**Supporting Information for**

**Quantum Tunneling Mediated Low-Temperature Synthesis of Interstellar Hemiacetals**

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**METHODS**

**Experimental.** The experiments were conducted in a stainless steel chamber under ultrahigh vacuum (UHV) conditions at pressures of about 8 × 10−11 Torr using turbomolecular pumps (Osaka, TG1300MUCWB and TG420MCAB) backed by a dry scroll pump (Edwards GVSP30).[1](#_ENREF_1) Acetaldehyde (Sigma Aldrich, anhydrous, ≥99.5% purity) and methanol (Sigma-Aldrich, HPLC grade) samples were stored in separate glass vials connected to a high vacuum chamber at pressures of a few 10−8 Torr and repeatedly frozen and thawed using liquid nitrogen to remove residual atmospheric gases. To prepare each ice mixture, methanol and acetaldehyde vapors were deposited via separate glass capillary arrays onto a polished silver substrate, which was mounted on a cold finger maintained at 5.0 ± 0.1 K using a two-stage closed-cycle helium refrigerator (Sumitomo Heavy Industries, RDK-415E). The substrate can be rotated in the horizontal plane or translated vertically with a rotational feedthrough or a linear translator, respectively. The deuterated samples used in the experiment are acetaldehyde-d3 (CD3CHO, CDN isotopes, ≥98 atom % D), acetaldehyde-d4 (CD3CDO, Sigma Aldrich, ≥99 atom % D), methanol-d3 (CD3OH, Sigma Aldrich, ≥98 atom % D), and methanol-d4 (CD3OD, Cambridge Isotope Laboratories Inc., 99.96% D atom). Utilizing a He-Ne laser (CVI Melles Griot, 25-LHP-230) of 632.8 nm wavelength at an angle of incidence equal to 4°, the thickness of each ice was monitored online and in situ via laser interferometry.[2](#_ENREF_2) The average refractive index of the acetaldehyde–methanol ice was determined to be 1.32 ± 0.04 based on the refractive index of amorphous acetaldehyde (n = 1.303)[3](#_ENREF_3) and that of methanol ice (n = 1.33 ± 0.04).[4](#_ENREF_4) By accounting for the densities of methanol (0.779 g cm−3) and acetaldehyde (0.787 g cm−3),[5](#_ENREF_5) the ice thicknesses of 750 ± 30 nm were calculated. Note that thicker ices (2300 ± 200 nm) were used for CH3CHO−CH3OH and CD3CDO−CD3OD systems to obtain better signal-to-noise infrared spectra (Figure 2). The infrared spectra of the ice mixtures were collected in the 6000–500 cm−1 region using a Fourier transform infrared (FTIR) spectrometer (Nicolet 6700) operated at a spectral resolution of 4 cm−1. The ratio of acetaldehyde to methanol in the ice mixture was determined to be (1.1 ± 0.3):1 based on integrating the infrared features of acetaldehyde at 1128, 1350, and methanol at 2827, 3270 cm−1 and their absorption coefficients of 6.6 × 10−19, 1.1 × 10−18, 5.3 × 10−18, and 1.01 × 10−16 cm molecule−1, respectively.[4](#_ENREF_4),[6](#_ENREF_6),[7](#_ENREF_7)

After the deposition, temperature-programmed desorption (TPD) was conducted by heating the sample from 5 K to 320 K at a rate of 0.5 K minute−1. During the TPD phase, either IR spectra were used to track chemical changes induced by the thermal reaction or the sublimed molecules from the ices were analyzed using vacuum ultraviolet (VUV) photoionization reflectron time-of-flight mass spectrometry (PI-ReToF-MS). The pure IR spectra of 1-methoxyethanol and fully deuterated 1-methoxyethanol-d8 at 150 K were achieved after the sublimation of both reactants (Figure 2). In PI-ReToF-MS mode, sublimed hemiacetal molecules were photoionized by pulsed VUV photons at 10.49 eV (118.222 nm), 9.70 eV (127.819 nm) and 9.20 eV (134.765 nm), which were generated by resonant or non-resonant four-wave mixing processes (Table S5). The third harmonic (355 nm) of a pulsed Nd:YAG laser (Spectra-Physics, Quanta Ray Pro 250-30) was used to generate the 10.49 eV (118.222 nm) photons via frequency tripling in pulsed gas jets of Xe gas. To produce 9.70 eV light, a second harmonic (532 nm) from another pulsed Nd: YAG laser (Spectra-Physics, Quanta Ray Pro 270-30) was used to pump a dye laser (Sirah, Cobra-Stretch) containing Rhodamine 610/640 dye mixture (0.17/0.04 g L−1 ethanol) to obtain 606.948 nm (2.04 eV), which undergoes frequency tripling to generate 202.316 nm (ω1, 6.13 eV) (β-BaB2O4 (BBO) crystals, 44° and 77°). The third harmonic (355 nm) of an Nd:YAG laser pumped a dye laser (Coumarin 480, 0.4 g L−1 ethanol) to produce 484.982 nm (ω2, 2.56 eV). The 9.20 eV light was produced in pulsed jets of Xe gas with ω2 = 638.667 nm and ω1 = 222.566 nm, which was obtained via a double frequency of 445.132 nm from a dye laser. The ω1 and ω2 lights were spatially and temporally overlapped in a non-linear medium of Kr or Xe for the generation of 9.70 eV or 9.20 eV photons. Using a biconvex lithium fluoride lens (ISP Optics) in an off-axis geometry, the VUV photons (ωvuv) were spatially separated from the dye lasers (ω1 and ω2) and other wavelengths generated via multiple resonant and non-resonant processes (3ω1; 3ω2; 2ω1 + ω2) and passed at 2.0 ± 0.5 mm above the ice surface for ionizing the sublimed molecules. The resulting ions were extracted and separated based on their mass-to-charge (*m/z*) ratio before reaching the microchannel plate (MCP) detector (Jordan TOF Products, Inc.). The ion signal generated from MCP is first amplified by a preamplifier (Ortec 9305), converted to 4 V with a 100 MHz discriminator (3.2 ns bins, 30 Hz), and then recorded with a dedicated multichannel scaler (FAST ComTec, MCS6A) with accumulation times of 3600 sweeps (2 minutes) for each recorded mass spectra.

**Computational.** All computations were carried out with Gaussian 16, Revision C.01.[8](#_ENREF_8) For geometry optimizations of neutral conformers of 1-methoxyethanol (**1**) and their ions and their frequency computations, the density functional theory (DFT) B3LYP functional[9-11](#_ENREF_9) was employed utilizing the Dunning correlation consistent split valence basis set cc‑Pvtz.[12](#_ENREF_12) Based on these geometries, the corresponding frozen-core coupled cluster[13-16](#_ENREF_13) CCSD(T)/cc‑pVTZ, and CCSD(T)/cc‑pVQZ single point energies were computed and extrapolated to complete basis set limit[17](#_ENREF_17) CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point vibrational energy (ZPVE) corrections. The adiabatic ionization energies were computed by taking the ZPVE corrected energy difference between the neutral and ionic species that correspond to similar conformations. As in general the difference between heavier isotopologues and standard isotopologues in the zero-point vibrational energy is marginal, we used the ZPVEs of standard isotopologues for IE calculations and assumed them to be the same for our experiments with heavier isotopologues.The electric field of ion optics lowers the ionization energy by 0.03 eV,[18](#_ENREF_18) which was considered during the IE error analysis (Table S3). The computed Cartesian coordinates and vibration frequencies for the structures of 1-methoxynethanol are listed in Table S6. For the calculation of the Gibbs free energies depicted in Figure S4, all geometries were optimized at the B3LYP/cc-pVTZ level of theory and augmented CBS-QB3[19](#_ENREF_19) energies (Table S7). Potential energy surfaces for the reaction of methanol and acetaldehyde in mixed ices were computed using the ωB97X-D density functional[20](#_ENREF_20) with the 6-311G(d,p) basis set. Implicit solvent effects were taken into account by applying the universal continuum SCRF SMD model[21](#_ENREF_21) considering methanol below its freezing temperature as a solvent, with the dielectric constant 82.17[22](#_ENREF_22) the refractive index 1.35.[23](#_ENREF_23) Note that this value of the refractive index is close to 1.32 ± 0.04 for the acetaldehyde–methanol ice in the present study. The variation of the dielectric constant had very little effect on the reaction energetics. Optimized Cartesian coordinates and harmonic frequencies involved in the potential energy surfaces illustrated in Figure 5 and S6 are detailed in Table S8.

**Calculations of the tunneling transmission coefficient**

At low temperatures, reactions that involve the transfer of light atoms, such as hydrogen atoms, may exhibit quantum mechanical tunneling. The ratio of thermally averaged quantum tunneling probability to quasiclassical transmission probability defines the tunneling transmission coefficient *κ*(T). For a one-dimensional truncated parabolic-type barrier, the Skodje–Truhlar tunneling transmission coefficient *κ*(T) can be calculated using the following equation:[24](#_ENREF_24)

(S1)

where h is the Planck constant, *ν* the absolute value of the imaginary frequency of the transition state, *k*B the Boltzmann constant, and T the temperature of reaction. The intrinsic barrier *V*b is given by:[24](#_ENREF_24)

(S2)

where ∆*V* is the value of the potential of products relative to the reactants, *V*max is the value of the potential at its maximum relative to reactants. At temperature of 113 K, *κ*(T)s are calculated based on their barriers, reaction energies, and imaginary frequencies at the transition states. These tunneling transmission coefficients range from 214 to several orders of magnitude higher, corroborating the fact that the reaction is dominated by tunneling.

Diagram, schematic

Description automatically generated **Figure S1.** FTIR spectrum of an CH3CHO–CH3OH ice after deposition at 5 K.

 **Figure S2.** Overlay of FTIR spectra of CH3CHO–CH3OH ice measured at 5 K (black) and 150 K (red).

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**Figure S3.** PI-ReToF-MS mass spectra collected during the temperature-programmed desorption (TPD) phase of the acetaldehyde–methanol ice mixtures.TheCH3CHO–CH3OH ice was photoionized at 10.49 eV (**a**) and 9.70 eV (**b**); CD3CHO–CH3OH ice was photoionized at 10.49 eV (**c**) and 9.70 eV (**d**); CD3CDO–CD3OH ice was photoionized at 10.49 eV (**e**) and 9.70 eV (**f**).

Chart

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**Figure S4.** Calculated dissociation pathways of the 1-methoxyethanol radical cation (**1∙**+), leading to the methyl radical and fragment ion, hydroxymethylmethylium (**2**+).The Gibbs free energies calculated (151 K) at the CBS-QB3 level are given in kJ mol−1 relative to the 1-methoxyethanol radical cation (**1∙+**).



**Figure S5.** Formation mechanisms of 1-methoxyethanol (**1**) via nucleophilic addition and its photoionization fragment, hydroxymethylmethylium (**2**+). Reactions [1] and [2] for CH3CHO–CH3OH ice; reactions [3] and [4] for CD3CHO–CH3OH ice; reactions [5] and [6] for CD3CDO–CD3OH ice.

Chart, scatter chart

Description automatically generated

**Figure S6.** Potential energy surfaces of the reactions between various combinations of acetaldehyde (CH3CHO) and methanol (CH3OH) molecules leading to the formation of 1-methoxyethanol (**1**). Panels **a** to **d** illustrate the reaction pathways for the systems (CH3CHO)2−CH3OH, (CH3CHO)2−(CH3OH)2, (CH3CHO)2−(CH3OH)3, and (CH3CHO)3− (CH3OH)2, respectively. The reactants, transition states, intermediates, and products are labelled as “**R**”, “**TS**”, “**I**” and “**P**”, respectively. Energies, computed at the SCRF/SMD//ωB97X-D/6-311G(d,p) + ZPVE level of theory, are shown in kJ mol−1 and are relative to the energy of the reactants. The atoms are depicted with a color code of white for hydrogen, gray for carbon, and red for oxygen.

**Table S1.** Absorption peaks observed in CH3CHO−CH3OH ices after deposition at 5 K.

|  |  |
| --- | --- |
| Absorption position (cm−1) |  |
| **CH3OH** | Assignment[25](#_ENREF_25),[26](#_ENREF_26) |
| 3402, 3261, 3048 | ν1 |
| 2957 | ν9 |
| 2917 | 2ν4 / 2ν5 / 2ν10 |
| 2826 | ν3 |
| 2598 | ν4 + ν11 |
| 2521 | ν6 + ν11 |
| 2233 | 2ν11 / 2ν7 |
| 2041 | 2ν8 |
| 1476 | ν4 |
| 1455 | ν5 |
| 1031 | ν8 |
| **CH3CHO** | Assignment[27](#_ENREF_27) |
| 2869 | 2ν6 |
| 2761 | ν3 |
| 1768 | 2ν9 |
| 1716 | ν4 |
| 1427 | ν12 / ν5 |
| 1392 | ν6 |
| 1347 | ν7 |
| 1123 | ν8 |
| 887 | ν14 + ν15 |
| 775 | ν14 |

**Table S2.** Absorption peak positions (cm-1) of 1-methoxyethanol (**1**) in CH3CHO–CH3OH and CD3CDO–CD3OD ices measured after the sublimation of acetaldehyde and methanol. Assignment labels: stretching (*ν*), bending (*δ*), rocking (*ρ*).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| CH3CHO–CH3OH ice | | |  | |
| Experimental (this work) | Reported  Position | | Assignment c | |
| 3310 |  | | *ν*(OH) | |
| 2988 |  | | *ν*(CH) | |
| 2932 |  | | *ν*(CH) | |
| 2832 |  | | *ν*(CH) | |
| 1511 |  | | *δ*(CH) | |
| 1456 |  | | *δ*(CH) | |
| 1384 |  | | *δ*(CH) | |
| 1204 | 1210a | | *ρ*(CH3) | |
| 1137 | 1140a, 1150b | | *ν*(CO) | |
| 1107 | 1087b | | *ν*(CO) | |
| 909 | 920a, 917b | | *ρ*(CH3) | |
| CD3CDO–CD3OD ice | | |  | |
| Experimental (this work) | Reported  Position | | Assignment c | |
| 2461 |  |  |  | *ν*(OD) | |
| 2244 |  |  |  | *ν*(CD) | |
| 2215 |  |  |  | *ν*(CD) | |
| 2069 |  |  |  | *ν*(CD) | |
| 1274 |  |  |  | *δ*(CD) | |
| 1256 |  |  |  | *δ*(CD) | |
| 1141 |  |  |  | *ν*(CO) | |
| 1097 |  |  |  | *ν*(CO) | |
| 978 |  |  |  | *ρ*(CD3) | |

a From Meadows et al.,[28](#_ENREF_28) measured in methanol.

b From Dutta et al.,[29](#_ENREF_29) calculated at B3LYP/6-31++G(d,p) level of theory.

c Calculated at the B3LYP/cc-pVTZ level of theory.

