 -0.098666 0.073350

C -1.385163 1.105623 0.004463

C 3.982542 -0.108583 -0.641758

C 3.130530 0.067368 0.334573

C 1.702727 0.448275 0.162450

C 0.697217 -0.426121 0.203506

H -3.567772 1.542496 -0.193691

H -3.787159 -1.161548 -0.196939

H -1.462668 -2.072925 0.008525

H -0.928067 2.081993 0.049349

H 5.027905 -0.365716 -0.741742

H 3.487803 -0.051536 1.365305

H 1.496977 1.505251 0.011196

H 0.933525 -1.480004 0.343369

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -175.697 | 54.1544 | 94.3057 |
| 137.8535 | 272.5889 | 320.2014 |
| 405.8302 | 467.0706 | 505.6712 |
| 632.2224 | 643.0186 | 677.3347 |
| 729.9713 | 770.6848 | 803.1279 |
| 821.335 | 845.8424 | 892.9853 |
| 896.117 | 907.5336 | 996.0984 |
| 1000.217 | 1065.866 | 1067.605 |
| 1135.423 | 1145.27 | 1238.898 |
| 1242.468 | 1302.305 | 1326.739 |
| 1354.308 | 1470.882 | 1488.749 |
| 1508.101 | 1628.154 | 1686.811 |
| 1749.191 | 3039.805 | 3152.851 |
| 3168.155 | 3255.137 | 3257.155 |
| 3270.339 | 3286.171 | 3706.85 |

***i51 – i52***

**Cartesian coordinates**

C 2.633663 0.895982 0.071081

C 2.846161 -0.461679 0.137168

N 1.632151 -1.078382 0.047820

C 0.625450 -0.144769 -0.077290

C 1.244188 1.101528 -0.064248

C -0.744397 -0.537272 -0.190912

C -1.803556 0.337292 -0.349061

C -3.225048 -0.095091 -0.433705

C -3.329095 0.150807 0.826670

H 3.398265 1.655550 0.117311

H 3.757565 -1.028072 0.240287

H 1.484957 -2.071905 0.066993

H 0.738739 2.051701 -0.138031

H -0.966543 -1.599095 -0.112181

H -1.592573 1.390624 -0.506564

H -3.826708 -0.462639 -1.259491

H -3.902959 0.131719 1.738720

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -723.667 | 66.3853 | 95.6949 |
| 155.4244 | 225.1033 | 328.627 |
| 355.4485 | 427.0609 | 480.6035 |
| 572.1966 | 624.9505 | 663.1783 |
| 678.4931 | 725.7211 | 770.1827 |
| 783.5041 | 805.8067 | 867.3782 |
| 893.0396 | 903.6121 | 929.2659 |
| 998.2468 | 1052.339 | 1073.396 |
| 1136.286 | 1145.032 | 1174.458 |
| 1238.304 | 1276.658 | 1308.005 |
| 1338.772 | 1452.275 | 1460.203 |
| 1503.261 | 1535.893 | 1599.633 |
| 1723.474 | 3163.422 | 3164.629 |
| 3178.604 | 3258.711 | 3271.002 |
| 3285.964 | 3288.254 | 3707.811 |

***i51 – i54***

**Cartesian coordinates**

C -2.516329 0.815433 0.339602

C -2.699910 -0.509834 0.016293

N -1.481023 -1.046511 -0.265045

C -0.499898 -0.089204 -0.136013

C -1.131682 1.079190 0.253011

C 0.896041 -0.367327 -0.369209

C 2.615267 -0.588118 0.920285

C 3.046061 0.251657 -0.045366

C 1.843207 0.634218 -0.696371

H -3.293542 1.508671 0.620361

H -3.598592 -1.103961 -0.030093

H -1.316406 -1.996389 -0.548657

H -0.629726 2.008957 0.472206

H 1.146027 -1.392979 -0.620430

H 3.086673 -1.214019 1.672609

H 4.061880 0.562363 -0.273584

H 1.594308 1.596851 -1.130483

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -624.978 | 84.2994 | 115.8074 |
| 156.768 | 372.2784 | 400.2379 |
| 433.4821 | 506.2782 | 582.3149 |
| 633.8786 | 668.3419 | 696.9407 |
| 720.384 | 745.7892 | 775.1638 |
| 832.8783 | 842.3627 | 892.0437 |
| 904.9307 | 905.3345 | 917.557 |
| 1004.468 | 1060.357 | 1064.935 |
| 1135.37 | 1145.628 | 1170.499 |
| 1240.051 | 1255.657 | 1307.371 |
| 1363.116 | 1446.088 | 1482.439 |
| 1489.293 | 1504.734 | 1537.742 |
| 1624.53 | 3163.627 | 3172.735 |
| 3195.658 | 3205.008 | 3259.218 |
| 3269.141 | 3284.394 | 3708.041 |

***i52 – i53***

**Cartesian coordinates**

C 2.283267 1.080485 0.018201

C 2.739308 -0.196264 -0.240150

N 1.674684 -1.048152 -0.175263

C 0.511550 -0.351441 0.121826

C 0.899855 1.000067 0.244372

C -0.735513 -0.954626 0.252030

C -1.970560 -0.183132 0.558945

C -2.445522 0.935940 -0.340954

C -3.129576 -0.152685 -0.409746

H 2.893221 1.970210 0.041138

H 3.731743 -0.555587 -0.460835

H 1.714951 -2.039696 -0.327523

H 0.231121 1.810091 0.488064

H -0.811485 -2.034540 0.150593

H -2.203755 -0.105533 1.625329

H -2.258173 1.940737 -0.676864

H -3.937260 -0.718691 -0.840204

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -54.3622 | 99.5718 | 140.1054 |
| 236.8084 | 326.169 | 375.7637 |
| 431.1661 | 514.6747 | 593.3307 |
| 613.6562 | 660.2849 | 701.9476 |
| 719.3796 | 737.6335 | 780.3046 |
| 842.6559 | 880.6631 | 889.5596 |
| 890.7537 | 911.1135 | 966.3444 |
| 1014.419 | 1033.783 | 1052.478 |
| 1059.614 | 1126.546 | 1144.52 |
| 1218.485 | 1225.916 | 1293.06 |
| 1364.193 | 1398.671 | 1416.256 |
| 1488.32 | 1505.765 | 1567.147 |
| 1743.771 | 3047.629 | 3159.001 |
| 3252.113 | 3274.674 | 3277.359 |
| 3284.244 | 3325.745 | 3715.29 |

***i44 – i53***

**Cartesian coordinates**

C 2.098811 -1.203033 -0.060499

C 2.700905 0.019281 0.127758

N 1.723278 0.968742 0.136161

C 0.482956 0.390013 -0.048395

C 0.709837 -0.979623 -0.170552

C -0.694313 1.199508 -0.072551

C -2.004706 0.782587 -0.248966

C -2.449396 -0.616814 -0.480784

C -2.750042 -0.670150 0.770689

H 2.605731 -2.153982 -0.110226

H 3.738801 0.281078 0.256521

H 1.875956 1.955158 0.249556

H -0.051944 -1.728426 -0.307139

H -0.544387 2.262984 0.097421

H -2.760685 1.556981 -0.318188

H -2.429356 -1.256057 -1.358475

H -3.061366 -1.229537 1.637193

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -710.674 | 60.8989 | 117.3284 |
| 163.0068 | 233.158 | 306.3963 |
| 412.9059 | 483.4287 | 523.3266 |
| 605.932 | 627.6058 | 664.4155 |
| 679.7452 | 732.6921 | 756.7748 |
| 778.6965 | 812.603 | 869.2607 |
| 893.0119 | 901.8441 | 918.6341 |
| 962.306 | 1020.329 | 1056.881 |
| 1127.271 | 1143.639 | 1152.247 |
| 1249.323 | 1256.57 | 1304.212 |
| 1408.489 | 1443.151 | 1462.629 |
| 1508.346 | 1527.389 | 1598.17 |
| 1722.273 | 3153.719 | 3159.966 |
| 3188.885 | 3260.839 | 3278.822 |
| 3288.599 | 3289.507 | 3709.934 |

***i46 – i54***

**Cartesian coordinates**

C 2.239118 0.940998 -0.247896

C 2.477996 -0.408909 -0.270043

N 1.329318 -1.041110 0.126671

C 0.347475 -0.117644 0.382369

C 0.895553 1.128208 0.168866

C -0.977655 -0.521964 0.857692

C -1.882108 -0.617922 -1.156247

C -2.430827 0.472647 -0.589384

C -2.124582 0.300672 0.793666

H 2.955696 1.711323 -0.486834

H 3.366519 -0.966458 -0.518456

H 1.190481 -2.035928 0.140653

H 0.379812 2.064196 0.315503

H -0.935391 -1.283425 1.642390

H -1.732169 -0.980776 -2.169618

H -2.990562 1.272143 -1.066970

H -2.809430 0.450181 1.622509

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -685.224 | 56.1621 | 122.1899 |
| 173.8398 | 280.4473 | 371.2269 |
| 450.9208 | 484.3741 | 579.4585 |
| 632.285 | 657.9826 | 713.5861 |
| 726.8637 | 740.8624 | 796.3405 |
| 820.1241 | 882.9233 | 888.2053 |
| 904.2771 | 906.6738 | 951.3065 |
| 991.8901 | 1058.602 | 1063.246 |
| 1112.873 | 1142.645 | 1152.089 |
| 1243.806 | 1260.239 | 1294.878 |
| 1415.828 | 1432.773 | 1472.388 |
| 1490.061 | 1519.467 | 1527.044 |
| 1627.745 | 3085.534 | 3158.141 |
| 3186.425 | 3194.891 | 3257.132 |
| 3269.29 | 3282.985 | 3707.365 |

***i55 – i56***

**Cartesian coordinates**

N -2.108613 -1.230147 0.100601

C -2.995464 -0.198909 -0.040998

C -2.288865 0.981385 -0.114644

C -0.932237 0.606790 -0.011894

C -0.821372 -0.745049 0.121195

H -2.362380 -2.199099 0.176185

H -4.058520 -0.378618 -0.080451

H -2.708342 1.967785 -0.229980

H 0.037695 -1.388474 0.219367

C 3.211310 -1.444202 -0.280851

C 2.746787 -0.388706 0.060846

C 2.191444 0.848771 0.492833

C 1.467968 1.649746 -0.301709

H 3.632278 -2.369063 -0.593753

H 2.350056 1.110825 1.534281

H 1.075663 2.587662 0.070665

H 1.316418 1.421054 -1.349198

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -108.15 | 34.1861 | 58.3196 |
| 66.4784 | 91.6956 | 168.7454 |
| 231.0765 | 364.6825 | 476.5817 |
| 567.4106 | 574.0887 | 645.2328 |
| 680.5686 | 686.655 | 694.2332 |
| 725.3502 | 776.7231 | 848.6333 |
| 857.004 | 896.3201 | 900.1022 |
| 961.6073 | 1006.233 | 1048.619 |
| 1085.19 | 1118.848 | 1168.018 |
| 1187.5 | 1248.335 | 1318.112 |
| 1402.338 | 1442.507 | 1468.162 |
| 1508.075 | 1561.837 | 1652.137 |
| 2226.351 | 3172.489 | 3189.875 |
| 3258.328 | 3272.013 | 3277.302 |
| 3285.338 | 3486.16 | 3709.656 |