**Table S3.** Error analysis of adiabatic ionization energies (IE) and relative energies (*Δ*E) of 1-methoxyethanol (**1**); IEs and *Δ*E were computed at the CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory including the zero-point vibrational energy corrections. Their computed Cartesian coordinates and vibrational frequencies are shown in TableS6. The IE ranges are calculated based on the electrical effect of −0.03 eV and computed IE error limits of −0.05 - +0.03 eV.[30](#_ENREF_30)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Isomer | Structure | *Δ*E  (kJ mol-1) | Dipole moment (Debye) | Computed IE (eV) | IE range after error analysis (eV) | Corrected IE with electric field effect (eV) |
| **1a** | D:\Dropbox\Astrochemistry\4 Hemiacetal\Figures\Hemiactal\01.PNG | 0 | 0.37 | 9.98 | 9.93 – 10.01 | 9.90 – 9.98 |
| **1b** | D:\Dropbox\Astrochemistry\4 Hemiacetal\Figures\Hemiactal\04-1b.PNG | 10.2 | 1.99 | 9.76 | 9.71 – 9.79 | 9.68 – 9.76 |
| **1c** | D:\Dropbox\Astrochemistry\4 Hemiacetal\Figures\Hemiactal\05-1c.PNG | 6.6 | 2.12 | 9.73 | 9.68 – 9.76 | 9.65 – 9.73 |
| **1d** | D:\Dropbox\Astrochemistry\4 Hemiacetal\Figures\Hemiactal\02-1d.PNG | 7.2 | 0.20 | 9.72 | 9.67 – 9.70 | 9.64 – 9.72 |
| **1e** | D:\Dropbox\Astrochemistry\4 Hemiacetal\Figures\Hemiactal\03-1e.PNG | 14.1 | 1.75 | 9.72 | 9.67 – 9.70 | 9.64 – 9.72 |
| **1f** | D:\Dropbox\Astrochemistry\4 Hemiacetal\Figures\Hemiactal\06.PNG | 17.2 | 2.35 | 9.62 | 9.57 – 9.65 | 9.54 – 9.62 |

**Table S4.** Calculated Gibbs free energies (kJ mol−1) for the structures involved in the dissociation pathways of 1-methoxyethanol, 1-methoxyethanol-d3, and1-methoxyethanol-d7 cations. The Gibbs free energies calculated at the CBS-QB3 level are relative to the corresponding 1-methoxyethanol cation (**1∙+**).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Reactant (**1∙**+) | Transition state (**TS**) | Complex (**3**) | Methyl radical and **2+** |
| 1-methoxyethanol cation | 0.0 | 2.0 | -12.8 | -12.0 |
| 1-methoxyethanol-d3 cation | 0.0 | 3.6 | -10.0 | -8.5 |
| 1-methoxyethanol-d7  cation | 0.0 | 2.5 | -11.1 | -9.6 |

**Table S5.** Parameters for the generation of vacuum ultraviolet (VUV) light.The uncertainty for VUV photon energies is less than 0.0001 eV.

|  |  |  |  |
| --- | --- | --- | --- |
| VUV energy (eV) | 10.49  (3ω1) | 9.70  (2ω1 – ω2) | 9.20  (2ω1 – ω2) |
| VUV wavelength (nm) | 118.222 | 127.819 | 134.765 |
| Nonlinear medium | Xenon | Krypton | Xenon |
| ω1 wavelength (nm) | 355 | 202.316 | 222.566 |
| Nd:YAG output (nm) | 355 | 532 | 355 |
| Dye laser output (nm) | - | 606.948 | 445.132 |
| Dye | - | Rhodamine 610/640  (0.17/0.04 g L−1 ethanol) | Coumarin 450  (0.2 g L−1 ethanol) |
| ω2 wavelength (nm) | - | 484.982 | 638.667 |
| Nd:YAG output (nm) | - | 355 | 532 |
| Dye laser output (nm) | - | 484.982 | 638.667 |
| Dye | - | Coumarin 480  (0.4 g L−1 ethanol) | DCM  (0.3 g L−1 DMSO) |

**Table S6.** Cartesian coordinates for structures of 1-methoxyethanol. B3LYP/cc-pVTZ optimized Cartesian geometry (Å), electronic energies (hartree) and vibrational frequencies (cm-1) & intensities (km mol-1), zero-point vibrational energies (ZPVE) (hartree), extrapolated CCSD(T)/CBS energies (hartree) and adiabatic ionization energies (IE) at CCSD(T)/CBS level of theory.

|  |
| --- |
| **1a**  C 1.647038 –0.821182 –0.010227  C 0.424238 0.007841 0.328106  H 1.776570 –0.864635 –1.093537  H 1.532016 –1.839703 0.358062  H 2.534857 –0.376363 0.435978  O 0.564738 1.362405 –0.056893  H 0.775499 1.381035 –0.997884  O –0.680506 –0.604913 –0.290563  H 0.264574 0.056167 1.411399  C –1.936466 –0.074033 0.105511  H –2.093665 –0.198903 1.182970  H –2.699612 –0.633227 –0.431100  H –2.020081 0.986020 –0.141838  E = –269.6821552  E[CCSD(T)/CBS] = –269.2985145  ZPVE = 0.1124990  Frequency Intensity  125.3641 3.6050  180.1028 3.4604  227.1570 0.7761  284.7352 2.1192  343.8847 82.8704  391.3748 25.2400  535.5502 10.6963  565.8097 24.8806  840.9693 9.2036  907.9046 65.5176  1052.4975 81.1241  1070.1458 34.1794  1118.2683 120.4363  1145.3900 140.0426  1177.9719 1.5567  1218.8900 24.4913  1306.3715 13.4142  1382.2524 14.2715  1410.6997 22.1698  1433.4828 60.3724  1473.2606 2.7108  1484.6364 0.9629  1487.1137 6.3180  1495.8970 6.5346  1513.8741 7.0383  2989.5222 43.1353  3000.8652 57.5555  3035.6276 13.2766  3058.7598 40.5221  3102.8858 27.1003  3116.9759 23.3948  3122.4663 17.7593  3780.6383 20.8598 |
| **1a-d8**  Frequency Intensity  98.1193 1.3743  146.4724 3.6522  165.6843 0.4119  244.3285 13.6234  254.9121 40.3063  344.1516 9.9886  458.2172 6.9165  524.1276 20.9629  705.1611 1.7651  755.9242 6.5977  857.6289 38.8253  880.8878 17.6963  913.8787 7.2581  945.5429 26.6681  1008.3837 10.9410  1041.0891 12.7320  1066.5611 23.6642  1070.1544 12.1966  1074.4516 3.4305  1089.6373 10.5514  1093.3914 10.4779  1105.6532 70.6995  1135.2762 123.3380  1160.0427 52.1267  1253.5156 116.5193  2147.8376 36.9228  2181.8387 3.9567  2211.2097 32.3647  2263.5260 25.9051  2297.0023 13.6068  2311.0230 15.0989  2314.6021 7.4509  2751.1325 13.3162 |
| **1a+**  C 1.621825 –0.768144 –0.030704  C 0.500052 0.161037 0.309487  H 1.803488 –0.787883 –1.105652  H 1.405116 –1.778975 0.312773  H 2.519340 –0.421933 0.484879  O 0.581029 1.458073 –0.150942  H 1.144126 1.524285 –0.940889  O –0.714017 –0.258508 –0.470053  H 0.221012 0.185470 1.360714  C –1.981693 –0.206441 0.132858  H –1.936057 –0.376260 1.207237  H –2.607336 –0.918528 –0.412272  H –2.404152 0.792595 –0.077257  E = –269.3306659  E[CCSD(T)/CBS] = –268.9286049  ZPVE = 0.1094960  Frequency Intensity  56.2687 4.7597  106.9933 15.9249  225.2812 0.3918  297.7567 12.8753  340.8625 5.0425  362.5005 4.5039  441.1438 43.9397  528.5316 74.1453  624.5186 38.2128  866.1477 12.8284  919.6565 39.9703  1026.9209 11.3672  1050.2738 38.4849  1077.5016 49.9444  1150.7270 41.3304  1174.5588 24.1295  1293.2245 45.2903  1338.0519 17.4897  1350.3114 77.0186  1390.1917 22.5697  1414.0514 4.6325  1430.8676 65.2497  1466.9328 17.9346  1475.8854 16.6938  1485.8855 20.5422  2912.1783 159.4211  3035.5016 14.6195  3040.2284 7.5360  3108.7388 1.5545  3117.9061 3.0805  3128.6702 5.7240  3130.4551 9.2008  3694.4238 260.1255 |
| **1b**  C 1.357275 –0.943760 0.056520  C 0.370359 0.190634 0.245816  H 0.948032 –1.881043 0.432412  H 2.280169 –0.730526 0.594752  H 1.580686 –1.050694 –1.004215  O 0.956300 1.352410 –0.266643  H 0.283544 2.042034 –0.267801  O –0.846617 –0.017682 –0.458541  H 0.122515 0.314292 1.313311  C –1.781013 –0.844707 0.205627  H –2.697589 –0.822952 –0.380055  H –1.996366 –0.477401 1.216510  H –1.439624 –1.882608 0.278901  E = –269.6777963  E[CCSD(T)/CBS] = –269.2943452  ZPVE = 0.1122190  Frequency Intensity  95.3946 1.4173  188.8079 0.7842  216.2003 5.7505  302.9790 48.5681  327.5976 57.1886  410.1554 5.6335  459.6311 16.3741  566.5570 8.4638  840.4638 21.0482  932.9774 34.4070  1026.0729 87.5825  1111.8091 41.7130  1117.1322 95.0237  1162.3109 114.8680  1178.8777 3.9660  1228.1389 21.4197  1290.0048 101.1700  1392.9336 26.6415  1397.4542 4.3488  1451.7210 50.2164  1474.6595 7.1062  1485.5003 12.2565  1489.2787 1.4923  1499.0469 2.7380  1512.4443 5.7598  2911.5101 75.4386  2977.0583 64.3646  3022.9218 52.3801  3044.6035 13.0753  3110.1904 32.2490  3112.5942 14.6982  3120.4844 18.8039  3800.9425 29.9916 |
| **1b-d8**  Frequency Intensity  78.9068 0.7782  143.5790 0.8345  157.5072 2.7860  229.0961 57.2821  282.1733 3.1494  359.0458 2.5525  402.7982 12.0660  515.0491 4.2512  705.0685 7.0611  781.2713 13.0344  835.7372 35.6328  889.1456 3.5184  917.2890 4.9051  949.2732 8.5935  1017.9023 26.6883  1021.4142 21.1813  1064.2227 11.8753  1069.8934 13.0312  1076.6716 5.4089  1079.2845 1.5255  1090.0584 0.2395  1113.4743 73.4463  1146.6728 151.1557  1185.0840 103.5173  1277.5961 79.0462  2135.0992 18.0364  2144.7676 74.9279  2186.7944 2.6744  2240.7916 33.8483  2302.8864 17.0364  2305.9410 8.5286  2312.8158 9.2077  2766.0157 20.0331 |
| **1b+**  C –0.922645 1.341289 0.014363  C –0.395224 –0.239808 0.409061  H –0.121619 2.003632 0.325028  H –1.834026 1.460690 0.589054  H –1.083595 1.314341 –1.058051  O –1.425531 –1.059023 0.162400  H –1.262726 –1.643782 –0.598342  O 0.710361 –0.509499 –0.286389  H –0.249664 –0.100431 1.494531  C 1.972167 0.113408 0.066636  H 2.720125 –0.669023 –0.034919  H 1.944445 0.498006 1.083359  H 2.168760 0.902103 –0.658745  E = –269.3339565  E[CCSD(T)/CBS] = –268.9325881  ZPVE = 0.1092140  Frequency Intensity  87.7447 3.4675  139.4058 1.3396  220.5534 0.0763  256.9591 9.1757  303.5157 112.3772  352.7757 35.5306  366.7758 5.5021  536.2020 34.4015  552.4660 21.1152  885.8645 9.2572  901.1724 40.9329  932.5115 78.4570  995.5942 18.0749  1124.6151 27.6146  1148.1654 8.4374  1179.1749 103.1539  1249.7105 79.1694  1302.3013 7.0858  1329.2031 7.3998  1346.9602 39.3949  1438.4595 13.1323  1444.6245 9.1500  1459.1170 13.4405  1470.5811 15.9534  1491.0785 52.3045  2914.3048 18.8587  3045.3880 11.5419  3070.1137 4.9311  3135.4645 1.9959  3157.3667 13.5646  3202.9978 0.6771  3208.9001 3.1325  3689.1964 268.2465 |
| **1c**  C 1.649122 –0.786742 –0.033557  C 0.406929 –0.001080 0.315308  H 1.552874 –1.814842 0.310691  H 2.522689 –0.330276 0.428207  H 1.780236 –0.786678 –1.115066  O 0.568295 1.312650 –0.188471  H –0.023545 1.909797 0.276765  O –0.691534 –0.670533 –0.260021  H 0.254693 0.047003 1.404361  C –1.952652 –0.130688 0.078213  H –2.104128 0.860932 –0.360290  H –2.081175 –0.064166 1.166544  H –2.707925 –0.803314 –0.322246  E = –269.6791074  E[CCSD(T)/CBS] = –269.2957249  ZPVE = 0.1122370  Frequency Intensity  113.9842 4.1829  191.1030 7.6228  212.7047 2.5786  279.4805 10.2074  292.0185 81.5400  391.7327 9.3512  522.9182 7.7126  573.3771 3.1647  846.5114 13.3961  910.0749 92.9995  1047.0316 52.2764  1086.6577 11.2655  1121.7567 114.7207  1138.3006 123.6245  1174.3659 3.8132  1218.9466 68.6896  1279.1040 51.9493  1382.7718 16.9443  1402.2539 3.4056  1451.9164 44.1758  1472.6888 2.6882  1485.2261 4.4089  1489.9935 3.0874  1493.1528 1.8223  1513.7728 5.5815  2936.8754 66.1257  2969.6491 70.6755  3024.1952 54.5055  3050.7077 9.6589  3112.0526 23.4172  3122.3210 18.0162  3127.1793 17.1993  3831.3310 24.6281 |
| **1c-d8**  Frequency Intensity  95.8160 2.1758  143.7275 4.2946  156.3754 4.4323  210.8215 41.0665  248.0821 10.1252  340.2033 3.0345  452.8341 5.1994  538.7269 5.3499  708.0674 3.3873  772.4999 37.5428  829.3622 11.2548  877.2430 4.2055  909.6745 11.8134  936.7464 4.8835  1011.5911 41.0047  1033.0601 14.0442  1065.4167 30.9767  1068.5744 31.1552  1076.4114 3.3158  1085.7264 36.6794  1092.5225 2.0599  1097.4726 31.4962  1129.1039 172.1395  1160.4539 31.5163  1290.6574 79.7754  2132.9388 36.1904  2162.7022 55.0151  2191.6732 3.2114  2240.0705 33.1398  2303.7193 14.7623  2313.4736 8.5670  2318.1657 8.0619  2789.4659 17.0849 |
| **1c+**  C 1.569632 –0.613545 –0.149477  C 0.333768 0.025447 0.633195  H 1.647884 –1.660415 0.125851  H 2.457460 –0.066751 0.158650  H 1.372784 –0.491586 –1.211738  O 0.098849 1.330467 0.347039  H 0.859951 1.893459 0.550679  O –0.756751 –0.758342 0.405380  H 0.600351 –0.149265 1.702776  C –1.952728 –0.195887 –0.145648  H –1.721820 0.268322 –1.110361  H –2.315109 0.593777 0.520761  H –2.652495 –1.016689 –0.238257  E = –269.3387711  E[CCSD(T)/CBS] = –268.9352339  ZPVE = 0.1091750  Frequency Intensity  110.5015 8.1210  156.9752 1.4252  239.2617 1.2685  286.9879 15.5166  325.0052 86.5269  369.3747 26.3233  458.2807 36.3359  624.1289 7.5646  724.9052 81.8222  851.7991 83.7811  891.2320 30.0141  985.2395 13.2086  990.7251 9.2721  1080.5598 1.8373  1116.1992 45.0240  1189.6306 41.2657  1202.0043 106.9119  1224.1111 101.0830  1315.1692 7.1584  1373.1033 7.1002  1407.3974 46.8047  1435.2851 27.2667  1452.9384 16.2519  1470.3271 0.9372  1472.0346 14.5979  2772.2575 69.4118  2993.8279 65.9888  3045.1534 2.4210  3061.3553 2.3405  3162.9986 0.2545  3179.8825 1.7048  3197.0212 8.6355  3756.6631 303.1346 |
| **1d**  C 1.327187 –0.860470 –0.408246  C 0.508469 0.069260 0.468073  H 2.380974 –0.597059 –0.331453  H 1.034092 –0.771920 –1.453493  H 1.196529 –1.892186 –0.084154  O 0.651495 1.373361 –0.061778  H 0.203392 1.983135 0.534010  O –0.850616 –0.294992 0.604716  H 0.875198 0.036179 1.497997  C –1.597559 –0.407469 –0.600306  H –1.467701 0.470043 –1.236848  H –2.642428 –0.484059 –0.307112  H –1.327108 –1.303970 –1.165174  E = –269.6790369  E[CCSD(T)/CBS] = –269.2960108  ZPVE = 0.1127460  Frequency Intensity  127.1942 4.5168  174.8104 1.7438  240.1150 3.4836  297.0313 2.7444  378.6190 91.2602  406.1282 11.3107  475.0742 36.2619  643.9788 7.0871  821.4752 15.5616  908.9175 66.0737  998.9467 56.2569  1058.6555 56.4679  1120.7460 79.7564  1162.1969 151.5826  1175.2642 3.8318  1216.0483 4.5555  1281.0169 67.2644  1396.8352 2.1599  1402.3373 4.7933  1447.1607 39.9308  1468.5084 3.5765  1485.6308 2.0107  1492.7767 6.6821  1504.7098 2.2325  1515.0044 7.9281  3006.4383 61.6384  3018.7409 36.4410  3047.8793 6.9386  3065.2312 40.6983  3111.9742 28.1279  3117.8961 17.2997  3120.3424 20.5159  3802.3069 28.3822 |
| **1d-d8**  Frequency Intensity  101.9735 1.8045  133.0290 1.7929  181.4868 2.6723  259.7570 0.7034  279.2696 61.9132  355.3013 2.9819  420.9170 18.9719  571.1796 6.7500  708.5907 6.4377  770.7454 26.3780  826.6040 13.9565  869.7595 8.1459  911.2214 3.1646  933.3231 12.9996  986.5963 21.1839  1040.3064 20.1349  1067.8675 27.1808  1070.4380 23.4223  1081.8800 3.1632  1086.4752 17.2045  1093.5849 1.0222  1101.7751 63.7735  1120.2420 147.6512  1157.1330 42.8800  1265.1400 77.0105  2156.0978 33.2980  2189.4492 3.0640  2225.5059 33.5356  2272.1185 25.0996  2307.1361 15.5462  2309.9054 7.7750  2312.6879 9.8610  2767.4053 19.1277 |
| **1d+**  C –1.366465 1.207812 0.026418  C –0.397967 –0.032387 0.294671  H –2.383862 0.824522 0.038429  H –1.103133 1.614170 –0.947007  H –1.220651 1.936427 0.817453  O –0.452437 –1.004943 –0.649532  H –1.340994 –1.379144 –0.739824  O 0.863785 0.450872 0.466969  H –0.717002 –0.382326 1.305315  C 1.939712 –0.020349 –0.351930  H 2.038258 –1.103189 –0.222649  H 2.819836 0.519903 –0.027135  H 1.699658 0.164716 –1.404366  E = –269.3387711  E[CCSD(T)/CBS] = –268.9352342  ZPVE = 0.1091760  Frequency Intensity  110.4643 8.1179  157.0850 1.4249  239.2821 1.2671  287.0444 15.4685  325.1809 86.3874  369.4858 26.5075  458.3517 36.2538  624.1086 7.5669  725.0316 81.7655  851.9728 83.8827  891.3091 30.0255  985.3010 13.2421  990.7195 9.2759  1080.6006 1.8553  1116.1923 44.9042  1189.5370 41.9517  1202.0068 106.2089  1224.0968 101.0249  1315.1562 7.1872  1373.1287 7.0938  1407.4001 46.7996  1435.3211 27.2922  1452.9492 16.2443  1470.3360 0.9259  1472.0273 14.6014  2772.0337 69.4209  2993.8173 65.9867  3045.1785 2.4268  3061.3612 2.3396  3163.0171 0.2542  3179.8391 1.7038  3196.9477 8.6320  3756.6100 303.1168 |
| **1e**  C 1.314544 –0.925161 0.143266  C 0.356862 0.250943 0.274430  H 0.878544 –1.839691 0.546650  H 2.239223 –0.718276 0.680930  H 1.546238 –1.094641 –0.910237  O 0.915538 1.439895 –0.205954  H 1.110145 1.320987 –1.142684  O –0.848146 0.013418 –0.437194  H 0.123188 0.445884 1.327439  C –1.807880 –0.761053 0.252206  H –1.476851 –1.793068 0.413540  H –2.704855 –0.778991 –0.363310  H –2.054690 –0.317594 1.224158  E = –269.6762414  E[CCSD(T)/CBS] = –269.2926981  ZPVE = 0.1120400  Frequency Intensity  68.1433 2.6170  185.4027 1.4309  230.9550 34.1368  253.6802 60.8705  320.0520 13.5479  412.1106 2.8085  478.4663 30.8949  548.1702 1.8097  833.3364 13.9260  927.5232 40.5586  1060.4437 78.9972  1079.8721 9.6402  1119.8356 192.9289  1140.3732 148.2043  1177.5777 3.6254  1214.4389 29.7381  1333.0799 6.4252  1376.3457 18.1569  1405.7222 25.3047  1425.7850 67.8672  1476.1702 1.1064  1483.8961 0.8941  1489.8544 7.7953  1500.4723 7.2710  1510.8184 6.8026  2976.1095 47.3921  2998.6236 52.0847  3019.4179 47.8910  3030.1041 20.3147  3095.3117 30.9557  3109.1514 44.8326  3109.7015 4.4725  3788.8382 27.2050 |
| **1e-d8**  Frequency Intensity  57.2335 1.6965  140.7479 1.6243  168.5429 14.1220  183.2063 41.0819  276.9561 3.5583  362.2998 0.7486  432.8830 19.1115  488.3039 5.9358  703.5895 3.0948  762.1342 7.5093  864.1118 26.3963  879.0094 25.2219  912.3065 4.0416  952.9939 35.4927  993.9455 22.1184  1040.4334 2.7063  1065.6828 16.3848  1069.8385 4.9501  1078.7115 3.1554  1086.2557 3.4025  1090.4882 3.7224  1135.4769 211.2345  1154.2515 41.9941  1172.3478 61.2397  1225.3405 116.6520  2135.9105 36.7064  2176.8428 2.9775  2210.5343 32.5320  2239.2301 33.2733  2292.3108 14.1792  2302.1476 19.6586  2303.9890 7.9339  2757.0929 16.8265 |
| **1e+**  C –0.878750 1.460966 0.058102  C –0.458452 –0.186768 0.265683  H –0.050201 2.028858 0.467802  H –1.799091 1.565430 0.621293  H –1.007157 1.575847 –1.012889  O –1.527836 –0.903464 –0.103445  H –1.377475 –1.399852 –0.926957  O 0.649378 –0.438358 –0.433108  H –0.337098 –0.190671 1.362958  C 1.934757 0.057401 0.021796  H 2.198331 0.915309 –0.595779  H 2.638124 –0.751464 –0.159767  H 1.900064 0.315455 1.077553  E = –269.3339565  E[CCSD(T)/CBS] = –268.9325891  ZPVE = 0.1092120  Frequency Intensity  88.2444 3.4868  139.5601 1.3362  220.3853 0.0640  256.8740 9.2973  303.2836 112.4868  352.6525 35.2170  366.7032 5.3966  536.1148 34.6958  552.3974 20.9487  885.7589 9.2088  901.0055 40.8019  932.4480 78.5425  995.3582 18.1041  1124.5242 27.6011  1148.1977 8.4973  1179.1493 103.1312  1249.5873 79.2351  1302.2053 7.0975  1329.1510 7.3787  1346.8412 39.4514  1438.4723 13.1863  1444.5709 9.1487  1459.1273 13.4602  1470.5641 15.8753  1491.0879 52.2385  2914.7641 18.8761  3045.3566 11.5216  3070.1270 4.9389  3135.4657 2.0046  3157.3586 13.5216  3203.0310 0.6850  3208.9795 3.1327  3689.1543 268.2177 |
| **1f**  C 1.349909 –0.848810 –0.393675  C 0.494793 0.077374 0.462002  H 1.280269 –1.872872 –0.028977  H 2.391097 –0.530493 –0.352743  H 1.032143 –0.836325 –1.438700  O 0.555819 1.413464 0.006766  H 0.614436 1.421178 –0.953557  O –0.834823 –0.381448 0.618239  H 0.872326 0.100206 1.483606  C –1.648374 –0.381170 –0.540552  H –1.724758 0.617030 –0.980721  H –2.639990 –0.692299 –0.219404  H –1.296294 –1.085244 –1.301941  E = –269.6750403  E[CCSD(T)/CBS] = –269.2918705  ZPVE = 0.1124100  Frequency Intensity  87.8113 2.7041  183.6234 6.8338  243.8844 4.9409  297.5491 19.9921  307.0787 72.4185  401.2408 3.1482  470.9207 8.7878  631.7143 5.6638  812.1377 9.3681  908.2047 75.1323  1013.8206 42.4615  1057.7560 63.9672  1115.0889 98.7587  1149.0696 167.9441  1173.8494 15.0712  1214.9953 22.9952  1298.6593 11.2350  1397.8974 3.2769  1414.6153 17.2072  1422.2146 62.3972  1469.1110 0.4501  1489.0858 4.1002  1494.2670 2.5010  1503.3793 1.6723  1512.2657 10.8052  2990.6282 48.9555  3030.4301 10.0944  3043.6047 53.2467  3072.4477 9.8273  3099.0706 45.5222  3111.4073 21.6343  3115.3025 16.7110  3809.3522 19.8022 |
| **1f-d8**  Frequency Intensity  71.1320 1.4260  139.9346 4.1839  181.8423 3.8694  219.7859 45.4145  264.9183 4.2330  347.8438 2.9022  426.1768 8.5519  557.8019 6.0090  703.3648 5.7705  755.4994 5.8615  852.4157 51.6240  863.8965 7.7976  910.4477 2.9424  940.9212 41.6342  973.9581 3.7409  1059.7916 4.5787  1068.5719 26.1862  1071.3793 4.0149  1082.7564 6.0174  1087.6962 11.8211  1092.5297 8.7903  1103.5584 103.0466  1122.7659 102.2404  1166.9369 41.8482  1220.3544 113.0889  2146.2837 33.2315  2179.0249 3.7820  2255.5579 31.6624  2268.0350 11.5451  2291.7914 20.3313  2304.4325 14.7578  2309.0559 7.3754  2773.0956 12.8642 |
| **1f+**  C 1.391350 –1.242946 –0.139706  C 0.456464 0.015581 0.161442  H 1.285943 –1.953052 0.674240  H 2.412127 –0.873256 –0.198741  H 1.063083 –1.665556 –1.086104  O 0.463989 0.967644 –0.804871  H 1.349791 1.327487 –0.958405  O –0.797835 –0.446819 0.421872  H 0.842346 0.381752 1.142610  C –1.916908 0.021971 –0.338505  H –1.993760 1.108507 –0.226903  H –2.781604 –0.499404 0.051920  H –1.745436 –0.188220 –1.399622  E = –269.3387711  E[CCSD(T)/CBS] = –268.9352343  ZPVE = 0.1091770  Frequency Intensity  110.4851 8.1385  157.0907 1.4176  239.2526 1.2666  287.0212 15.4245  325.1972 86.3492  369.4219 26.5678  458.2382 36.3711  624.0609 7.6266  724.7770 81.6695  852.1724 83.7771  891.3299 30.2285  985.3182 13.2983  990.6877 9.2790  1080.6646 1.8590  1116.1636 44.8702  1189.5971 41.6952  1202.0588 106.4847  1224.1220 101.0950  1315.2716 7.1105  1373.0643 7.1144  1407.4897 46.7721  1435.3241 27.2945  1452.9332 16.2377  1470.3630 0.9246  1472.0098 14.5916  2771.8545 69.4012  2993.8131 65.9315  3045.1658 2.4338  3061.3676 2.3410  3163.0690 0.2550  3179.8924 1.7052  3197.0269 8.6262  3756.6846 303.0340 |

**Table S7.** Cartesian coordinates of structures in the dissociation pathways of 1-methoxyethanol cation (**1∙+**). B3LYP/cc-pVTZ optimized Cartesian geometry, enthalpy, and Gibbs free energies (hartree) at CBS-QB3 level of theory.