***i56 – i57***

**Cartesian coordinates**

N -1.991945 -1.237983 0.070284

C -2.809345 -0.179085 -0.257021

C -2.051049 0.966619 -0.309945

C -0.714235 0.586957 -0.006505

C -0.722476 -0.761684 0.202465

C 3.731770 -0.512338 -0.604269

C 2.728974 -0.226110 -0.003688

C 1.518025 0.083972 0.690190

C 0.634490 1.225871 0.143422

H -2.281249 -2.196160 0.142850

H -3.862239 -0.330610 -0.437849

H -2.425876 1.952656 -0.539502

H 0.685011 -0.879708 0.540353

H 4.622075 -0.757433 -1.131248

H 1.651308 0.113005 1.772610

H 0.629711 2.068122 0.841722

H 1.027945 1.590801 -0.808815

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1788.76 | 50.7341 | 124.5473 |
| 174.4043 | 244.5287 | 365.3832 |
| 402.749 | 433.1868 | 477.2247 |
| 559.7475 | 597.4308 | 642.9082 |
| 668.2701 | 705.5821 | 717.4152 |
| 722.9921 | 852.2895 | 862.0361 |
| 903.8638 | 928.2629 | 994.3496 |
| 1027.263 | 1075.936 | 1078.672 |
| 1132.827 | 1189.626 | 1219.857 |
| 1247.897 | 1271.134 | 1331.346 |
| 1355.752 | 1437.31 | 1447.965 |
| 1496.811 | 1521.737 | 1605.251 |
| 1659.672 | 2204.013 | 3062.515 |
| 3101.236 | 3126.114 | 3252.857 |
| 3273.333 | 3481.461 | 3723.556 |

***i57 – i58***

**Cartesian coordinates**

N -1.754122 1.106485 -0.041900

C -2.507484 -0.038504 -0.171794

C -1.659098 -1.108416 -0.048274

C -0.337861 -0.607161 0.162970

C -0.457442 0.758528 0.177548

C 1.631674 1.743425 0.120707

C 2.155570 0.672262 -0.129067

C 2.137380 -0.766042 -0.380619

C 0.929322 -1.387210 0.363059

H -2.107927 2.044502 -0.085240

H -3.572558 0.007926 -0.334170

H -1.944869 -2.149052 -0.102874

H 1.475788 2.777474 0.325484

H 2.037967 -0.926030 -1.459111

H 3.067291 -1.243536 -0.060742

H 0.797131 -2.414748 0.013248

H 1.173656 -1.443218 1.429527

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -398.492 | 72.8325 | 135.442 |
| 232.043 | 299.5451 | 343.887 |
| 396.1271 | 446.9239 | 534.3928 |
| 593.8257 | 633.1433 | 676.6287 |
| 680.2564 | 717.391 | 747.6249 |
| 843.1436 | 849.4717 | 893.3566 |
| 913.9627 | 986.8471 | 1007.197 |
| 1026.591 | 1079.404 | 1118.462 |
| 1181.336 | 1219.387 | 1250.202 |
| 1290.16 | 1342.721 | 1370.979 |
| 1415.02 | 1443.413 | 1474.084 |
| 1486.54 | 1512.929 | 1599.733 |
| 2095.563 | 3048.042 | 3061.313 |
| 3101.601 | 3111.004 | 3242.35 |
| 3276.792 | 3447.726 | 3721.319 |

***i58 – i49***

**Cartesian coordinates**

N -1.632086 1.036577 -0.03155

C -2.408896 -0.086781 -0.04515

C -1.582722 -1.191033 -0.00491

C -0.255748 -0.718564 0.02563

C -0.304314 0.681018 0.01346

C 0.836272 1.506461 0.10729

C 2.099368 0.932912 -0.18651

C 2.209157 -0.471051 -0.11823

C 1.051700 -1.440741 0.10195

H -1.972457 1.980928 -0.06304

H -3.484499 -0.020573 -0.08413

H -1.911289 -2.219168 0.00067

H 0.744564 2.560581 0.35014

H 3.130125 -0.918709 -0.49167

H 2.774979 0.275509 0.76997

H 1.117011 -2.210955 -0.67624

H 1.157266 -1.976976 1.05402

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1402.97 | 88.7998 | 216.544 |
| 268.5882 | 385.9488 | 479.7169 |
| 489.0827 | 503.6732 | 584.5073 |
| 624.3191 | 644.2735 | 694.6451 |
| 720.5887 | 734.9178 | 761.2866 |
| 847.3845 | 861.018 | 912.2868 |
| 920.6684 | 970.1634 | 1066.937 |
| 1078.46 | 1125.372 | 1198.339 |
| 1207.051 | 1238.478 | 1253.991 |
| 1271.822 | 1339.54 | 1370.47 |
| 1395.67 | 1428.147 | 1461.171 |
| 1475.509 | 1505.054 | 1544.707 |
| 1578.116 | 2168.086 | 3023.866 |
| 3051.707 | 3130.177 | 3178.411 |
| 3253.836 | 3280.319 | 3713.519 |

***i59 – i60***

**Cartesian coordinates**

N 2.182707 -1.249310 0.001797

C 3.043650 -0.189859 -0.072979

C 2.307734 0.974314 -0.045724

C 0.959731 0.565373 0.052821

C 0.885851 -0.795053 0.079099

C -1.221622 1.731960 0.230551

C -2.026289 0.888880 -0.093627

C -2.862446 -0.179649 -0.509878

C -3.364276 -1.098097 0.320459

H 2.459721 -2.214721 0.002879

H 4.109599 -0.341647 -0.141716

H 2.704374 1.976082 -0.092950

H 0.045143 -1.466412 0.141300

H -0.691187 2.596065 0.552744

H -3.084067 -0.228076 -1.572471

H -3.996656 -1.895406 -0.051274

H -3.159878 -1.067931 1.384578

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -210.238 | 12.1477 | 37.2349 |
| 57.222 | 81.6405 | 114.6697 |
| 226.6014 | 333.7453 | 483.1769 |
| 563.4937 | 583.1009 | 646.1139 |
| 663.7613 | 685.8318 | 691.0507 |
| 703.919 | 769.0561 | 848.8014 |
| 857.1462 | 897.5937 | 902.563 |
| 957.5149 | 1016.067 | 1045.756 |
| 1083.624 | 1115.812 | 1167.762 |
| 1185.659 | 1247.026 | 1321.359 |
| 1400.837 | 1443.828 | 1470.311 |
| 1509.113 | 1563.509 | 1676.127 |
| 2158.307 | 3165.715 | 3179.317 |
| 3258.358 | 3264.592 | 3277.109 |
| 3281.307 | 3470.602 | 3714.124 |

***i60 – i61***

**Cartesian coordinates**

N 2.192111 -1.075530 0.243142

C 2.829072 0.142644 0.404992

C 1.958469 1.144769 0.056115

C 0.758512 0.498398 -0.340404

C 0.968661 -0.882042 -0.312102

C -0.646651 0.826045 -0.494377

C -1.408070 -0.268736 -0.340415

C -2.796208 -0.532041 -0.133965

C -3.591915 0.213636 0.653143

H 2.669308 -1.960281 0.277583

H 3.869039 0.191194 0.692527

H 2.155569 2.203455 0.128344

H -0.392557 -1.208906 -0.374314

H -1.023854 1.814992 -0.739898

H -3.210074 -1.416762 -0.613277

H -4.640575 -0.027782 0.786366

H -3.202851 1.076761 1.182756

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1852.3 | 84.8584 | 115.8038 |
| 165.8529 | 258.0464 | 309.7041 |
| 403.4472 | 455.4966 | 571.5874 |
| 589.8727 | 627.193 | 659.4509 |
| 697.2788 | 739.3893 | 755.9177 |
| 866.387 | 891.5243 | 912.8911 |
| 944.8097 | 979.6453 | 1007.394 |
| 1025.404 | 1077.5 | 1087.05 |
| 1095.924 | 1124.346 | 1185.457 |
| 1258.325 | 1318.945 | 1339.307 |
| 1378.817 | 1433.468 | 1438.62 |
| 1501.108 | 1546.281 | 1610.054 |
| 1639.475 | 1780.321 | 3155.036 |
| 3165.112 | 3181.782 | 3248.073 |
| 3255.598 | 3268.779 | 3687.502 |

***i60 – i62***

**Cartesian coordinates**

C 1.905529 1.060225 -0.184333

C 2.863219 0.082404 -0.210639

N 2.248855 -1.109914 0.057513

C 0.911868 -0.909475 0.256005

C 0.654734 0.437181 0.106694

C -0.631591 1.127565 0.221671

C -1.824678 0.560434 0.085317

C -2.489183 -0.694720 -0.207008

C -3.745680 -0.260700 -0.106872

H 2.066982 2.112236 -0.363523

H 3.923544 0.137250 -0.396732

H 2.713500 -1.997057 0.125608

H 0.256630 -1.723411 0.520529

H -0.587666 2.193986 0.422927

H -2.082985 -1.671241 -0.444964

H -4.741662 -0.680615 -0.212842

H -3.155642 0.980767 0.181403

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -2278.81 | 40.7885 | 96.6263 |
| 120.0296 | 230.1558 | 286.2089 |
| 408.5442 | 416.0579 | 499.8108 |
| 643.698 | 650.5299 | 694.3728 |
| 703.4394 | 723.2772 | 769.3177 |
| 795.6711 | 856.8289 | 887.5834 |
| 905.1919 | 914.7446 | 926.8359 |
| 986.3242 | 1025.741 | 1061.793 |
| 1098.866 | 1106.361 | 1175.56 |
| 1204.054 | 1245.615 | 1313.813 |
| 1374.092 | 1436.814 | 1497.186 |
| 1542.685 | 1604.494 | 1622.544 |
| 1737.059 | 1933.606 | 3178.113 |
| 3178.866 | 3221.056 | 3256.852 |
| 3279.652 | 3285.714 | 3721.074 |

***i61 – i63***

**Cartesian coordinates**

N 1.838385 -1.212020 -0.132066

C 2.746329 -0.154979 -0.197761

C 2.084339 1.031864 -0.101879

C 0.699621 0.678445 0.044558

C 0.574981 -0.722053 -0.013637

C -0.606448 1.099115 0.299953

C -1.286110 -0.086644 0.760568

C -2.630311 -0.436846 0.313860

C -3.134921 -0.033437 -0.854872

H 2.090387 -2.179490 -0.231834

H 3.803896 -0.348937 -0.301106

H 2.541126 2.009005 -0.104947

H -1.092995 2.041800 0.075805

H -0.984384 -0.488881 1.719333

H -3.227355 -1.070207 0.965017

H -4.147385 -0.280413 -1.152950

H -2.536861 0.548464 -1.549598

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -378.131 | 87.2545 | 133.2922 |
| 203.2597 | 298.7109 | 338.187 |
| 485.3479 | 536.4851 | 590.5341 |
| 633.6277 | 679.286 | 700.441 |
| 707.4613 | 742.8554 | 781.3188 |
| 809.2345 | 879.7939 | 891.9345 |
| 966.5489 | 973.3647 | 1015.783 |
| 1042.553 | 1057 | 1078.355 |
| 1111.217 | 1175.152 | 1181.539 |
| 1259.097 | 1329.863 | 1339.557 |
| 1370.146 | 1426.46 | 1443.826 |
| 1459.287 | 1566.054 | 1585.921 |
| 1695.62 | 3152.675 | 3167.06 |
| 3206.27 | 3208.723 | 3248.984 |
| 3252.178 | 3277.965 | 3703.051 |

***i62 – i64***

**Cartesian coordinates**

N -1.954871 -1.208132 0.095444

C -2.723641 -0.082143 -0.030985

C -1.875143 0.987007 -0.114036

C -0.535488 0.495131 -0.033778

C -0.632231 -0.877359 0.093591

C 0.641954 1.356119 -0.072755

C 1.932401 1.054726 0.090135

C 2.808765 -1.188553 -0.533188

C 2.510389 -0.285866 0.365317

H -2.310135 -2.144525 0.165531

H -3.799789 -0.138250 -0.051657

H -2.165014 2.021765 -0.218954

H 0.133639 -1.629426 0.167412

H 0.411718 2.405013 -0.245846

H 2.655461 1.865711 0.052818

H 3.251916 -2.175139 -0.539752

H 2.744264 -0.502593 1.416536

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -111.044 | 42.0804 | 142.0268 |
| 176.3488 | 259.0249 | 345.334 |
| 499.0057 | 516.6944 | 540.5519 |
| 646.8094 | 659.734 | 671.458 |
| 712.5352 | 745.9315 | 763.2928 |
| 824.7429 | 830.2233 | 871.5618 |
| 897.0907 | 913.1201 | 975.6609 |
| 1017.408 | 1024.671 | 1087.474 |
| 1107.737 | 1179.065 | 1239.855 |
| 1254.799 | 1262.377 | 1332.622 |
| 1419.01 | 1451.205 | 1496.756 |
| 1542.909 | 1621.32 | 1687.555 |
| 1743.838 | 3021.263 | 3153.571 |
| 3176.789 | 3250.562 | 3257.164 |
| 3285.263 | 3303.292 | 3718.129 |

***i63 – i65***

**Cartesian coordinates**

N -1.562260 -1.047138 -0.625066

C -2.344152 -0.456256 0.381567

C -1.780137 0.709708 0.774894

C -0.568030 0.816382 -0.004914

C -0.507221 -0.266710 -0.951918

C 0.637169 1.459016 -0.086444

C 1.529938 0.549454 -0.798094

C 2.211451 -0.549720 -0.141571

C 2.173716 -0.842637 1.167223

H -1.852480 -1.861432 -1.139539

H -3.254809 -0.931508 0.717598

H -2.140813 1.358635 1.557284

H 0.911392 2.447725 0.268183

H 2.018866 0.905931 -1.705557

H 2.829545 -1.161005 -0.795027

H 2.722928 -1.687757 1.563896

H 1.584793 -0.256042 1.864165

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -474.055 | 62.5445 | 98.8967 |
| 151.1058 | 206.8851 | 298.4845 |
| 476.7285 | 569.3046 | 612.0249 |
| 624.9646 | 633.1332 | 709.3413 |
| 737.2275 | 744.5402 | 761.244 |
| 835.2101 | 885.9282 | 897.7764 |
| 911.6623 | 943.8259 | 978.2975 |
| 1036.481 | 1053.65 | 1060.467 |
| 1103.515 | 1128.108 | 1177.287 |
| 1232.736 | 1292.018 | 1334.967 |
| 1366.625 | 1417.337 | 1427.544 |
| 1442.695 | 1597.792 | 1615.356 |
| 1645.36 | 3127.796 | 3156.746 |
| 3167.966 | 3191.437 | 3247.55 |
| 3256.705 | 3274.78 | 3686.31 |

***i64 – i65***

**Cartesian coordinates**

N 1.825290 1.170421 -0.000077

C 2.628201 0.048342 0.000097

C 1.817777 -1.050154 0.000131

C 0.456081 -0.594197 -0.000028

C 0.526456 0.783409 -0.000134

C -0.731971 -1.411156 -0.000102

C -2.022755 -1.015423 -0.000075

C -1.908284 1.498556 0.000014

C -2.560795 0.335521 0.000125

H 2.150817 2.120115 -0.000143

H 3.702986 0.135833 0.000193

H 2.145098 -2.079204 0.000260

H -0.671796 1.468934 -0.000402

H -0.550002 -2.482834 -0.000185

H -2.771913 -1.800555 -0.000126

H -2.360732 2.484103 0.000323

H -3.649758 0.391267 0.000460

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1263.59 | 75.7371 | 181.2403 |
| 273.9676 | 276.242 | 399.8291 |
| 453.0037 | 477.4223 | 482.9292 |
| 596.5119 | 627.2643 | 677.4407 |
| 694.681 | 724.2616 | 798.089 |
| 816.5287 | 861.3998 | 887.2924 |
| 912.1131 | 948.5015 | 952.1093 |
| 999.3258 | 1018.192 | 1082.957 |
| 1112.908 | 1129.334 | 1220.137 |
| 1270.521 | 1299.543 | 1325.341 |
| 1403.968 | 1437.806 | 1467.563 |
| 1498.786 | 1545.925 | 1610.903 |
| 1657.138 | 1711.684 | 3128.932 |
| 3169.42 | 3197.994 | 3213.309 |
| 3249.504 | 3279.083 | 3718.583 |

***i64 – i66***

**Cartesian coordinates**

N 1.816150 -0.961414 0.290223

C 2.388747 0.067521 -0.410902

C 1.498413 1.108097 -0.451666

C 0.319559 0.693660 0.226661

C 0.539102 -0.622326 0.664314

C -0.949164 1.378835 0.313544

C -2.129560 0.758885 0.108454

C -1.321889 -1.547706 -0.319277

C -2.268268 -0.620705 -0.355306

H 2.265913 -1.830719 0.510968

H 3.369401 -0.033273 -0.847826

H 1.646540 2.048307 -0.960130

H 0.073345 -1.126567 1.495102

H -0.939694 2.454064 0.469214

H -3.040326 1.347067 0.160869

H -1.325589 -2.567393 -0.686387

H -3.224288 -0.859150 -0.828304

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -364.152 | 117.058 | 164.5887 |
| 272.1659 | 303.4923 | 430.5515 |
| 455.6 | 468.1292 | 593.861 |
| 634.5587 | 637.4554 | 682.0593 |
| 742.5821 | 760.6106 | 783.8782 |
| 807.9667 | 888.4475 | 898.6379 |
| 916.81 | 921.2307 | 979.3535 |
| 991.9996 | 1016.649 | 1092.165 |
| 1100.934 | 1175.358 | 1203.843 |
| 1260.081 | 1269.785 | 1302.799 |
| 1398.155 | 1439.664 | 1490.514 |
| 1539.065 | 1561.783 | 1605.795 |
| 1674.906 | 3092.319 | 3169.673 |
| 3193.089 | 3214.471 | 3256.499 |
| 3264.548 | 3278.045 | 3722.727 |

***i22 – i65***

**Cartesian coordinates**

N 1.800586 1.161879 -0.072515

C 2.600974 0.033217 -0.066217

C 1.784161 -1.056927 0.019260

C 0.426863 -0.589031 0.066569

C 0.499835 0.789909 -0.049031

C -0.761203 -1.403324 0.141846

C -2.038055 -0.993381 -0.045558

C -1.846391 1.446559 0.304286

C -2.422067 0.377073 -0.287148

H 2.129579 2.101692 -0.203929

H 3.672055 0.110357 -0.166673

H 2.104630 -2.088044 0.048882

H -0.589448 -2.469524 0.264634

H -2.808857 -1.753533 -0.133677

H -2.107566 2.457075 0.011225

H -1.273940 1.338374 1.217478

H -3.195260 0.545877 -1.034380

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -199.019 | 97.3654 | 171.3478 |
| 245.2653 | 275.7546 | 401.9812 |
| 450.4513 | 511.6312 | 588.692 |
| 608.5652 | 616.0642 | 674.4244 |
| 729.1449 | 805.5337 | 812.0425 |
| 863.7987 | 866.705 | 912.7279 |
| 948.3253 | 976.9591 | 1006.017 |
| 1020.98 | 1079.421 | 1092.736 |
| 1109.129 | 1197.918 | 1242.692 |
| 1286.958 | 1308.409 | 1374.339 |
| 1429.537 | 1433.123 | 1457.083 |
| 1524.243 | 1569.582 | 1624.507 |
| 1667.069 | 3144.178 | 3161.843 |
| 3165.957 | 3185.678 | 3245.655 |
| 3251.318 | 3275.589 | 3710.145 |