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| --- |
| 1-methoxyethanol cation (**1∙+**)  C 1.665286 -0.700920 0.303618  C 0.480028 0.102516 -0.403889  H 2.584618 -0.144438 0.121590  H 1.722686 -1.693721 -0.137243  H 1.430958 -0.747816 1.366804  O 0.262321 1.344966 0.099256  H 1.044709 1.910618 0.020377  O -0.640496 -0.675652 -0.349859  H 0.778576 0.106963 -1.480834  C -1.842140 -0.175856 0.253655  H -1.632489 0.105449 1.293627  H -2.567674 -0.978397 0.176945  H -2.155032 0.732385 -0.276744  Temperature = 151.000000 Pressure = 1.000000  E(ZPE) = 0.108208 E(Thermal) = 0.110499  E(SCF) = -267.746393 DE(MP2) = -0.938668  DE(CBS) = -0.095969 DE(MP34) = -0.057109  DE(CCSD) = -0.032560 DE(Int) = 0.030137  DE(Empirical) = -0.048189  CBS-QB3 (0 K) = -268.780545 CBS-QB3 Energy = -268.778254  CBS-QB3 Enthalpy = -268.777776 CBS-QB3 Free Energy = -268.793634 |
| Transition state (**TS**)  C -1.838259 -0.871587 -0.310740  C -0.303051 0.358158 0.538696  H -1.757120 -1.728673 0.347493  H -1.420860 -0.959407 -1.307426  H -2.702624 -0.227172 -0.188921  O -0.208159 1.375017 -0.286843  H -0.910421 2.031624 -0.160111  O 0.680797 -0.470413 0.600954  H -0.904126 0.426906 1.444906  C 1.779374 -0.411609 -0.376414  H 1.383223 -0.601331 -1.373453  H 2.455855 -1.198672 -0.062118  H 2.246580 0.570111 -0.322504  vi=-209.3049  Temperature = 151.000000 Pressure = 1.000000  E(ZPE) = 0.107241 E(Thermal) = 0.109731  E(SCF) = -267.752659 DE(MP2) = -0.946650  DE(CBS) = -0.094342 DE(MP34) = -0.050898  DE(CCSD) = -0.024124 DE(Int) = 0.030199  DE(Empirical) = -0.048273  CBS-QB3 (0 K) = -268.779507 CBS-QB3 Energy = -268.777018  CBS-QB3 Enthalpy = -268.776539 CBS-QB3 Free Energy = -268.792857 |
| Complex (**3**)  C 2.430183 -0.710017 0.230401  C 0.019136 0.521939 -0.570934  H 2.240619 -1.59199 0 -0.368105  H 2.177029 -0.724023 1.283271  H 3.151304 0.016817 -0.123508  O -0.110434 1.394655 0.369320  H 0.519493 2.131405 0.299407  O -0.751163 -0.472886 -0.628963  H 0.708138 0.655542 -1.399718  C -1.770885 -0.725995 0.420181  H -1.256382 -0.885892 1.365497  H -2.277074 -1.621284 0.077850  H -2.440958 0.129708 0.464554  Temperature = 151.000000 Pressure = 1.000000  E(ZPE) = 0.105582 E(Thermal) = 0.108917  E(SCF) = -267.769733 DE(MP2) = -0.934561  DE(CBS) = -0.092298 DE(MP34) = -0.051780  DE(CCSD) = -0.023024 DE(Int) = 0.030003  DE(Empirical) = -0.048265  CBS-QB3 (0 K) = -268.784076 CBS-QB3 Energy = -268.780741  CBS-QB3 Enthalpy = -268.780263 CBS-QB3 Free Energy = -268.798523 |
| CH3 radical  C 0. 000000 0.000000 0.000000  H 0.000000 1.080506 0.000000  H 0.935745 -0.540253 0.000000  H -0.935745 -0.540253 0.000000  Temperature = 151.000000 Pressure = 1.000000  E(ZPE) = 0.029274 E(Thermal) = 0.030728  E(SCF) = -39.576432 DE(MP2) = -0.153698  DE(CBS) = -0.015807 DE(MP34) = -0.021303  DE(CCSD) = -0.003287 DE(Int) = 0.005779  DE(Empirical) = -0.009324  CBS-QB3 (0 K) = -39.744799 CBS-QB3 Energy = -39.743345  CBS-QB3 Enthalpy = -39.742866 CBS-QB3 Free Energy = -39.752625 |
| Fragment ion (**2+**)  C -0.909628 0.013397 0.000000  O -0.637556 -1.239456 0.000000  H -1.422908 -1.814797 0.000000  O 0.00000 0 0.872348 0.000000  H -1.934437 0.385908 0.000000  C 1.444927 0.497381 0. 000000  H 1.645073 -0.076102 0.902453  H 1.955852 1.453286 0.000000  H 1.645073 -0.076102 -0.902453  Temperature = 151.000000 Pressure = 1.000000  E(ZPE) = 0.073863 E(Thermal) = 0.075793  E(SCF) = -228.190522 DE(MP2) = -0.775818  DE(CBS) = -0.076144 DE(MP34) = -0.030745  DE(CCSD) = -0.019300 DE(Int) = 0.024159  DE(Empirical) = -0.039004  CBS-QB3 (0 K) = -229.033511 CBS-QB3 Energy = -229.031581  CBS-QB3 Enthalpy = -229.031103 CBS-QB3 Free Energy = -229.045597 |

**Table S8.** The ωB97X-D/6-311G(d,p) optimized geometries and harmonic frequencies of the reactants, transition states, intermediates, and products depicted in Figures 5 and S6.