***i22 – i66***

**Cartesian coordinates**

N 1.593752 -1.079903 -0.075138

C 2.392045 0.028814 -0.109826

C 1.644169 1.166672 -0.017068

C 0.266209 0.777359 0.093798

C 0.275786 -0.660794 0.154358

C -0.929592 1.474260 0.066618

C -2.154687 0.715197 -0.062777

C -0.999526 -1.453056 0.018703

C -2.184087 -0.643523 -0.118897

H 1.926083 -2.020147 0.034524

H 3.462565 -0.077229 -0.205419

H 2.021896 2.175067 -0.076230

H -0.305540 -1.087222 1.161592

H -0.946868 2.555640 0.044836

H -3.088782 1.257651 -0.158671

H -0.960169 -2.518782 -0.151575

H -3.127353 -1.155222 -0.272541

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -3401.36 | 161.1858 | 203.7743 |
| 251.5592 | 325.8193 | 377.596 |
| 475.8229 | 528.7769 | 533.8137 |
| 584.2505 | 601.2067 | 662.1267 |
| 718.7921 | 744.7061 | 763.9731 |
| 777.5113 | 867.5867 | 889.2202 |
| 899.384 | 965.2552 | 997.2556 |
| 1015.55 | 1094.189 | 1113.218 |
| 1143.681 | 1181.214 | 1199.705 |
| 1230.639 | 1266.267 | 1316.118 |
| 1374.81 | 1426.602 | 1431.728 |
| 1482.634 | 1498.889 | 1582.87 |
| 1635.011 | 2233.856 | 3188.939 |
| 3209.722 | 3228.131 | 3246.095 |
| 3253.326 | 3275.126 | 3721.301 |

***i66 – indole (2) + H***

**Cartesian coordinates**

N 1.563310 -1.067032 -0.083411

C 2.367490 0.045849 -0.089252

C 1.609282 1.178277 -0.039111

C 0.244094 0.765158 0.035147

C 0.248626 -0.664786 0.121238

C -0.983166 1.436334 0.018703

C -2.150004 0.699876 -0.014356

C -0.944756 -1.407400 -0.072677

C -2.126619 -0.711157 -0.087806

H 1.895667 -1.999123 0.087429

H 3.439991 -0.059073 -0.149788

H 1.980982 2.190004 -0.076546

H 0.253255 -0.707247 1.832088

H -1.013962 2.520057 0.004515

H -3.106098 1.210206 -0.030363

H -0.919512 -2.488763 -0.139037

H -3.063172 -1.249742 -0.175734

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1028.98 | 213.8488 | 231.0279 |
| 383.0114 | 412.6863 | 448.049 |
| 512.1488 | 545.9072 | 565.9965 |
| 594.5746 | 623.3671 | 661.0966 |
| 736.5646 | 757.4359 | 771.7426 |
| 806.9484 | 869.7326 | 890.8347 |
| 894.4313 | 909.2093 | 955.0578 |
| 990.7 | 1035.92 | 1091.441 |
| 1128.658 | 1153.691 | 1178.008 |
| 1229.414 | 1266.506 | 1308.698 |
| 1361.26 | 1388.877 | 1461.791 |
| 1482.3 | 1538.171 | 1566.752 |
| 1622.398 | 1670.948 | 3194.376 |
| 3201.97 | 3213.03 | 3223.222 |
| 3258.662 | 3278.604 | 3712.083 |

***i56 – i67***

**Cartesian coordinates**

N -2.486959 -0.954013 -0.136452

C -2.903469 0.353561 -0.142382

C -1.795046 1.146238 -0.040185

C -0.655137 0.286931 0.038354

C -1.130786 -1.008931 -0.036418

H -3.091528 -1.751721 -0.217938

H -3.949290 0.603702 -0.217156

H -1.785472 2.225080 -0.010011

H -0.596651 -1.945587 -0.051679

C 4.035489 -0.285342 -0.450866

C 2.891729 0.030567 -0.013828

C 1.729429 -0.190566 0.735316

C 0.739210 0.668427 0.172744

H 4.881170 -0.077083 -1.072404

H 1.583983 -0.928546 1.518964

H 0.921475 1.740114 0.234452

H 1.976514 0.806826 -0.805472

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -2155.46 | 70.7439 | 79.0822 |
| 172.3666 | 227.3971 | 309.357 |
| 394.5107 | 415.8886 | 499.673 |
| 517.6897 | 523.2868 | 573.8453 |
| 645.5497 | 654.5329 | 718.0734 |
| 726.7542 | 762.0985 | 805.5397 |
| 837.9286 | 874.3815 | 909.2635 |
| 994.1551 | 1013.877 | 1080.451 |
| 1101.854 | 1109.531 | 1159.936 |
| 1170.901 | 1234.913 | 1312.32 |
| 1332.039 | 1421.027 | 1466.379 |
| 1488.63 | 1498.306 | 1561.773 |
| 1612.79 | 1813.069 | 3137.458 |
| 3173.688 | 3260.096 | 3279.825 |
| 3286.697 | 3382.539 | 3715.65 |

***i67 – i68***

**Cartesian coordinates**

N 2.653213 -0.845180 -0.065586

C 2.941468 0.492797 -0.069558

C 1.753716 1.172213 -0.030492

C 0.700463 0.210058 0.003354

C 1.302046 -1.030827 -0.025521

C -0.725705 0.520663 0.054477

C -1.711783 -0.336171 0.318251

C -3.149306 0.049571 0.350601

C -4.000219 -0.131532 -0.625761

H 3.333583 -1.582169 -0.108815

H 3.959119 0.846644 -0.100221

H 1.635679 2.245220 -0.019217

H 0.872413 -2.019533 -0.039975

H -0.984018 1.558480 -0.146305

H -1.488206 -1.376705 0.544754

H -3.515628 0.503750 1.280139

H -5.049515 0.059942 -0.803359

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -181.16 | 40.5977 | 97.2631 |
| 146.5275 | 274.4494 | 331.868 |
| 392.8098 | 475.2001 | 504.1224 |
| 641.3186 | 644.4876 | 661.0545 |
| 705.0515 | 768.0211 | 786.7034 |
| 821.8351 | 847.5002 | 862.5258 |
| 902.7392 | 914.0688 | 998.5973 |
| 1008.943 | 1066.677 | 1095.794 |
| 1106.545 | 1176.804 | 1233.687 |
| 1250.006 | 1309.366 | 1336.472 |
| 1349.904 | 1436.753 | 1496.822 |
| 1540.575 | 1624.635 | 1686.126 |
| 1748.756 | 3034.22 | 3149.779 |
| 3158.798 | 3247.839 | 3255.277 |
| 3281.025 | 3284.848 | 3718.368 |

***i68 – i69***

**Cartesian coordinates**

N -2.542548 -0.871850 0.04729

C -2.860462 0.457775 0.13676

C -1.696524 1.170588 0.06852

C -0.615672 0.240429 -0.06948

C -1.191351 -1.020950 -0.07734

C 0.777557 0.588832 -0.17361

C 1.817354 -0.305989 -0.35463

C 3.249171 0.095443 -0.43150

C 3.331438 -0.203106 0.81892

H -3.203740 -1.626504 0.07732

H -3.883274 0.781437 0.24236

H -1.605314 2.245296 0.11100

H -0.742779 -1.998158 -0.15194

H 1.024503 1.641515 -0.06514

H 1.586034 -1.349187 -0.55077

H 3.859353 0.489556 -1.23805

H 3.893993 -0.219126 1.73847

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -717.6 | 57.8342 | 94.2292 |
| 153.9602 | 233.3548 | 345.4841 |
| 351.8523 | 417.762 | 484.1564 |
| 568.9153 | 635.4104 | 649.8693 |
| 683.7325 | 707.5834 | 765.9656 |
| 772.4591 | 809.8769 | 867.0209 |
| 867.8109 | 909.6653 | 934.0475 |
| 995.4062 | 1048.212 | 1092.114 |
| 1106.468 | 1166.7 | 1176.489 |
| 1234.826 | 1272.904 | 1310.596 |
| 1344.664 | 1420.581 | 1493.971 |
| 1502.964 | 1556.653 | 1598.816 |
| 1725.033 | 3162.438 | 3170.118 |
| 3178.198 | 3255.933 | 3277.557 |
| 3282.341 | 3285.832 | 3718.802 |

***i68 – i71***

**Cartesian coordinates**

N -2.415487 0.812396 0.301943

C -2.723463 -0.494179 0.015135

C -1.554977 -1.147628 -0.258937

C -0.490790 -0.200615 -0.141905

C -1.070005 1.000659 0.218380

C 0.926139 -0.434470 -0.351403

C 2.649753 -0.508896 0.952819

C 3.058889 0.269148 -0.070925

C 1.841588 0.570565 -0.742333

H -3.081555 1.517897 0.560680

H -3.743528 -0.842482 0.029250

H -1.455453 -2.188670 -0.525839

H -0.613617 1.951488 0.442858

H 1.211266 -1.464937 -0.529746

H 3.138901 -1.071553 1.743270

H 4.066573 0.584900 -0.327683

H 1.563005 1.499085 -1.231377

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -619.706 | 79.6628 | 118.8136 |
| 154.6351 | 386.1194 | 397.884 |
| 435.5721 | 515.1791 | 579.8734 |
| 645.6905 | 663.8749 | 683.4984 |
| 714.4237 | 729.0014 | 777.9058 |
| 817.5341 | 842.0909 | 874.6819 |
| 903.9763 | 911.4926 | 914.8721 |
| 1003.879 | 1056.705 | 1092.591 |
| 1104.802 | 1163.21 | 1174.737 |
| 1235.064 | 1254.779 | 1322.668 |
| 1361.284 | 1428.163 | 1480.696 |
| 1491.67 | 1520.006 | 1566.15 |
| 1618.48 | 3158.06 | 3185.527 |
| 3194.06 | 3195.78 | 3260.402 |
| 3280.824 | 3284.81 | 3715.52 |

***i69 – i70***

**Cartesian coordinates**

N 2.204139 1.024843 0.030632

C 2.740200 -0.209291 -0.244413

C 1.735790 -1.128966 -0.203992

C 0.509461 -0.437509 0.110362

C 0.859866 0.909802 0.247435

C -0.773347 -1.004515 0.251394

C -1.990644 -0.206657 0.555782

C -2.416611 0.956293 -0.315397

C -3.126920 -0.111087 -0.437025

H 2.722971 1.882773 0.071025

H 3.793309 -0.325706 -0.444932

H 1.837684 -2.189105 -0.378250

H 0.254701 1.765070 0.497935

H -0.873270 -2.082605 0.162548

H -2.250531 -0.159046 1.618644

H -2.203175 1.966428 -0.618967

H -3.937423 -0.640122 -0.907298

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -53.0403 | 94.866 | 141.773 |
| 253.8344 | 320.2085 | 371.5612 |
| 455.3022 | 494.8932 | 573.7737 |
| 623.6438 | 649.2945 | 672.2398 |
| 705.6376 | 737.8816 | 773.6768 |
| 841.8876 | 879.7019 | 881.8778 |
| 899.3941 | 911.2125 | 972.395 |
| 1012.115 | 1037.645 | 1053.219 |
| 1100.642 | 1100.951 | 1167.083 |
| 1219.082 | 1225.948 | 1299.292 |
| 1358.274 | 1390.616 | 1453.008 |
| 1492.031 | 1532.923 | 1578.965 |
| 1741.649 | 3033.594 | 3170.197 |
| 3257.779 | 3271.418 | 3279.706 |
| 3282.914 | 3319.586 | 3723.74 |