|  |
| --- |
| **R1**  C -1.329779 -0.309798 0.306216  C -1.415721 1.142755 -0.053559  O -1.104293 -1.199617 -0.472110  H -1.483523 -0.532620 1.383208  H -0.598237 1.659164 0.458405  H -2.355666 1.566897 0.311353  H -1.330161 1.279247 -1.131484  C 1.931742 0.236727 -0.527190  O 1.510684 -0.101395 0.781464  H 2.139355 1.307760 -0.531496  H 1.155919 0.024122 -1.272694  H 2.850192 -0.290422 -0.812557  H 1.253543 -1.024156 0.767626  **Frequencies**  63.7147 81.3862 105.6514  116.2358 149.9844 161.7214  178.5517 487.3129 516.8849  784.8979 903.4662 1081.0503  1111.1576 1139.6672 1144.7354  1190.9162 1375.4236 1399.3824  1437.4652 1466.5220 1475.5095  1496.0856 1501.2066 1526.8254  1852.0457 2912.7724 3010.7727  3045.8338 3070.4016 3122.4603  3127.6907 3161.5188 3916.9667  **TS1**  C 0.821763 -0.168981 -0.381147  C 1.067547 1.242303 0.077578  O 1.015664 -1.159247 0.441938  H 1.040426 -0.326048 -1.447631  H 0.597539 1.978504 -0.578411  H 2.149443 1.400711 0.048417  H 0.736918 1.375168 1.108184  C -1.785737 0.336043 0.225550  O -0.863574 -0.501822 -0.449825  H -1.867622 1.288800 -0.302626  H -1.484671 0.518204 1.263020  H -2.760743 -0.154500 0.218482  H -0.249445 -1.248471 0.221772  **Frequencies**  -1756.7334 109.1502 171.9935  210.0332 235.1665 369.1272  500.4511 508.2290 696.2759  910.6706 960.0773 1067.5703  1092.0966 1164.0080 1193.4032  1235.7242 1279.5662 1360.7920  1398.4265 1464.3470 1467.8494  1482.3619 1501.1209 1507.8575  1545.1542 2032.0097 3015.1173  3035.6478 3060.1678 3115.2148  3136.0848 3139.6794 3165.4872  **P1**  C -0.552824 -0.119919 0.442263  C -1.082780 1.163378 -0.167424  O -0.899998 -1.165828 -0.430522  H -0.998958 -0.278158 1.430954  H -0.775467 2.019401 0.436382  H -2.172284 1.125532 -0.205656  H -0.713267 1.289583 -1.186987  C 1.662253 0.172907 -0.391703  O 0.826300 -0.108475 0.713577  H 1.653869 1.239467 -0.646448  H 1.370527 -0.409777 -1.271375  H 2.673708 -0.106022 -0.096849  H -0.608439 -1.983797 -0.023269  **Frequencies**  138.2421 166.7575 251.1452  312.2554 392.8204 412.1547  488.5757 660.3627 845.4841  938.4233 1030.6731 1085.8634  1153.3113 1181.2918 1199.0773  1225.7504 1305.4469 1397.8221  1430.3292 1466.4659 1475.0610  1488.1526 1496.0628 1505.2752  1516.5601 3019.7788 3048.3558  3067.0945 3088.4660 3145.4951  3152.2779 3155.8175 3901.6918  **R2**  C 1.467904 -0.914024 -0.257103  C 2.769928 -0.253213 0.055740  O 0.711024 -1.354307 0.578629  H 1.217691 -0.989192 -1.330720  H 2.721804 0.765238 -0.339470  H 3.584744 -0.769896 -0.460114  H 2.947971 -0.239387 1.130494  C -0.065395 1.919113 0.557094  O 0.096312 1.435740 -0.756948  H 0.723317 2.650476 0.745430  H 0.021602 1.117520 1.304709  H -1.031720 2.420718 0.697616  H -0.619303 0.797341 -0.904743  C -2.817608 -0.494137 0.285419  O -1.718506 -0.683143 -0.583477  H -3.556054 0.107971 -0.245526  H -2.532331 0.035270 1.203133  H -3.283919 -1.447304 0.559700  H -1.033410 -1.181512 -0.113050  **Frequencies**  40.7116 79.8489 85.2921  106.1497 112.2427 122.4045  138.6965 151.1289 162.5008  174.1485 197.3306 225.0528  236.8942 525.3713 657.9622  800.0673 847.3546 912.7017  1098.1664 1106.8361 1136.2659  1140.7794 1143.1899 1156.5354  1187.9937 1192.5748 1378.1383  1443.0918 1454.1900 1467.2272  1472.7176 1475.3875 1492.3758  1497.8810 1499.8418 1505.9542  1520.0115 1528.3262 1824.0633  2975.8768 2990.9073 3009.3358  3044.4439 3048.7077 3069.6030  3112.2511 3125.4396 3129.5728  3166.6546 3673.2365 3723.3579  **TS2**  C 1.087922 -0.682675 -0.290677  C 2.496828 -0.340142 0.109563  O 0.336628 -1.239069 0.598884  H 1.010242 -1.053913 -1.323458  H 2.970556 0.314947 -0.623469  H 3.062231 -1.273384 0.167033  H 2.511456 0.122142 1.097825  C 0.363609 1.750183 0.373748  O 0.342426 0.817602 -0.696450  H 1.324443 2.267745 0.390589  H 0.202079 1.241697 1.331220  H -0.429369 2.484658 0.216128  H -0.725517 0.339875 -0.722343  C -2.709346 -0.072296 0.272836  O -1.617619 -0.507041 -0.510692  H -3.307551 0.641780 -0.299069  H -2.381217 0.407924 1.203886  H -3.344291 -0.924447 0.529675  H -0.818622 -1.071384 0.105221  **Frequencies**  -1450.5867 67.1973 110.5955  131.8856 177.9587 210.9735  218.8128 241.8228 282.4647  336.3645 378.3028 475.6947  575.1472 616.5879 686.2285  932.8900 1011.1134 1053.2421  1089.0018 1149.5389 1155.5678  1187.8827 1194.6779 1202.8486  1237.3021 1295.6383 1349.8040  1353.3030 1401.8643 1472.5670  1482.4279 1493.9198 1500.3095  1506.6125 1514.8970 1519.3955  1535.7812 1558.9970 1593.4510  1755.7046 1950.1949 3009.1070  3017.3484 3032.8503 3065.3471  3089.2186 3113.4739 3116.3390  3136.8031 3145.5807 3162.6963  **P2**  C 1.098386 -0.536713 -0.329530  C 2.562977 -0.398606 0.028206  O 0.443083 -1.149211 0.734019  H 0.984016 -1.114869 -1.253616  H 3.090078 0.166267 -0.742955  H 3.007291 -1.391307 0.110496  H 2.679796 0.103012 0.990894  C 0.541477 1.705065 0.331445  O 0.484815 0.707955 -0.673799  H 1.535482 2.161701 0.385811  H 0.276951 1.292639 1.309880  H -0.180388 2.473719 0.054336  H -1.324567 0.038037 -0.890474  C -2.845321 0.083230 0.316063  O -1.988272 -0.595063 -0.581272  H -3.394800 0.892787 -0.178678  H -2.299170 0.499628 1.172625  H -3.569219 -0.641492 0.690384  H -0.467591 -1.307427 0.442608  **Frequencies**  51.1282 73.5291 103.6115  121.2530 148.3475 177.4800  196.1576 201.0103 266.2451  319.8241 421.2509 495.8251  633.6555 656.0264 782.7374  832.2638 940.6050 1039.1795  1090.6262 1108.9975 1137.1994  1162.2662 1185.0852 1186.0784  1187.5152 1230.1434 1358.5887  1404.5892 1422.4913 1458.8631  1474.0451 1484.7126 1490.9271  1496.1110 1501.1621 1508.9585  1519.8613 1520.6616 1525.4722  3003.6424 3026.7775 3050.4737  3062.0107 3062.9532 3097.8268  3130.6794 3138.4049 3146.8546  3150.9908 3706.2250 3745.6237  **R3**  C -1.737740 0.766727 -0.355093  C -3.122602 0.310035 -0.670348  O -1.399671 1.210633 0.721885  H -1.011587 0.717349 -1.186006  H -3.062542 -0.728990 -1.000914  H -3.524401 0.905808 -1.496028  H -3.763507 0.400800 0.206016  C -0.763308 -2.031078 1.072398  O -0.866710 -1.771296 -0.308320  H -1.748157 -2.335233 1.433183  H -0.454111 -1.142502 1.640002  H -0.057400 -2.844239 1.286102  H 0.024884 -1.527517 -0.616626  C 1.595300 2.712023 -0.039794  O 1.308251 1.462812 0.556826  H 1.014665 2.875020 -0.956287  H 2.655265 2.721916 -0.297059  H 1.399685 3.538507 0.651881  H 0.358558 1.437074 0.777173  C 2.699647 -1.597687 -0.214627  O 1.657396 -0.846331 -0.801798  H 2.706906 -2.583022 -0.683682  H 2.556622 -1.727264 0.865393  H 3.676871 -1.130082 -0.382949  H 1.606343 0.015711 -0.344168  **Frequencies**  11.8604 30.2866 44.2578  56.4348 69.4681 78.0247  95.8924 101.0220 106.3919  113.0035 122.1198 132.1011  135.9093 152.2461 172.2421  215.8484 249.1870 266.9392  294.0540 536.4371 780.5636  814.7429 836.3718 915.7933  945.8478 1098.6653 1105.4122  1111.8614 1139.8804 1141.5867  1148.2550 1154.8379 1164.8737  1188.1355 1188.9144 1189.1749  1375.4414 1439.3993 1463.4415  1471.1355 1479.3556 1480.8320  1486.3301 1490.2570 1496.3956  1499.2969 1501.0765 1501.9792  1505.8842 1520.5177 1525.6123  1535.3506 1812.3178 2978.2294  2992.9442 3006.5864 3010.5867  3046.4590 3049.2533 3065.8314  3074.2927 3111.4258 3122.8681  3130.1408 3130.7028 3168.9809  3516.0139 3603.1834 3616.9173  **TS3**  C 1.298412 -0.687904 -0.324992  C 2.788179 -0.846452 -0.511364  O 0.814061 -1.146583 0.783856  H 0.731225 -0.914467 -1.243340  H 3.145370 -0.290762 -1.379591  H 3.001779 -1.908454 -0.651341  H 3.313903 -0.516874 0.387039  C 1.458090 1.633478 0.761902  O 1.058717 0.949853 -0.419245  H 2.527324 1.848089 0.716070  H 1.236527 1.020847 1.640382  H 0.910048 2.576002 0.818168  H -0.100302 1.054396 -0.558393  C -2.092695 -2.161378 -0.136779  O -1.568616 -1.048512 0.551302  H -1.817705 -2.155616 -1.200628  H -3.184113 -2.163467 -0.063775  H -1.718273 -3.088653 0.307800  H -0.442177 -1.164086 0.723815  C -2.004943 2.112040 -0.076456  O -1.323643 1.010382 -0.647821  H -1.645548 3.034704 -0.538148  H -1.848086 2.167964 1.007055  H -3.076483 2.023576 -0.271062  H -1.559898 0.056981 -0.112663  **Frequencies**  -1257.0361 41.3197 52.2013  75.1522 98.5514 102.7045  111.8360 142.1298 142.8320  162.7920 179.5582 202.9314  244.2485 286.3263 334.4321  386.5425 453.1526 549.5906  595.1896 642.4778 677.0852  936.9240 985.8087 1050.5279  1066.0151 1099.8831 1138.5627  1151.5453 1171.7457 1181.8803  1194.0250 1197.6596 1202.8278  1220.1042 1321.7970 1325.8197  1345.9859 1400.4185 1407.0773  1470.6677 1482.6559 1484.1877  1496.0817 1499.3877 1502.3474  1503.3989 1506.6679 1512.9115  1524.1978 1525.0644 1544.3726  1567.8923 1604.0676 1706.5559  1767.1654 1838.9679 2973.8490  3000.9350 3024.8394 3044.4753  3059.2522 3071.5013 3098.9578  3101.2345 3122.4612 3129.5374  3135.3073 3141.0579 3153.9053  **P3**  C 1.375272 -0.537903 -0.312707  C 2.854789 -0.746989 -0.564520  O 1.047093 -1.084866 0.909722  H 0.782176 -0.975438 -1.125387  H 3.165124 -0.229359 -1.474075  H 3.053927 -1.814070 -0.672245  H 3.441550 -0.381036 0.280603  C 1.600018 1.689707 0.584443  O 1.013668 0.851877 -0.397099  H 2.652694 1.890200 0.358807  H 1.516288 1.241749 1.577795  H 1.053600 2.633280 0.562104  H -0.712758 1.094179 -0.681823  C -2.024813 -2.332502 -0.259171  O -1.651875 -1.292020 0.621085  H -1.523295 -2.251038 -1.231982  H -3.107656 -2.347951 -0.426510  H -1.733677 -3.277972 0.200637  H 0.076024 -1.196077 0.939816  C -2.114143 2.240503 0.048882  O -1.687877 1.091468 -0.656291  H -1.808655 3.159937 -0.463866  H -1.726804 2.262093 1.075329  H -3.203794 2.220064 0.092493  H -1.839553 -0.437141 0.187404  **Frequencies**  19.9020 43.2449 51.5802  74.7118 93.6010 96.9272  111.7061 113.4777 125.2260  130.1646 179.1227 216.6414  228.4528 265.0507 272.0760  316.3411 433.1060 497.3519  653.3008 735.6663 817.6303  850.0073 937.9278 957.6662  1043.5449 1099.0114 1103.5701  1115.2135 1147.3098 1154.0376  1163.3845 1185.6922 1188.3396  1189.1205 1197.7523 1231.9234  1372.0569 1405.8792 1424.4526  1470.9085 1476.2776 1485.8845  1487.9900 1492.8547 1493.9934  1497.9616 1502.0293 1503.5646  1512.1390 1521.1766 1523.4703  1529.7079 1543.5172 3005.6090  3006.9955 3030.5565 3037.2288  3060.6742 3067.5750 3067.7619  3106.7822 3127.7606 3129.5897  3139.5799 3144.9418 3149.8269  3497.2420 3570.0722 3604.3580  **R4**  C -1.726059 1.065462 -0.722331  C -3.040535 0.923680 -1.413048  O -1.588636 1.630574 0.345234  H -0.847851 0.648624 -1.242341  H -3.259505 -0.145714 -1.467063  H -2.968857 1.306552 -2.435317  H -3.822441 1.445624 -0.862084  C -1.767434 -1.408857 1.394217  O -1.781235 -1.532781 -0.009359  H -2.704219 -0.937822 1.699444  H -0.940971 -0.776946 1.745376  H -1.697810 -2.385184 1.892242  H -0.919319 -1.897444 -0.278461  C 1.523966 2.106698 1.997196  O 0.917978 1.109180 1.200387  H 1.525271 3.084000 1.500043  H 2.557276 1.806657 2.178075  H 1.019279 2.204376 2.964154  H -0.008309 1.363854 1.007543  C 1.544589 -2.416891 0.628179  O 0.813809 -2.271045 -0.575253  H 1.101897 -3.241905 1.188967  H 1.500408 -1.509084 1.241821  H 2.595474 -2.662364 0.431228  H 1.138015 -1.460201 -1.004752  C 2.737478 0.786875 -1.844607  O 1.575141 0.242367 -1.258642  H 2.669379 1.877370 -1.935538  H 2.835518 0.365920 -2.846040  H 3.640964 0.536685 -1.275001  H 1.457322 0.608843 -0.358885  **Frequencies**  24.7947 27.0544 38.9914  40.5445 61.9153 71.4516  76.6823 82.5024 98.2806  101.2249 110.2960 114.5683  117.2178 118.8999 127.8746  142.9708 157.1729 159.7176  166.6850 175.1186 212.5057  237.8599 259.4503 271.2954  290.9847 539.0863 716.7214  766.7628 818.9118 887.2494  919.1441 943.7541 1092.7631  1102.6056 1108.6844 1116.6764  1139.4628 1147.2325 1150.4446  1154.4706 1157.7259 1172.8958  1185.7674 1187.4553 1188.3466  1194.9656 1375.0739 1458.4316  1463.9191 1470.8195 1479.4624  1480.1664 1486.9745 1488.7915  1490.7674 1492.2034 1496.4713  1500.9519 1502.3411 1502.7445  1503.1743 1511.4446 1527.9642  1531.1176 1535.8709 1548.7040  1800.8921 2995.3630 3005.8066  3007.6954 3014.3085 3015.4101  3048.9486 3051.8303 3066.7526  3068.6077 3079.5466 3112.3570  3122.5615 3126.6045 3128.9395  3129.4249 3165.1628 3468.5613  3540.9558 3601.4716 3656.2426  **TS4**  C 1.448409 -0.736393 -0.406552  C 2.696736 -1.513928 -0.787306  O 1.012403 -0.952686 0.816808  H 0.678575 -0.836532 -1.194086  H 3.102359 -1.187259 -1.747834  H 2.431394 -2.570963 -0.853486  H 3.456158 -1.413082 -0.008748  C 2.773865 1.254022 0.274861  O 1.780881 0.761580 -0.614735  H 3.771118 1.017478 -0.103240  H 2.635552 0.818121 1.268365  H 2.667315 2.339648 0.325677  H 0.648408 1.417539 -0.434226  C -1.598410 -2.681098 0.464695  O -1.356877 -1.315541 0.698114  H -1.484414 -2.946440 -0.596571  H -2.615957 -2.941940 0.774462  H -0.898912 -3.295741 1.041708  H -0.251988 -1.146462 0.801569  C -0.440484 1.989122 1.228014  O -0.307155 1.912268 -0.201698  H 0.170564 2.818160 1.584537  H -0.117800 1.049764 1.681254  H -1.486167 2.184134 1.465291  H -1.111117 1.280079 -0.579309  C -3.396330 0.801767 -0.700200  O -2.055906 0.394449 -0.903503  H -4.082064 0.096801 -1.178261  H -3.539947 1.784771 -1.153508  H -3.640037 0.860430 0.366968  H -1.822527 -0.410021 -0.261516  **Frequencies**  -678.1938 23.1690 37.0644  44.7874 61.2696 73.5305  88.5544 92.0300 107.0619  120.3178 126.8032 133.3424  153.8814 177.9364 183.8485  197.9262 204.9759 260.7605  287.4363 334.6245 377.4668  469.3889 472.6808 514.3980  607.3498 678.2610 848.0911  948.1324 1011.3781 1051.3479  1070.0992 1095.1729 1117.6559  1137.7898 1141.7815 1164.7526  1172.0695 1186.5951 1189.9727  1192.2149 1198.2755 1222.6377  1256.7079 1307.3592 1318.4677  1380.5874 1401.4449 1406.3615  1424.1662 1453.0444 1467.5865  1474.2267 1481.4844 1484.3683  1489.7054 1494.2078 1500.4395  1503.6998 1503.8891 1510.5863  1513.0154 1515.2304 1523.2222  1526.3149 1554.3654 1589.4079  1627.5268 1706.0869 1813.4113  1926.9651 2284.3792 2938.5400  2989.1552 3024.4813 3039.1742  3052.2445 3055.1229 3060.5641  3085.9075 3094.1547 3122.4624  3123.3686 3129.1169 3138.6950  3140.1153 3155.0804 3161.2116  **P4**  C -1.783534 0.565100 -0.475337  C -3.114354 1.122564 -0.941305  O -1.497163 1.057593 0.782458  H -0.989478 0.812296 -1.189343  H -3.420377 0.654816 -1.879080  H -3.019657 2.198984 -1.091091  H -3.884275 0.957548 -0.184590  C -2.707369 -1.495172 0.371241  O -1.777426 -0.870593 -0.497505  H -3.725409 -1.437175 -0.027610  H -2.673774 -1.042480 1.365769  H -2.417787 -2.544568 0.436658  H -0.210240 -1.626288 -0.429516  C 1.381268 2.816536 0.488876  O 1.171878 1.442365 0.745768  H 1.132528 3.081908 -0.545633  H 2.419168 3.107356 0.687139  H 0.730412 3.383759 1.155850  H -0.525329 1.107897 0.873896  C 0.808313 -1.943019 1.195415  O 0.671383 -1.986918 -0.215567  H 0.022399 -2.524580 1.689659  H 0.784394 -0.917064 1.579475  H 1.771723 -2.389512 1.447872  H 1.840078 -0.899466 -0.876416  C 3.750772 -0.549477 -0.631895  O 2.449791 -0.143226 -1.007502  H 4.424950 0.292915 -0.794573  H 4.097287 -1.390653 -1.241818  H 3.802768 -0.836227 0.426169  H 1.682340 0.917560 0.093992  **Frequencies**  15.0911 29.3081 44.3664  51.4111 66.9951 75.2406  86.8889 89.9183 100.3040  103.8891 117.6794 126.4582  135.1125 142.7441 151.1098  188.1687 213.8107 226.5883  268.7440 297.1387 303.9055  319.7067 437.1875 496.6125  655.3365 816.3964 844.8192  874.0500 881.7324 911.6843  951.0184 1045.6688 1087.0466  1098.8469 1105.1026 1116.5720  1138.1816 1149.5895 1161.0012  1168.5680 1186.6398 1188.0224  1190.0643 1192.8295 1199.1987  1232.7365 1373.4601 1405.6187  1426.2811 1463.8480 1473.4169  1484.4751 1486.1855 1488.6319  1491.3846 1493.0122 1499.0228  1500.6078 1504.5027 1506.1009  1509.7836 1512.8349 1518.6956  1521.4630 1526.5548 1536.9503  1564.4903 3007.6374 3010.8473  3020.0165 3031.1152 3050.6894  3059.5677 3071.8385 3073.3324  3086.5179 3106.7323 3124.1202  3125.7028 3128.2486 3139.3226  3144.0211 3148.2161 3428.3938  3515.4070 3553.6973 3583.2952  **R5**  C 0.416982 -0.065779 1.631314  C -0.011447 -1.009047 2.697898  O 0.947734 1.008970 1.832468  C 3.060167 -1.086717 -0.121060  O 2.184135 -1.988448 0.513157  H 0.214008 -0.391300 0.601353  H 0.590657 -1.914966 2.584979  H -1.055343 -1.281934 2.520555  H 0.127892 -0.575664 3.687656  H 3.839468 -0.817378 0.594544  H 2.550267 -0.163781 -0.433384  H 3.544117 -1.528298 -1.002636  H 1.468057 -2.188566 -0.112907  C 1.915609 2.792780 -1.231867  O 0.931870 1.929397 -0.701021  H 1.943893 3.752114 -0.703216  H 1.666444 2.978615 -2.277185  H 2.909798 2.333940 -1.190026  H 1.122141 1.729053 0.237099  C 0.205705 -1.207549 -2.309315  O 0.033606 -2.123176 -1.242116  H 1.086732 -1.518446 -2.873541  H 0.368014 -0.184511 -1.948508  H -0.655438 -1.215733 -2.987619  H -0.784515 -1.871548 -0.775085  C -2.072696 2.449740 0.591647  O -1.731497 1.570621 -0.465802  H -1.321034 2.436364 1.388158  H -3.026501 2.117674 1.004965  H -2.191422 3.476637 0.229641  H -0.818378 1.772401 -0.741191  C -3.464843 -1.400133 -0.456874  O -2.166246 -1.042872 -0.026733  H -3.590528 -2.470721 -0.289909  H -3.614348 -1.193598 -1.523034  H -4.235552 -0.869700 0.114045  H -2.032112 -0.086353 -0.194834  **Frequencies**  31.6736 39.7464 46.1553  55.4389 59.3437 66.5351  71.6052 81.0624 89.4443  95.1870 102.3828 104.7566  114.7096 119.5797 131.3956  133.4453 140.7216 146.6928  151.0224 152.4882 156.8805  158.5640 170.9423 182.2671  188.7176 211.5681 227.3935  260.8274 284.3175 313.8222  319.1638 540.3146 767.6963  785.1497 842.7559 861.3960  887.5033 930.7852 933.1109  1089.2637 1093.6417 1103.9619  1110.4735 1112.9368 1138.8836  1144.8334 1156.2062 1157.8257  1164.7037 1172.5263 1178.2780  1188.2129 1191.2153 1191.5554  1194.8050 1196.4466 1384.2329  1452.8055 1462.3236 1469.0382  1472.7233 1475.5145 1485.2158  1487.2634 1488.6753 1493.5843  1494.6858 1497.0118 1503.3859  1503.6311 1507.4667 1508.6582  1509.7418 1510.0269 1512.6286  1525.3715 1528.3828 1531.0008  1534.6689 1549.9998 1806.9247  2997.5765 3016.7423 3018.9281  3022.6752 3027.8051 3047.8807  3059.8016 3079.4687 3079.5966  3082.3804 3085.8385 3094.2339  3121.6688 3125.4215 3131.3870  3135.6454 3137.1659 3142.7601  3171.9097 3464.2827 3530.6929  3595.5263 3618.0262 3664.0566  **TS5**  C 1.712629 -0.927347 -0.283444  C 2.828936 -1.841510 -0.734957  O 1.519564 -0.927761 1.033306  C 3.255111 1.040506 -0.160608  O 2.080401 0.495649 -0.762819  H 0.797620 -1.078864 -0.867742  H 3.061279 -1.695191 -1.791638  H 2.502348 -2.871379 -0.582292  H 3.724853 -1.685265 -0.130349  H 4.139885 0.661650 -0.673061  H 3.283341 0.776843 0.899326  H 3.206325 2.123288 -0.280952  H 1.164590 1.248600 -0.554425  C -1.451480 -1.436782 2.287387  O -0.876605 -0.642112 1.295905  H -1.310163 -2.515511 2.103402  H -2.536010 -1.261370 2.362380  H -1.023638 -1.225228 3.279176  H 0.451611 -0.798895 1.223540  C 0.192881 2.257771 1.113832  O 0.343471 2.069082 -0.307378  H 1.191019 2.371390 1.536490  H -0.305733 1.387288 1.547200  H -0.371427 3.176274 1.279760  H -0.566467 1.854726 -0.714851  C -2.430688 -2.174096 -1.238918  O -1.555171 -1.086172 -1.073555  H -1.991207 -3.101090 -0.850721  H -2.625467 -2.311678 -2.305197  H -3.392017 -2.013122 -0.732127  H -1.320786 -0.968831 -0.076887  C -2.947857 1.637545 -0.201716  O -1.954423 1.468259 -1.206753  H -2.988592 2.697084 0.056851  H -2.700875 1.048586 0.688192  H -3.929536 1.337792 -0.580927  H -1.876045 0.490812 -1.354236  **Frequencies**  -507.1544 33.1038 39.4006  57.1045 61.8967 75.9739  83.3013 90.6474 101.0073  117.9031 124.5330 130.4450  140.6153 158.2782 161.0859  163.4336 167.8851 181.3434  190.0091 199.1970 211.9441  231.2270 258.3745 276.7039  298.2157 322.5173 341.9513  377.7175 479.6210 494.2863  586.3709 661.4779 800.7789  938.4935 942.9608 1027.8591  1051.5236 1068.5919 1090.6282  1103.5017 1105.0764 1128.4053  1138.1902 1167.3448 1174.6252  1185.3771 1189.3388 1193.1081  1195.3630 1199.5602 1201.9967  1212.5222 1228.0747 1240.6222  1287.0970 1325.9828 1391.5820  1399.7056 1430.8808 1460.9340  1475.5818 1477.6788 1480.9016  1485.3840 1488.5428 1494.3057  1497.7776 1502.0186 1502.3475  1506.4952 1509.3835 1511.1127  1515.5325 1518.5120 1521.4759  1522.9955 1529.8282 1554.6367  1575.5542 1615.1484 1683.0605  1751.2070 1806.8303 2533.9486  2764.2376 2951.8532 2991.6502  3000.3424 3009.1699 3029.9867  3047.2571 3056.6381 3057.3809  3066.7234 3072.5952 3105.3228  3110.6880 3132.0690 3147.3178  3149.9184 3151.6182 3155.3170  3158.4385 3160.2475 3305.2743  **P5**  C 1.944587 -0.764997 -0.374106  C 3.091676 -1.571120 -0.950303  O 1.907938 -0.953937 0.998738  C 3.206435 1.285750 -0.218126  O 2.052991 0.625171 -0.709936  H 0.995834 -1.046830 -0.841864  H 3.219946 -1.348776 -2.011416  H 2.878477 -2.634327 -0.830820  H 4.020809 -1.354227 -0.418656  H 4.093393 1.030707 -0.807457  H 3.377574 1.037910 0.832952  H 3.017008 2.355483 -0.315291  H 0.667227 1.667657 -0.519894  C -1.169823 -2.000375 2.251078  O -0.792813 -0.858370 1.507441  H -0.669325 -2.905826 1.887259  H -2.254260 -2.157830 2.222800  H -0.873603 -1.837392 3.288022  H 0.993050 -0.805965 1.297080  C 0.035198 2.406681 1.165374  O -0.021034 2.303937 -0.248554  H 1.023936 2.743547 1.497753  H -0.201160 1.454693 1.651480  H -0.698751 3.154434 1.471452  H -1.554583 1.822842 -0.880585  C -2.409548 -2.074187 -1.562828  O -1.479564 -1.127113 -1.080116  H -2.022650 -3.069890 -1.339857  H -2.537269 -1.988574 -2.647101  H -3.391046 -1.966489 -1.084544  H -1.076811 -0.991441 0.578748  C -3.208097 1.391815 0.058059  O -2.393627 1.365145 -1.101105  H -3.440675 2.419623 0.357041  H -2.732779 0.873689 0.900322  H -4.145949 0.887097 -0.181893  H -1.822083 -0.220166 -1.252152  **Frequencies**  26.2984 31.0684 37.2316  44.1285 51.8247 60.6379  71.2797 74.7097 85.6401  92.0651 102.5428 104.9408  116.5444 124.5860 126.3801  145.5905 149.9855 154.1650  161.6698 178.5686 197.1862  213.7258 215.7229 259.5993  280.2740 292.9606 309.4261  317.5814 434.5687 496.3983  652.7625 757.0692 807.4899  832.0583 851.7128 924.5965  945.5461 986.5583 1045.1966  1085.4958 1094.3332 1097.8996  1108.8132 1115.5501 1139.5402  1145.7270 1153.4423 1163.6957  1170.9097 1186.8059 1187.2382  1188.6658 1190.6548 1198.3965  1200.7406 1234.2035 1389.8001  1406.9878 1442.1203 1467.8141  1475.2942 1479.2690 1485.4409  1486.6838 1488.7029 1491.1285  1493.3632 1497.0086 1501.5162  1502.2650 1503.8074 1507.0575  1510.9836 1512.1784 1515.0595  1521.3294 1526.3439 1532.9279  1535.5564 1552.1798 1576.2023  3008.1038 3009.8586 3011.8876  3018.7160 3029.8238 3058.7378  3071.1718 3075.6239 3076.4406  3077.8052 3090.1354 3104.9903  3119.0073 3124.5015 3124.9056  3129.9871 3138.3392 3142.9813  3147.6949 3367.4523 3487.0144  3500.5886 3580.5408 3627.0914  **R6**  C 1.270110 -1.105336 -0.165067  C 2.720081 -0.783090 0.014341  O 0.510207 -1.359458 0.738308  H 0.904993 -1.097956 -1.209732  H 2.883119 0.221664 -0.384342  H 3.330038 -1.476841 -0.572260  H 2.999048 -0.829777 1.066781  C 0.487175 2.078804 0.625830  O 0.694134 1.630898 -0.693697  H 0.333801 1.246348 1.326667  H -0.367276 2.764530 0.703029  H 1.381276 2.623693 0.934746  H -0.120427 1.208146 -0.995193  C -1.995505 -0.723612 -0.403990  C -2.384444 -0.158032 0.924465  O -1.489162 -0.095795 -1.303544  H -2.217588 -1.798563 -0.545093  H -3.433756 -0.389443 1.130455  H -2.222229 0.919179 0.953295  H -1.776935 -0.648541 1.689635  **Frequencies**  59.8219 72.1924 82.1952  94.3702 109.9562 114.6104  128.4035 134.0506 142.4336  161.3303 