***i62 – i70***

**Cartesian coordinates**

N 2.023398 -1.133740 -0.060686

C 2.705477 0.043599 0.105156

C 1.788521 1.054461 0.132226

C 0.484427 0.478201 -0.026580

C 0.682704 -0.891808 -0.139911

C -0.736547 1.238218 -0.045520

C -2.034350 0.780912 -0.227083

C -2.436418 -0.624364 -0.504198

C -2.704783 -0.711072 0.753000

H 2.444674 -2.043691 -0.106757

H 3.779940 0.060223 0.190363

H 2.003828 2.105672 0.249855

H -0.022763 -1.696728 -0.250776

H -0.622240 2.303033 0.136462

H -2.815590 1.532006 -0.279566

H -2.428332 -1.232529 -1.403914

H -2.997488 -1.300689 1.606591

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -701.104 | 61.1915 | 122.8166 |
| 173.8483 | 242.2535 | 299.3211 |
| 420.5596 | 490.5708 | 516.0715 |
| 604.2039 | 637.605 | 653.7011 |
| 680.4696 | 716.0804 | 756.8146 |
| 776.4532 | 806.7668 | 874.0098 |
| 877.7426 | 908.4951 | 930.9628 |
| 956.3611 | 1018.16 | 1095.485 |
| 1106.436 | 1138.934 | 1179.878 |
| 1243.141 | 1256.482 | 1322.686 |
| 1408.058 | 1422.935 | 1488.662 |
| 1498.466 | 1556.345 | 1599.294 |
| 1722.07 | 3151.349 | 3168.943 |
| 3188.871 | 3256.71 | 3277.053 |
| 3283.548 | 3304.239 | 3721.491 |

***i64 – i71***

**Cartesian coordinates**

N 2.150627 0.939053 -0.105899

C 2.507920 -0.367994 -0.291099

C 1.412511 -1.143847 -0.018550

C 0.342616 -0.271045 0.339206

C 0.842032 1.010066 0.287684

H 2.766840 1.725507 -0.200153

H 3.505686 -0.637041 -0.598306

H 1.363770 -2.220020 -0.086353

H 0.363408 1.951240 0.503720

C -1.008317 -0.680034 0.759294

C -1.927766 -0.426175 -1.230694

C -2.445977 0.572648 -0.495094

C -2.134087 0.168275 0.841355

H -0.988676 -1.558311 1.410381

H -1.786458 -0.631096 -2.288578

H -2.987257 1.453247 -0.831469

H -2.825294 0.171738 1.679442

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -701.851 | 49.4391 | 130.2543 |
| 170.4309 | 293.4601 | 366.018 |
| 452.3366 | 474.1968 | 586.7101 |
| 638.2486 | 646.9462 | 703.4451 |
| 710.3877 | 743.4428 | 783.2912 |
| 808.5062 | 859.452 | 888.1518 |
| 903.2526 | 911.8677 | 944.1024 |
| 984.5386 | 1059.674 | 1077.976 |
| 1095.224 | 1139.361 | 1171.022 |
| 1240.408 | 1252.803 | 1313.781 |
| 1408.319 | 1423.039 | 1464.777 |
| 1493.068 | 1524.423 | 1550.508 |
| 1621.855 | 3093.037 | 3153.637 |
| 3176.799 | 3191.155 | 3254.515 |
| 3280.608 | 3283.725 | 3721.632 |

***Reaction steps with extra ammonia molecules***

**1)**

***i2 + NH3***

**Cartesian coordinates**

C 0.397016 -0.285947 1.159658

C 0.866534 0.990408 0.556783

N 0.464271 -1.163821 -0.004157

C 1.107375 0.790454 -0.746889

C 0.832072 -0.617860 -1.150981

H -0.644115 -0.209115 1.494563

H 1.030688 -0.641309 1.979018

H 0.968945 1.907862 1.121868

H 0.171082 -2.125764 0.059338

H 1.452954 1.539840 -1.446885

N -2.505741 0.213393 -0.105967

H -3.398221 -0.226141 -0.297934

H -2.639202 1.212960 -0.204777

H -1.869821 -0.067672 -0.845751

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 35.4321 | 71.4887 | 89.5409 |
| 158.5417 | 174.1515 | 227.7499 |
| 374.2394 | 464.2956 | 719.7899 |
| 744.1377 | 832.3217 | 863.9683 |
| 965.8086 | 971.2871 | 1002.229 |
| 1004.145 | 1022.432 | 1089.089 |
| 1126.682 | 1195.539 | 1302.681 |
| 1337.416 | 1368.8 | 1443.826 |
| 1514.795 | 1618.339 | 1673.508 |
| 1687.966 | 3045.45 | 3100.516 |
| 3216.521 | 3239.988 | 3506.298 |
| 3626.454 | 3642.349 | 3658.904 |

***i2 + NH3 – pyrrole (3) + NH3***

**Cartesian coordinates**

C -0.285554 0.445891 1.093218

C -0.761436 -0.841145 0.755917

N -0.410801 1.174338 -0.108912

C -0.959909 -0.862539 -0.618857

C -0.708113 0.423588 -1.205728

H 1.110656 -0.015882 0.667236

H -0.337198 0.933887 2.059303

H -0.858512 -1.658346 1.460212

H -0.148297 2.143622 -0.178419

H -1.253642 -1.734150 -1.190219

N 2.006742 -0.269883 -0.145274

H 2.775578 0.387384 -0.100940

H 2.343697 -1.220766 -0.060266

H 1.486204 -0.161709 -1.024904

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1082.82 | 175.6353 | 195.6927 |
| 265.3575 | 432.1453 | 469.7818 |
| 586.7273 | 611.6169 | 674.3764 |
| 724.0266 | 772.7104 | 846.8163 |
| 868.8377 | 906.6337 | 936.9374 |
| 1032.085 | 1053.583 | 1103.966 |
| 1132.297 | 1232.629 | 1275.67 |
| 1340.256 | 1388.417 | 1453.65 |
| 1472.584 | 1503.119 | 1568.61 |
| 1655.127 | 1706.82 | 3201.788 |
| 3208.824 | 3229.628 | 3376.221 |
| 3587.073 | 3662.807 | 3666.175 |

***Pyrrole (3) + NH3***

**Cartesian coordinates**

C -0.585064 -1.112578 0.000007

C -1.899706 -0.711786 0.000057

N 0.202358 0.002168 -0.000033

C -1.902392 0.708145 0.000055

C -0.589272 1.113915 0.000003

H 3.564553 -0.142021 -0.932551

H -0.151659 -2.100335 -0.000253

H -2.760718 -1.362404 0.000022

H 1.223914 0.003781 0.000279

H -2.765852 1.355510 0.000016

N 3.193810 0.000221 -0.000080

H 3.564444 -0.736783 0.588761

H 3.570425 0.876026 0.344040

H -0.159672 2.103326 -0.000250

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 29.2729 | 50.1472 | 62.138 |
| 180.6241 | 276.9531 | 302.1805 |
| 629.8918 | 638.773 | 715.7773 |
| 737.3557 | 825.8811 | 891.1997 |
| 892.4632 | 904.5808 | 920.9019 |
| 1044.289 | 1081.47 | 1103.974 |
| 1108.236 | 1196.448 | 1219.821 |
| 1335.531 | 1441.242 | 1528.261 |
| 1529.485 | 1618.387 | 1678.353 |
| 1679.107 | 3243.62 | 3254.532 |
| 3268.346 | 3276.843 | 3427.251 |
| 3518.424 | 3643.724 | 3645.267 |

***i2 + 2 NH3***

**Cartesian coordinates**

N 0.384972 0.458218 0.000098

C 0.395323 -0.858736 0.000503

C 1.690329 1.103093 -0.000416

C 1.848736 -1.188227 0.000355

C 2.598528 -0.078228 -0.000169

H -0.495454 1.000332 0.000063

H 1.817168 1.735319 -0.886419

H 1.817569 1.736027 0.885017

H 2.223968 -2.203313 0.000614

H 3.678083 0.000639 -0.000447

N -2.290560 1.573786 0.000287

H -2.659450 0.611598 0.000049

H -2.662600 2.046468 0.815936

H -2.662601 2.046954 -0.815080

N -2.727689 -1.399456 -0.000393

H -1.699042 -1.462485 0.000082

H -3.061518 -1.903621 0.813420

H -3.060690 -1.903172 -0.814823

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 33.0113 | 74.7515 | 99.0718 |
| 154.4523 | 183.4263 | 199.1697 |
| 232.7614 | 248.8419 | 290.8677 |
| 360.6117 | 398.8889 | 456.0546 |
| 507.9403 | 600.4547 | 711.2985 |
| 840.571 | 861.1992 | 958.0317 |
| 970.3599 | 975.7095 | 1003.732 |
| 1032.638 | 1070.332 | 1123.085 |
| 1165.921 | 1175.837 | 1206.326 |
| 1296.698 | 1355.733 | 1416.708 |
| 1457.696 | 1592.249 | 1627.695 |
| 1658.561 | 1681.363 | 1718.538 |
| 1730.8 | 3055.617 | 3096.523 |
| 3218.527 | 3221.739 | 3244.718 |
| 3298.752 | 3333.383 | 3561.116 |
| 3568.403 | 3631.299 | 3637.689 |