170.8098 182.6944  201.6687 224.6036 521.2365  523.0941 675.2135 789.1434  802.6298 908.2604 909.8652  1105.4991 1129.3331 1140.0812  1144.6272 1147.0378 1147.7151  1192.1705 1375.8147 1378.6871  1436.5803 1441.8762 1443.1051  1466.6346 1468.0554 1472.9210  1478.4906 1495.4677 1504.5673  1522.7265 1827.5380 1839.4550  2957.9503 2961.2188 2992.0502  3045.0497 3047.1463 3049.2996  3115.3222 3125.8744 3126.9908  3163.8142 3165.1619 3768.9790  **TS6**  C 1.032434 -0.683312 -0.376091  C 2.523434 -0.630978 -0.548753  O 0.597883 -1.243293 0.695405  H 0.468426 -0.854749 -1.301368  H 2.803280 0.019969 -1.376806  H 2.875693 -1.644869 -0.753281  H 2.994188 -0.290204 0.375073  C 0.800784 1.625278 0.934736  O 0.605724 1.008932 -0.334888  H 0.713724 0.876217 1.726871  H 0.038278 2.393708 1.068630  H 1.790143 2.082349 0.955282  H -0.423875 1.006928 -0.574156  C -2.246577 -0.260933 -0.446652  C -1.956772 -0.748589 0.842178  O -1.746077 0.758346 -0.983357  H -2.915719 -0.865640 -1.081868  H -2.587758 -1.557285 1.198793  H -1.731557 0.011001 1.591442  H -0.604882 -1.178100 0.721588  **Frequencies**  -1290.4314 84.4335 99.6898  125.6519 151.5355 175.8713  203.0938 231.8606 259.5717  296.5114 367.7785 389.1199  473.3475 555.8287 580.0965  593.9242 704.0864 898.8801  939.1599 1021.0718 1030.6941  1055.5288 1071.1702 1145.5191  1175.8763 1188.9663 1239.7813  1289.0632 1336.9089 1343.3864  1379.4489 1406.6226 1412.3238  1451.8962 1474.3877 1481.9308  1484.1910 1496.5713 1518.5183  1545.2227 1585.9981 1602.3218  1682.4389 2159.4493 2993.5338  3047.1009 3049.6365 3063.3827  3107.0976 3134.4549 3143.0145  3154.8857 3165.5788 3202.2843  **P6**  C 1.106573 -0.598750 -0.247239  C 2.612461 -0.704454 -0.354033  O 0.729127 -1.060356 1.010718  H 0.619355 -1.169752 -1.044413  H 2.955897 -0.261096 -1.290274  H 2.902525 -1.755485 -0.328452  H 3.094955 -0.200949 0.486090  C 1.103555 1.724613 0.401989  O 0.627776 0.726095 -0.485064  H 1.056394 1.379783 1.438646  H 0.454953 2.591465 0.276469  H 2.130735 2.013470 0.157876  H -1.057247 0.520594 -1.059099  C -2.532547 -0.329401 -0.204537  C -2.303214 0.068291 1.049967  O -1.861081 0.026483 -1.308418  H -3.337632 -1.020345 -0.437411  H -2.933042 -0.297601 1.849152  H -1.539914 0.798270 1.294081  H -0.234524 -1.097924 1.042561  **Frequencies**  60.3437 77.1655 95.9182  117.8711 143.0334 173.7296  197.1281 200.3482 259.9867  315.1310 423.5827 483.9444  524.3623 558.1543 661.4166  738.6269 826.5419 838.0761  853.4827 943.9361 983.2579  1035.0179 1046.9997 1098.2234  1159.4936 1184.4239 1187.8051  1206.1922 1231.0617 1330.3634  1350.7502 1402.7119 1425.0953  1431.9417 1470.0429 1475.2579  1482.6909 1490.6960 1499.5689  1510.5766 1523.4497 1712.1428  3033.5567 3062.9362 3066.5434  3107.4162 3144.9997 3148.3861  3153.0973 3167.5893 3185.7624  3266.2140 3587.4263 3793.6562  **R7**  C 0.693553 -1.584223 -0.857914  C 1.923365 -2.433800 -0.910524  O -0.331616 -1.906931 -0.303839  H 0.761825 -0.606161 -1.370719  H 2.710667 -1.890042 -0.381971  H 2.242733 -2.565142 -1.948854  H 1.742950 -3.400507 -0.440766  C 1.363172 0.093599 2.051461  O 2.125756 0.182693 0.868653  H 1.820962 -0.667146 2.686922  H 0.324914 -0.203136 1.853955  H 1.352580 1.040207 2.608338  H 1.693990 0.838609 0.299042  C -2.277802 0.052922 -0.187733  C -3.286074 -0.922021 0.320781  O -1.816927 0.955300 0.475895  H -1.963941 -0.078273 -1.238356  H -4.157264 -0.935235 -0.340850  H -3.582273 -0.671874 1.338788  H -2.830041 -1.914810 0.289724  C 0.632772 3.195770 -0.914554  O 0.508655 1.807329 -0.685519  H 0.600780 3.770596 0.018565  H -0.153324 3.565696 -1.583177  H 1.598054 3.367552 -1.392505  H -0.343476 1.629060 -0.248747  **Frequencies**  27.2893 32.3765 45.6924  51.1045 61.7026 63.5113  85.3807 93.3299 97.3328  102.2508 115.2157 125.5469  133.9614 142.9099 152.5661  165.6350 201.0238 221.2788  235.4797 266.0105 521.1688  533.7933 774.1620 799.8027  809.6880 820.0614 910.7194  917.7938 1102.0723 1107.2262  1136.3971 1141.0449 1145.6502  1149.6449 1151.9890 1157.8123  1187.1820 1188.1506 1373.9927  1380.6923 1439.6215 1449.1299  1456.5118 1466.8005 1467.4574  1476.7587 1480.6178 1483.0188  1494.7439 1497.0914 1501.8041  1503.7278 1520.6112 1529.0577  1819.6657 1829.9864 2965.5719  2982.4588 2996.7312 3010.9240  3046.7976 3051.0251 3052.9863  3071.0944 3114.1772 3128.2436  3129.4723 3129.6176 3163.7370  3168.9414 3601.7143 3689.5309  **TS7**  C 1.419529 0.701769 -0.502477  C 2.041827 2.009340 -0.887206  O 2.164864 -0.121420 0.147998  H 0.747972 0.258825 -1.248766  H 1.297256 2.704581 -1.274160  H 2.786373 1.813296 -1.663070  H 2.544162 2.447162 -0.024024  C 0.116823 0.627290 1.848611  O 0.147838 1.264786 0.560339  H 1.143263 0.538673 2.197734  H -0.340090 -0.360747 1.761320  H -0.451160 1.272529 2.519371  H -0.734708 1.068140 0.084467  C -0.160961 -2.168994 -0.525342  C 1.080857 -2.542536 -0.008307  O -1.146894 -1.740831 0.127024  H -0.241803 -2.171039 -1.632169  H 1.740246 -3.105453 -0.663439  H 1.120241 -2.797600 1.049312  H 1.731352 -1.153952 0.069880  C -3.248970 0.926452 -0.243714  O -1.946693 0.532671 -0.634073  H -3.447395 0.689835 0.807803  H -4.002613 0.432208 -0.863813  H -3.336394 2.004860 -0.386100  H -1.804260 -0.442881 -0.434040  **Frequencies**  -625.7765 36.8753 54.7354  88.6499 95.0992 108.6567  125.9575 130.4506 144.5156  161.0286 189.1621 226.1114  240.8949 260.5357 299.2046  319.9394 352.3724 429.9113  446.5797 555.0189 579.0741  655.4582 707.4759 936.7329  981.1573 995.4255 1025.4834  1031.5711 1046.7268 1090.6325  1104.6481 1151.0542 1163.3447  1186.2593 1192.4948 1202.5226  1257.3988 1289.7148 1311.1505  1323.2001 1357.9491 1403.4550  1413.0506 1463.0448 1472.3777  1477.2329 1483.7629 1488.4425  1501.3219 1503.2774 1511.4654  1524.8621 1544.1727 1564.7959  1587.7502 1613.3455 1732.4559  2686.7129 2908.0666 2999.9004  3052.8073 3054.6538 3065.0036  3066.6792 3093.6537 3114.2944  3130.0207 3147.1567 3156.0020  3168.4866 3183.1852 3207.4370  **P7**  C -1.698082 -0.301453 -0.538362  C -2.923497 -1.192162 -0.539658  O -2.029311 0.888392 0.084844  H -1.336469 -0.138128 -1.560902  H -2.678073 -2.172350 -0.951925  H -3.707224 -0.733490 -1.144100  H -3.306728 -1.311977 0.475841  C -0.662558 -1.121347 1.488381  O -0.577389 -0.939713 0.083435  H -1.339921 -1.943069 1.744116  H -0.990955 -0.203386 1.977823  H 0.343309 -1.366830 1.829251  H 1.076120 -1.043419 -0.471428  C 1.074551 2.008824 -0.307749  C 0.284417 3.080232 -0.211207  O 1.635639 1.402967 0.746588  H 1.299770 1.561494 -1.275493  H -0.099482 3.547832 -1.107657  H 0.075191 3.535518 0.749689  H -1.301824 1.519007 -0.030943  C 2.708244 -2.136888 -0.349852  O 2.038621 -0.908068 -0.540790  H 2.494768 -2.575087 0.633044  H 3.779643 -1.945379 -0.416881  H 2.438443 -2.863673 -1.124176  H 2.014499 0.561078 0.431798  **Frequencies**  36.2397 42.2077 52.2154  65.3890 70.6253 84.8505  95.4354 111.4825 127.1572  139.6114 159.0925 172.2769  215.7961 246.2527 251.5308  319.2555 421.3286 481.1492  506.3989 615.2557 678.0308  713.2766 771.4466 821.3586  844.6869 919.5026 949.5613  989.7920 1033.0414 1037.2694  1099.4190 1110.0376 1148.8678  1156.9864 1185.5732 1188.1760  1196.1524 1222.8327 1232.6034  1334.8364 1347.0060 1400.5122  1420.9729 1433.8875 1454.5344  1472.3695 1478.3763 1480.7242  1486.4501 1494.5131 1498.0783  1503.2368 1510.2566 1519.7833  1521.9254 1746.4435 3009.5047  3034.5671 3039.9606 3061.7192  3071.3085 3120.4738 3133.3322  3141.6208 3145.8506 3151.4927  3152.0955 3170.1706 3268.8030  3560.0234 3624.4506 3696.6661  **R8**  C 2.066234 -1.112124 -0.346315  C 3.521942 -0.827411 -0.517356  O 1.638784 -2.087419 0.233835  H 1.369536 -0.374803 -0.783701  H 3.742240 0.060619 0.081298  H 3.741455 -0.593153 -1.562821  H 4.121147 -1.670728 -0.175304  C 0.858737 0.662113 2.209623  O 1.873769 1.132545 1.348602  H 1.339992 0.127848 3.030488  H 0.174914 -0.031838 1.703013  H 0.262370 1.481699 2.630540  H 1.433815 1.533892 0.583884  C -2.605677 0.436762 -0.076633  C -3.684638 -0.326104 0.613579  O -2.052425 1.405065 0.395749  H -2.317495 0.072777 -1.078845  H -4.543975 -0.451487 -0.051246  H -3.979799 0.172994 1.535781  H -0.164412 -2.061164 0.289230  C 0.389666 3.052339 -1.601501  O 0.335653 1.857782 -0.848766  H 0.223506 3.938091 -0.977443  H -0.346463 3.050640 -2.413956  H 1.385208 3.122773 -2.041884  H -0.539625 1.788404 -0.425384  C -1.252902 -2.500485 -1.244507  O -1.100908 -1.960083 0.046497  H -0.696238 -1.932382 -2.003397  H -2.314899 -2.461440 -1.503439  H -0.932910 -3.548031 -1.296004  H -3.277519 -1.318365 0.830509  **Frequencies**  14.8547 22.9728 32.2227  39.5015 54.3892 56.5807  67.6317 68.7551 75.9318  80.0015 99.5629 106.1467  110.0522 115.8387 120.6206  132.9662 139.0931 139.7298  146.7757 159.8539 172.8963  200.7100 220.8510 245.3738  248.0248 276.8990 532.8638  534.8893 733.7907 794.3904  803.2923 820.8829 838.1829  921.3123 922.6192 1097.5095  1104.2559 1107.0587 1135.1857  1139.5854 1143.5974 1149.5876  1155.4171 1157.7065 1159.9935  1186.4075 1187.0133 1187.4431  1374.1243 1375.6341 1443.5364  1451.1567 1457.2992 1465.2506  1468.0819 1471.0514 1478.9999  1479.9941 1485.4899 1493.9413  1495.8590 1498.4895 1500.3288  1501.6605 1505.4691 1521.1369  1525.7539 1533.3840 1814.8422  1823.9799 2981.7490 2989.0555  2991.1484 3000.5215 3011.7884  3045.1514 3048.7209 3052.8404  3054.5300 3072.5605 3094.9782  3121.5063 3123.3812 3127.9235  3129.0614 3165.0506 3166.7417  3583.6625 3632.6200 3706.4318  **TS8**  C 0.062243 1.520046 -0.526157  C -0.783672 2.541010 -1.205876  O 1.158318 1.859616 -0.008348  H -0.060119 0.477026 -0.834459  H -1.790119 2.157432 -1.369146  H -0.325759 2.753487 -2.177586  H -0.807543 3.458259 -0.618799  C -0.565791 0.486907 2.039624  O -1.184430 1.220911 0.984946  H 0.398794 0.955592 2.241788  H -0.423620 -0.555966 1.744005  H -1.182966 0.554777 2.938865  H -1.872359 0.653082 0.551035  C 0.492795 -2.164130 -0.657847  C 1.682433 -2.467452 0.000219  O -0.598658 -1.851729 -0.120688  H 0.552129 -2.119622 -1.765570  H 2.471523 -2.930123 -0.587060  H 1.616409 -2.764472 1.044984  H 1.857864 0.928115 0.226245  C -3.865109 -1.000283 -0.191393  O -2.649059 -0.350588 -0.502018  H -3.785724 -1.594262 0.726287  H -4.179260 -1.659373 -1.008039  H -4.632485 -0.236944 -0.050858  H -1.920388 -1.024225 -0.529859  C 3.796508 0.136266 -0.346821  O 2.605876 0.008153 0.418068  H 3.623696 -0.122645 -1.396863  H 4.564394 -0.522239 0.063166  H 4.141464 1.168999 -0.282807  H 2.181253 -0.981978 0.238500  **Frequencies**  -834.1617 11.2091 26.5211  44.2764 46.3948 52.2407  68.0618 97.9058 103.6560  112.7011 120.8998 132.3659  140.9247 154.4692 170.4799  182.3685 205.6956 212.2248  225.6542 243.1233 276.5774  305.1190 334.4258 391.7431  470.1303 525.2938 559.0728  670.6602 729.0587 793.8946  905.6591 937.7486 1014.3509  1027.3695 1037.8454 1056.7942  1079.1321 1093.4813 1120.3989  1144.2886 1165.3321 1173.0365  1174.0448 1177.2536 1186.8719  1198.2705 1205.5098 1211.6654  1259.5706 1386.8058 1397.6396  1405.8912 1427.9950 1435.3253  1469.5406 1473.5750 1480.6796  1485.1780 1490.6014 1496.5677  1499.1549 1500.8084 1508.5675  1511.2303 1516.0358 1534.3462  1553.2446 1570.0623 1627.3547  1674.3596 1740.0447 1862.0805  2903.7792 3015.3970 3036.5493  3039.1102 3056.7976 3081.0041  3100.8383 3115.1546 3115.9586  3123.6648 3126.2956 3141.6466  3143.6562 3146.0420 3182.4093  3202.0703 3207.0158 3327.2282  **P8**  C -0.033142 -1.543365 -0.262047  C 0.569600 -2.296823 -1.423571  O -1.126876 -2.219215 0.241964  H -0.333431 -0.525363 -0.560655  H 1.438874 -1.765195 -1.815698  H -0.172670 -2.401400 -2.215998  H 0.872433 -3.290148 -1.087665  C 0.576829 -0.822462 1.932631  O 1.007838 -1.409236 