***i2 + 2 NH3 – pyrrole (3) + 2 NH3***

**Cartesian coordinates**

N 0.641612 -0.440013 1.140769

C 0.249484 -1.372857 0.243791

C 1.413024 0.619032 0.600629

C 0.964838 -0.977504 -0.939507

C 1.702976 0.168193 -0.714455

H 0.265163 -0.402559 2.073482

H 0.239179 1.381261 0.161168

H 2.082533 1.187469 1.238156

H 0.910448 -1.510216 -1.880442

H 2.331278 0.703746 -1.415949

N -0.907693 1.751968 -0.232855

H -1.590105 0.952441 -0.164748

H -1.246778 2.537177 0.312134

H -0.838146 2.036699 -1.203967

N -2.597157 -0.560286 -0.068096

H -1.786536 -1.186224 0.098478

H -3.262166 -0.708576 0.683047

H -3.044134 -0.874082 -0.922834

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1165.99 | 43.3262 | 134.27 |
| 160.9605 | 206.4274 | 236.0046 |
| 291.3893 | 307.6539 | 413.958 |
| 435.968 | 526.053 | 545.8227 |
| 601.6541 | 651.0327 | 713.2891 |
| 724.2884 | 770.5645 | 848.0175 |
| 871.4913 | 905.6764 | 945.1583 |
| 1032.193 | 1052.749 | 1109.498 |
| 1130.88 | 1226.239 | 1262.797 |
| 1341.285 | 1365.119 | 1396.817 |
| 1458.811 | 1494.132 | 1508.299 |
| 1555.27 | 1651.275 | 1692.369 |
| 1714.477 | 1733.619 | 2941.75 |
| 3182.889 | 3186.213 | 3210.978 |
| 3232.423 | 3554.317 | 3555.701 |
| 3629.479 | 3639.035 | 3664.406 |

***Pyrrole (3) + 2 NH3***

**Cartesian coordinates**

N -0.162224 -0.867513 -0.025889

C -0.843866 -0.507050 1.099706

C -0.849561 -0.439763 -1.123816

C -1.997294 0.140022 0.719540

C -2.000945 0.182558 -0.699778

H 0.815475 -1.179373 -0.036361

H 0.698702 1.660342 0.771616

H -0.471082 -0.617402 -2.118392

H -2.759166 0.520127 1.382844

H -2.766037 0.602437 -1.334775

N 1.362896 1.876889 0.033340

H 2.560398 0.134682 0.015678

H 0.827256 1.789354 -0.824867

H 1.614809 2.853664 0.131341

N 2.729973 -0.876523 -0.010647

H -0.460594 -0.744933 2.079750

H 3.299212 -1.078919 -0.823944

H 3.276513 -1.124554 0.805578

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 55.1256 | 61.5227 | 71.4473 |
| 143.8167 | 181.273 | 183.3674 |
| 215.0028 | 227.2016 | 263.2587 |
| 345.2602 | 374.9086 | 521.5999 |
| 637.8159 | 642.4723 | 726.5667 |
| 748.8268 | 839.9487 | 886.6105 |
| 893.0394 | 896.6776 | 962.1063 |
| 1043.489 | 1077.696 | 1104.763 |
| 1151.539 | 1161.937 | 1197.61 |
| 1221.81 | 1335.648 | 1439.178 |
| 1527.366 | 1529.096 | 1617.767 |
| 1667.939 | 1669.99 | 1710.461 |
| 1723.46 | 3247.556 | 3258.791 |
| 3273.077 | 3281.143 | 3344.326 |
| 3396.387 | 3501.84 | 3581.654 |
| 3607.19 | 3633.358 | 3642.735 |

**2)**

***i3 + NH3***

**Cartesian coordinates**

N 0.110630 -0.533455 0.636067

C -1.187641 1.126917 -0.103498

C -0.041016 1.004739 0.615082

C -1.766422 -0.149137 -0.518332

C -0.998713 -1.149639 -0.076599

H 0.168230 -0.823125 1.610854

H 1.053220 -0.701987 0.208919

H -1.631345 2.082494 -0.352237

H -2.671091 -0.280494 -1.098362

H -1.075921 -2.221255 -0.170139

N 2.668545 -0.015377 -0.391048

H 3.574885 -0.142978 0.042699

H 2.812199 0.060288 -1.391190

H 2.278349 0.871600 -0.065596

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 58.408 | 128.6633 | 174.0734 |
| 234.8591 | 311.8244 | 452.4989 |
| 515.2012 | 558.5855 | 670.6288 |
| 708.2952 | 803.2856 | 809.3786 |
| 868.5644 | 925.0964 | 961.9374 |
| 986.6156 | 1033.634 | 1127.327 |
| 1143.451 | 1180.105 | 1216.21 |
| 1316.477 | 1356.346 | 1514.036 |
| 1638.243 | 1665.817 | 1672.664 |
| 1693.656 | 3042.582 | 3223.529 |
| 3236.696 | 3275.361 | 3440.026 |
| 3539.754 | 3593.076 | 3648.764 |

***i3 + NH3 – pyrrole (3) + NH3***

**Cartesian coordinates**

N 0.112314 -0.647351 0.678112

C -0.958937 1.158831 -0.012768

C 0.066656 0.827673 0.832070

C -1.603373 -0.007074 -0.591888

C -0.970248 -1.101992 -0.129686

H 0.283422 -1.153051 1.539299

H 1.302345 -0.565399 -0.018042

H -1.260329 2.177644 -0.224099

H -2.434737 -0.012515 -1.284848

H -1.144707 -2.153813 -0.301847

N 2.268350 0.028413 -0.481084

H 3.194498 -0.307931 -0.244979

H 2.185488 0.194794 -1.477821

H 2.004780 0.888209 0.046775

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -991.445 | 45.6946 | 199.4668 |
| 264.6427 | 386.1657 | 446.1929 |
| 589.763 | 658.4343 | 679.8398 |
| 720.2598 | 796.4379 | 849.81 |
| 870.7731 | 881.451 | 914.1784 |
| 920.6587 | 1009.277 | 1075.237 |
| 1134.369 | 1216.207 | 1244.448 |
| 1299.767 | 1376.886 | 1476.237 |
| 1546.542 | 1631.299 | 1648.673 |
| 1691.573 | 1757.312 | 3151.928 |
| 3209.398 | 3228.027 | 3257.211 |
| 3562.57 | 3591.469 | 3652.877 |

***Pyrrole (3) + NH3***

**Cartesian coordinates**

N 0.202387 0.002464 0.005401

C -1.902512 0.707973 -0.002910

C -0.589504 1.113995 0.002207

C -1.899457 -0.712118 -0.002900

C -0.584713 -1.112458 0.002224

H 1.223968 0.004258 0.007692

H 3.556770 -0.749907 -0.578567

H -2.765932 1.355500 -0.006097

H -2.760038 -1.363413 -0.006076

H -0.149917 -2.099649 0.004235

N 3.193301 0.000250 -0.001901

H 3.575629 -0.121010 0.928831

H 3.565804 0.867829 -0.370430

H -0.158978 2.103054 0.004187

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 47.193 | 48.8703 | 70.1951 |
| 180.8137 | 280.7123 | 308.3389 |
| 629.787 | 638.0619 | 707.2158 |
| 737.0214 | 822.8168 | 892.3841 |
| 893.7454 | 902.5814 | 923.7 |
| 1038.042 | 1077.003 | 1104.908 |
| 1110.077 | 1196.897 | 1222.559 |
| 1332.924 | 1437.596 | 1528.723 |
| 1531.133 | 1619.226 | 1677.122 |
| 1681.937 | 3243.494 | 3256.204 |
| 3274.789 | 3281.439 | 3429.52 |
| 3517.343 | 3642.315 | 3643.522 |

***i3 + 2 NH3***

**Cartesian coordinates**

N 0.519882 0.468927 0.704717

C 1.433179 -1.272404 -0.349334

C 0.297416 -0.998077 0.342651

C 2.348875 -0.138106 -0.435003

C 1.814447 0.904925 0.207690

H 0.433239 0.560079 1.715545

H 1.642026 -2.236158 -0.795787

H 3.306622 -0.125723 -0.939272

H 2.159437 1.914323 0.367358

H -0.296309 1.021130 0.282567

N -1.739658 1.640678 -0.424482

H -2.237990 2.431097 -0.032243

H -1.632774 1.813190 -1.418004

H -2.323701 0.794246 -0.314903

N -2.803830 -1.081856 0.035786

H -3.343780 -1.379290 0.840854

H -3.093534 -1.664536 -0.741959

H -1.811493 -1.300633 0.227681

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 45.6546 | 67.6403 | 123.0406 |
| 166.6019 | 196.8222 | 238.5848 |
| 251.9268 | 263.8324 | 327.4975 |
| 406.2126 | 491.5606 | 534.149 |
| 561.6542 | 642.1149 | 680.279 |
| 762.1482 | 819.8224 | 827.5613 |
| 876.9719 | 938.5143 | 973.8351 |
| 989.2957 | 1037.314 | 1122.72 |
| 1196.432 | 1201.333 | 1221.05 |
| 1234.091 | 1351.174 | 1419.817 |
| 1516.848 | 1647.949 | 1654.575 |
| 1670.871 | 1683.955 | 1721.368 |
| 1728.763 | 2640.813 | 3220.049 |
| 3225.559 | 3236.138 | 3271.638 |
| 3276.733 | 3535.83 | 3557.121 |
| 3565.701 | 3629.967 | 3638.806 |

***i3 + 2 NH3 – pyrrole (3) + 2 NH3***

**Cartesian coordinates**

N -0.555016 -0.396676 0.869562

C -1.125064 1.287218 -0.444031

C -0.140407 0.964751 0.448444

C -2.162839 0.273424 -0.520675

C -1.837437 -0.723905 0.321063

H -0.426108 -0.575771 1.858999

H -1.144335 2.206470 -1.016458

H -3.047157 0.297520 -1.144480

H -2.331664 -1.654470 0.556879

H 0.320653 -1.055761 0.222541

N 1.256598 -1.527531 -0.575836

H 1.554897 -2.485714 -0.436569

H 0.920066 -1.420607 -1.527179

H 2.049601 -0.859778 -0.427146

N 2.874776 0.714615 0.066622

H 3.482818 0.796462 0.874070

H 3.245948 1.333591 -0.645872

H 1.935266 1.076262 0.333976

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -930.585 | 42.3986 | 79.5533 |
| 152.1068 | 181.5147 | 228.1516 |
| 287.7753 | 313.278 | 388.6121 |
| 443.0385 | 545.4117 | 568.1255 |
| 590.9049 | 669.9394 | 697.3748 |
| 737.5713 | 803.6325 | 847.974 |
| 878.5305 | 891.1118 | 922.1063 |
| 926.4323 | 1005.14 | 1062.613 |
| 1132.947 | 1219.445 | 1235.666 |
| 1289.55 | 1326.225 | 1372.229 |
| 1484.221 | 1533.086 | 1633.35 |
| 1642.33 | 1671.662 | 1709.025 |
| 1720.737 | 1739.866 | 3025.724 |
| 3132.627 | 3206.756 | 3222.473 |
| 3261.898 | 3552.948 | 3558.904 |
| 3585.662 | 3629.626 | 3642.724 |