0.713989  H -0.163247 -1.455771 2.425311  H 0.161805 0.178533 1.763693  H 1.458704 -0.737831 2.567514  H 2.097822 -0.246378 -0.016401  C -0.309696 2.295855 -0.423432  C -1.524507 2.819215 -0.237225  O 0.647565 2.305675 0.509679  H -0.039943 1.824311 -1.368745  H -2.238297 2.821850 -1.050111  H -1.781234 3.320294 0.688921  H -1.760292 -1.547318 0.544919  C 3.848784 0.585079 -0.413791  O 2.434157 0.571626 -0.432595  H 4.244477 0.562355 0.607879  H 4.177326 1.507436 -0.893588  H 4.259658 -0.261983 -0.973060  H 1.409263 1.776223 0.190674  C -3.490293 -0.068841 -0.660857  O -2.728421 -0.009700 0.532950  H -2.854446 -0.017471 -1.553255  H -4.230430 0.737075 -0.703500  H -4.013610 -1.025058 -0.665516  H -2.232315 0.820698 0.517140  **Frequencies**  17.4953 31.3124 42.9350  45.2494 61.4260 73.1414  93.5234 100.4490 104.1856  109.9756 118.7841 118.9200  134.5988 154.1521 158.2692  161.6882 192.0139 221.3693  228.9992 252.7028 280.5791  296.4516 402.4756 512.7451  524.4142 604.6170 613.9503  738.5208 788.2029 820.4030  842.4958 848.4217 945.3637  970.4614 992.8506 1025.8964  1083.6463 1087.1118 1106.7983  1109.1814 1120.3613 1141.3225  1161.2469 1187.6818 1188.0365  1191.6062 1205.4525 1226.1131  1232.4597 1340.3011 1375.3692  1405.7949 1420.0744 1422.4971  1436.1541 1466.6584 1472.0553  1483.2111 1489.7830 1492.2617  1493.4583 1498.5069 1499.7871  1500.3541 1503.6408 1515.7987  1518.2474 1525.1706 1529.5271  1742.6866 2983.2478 3013.4107  3018.9361 3028.7305 3060.6118  3078.7498 3084.0206 3116.0066  3134.0858 3135.7725 3140.8993  3147.2455 3149.4110 3152.3497  3167.6770 3266.2119 3450.3902  3550.6612 3649.8371 3740.5129  **R9**  C 0.806756 0.688024 1.474370  C 1.318139 -0.058133 2.660780  O 0.579161 1.876333 1.449443  H 0.640544 0.072181 0.573918  H 2.198271 -0.629187 2.354285  H 0.553150 -0.784260 2.953282  H 1.535995 0.615463 3.489083  H 1.760125 3.186991 -0.533319  C 2.505778 -1.172076 -1.226929  O 2.347541 -1.721698 0.059340  H 3.439173 -0.603898 -1.236418  H 1.684561 -0.490881 -1.492736  H 2.575330 -1.944851 -2.005357  H 1.467780 -2.129350 0.091085  C -2.399071 0.335547 0.712534  C -3.399646 0.137354 -0.378045  O -1.804383 -0.557636 1.269279  H -2.200948 1.382779 1.008217  H -4.327014 0.663656 -0.134385  H -3.593749 -0.922232 -0.542649  H -2.985232 0.590116 -1.283470  C -0.804315 -2.319795 -1.389460  O -0.325915 -2.533223 -0.072393  H -0.798827 -1.257570 -1.656550  H -1.816424 -2.722984 -1.517248  H -0.138947 -2.854831 -2.068592  H -0.887697 -2.022345 0.524325  C -0.055144 2.264754 -1.134560  C 1.339438 2.722544 -1.426777  O -0.486929 1.169479 -1.409684  H -0.715969 3.024268 -0.675623  H 1.302205 3.483178 -2.214321  H 1.960255 1.888404 -1.752883  **Frequencies**  39.9575 43.7315 50.9201  54.9958 63.4853 69.2053  75.8008 79.7794 84.5542  95.1084 102.4478 110.9666  119.3730 121.7968 125.8042  141.0839 143.8223 149.2856  160.6178 168.3738 179.4213  186.6411 204.5507 208.7515  227.4053 251.7828 260.6387  520.6825 521.9704 526.7112  639.9764 775.2192 791.3073  793.8028 815.9573 911.0053  913.3123 918.4653 1089.0010  1109.7960 1127.8490 1130.3588  1143.4336 1146.2473 1150.0320  1151.9810 1152.3095 1161.5127  1192.1880 1193.9137 1377.2462  1377.5607 1383.2630 1436.6867  1438.3441 1440.2133 1443.1636  1461.9358 1466.1777 1468.0949  1470.9506 1474.0492 1479.4100  1486.0468 1491.0065 1501.9742  1504.1695 1507.5053 1529.2565  1531.8775 1815.9899 1829.2709  1836.9523 2955.3788 2970.2102  2985.2311 3007.7377 3013.0219  3037.0925 3047.3849 3047.8459  3047.8894 3084.7151 3102.2164  3124.9398 3125.7809 3128.8619  3130.8670 3164.3804 3166.7099  3170.9213 3689.4526 3786.8310  **TS9a**  C 1.638635 -0.155992 0.939665  C 2.024506 -1.117799 2.021388  O 2.473238 0.800599 0.687188  H 0.580893 0.124886 0.924499  H 1.352090 -1.976060 2.046554  H 1.953806 -0.591709 2.976275  H 3.051965 -1.450775 1.873818  H 1.921309 1.609099 0.193339  C 1.874298 -0.569037 -1.680991  O 1.609884 -1.207562 -0.416522  H 2.791950 0.002521 -1.563869  H 1.043235 0.088221 -1.949167  H 2.022759 -1.360667 -2.415695  H 0.675241 -1.598924 -0.435493  C -2.448806 0.470989 1.461953  C -3.291588 0.669069 0.254728  O -1.719046 -0.484475 1.633005  H -2.462776 1.269920 2.226496  H -4.090475 1.391030 0.423190  H -3.694355 -0.284400 -0.093208  H -2.600494 1.040529 -0.526561  C -1.486339 -1.840762 -1.639897  O -0.793527 -2.059906 -0.410749  H -1.492538 -0.779081 -1.897724  H -2.508444 -2.225578 -1.572554  H -0.960411 -2.405443 -2.410655  H -1.244696 -1.566444 0.299962  C -0.220139 2.119076 -0.531830  C 1.060872 2.682145 -0.581069  O -0.722937 1.264258 -1.291673  H -0.828839 2.436889 0.352347  H 1.220555 3.578540 0.012559  H 1.579696 2.647992 -1.537791  **Frequencies**  -378.2774 40.8645 66.2385  69.9256 83.3132 89.5801  97.9609 103.3678 115.9668  133.6370 139.0611 158.7214  177.0249 187.1568 193.2983  202.5906 222.5343 229.7851  242.0431 256.8727 271.9843  278.9635 301.8495 351.4078  402.5008 471.9775 535.8519  550.1227 577.9901 690.6856  697.8324 763.3320 809.6143  932.4390 966.5644 999.3568  1024.3799 1036.7676 1045.0040  1068.5844 1108.9177 1123.4891  1133.4627 1149.6372 1153.7438  1198.7731 1200.0784 1205.2831  1232.0673 1251.7912 1291.0915  1338.4972 1387.0954 1396.8783  1411.4972 1430.3721 1438.5623  1468.6493 1469.1732 1470.8427  1474.5419 1478.3228 1483.5829  1486.8810 1494.9586 1503.7478  1512.7497 1531.0140 1544.5966  1545.9387 1633.4328 1645.0546  1789.9333 1806.2817 2802.4009  2863.2242 2917.6389 2967.9248  3038.2128 3051.6511 3065.0794  3095.7535 3100.8682 3111.1485  3120.6110 3146.2993 3147.8063  3152.7612 3163.5625 3167.1401  3186.9610 3201.4522 3580.6814  **I1**  C 1.540743 -0.284549 0.907247  C 1.782598 -1.275815 2.008266  O 2.487093 0.641096 0.793287  H 0.526956 0.119188 0.886965  H 1.048004 -2.081920 1.979620  H 1.688185 -0.753849 2.961931  H 2.789400 -1.686486 1.923043  C 1.891929 -0.517836 -1.640416  O 1.543437 -1.188902 -0.400767  H 2.860581 -0.050611 -1.489404  H 1.118739 0.218434 -1.876634  H 1.965295 -1.302030 -2.392719  H 0.576836 -1.565293 -0.484944  C -2.448419 0.433693 1.438151  C -3.217474 0.769972 0.215958  O -1.770792 -0.568424 1.560650  H -2.459712 1.166069 2.266159  H -3.967258 1.540059 0.394707  H -3.672092 -0.126557 -0.211329  H 2.068188 1.463437 0.375471  C -1.452442 -1.692873 -1.787939  O -0.810456 -1.991096 -0.543310  H -1.407469 -0.621143 -1.992505  H -2.488166 -2.041610 -1.763324  H -0.922430 -2.247800 -2.562634  H -1.281866 -1.527893 0.179727  C -0.101711 2.174025 -0.431168  C 1.136457 2.777350 -0.509819  O -0.589332 1.263737 -1.163779  H -0.720785 2.502740 0.440080  H 1.338615 3.635514 0.121915  H 1.723737 2.675883 -1.419229  H -2.454446 1.128779 -0.507225  **Frequencies**  32.9909 60.5426 68.8626  87.2135 90.1216 97.7108  100.5222 110.0255 127.7653  137.8145 161.9326 167.9243  185.0489 188.3601 197.0493  212.1385 218.5009 232.2423  237.9570 255.7290 282.3750  298.5853 324.2693 388.9147  486.1556 535.8176 537.6962  551.4995 608.0461 702.7296  733.2990 761.2306 837.9008  932.9966 972.4019 994.8843  1008.2423 1022.3079 1046.7277  1060.1134 1072.1747 1120.0045  1129.4187 1149.4537 1155.8311  1162.1134 1200.8204 1213.6475  1251.4980 1263.0123 1296.6691  1356.2236 1379.4204 1393.3952  1418.0020 1436.9886 1446.6299  1462.4626 1467.2096 1472.9578  1475.6942 1483.2877 1484.8746  1493.5411 1495.6828 1499.0561  1505.7977 1531.4895 1545.9320  1567.6714 1653.3784 1718.7691  1794.6865 2415.7471 2807.1476  2843.3151 2874.1257 2972.6345  3041.3441 3043.9018 3065.8470  3095.4145 3127.6464 3128.7521  3129.1847 3150.6164 3152.8018  3158.0970 3162.2914 3162.4068  3201.4269 3222.9509 3510.5974  **TS9b**  C 1.478666 0.565882 -0.769911  C 1.532310 1.661320 -1.804226  O 2.586078 -0.234048 -0.837530  H 0.563640 -0.029086 -0.850956  H 0.668157 2.322748 -1.718812  H 1.529673 1.213215 -2.798628  H 2.448799 2.239073 -1.673362  C 1.790856 0.463732 1.660314  O 1.392673 1.251730 0.531104  H 2.830222 0.160469 1.546444  H 1.142998 -0.411682 1.762784  H 1.698113 1.116473 2.529123  H 0.011183 1.616086 0.692228  C -2.405367 -0.207846 -1.435463  C -2.875139 -1.019235 -0.357499  O -1.895301 0.921610 -1.321395  H -2.409801 -0.634414 -2.449690  H -3.464015 -1.879272 -0.666053  H -3.341746 -0.453899 0.450725  H 2.316674 -1.130186 -0.552653  C -1.519930 1.185913 2.001937  O -1.019952 1.781095 0.785198  H -1.283667 0.120883 2.019879  H -2.595433 1.353798 2.029379  H -1.054186 1.708486 2.835870  H -1.495034 1.391923 -0.098382  C 0.123227 -2.362606 0.023905  C 1.378346 -2.838269 0.218816  O -0.576975 -1.616786 0.818551  H -0.352173 -2.608736 -0.945714  H 1.815203 -3.510415 -0.509707  H 1.876449 -2.721190 1.175770  H -1.815050 -1.386432 0.187094  **Frequencies**  -643.7969 39.9366 71.6016  82.6166 95.0009 101.2893  113.7052 119.1266 138.6928  146.1435 168.1345 178.7404  188.1885 192.7611 203.1109  220.3656 237.3387 258.2734  278.2191 288.0371 309.5344  376.1080 406.1662 506.0767  524.4129 555.7834 600.1411  618.0715 705.5572 732.0596  766.2774 783.1687 816.2531  910.1940 945.9431 1020.2231  1028.3560 1032.5172 1045.1987  1058.3746 1072.8064 1083.0894  1093.9156 1126.8891 1167.4102  1191.3350 1196.0318 1217.1338  1227.3300 1239.6879 1283.3762  1350.2243 1360.1819 1370.9813  1406.0392 1410.5418 1415.6398  1427.4651 1454.4949 1459.8979  1480.3119 1485.3380 1488.5875  1492.3427 1496.0492 1506.1084  1512.1728 1521.2848 1532.4080  1546.0915 1565.4925 1671.3525  1734.7457 1829.4562 1928.2119  2350.9391 2934.4437 3032.0790  3048.9888 3065.2296 3069.0015  3085.2019 3103.9596 3143.3431  3149.0548 3152.5348 3157.3157  3165.9327 3173.4709 3176.5737  3191.1937 3244.6676 3516.8363  **P9**  C -1.490272 -0.630951 -0.744855  C -1.410948 -1.595849 -1.901286  O -2.624049 0.161698 -0.869614  H -0.591963 0.000068 -0.693838  H -0.550059 -2.257896 -1.797093  H -1.312440 -1.038988 -2.833312  H -2.324564 -2.192352 -1.931592  C -1.774678 -0.673151 1.626637  O -1.524791 -1.422298 0.447937  H -2.787125 -0.262644 1.615923  H -1.048180 0.140481 1.740425  H -1.681661 -1.366329 2.463013  H 0.185692 -1.933883 0.550511  C 2.514858 0.609178 -1.329754  C 3.113067 0.949597 -0.179260  O 1.808957 -0.486704 -1.588315  H 2.565757 1.264230 -2.196099  H 3.687881 1.864531 -0.129587  H 3.141300 0.280103 0.673537  H -2.426543 1.024956 -0.488411  C 1.598461 -1.692105 1.885783  O 1.161640 -1.944766 0.563563  H 1.320087 -0.686485 2.223519  H 2.685994 -1.781955 1.899883  H 1.188206 -2.428112 2.584845  H 1.699994 -1.044234 -0.781959  C -0.287332 2.513423 0.145110  C -1.523594 2.933929 0.408881  O 0.473687 1.863173 1.044771  H 0.169036 2.669790 -0.831229  H -2.074886 3.483526 -0.342029  H -1.964218 2.798921 1.389591  H 1.316768 1.613020 0.629625  **Frequencies**  30.1921 41.2919 67.5057  71.8518 80.8001 86.3410  98.0763 103.9293 113.7103  125.9663 133.3823 136.1933  147.4630 167.8736 175.4573  181.6713 203.2648 212.5912  226.5072 253.1426 279.6915  296.4504 398.6912 504.3910  509.7066 534.6970 544.8351  601.4436 615.3766 747.8796  774.6991 787.5188 836.0829  843.6402 858.1533 918.7003  950.0195 985.7487 993.8528  1015.2575 1056.5504 1082.0510  1099.3319 1107.1715 1136.0336  1154.0845 1189.7600 1191.2478  1195.0562 1203.0211 1233.8122  1236.4903 1341.5802 1342.4313  1353.4503 1390.6855 1395.9272  1430.1512 1445.2683 1448.2460  1476.7423 1483.6461 1485.9048  1488.1000 1492.8690 1499.5212  1502.5662 1506.0256 1518.4888  1535.7431 1544.7123 1700.7191  1743.5478 3014.5563 3028.5842  3033.9059 3065.7728 3082.7026  3110.1444 3126.1422 3142.6825  3146.5982 3152.4930 3158.4269  3163.4657 3171.4764 3175.1001  3264.7881 3269.5955 3376.0953  3575.3702 3621.5158 3795.2645 |

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