***Pyrrole (3) + 2 NH3***

**Cartesian coordinates**

N 0.164639 -0.869815 0.042946

C 1.997775 0.125844 -0.723051

C 0.847125 -0.533900 -1.089928

C 1.998680 0.201967 0.694903

C 0.848444 -0.413589 1.131426

H -0.812658 -1.182641 0.058843

H 2.759664 0.492541 -1.393839

H 2.761204 0.639661 1.320878

H 0.468117 -0.568148 2.129133

H -0.882554 1.863531 0.831710

N -1.366857 1.877556 -0.060178

H -1.619599 2.840826 -0.248231

H -0.660232 1.611496 -0.741237

H -2.556916 0.130881 -0.022041

N -2.727128 -0.879748 0.019397

H -3.302951 -1.068898 0.831252

H -3.267399 -1.140413 -0.797095

H 0.466612 -0.796718 -2.064629

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 56.7607 | 64.5025 | 73.3663 |
| 117.4016 | 167.8376 | 181.7735 |
| 201.5116 | 221.4788 | 264.1089 |
| 309.7767 | 372.1533 | 518.5299 |
| 638.051 | 641.6542 | 726.4422 |
| 748.0802 | 840.1548 | 886.9301 |
| 893.1463 | 896.3007 | 963.7564 |
| 1043.621 | 1078.035 | 1104.885 |
| 1149.429 | 1161.988 | 1198.034 |
| 1222.069 | 1336.12 | 1439.579 |
| 1527.244 | 1529.961 | 1617.919 |
| 1667.522 | 1670.799 | 1695.717 |
| 1722.354 | 3247.551 | 3258.501 |
| 3272.841 | 3281.149 | 3344.808 |
| 3396.299 | 3501.875 | 3581.646 |
| 3607.962 | 3635.447 | 3642.812 |

***i37 + NH3***

**Cartesian coordinates**

N 0.144729 -0.532952 0.637257

C -1.178645 1.163861 -0.083704

C 0.032216 1.025884 0.596202

C -1.814239 -0.001974 -0.493871

C -0.981602 -1.184032 -0.112599

H 0.156768 -0.806783 1.615180

H -1.586620 2.148602 -0.284115

H -2.741800 -0.089655 -1.042070

H -1.491404 -1.911774 0.527329

H -0.569130 -1.728421 -0.970115

H 1.083790 -0.743759 0.247726

N 2.717284 -0.004675 -0.379224

H 3.604400 -0.069175 0.105522

H 2.915214 0.087973 -1.368485

H 2.248309 0.853955 -0.073367

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 46.9649 | 106.5947 | 168.2594 |
| 173.8724 | 249.1587 | 344.3351 |
| 442.105 | 520.6771 | 548.5135 |
| 669.7547 | 747.5794 | 840.2998 |
| 854.008 | 937.5135 | 949.5601 |
| 991.8522 | 1005.725 | 1074.996 |
| 1144.75 | 1151.913 | 1174.934 |
| 1287.824 | 1321.901 | 1363.209 |
| 1399.973 | 1421.254 | 1499.77 |
| 1661.181 | 1685.186 | 1696.635 |
| 3033.503 | 3073.06 | 3181.778 |
| 3202.442 | 3242.287 | 3399.645 |
| 3555.878 | 3582.746 | 3645.323 |

***i37 + NH3 – i39 + NH3***

**Cartesian coordinates**

N 0.204827 -0.663281 0.521064

C -0.985011 1.208660 0.020520

C 0.203343 0.838978 0.658533

C -1.745438 0.151996 -0.452889

C -1.051356 -1.132953 -0.122509

H 0.335611 -1.085447 1.433643

H -1.266040 2.248213 -0.109257

H -2.681387 0.203687 -0.992750

H -1.625180 -1.770718 0.563323

H -0.825380 -1.743459 -1.008093

H 1.455053 -0.651442 -0.121079

N 2.418558 0.027838 -0.400837

H 3.291709 -0.204517 0.055514

H 2.562656 0.212464 -1.385682

H 1.860029 0.839233 0.100862

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1158.01 | 76.9257 | 193.9245 |
| 338.6186 | 361.0405 | 450.0169 |
| 463.0018 | 579.5608 | 605.1681 |
| 740.7289 | 780.5691 | 806.7917 |
| 860.5987 | 905.2642 | 943.963 |
| 966.7982 | 1002.574 | 1045.294 |
| 1080.217 | 1170.892 | 1188.791 |
| 1230.269 | 1306.651 | 1347.514 |
| 1396.512 | 1426.436 | 1507.023 |
| 1550.273 | 1623.454 | 1713.483 |
| 1769.972 | 2396.527 | 2994.93 |
| 3019.555 | 3201.616 | 3233.685 |
| 3556.737 | 3564.597 | 3665.229 |

***i39 + NH3***

**Cartesian coordinates**

N 0.208103 -0.010589 -0.412961

C -1.825808 0.800528 0.182331

C -0.514177 1.130598 -0.141238

C -1.951336 -0.575571 0.199108

C -0.606883 -1.178829 -0.096197

H 1.214944 -0.034821 -0.261722

H -2.613204 1.516867 0.369563

H -2.842057 -1.150826 0.402376

H -0.193728 -1.728687 0.769989

H -0.625464 -1.891849 -0.934674

H 3.753585 0.283008 -0.636296

N 3.197307 0.013169 0.166410

H 3.555156 -0.874744 0.498216

H 3.364605 0.696516 0.895683

H -0.062477 2.106120 -0.241297

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 45.6125 | 60.6353 | 104.4608 |
| 170.4546 | 225.9677 | 264.8877 |
| 278.5659 | 526.3575 | 563.3064 |
| 646.7166 | 718.9836 | 826.3825 |
| 865.8423 | 878.7632 | 953.3669 |
| 976.6869 | 1010.454 | 1073.2 |
| 1089.442 | 1123.753 | 1165.088 |
| 1206.949 | 1304.569 | 1358.402 |
| 1418.582 | 1495.824 | 1535.674 |
| 1546.762 | 1679.638 | 1683.116 |
| 2907.015 | 2976.297 | 3232.79 |
| 3247.99 | 3263.039 | 3478.412 |
| 3518.982 | 3645.598 | 3646.53 |

***i37 + 2 NH3***

**Cartesian coordinates**

N 0.474249 0.464588 0.713614

C 1.455439 -1.297147 -0.323727

C 0.276256 -1.030113 0.369848

C 2.344755 -0.240312 -0.476509

C 1.769638 0.984465 0.158312

H 0.437140 0.551923 1.724856

H 1.651012 -2.286062 -0.723781

H 3.296723 -0.247346 -0.988481

H 2.383441 1.407831 0.960884

H 1.549574 1.791775 -0.550581

N -1.842653 1.638283 -0.405889

H -0.351767 0.996839 0.333821

H -2.369908 2.389916 0.023236

H -1.776880 1.846058 -1.396065

H -2.385541 0.763715 -0.308060

N -2.811629 -1.133658 0.019304

H -3.349732 -1.451448 0.817904

H -3.084642 -1.714111 -0.766157

H -1.815712 -1.334940 0.215672

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 38.9896 | 50.2604 | 106.5807 |
| 146.8249 | 185.3736 | 197.8088 |
| 240.3505 | 260.513 | 284.8415 |
| 344.8096 | 419.5219 | 478.2041 |
| 500.3532 | 557.6361 | 635.5418 |
| 708.0326 | 767.0743 | 848.2633 |
| 867.5649 | 934.3429 | 951.2456 |
| 1002.149 | 1008.695 | 1073.646 |
| 1162.484 | 1179.215 | 1200.468 |
| 1232.966 | 1293.12 | 1324.192 |
| 1388.618 | 1410.407 | 1474.919 |
| 1502.159 | 1653.086 | 1675.635 |
| 1705.696 | 1721.035 | 1731.318 |
| 2925.5 | 3029.863 | 3066.149 |
| 3201.879 | 3219.37 | 3244.986 |
| 3272.658 | 3550.808 | 3556.035 |
| 3565.729 | 3629.339 | 3637.961 |

***i37 + 2 NH3 – i39 + 2 NH3***

**Cartesian coordinates**

N 0.610432 0.343529 1.006212

C 0.847540 -1.180368 -0.613274

C 0.056391 -0.905475 0.511234

C 1.912487 -0.295535 -0.777952

C 1.944615 0.599923 0.422257

H 0.565998 0.439239 2.010451

H 0.641764 -2.004368 -1.289348

H 2.696518 -0.331376 -1.522585

H 2.746742 0.313385 1.127849

H 2.090965 1.666182 0.196666

N -1.324212 1.402027 -0.675229

H -0.566479 1.264837 0.058119

H -1.658866 2.357414 -0.715007

H -0.899832 1.140764 -1.561209

H -2.121836 0.590755 -0.360032

N -2.703901 -0.601002 0.201026

H -3.302998 -0.522381 1.015925

H -3.126109 -1.268808 -0.435154

H -1.708307 -0.968788 0.496662

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -571.569 | 53.4048 | 74.2382 |
| 132.0025 | 244.5027 | 282.524 |
| 332.0827 | 362.6223 | 384.8186 |
| 437.707 | 545.4863 | 562.8183 |
| 584.9432 | 663.6009 | 713.0068 |
| 763.9464 | 796.8855 | 858.5564 |
| 887.5079 | 912.3398 | 958.3124 |
| 963.9984 | 1003.533 | 1063.646 |
| 1076.042 | 1168.295 | 1189.748 |
| 1294.677 | 1304.326 | 1363.326 |
| 1403.386 | 1429.284 | 1452.584 |
| 1509.773 | 1535.513 | 1574.824 |
| 1684.116 | 1708.766 | 1755.997 |
| 1810.854 | 2218.675 | 2780.452 |
| 2911.433 | 2995.524 | 3185.417 |
| 3231.456 | 3539.908 | 3543.348 |
| 3613.472 | 3631.722 | 3637.467 |

***i39 + 2 NH3***

**Cartesian coordinates**

N 0.575507 0.266434 0.874214

C 1.333441 -1.047965 -0.815710

C 0.287563 -0.841078 0.071031

C 2.359041 -0.162181 -0.539667

C 1.977150 0.649449 0.664696

H 0.238787 0.240480 1.824307

H 1.325985 -1.783906 -1.607161

H 3.304819 -0.070006 -1.051986

H 2.594416 0.396512 1.544356

H 2.073048 1.732714 0.511738

N -1.851518 1.677353 -0.634609

H -0.996150 1.468229 -0.120920

H -2.105734 2.639256 -0.444159

H -1.618500 1.617273 -1.619152

H -2.821552 -0.107910 -0.000289

N -2.998683 -1.065517 0.314678

H -3.647737 -1.017070 1.091579

H -3.481403 -1.542316 -0.438434

H -0.686285 -1.310498 0.148042

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 30.271 | 41.8644 | 65.7461 |
| 122.1164 | 134.4179 | 145.7809 |
| 160.1645 | 190.8399 | 210.478 |
| 281.5023 | 318.4753 | 354.1078 |
| 482.7729 | 531.8864 | 583.6597 |
| 603.2324 | 788.7825 | 811.4066 |
| 855.9214 | 920.6439 | 949.7677 |
| 979.1195 | 1005.009 | 1077.363 |
| 1112.976 | 1121.57 | 1137.525 |
| 1173.321 | 1190.352 | 1307.544 |
| 1349.364 | 1402.661 | 1454.549 |
| 1506.911 | 1532.211 | 1665.324 |
| 1677.309 | 1703.637 | 1722.391 |
| 2938.831 | 3010.81 | 3205.789 |
| 3244.103 | 3262.466 | 3415.272 |
| 3464.162 | 3576.033 | 3594.744 |
| 3631.9 | 3637.922 | 3642.295 |

***i9b + NH3***

**Cartesian coordinates**

C -0.434379 1.173076 0.384953

C -1.202028 1.003032 -0.696379

N -0.009095 -0.152116 1.035708

C -1.376844 -0.480445 -0.734483

C -0.728243 -1.134419 0.236744

H 0.010003 2.035124 0.866347

H 1.015754 -0.250371 0.832973

H -0.200479 -0.219789 2.033849

H -1.972498 -0.999539 -1.478616

H -0.625975 -2.180183 0.485985

N 2.375843 -0.095231 -0.419438

H 1.749375 0.337002 -1.095411

H 3.129584 0.560766 -0.251800

H 2.775966 -0.919048 -0.852228

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 75.7763 | 103.2277 | 115.2902 |
| 253.3543 | 351.3028 | 366.4334 |
| 499.2825 | 504.8019 | 665.8936 |
| 690.1576 | 701.1234 | 808.7287 |
| 839.5269 | 926.9423 | 979.6392 |
| 992.4895 | 1011.554 | 1134.841 |
| 1149.183 | 1192.221 | 1256.816 |
| 1326.714 | 1346.071 | 1525.411 |
| 1585.18 | 1615.06 | 1673.761 |
| 1682.132 | 3031.995 | 3197.633 |
| 3223.247 | 3262.249 | 3496.692 |
| 3524.855 | 3613.752 | 3648.049 |

***i9b + NH3 – pyrrole (3) + NH3***

**Cartesian coordinates**

C 0.323995 1.159545 -0.439546

C 0.930932 1.017298 0.764400

N 0.025272 -0.129956 -1.089297

C 1.207061 -0.439495 0.787697

C 0.732949 -1.083585 -0.300891

H -0.107679 2.025970 -0.930815

H -1.184086 -0.251633 -0.489131

H 0.088338 -0.217716 -2.098283

H 1.729887 -0.950376 1.590188

H 0.746034 -2.121771 -0.603932

N -2.010809 -0.169145 0.445385

H -1.411779 0.318136 1.122247

H -2.803261 0.422507 0.224881

H -2.328315 -1.053988 0.822273

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -1017.48 | 164.0811 | 197.5985 |
| 219.0264 | 430.9 | 507.7228 |
| 582.7794 | 611.7739 | 681.413 |
| 717.3914 | 753.216 | 803.1826 |
| 842.5943 | 873.2088 | 934.2835 |
| 954.0085 | 1012.152 | 1060.077 |
| 1125.695 | 1237.434 | 1290.625 |
| 1306.541 | 1353.028 | 1486.658 |
| 1546.328 | 1581.852 | 1596.509 |
| 1671.052 | 1773.429 | 3177.902 |
| 3189.595 | 3234.017 | 3403.982 |
| 3560.217 | 3585.808 | 3655.423 |

***Pyrrole (3) + NH3***

**Cartesian coordinates**

C -0.589359 1.113949 0.002144

C -1.902420 0.708100 -0.002824

N 0.202384 0.002314 0.005234

C -1.899552 -0.711991 -0.002811

C -0.584861 -1.112508 0.002156

H -0.158703 2.102952 0.004077

H 3.557099 -0.750364 -0.577717

H 1.223966 0.004019 0.007441

H -2.760221 -1.363170 -0.005885

H -0.150192 -2.099755 0.004110

N 3.193305 0.000236 -0.001835

H -2.765753 1.355743 -0.005921

H 3.575372 -0.120134 0.929122

H 3.565759 0.867560 -0.371012

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 47.1614 | 48.4414 | 70.2146 |
| 180.811 | 280.5373 | 308.2735 |
| 629.7872 | 638.062 | 707.214 |
| 737.0211 | 822.8152 | 892.3847 |
| 893.7462 | 902.582 | 923.6989 |
| 1038.041 | 1077.004 | 1104.899 |
| 1110.053 | 1196.896 | 1222.559 |
| 1332.924 | 1437.596 | 1528.723 |
| 1531.131 | 1619.227 | 1677.104 |
| 1681.944 | 3243.494 | 3256.203 |
| 3274.793 | 3281.441 | 3429.52 |
| 3517.341 | 3642.329 | 3643.504 |

***i9b + 2 NH3***

**Cartesian coordinates**

C 0.707085 -0.250647 1.221399

C 0.848130 -1.386929 0.526236

N 1.017853 0.986218 0.406593

C 1.390315 -0.899605 -0.775488

C 1.504706 0.432139 -0.844467

H 0.302544 -0.028946 2.201184

H 0.063487 1.451576 0.221042

H 1.666090 1.641296 0.840830

H 1.665130 -1.549629 -1.599687

H 1.834830 1.108658 -1.618742

N -1.577684 1.681065 -0.170541

H -1.906886 0.699328 -0.209959

H -2.150370 2.165358 0.511995

H -1.768201 2.104569 -1.071929

N -2.255235 -1.248825 -0.179331

H -1.340083 -1.565163 0.159332

H -2.947063 -1.610278 0.468086

H -2.415436 -1.715716 -1.065277

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 45.2517 | 84.9458 | 106.3821 |
| 168.9925 | 185.6667 | 224.6146 |
| 260.8085 | 280.4756 | 356.75 |
| 433.1245 | 454.569 | 484.4846 |
| 532.7942 | 636.6039 | 694.8349 |
| 715.0014 | 748.606 | 827.5062 |
| 851.9202 | 954.6555 | 984.6924 |
| 1000.527 | 1022.529 | 1135.039 |
| 1184.809 | 1208.402 | 1260.115 |
| 1267.291 | 1346.722 | 1412.965 |
| 1531.64 | 1611.177 | 1623.885 |
| 1663.122 | 1684.211 | 1711.306 |
| 1733.856 | 2570.571 | 3196.957 |
| 3222.163 | 3231.579 | 3259.821 |
| 3382.852 | 3517.045 | 3561.92 |
| 3565.43 | 3628.939 | 3634.439 |

***i9b + 2 NH3 – pyrrole (3) + 2 NH3***

**Cartesian coordinates**

C 0.650210 -0.293424 1.227326

C 0.450627 -1.425879 0.521663

N 1.218430 0.802852 0.412590

C 1.084214 -1.094860 -0.778719

C 1.561354 0.162163 -0.823151

H 0.329544 0.002290 2.220439

H 0.153544 1.410330 0.131129

H 1.945915 1.378406 0.828108

H 1.156797 -1.781026 -1.616350

H 2.062697 0.730523 -1.594012

N -1.092383 1.751667 -0.220680

H -1.648752 0.858850 -0.231037

H -1.527112 2.386827 0.440060

H -1.141150 2.174156 -1.141341

N -2.449637 -0.801185 -0.141933

H -1.613406 -1.311192 0.189904

H -3.182859 -0.959144 0.540927

H -2.748516 -1.251362 -1.000384

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| -946 | 52.2602 | 124.8758 |
| 145.9663 | 202.0897 | 229.2262 |
| 296.4892 | 302.7531 | 427.0411 |
| 438.7598 | 534.075 | 545.7166 |
| 585.0717 | 658.1304 | 694.4672 |
| 702.8469 | 762.6495 | 804.9935 |
| 852.1609 | 903.5709 | 941.3845 |
| 958.6461 | 1010.256 | 1054.824 |
| 1128.143 | 1225.956 | 1230.776 |
| 1295.291 | 1351.782 | 1364.927 |
| 1505.393 | 1558.118 | 1599.513 |
| 1631.349 | 1661.588 | 1713.002 |
| 1733.148 | 1755.919 | 2967.293 |
| 3191.32 | 3198.266 | 3242.31 |
| 3247.985 | 3540.136 | 3554.873 |
| 3555.971 | 3627.876 | 3635.641 |

***Pyrrole (3) + 2 NH3***

**Cartesian coordinates**

C 1.145347 -0.721145 0.972393

C 0.294715 -0.765160 -0.103857

N 2.264897 -0.024400 0.601443

C 0.931732 -0.058929 -1.163832

C 2.144570 0.383838 -0.698690

H 1.047253 -1.133032 1.964052

H -0.983352 1.309781 0.287282

H 3.058102 0.152050 1.190670

H 0.541490 0.097207 -2.157838

H 2.927914 0.944809 -1.182797

N -1.884653 1.776888 0.346827

H -2.889393 -0.091427 0.006139

H -1.940905 2.207781 1.262076

H -1.879263 2.523655 -0.337919

N -3.091009 -1.080845 -0.153193

H -0.688140 -1.220138 -0.126025

H -3.765093 -1.370499 0.545836

H -3.551441 -1.153312 -1.053097

**Vibrational frequencies**

|  |  |  |
| --- | --- | --- |
| 31.5012 | 39.0804 | 48.3969 |
| 73.7789 | 98.8258 | 131.3393 |
| 141.64 | 159.8554 | 187.8819 |
| 261.3377 | 317.8211 | 457.1939 |
| 497.6169 | 643.7488 | 649.8733 |
| 719.312 | 773.8765 | 874.9177 |
| 882.9811 | 909.6617 | 975.8173 |
| 1049.989 | 1086.336 | 1095.74 |
| 1112.9 | 1123.195 | 1170.616 |
| 1189.9 | 1326.132 | 1442.332 |
| 1485.712 | 1523.001 | 1598.79 |
| 1666.888 | 1680.776 | 1685.27 |
| 1721.26 | 3216.24 | 3255.17 |
| 3272.47 | 3279.199 | 3433.757 |
| 3495.851 | 3582.718 | 3616.097 |
| 3635.785 | 3643.584 | 3720.951 |

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