# Supporting Information for

## Synthesis of Interstellar Propen-2-ol ($CH_3C(OH)CH_2$) – The Simplest Enol Tautomer of a Ketone

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**Ion signal of higher masses and assignment**

After the irradiation, several higher mass-to-charge ratios were observed at 9.43 eV, which were not present in the blank experiment. The ion signals at *m/z* = 72, 86, 100, 114, 116, and 158 in irradiated acetone ice shift to *m/z* = 80, 92, 108, 124, 128, and 172 in irradiated acetone-$d_6$ ice respectively (Figs. S1 and S4), confirming their respective formulae $C_4H_8O$, $C_4H_6O_2$, $C_5H_8O_2$, $C_6H_{10}O_2$, $C_6H_{12}O_2$, and $C_8H_{14}O_3$. Note that formula $C_{12}H_{14}$ is unlikely to be assigned to the signal at *m/z* = 158 due to the small dose (0.34 ± 0.05 eV molecule$^{-1}$) used in the experiment. The tentatively assigned molecules are listed in Table S7 and the proposed pathways for their formation are shown in Figs. S5 and S6. Upon irradiation, the acetyl radical (**7**, $CH_3\dot{C}O$), acetonyl radical (**8**, $CH_3CO\dot{C}H_2$) or methyl radical (**9**, $\dot{C}H_3$) can be produced via carbon-carbon single bond cleavage or H atom loss by acetone (**1**). Radical-radical reactions of two acetyl radicals (**7)** or two acetonyl radicals (**8**) can lead to the formation of 2,3-butanedione (**10**, $C_4H_6O_2$; IE = 9.20 – 9.27 eV) or 2,5-hexanedione (**11**, $C_6H_{10}O_2$). Our recent work demonstrated the recombination of two acetyl radicals (**7**) forms 2,3-butanedione (**10**) in irradiated acetaldehyde ice.[1] The recombination of **7** and **8** radicals can form 2,4-pentanedione (**12**, $C_5H_8O_2$; IE = 8.80 – 8.84 eV). Similarly, 2-butanone (**13**, $C_4H_8O$; IE = 9.45 – 9.53 eV) can be formed from the recombination reaction between acetonyl radical (**8**) and methyl radical (**9**). The ionization of 2-butanone (**13)** is possible as the lower limit of its ionization energy is only 0.02 eV higher than the energy of the ionizing photon (9.43 eV). Because the hydroxy (OH) group of propen-2-ol (**2**) is nucleophilic and the carbon of the carbonyl group (C=O) of acetone (**1**) or 2,4-pentanedione (**12**) acts as an electrophile, propen-2-ol (**2**) can react with acetone (**1**) or 2,4-pentanedione (**12**) via nucleophilic additions, forming the 2-prop-1-en-2-yloxypropan-2-ol (**14**, $C_6H_{12}O_2$) or 4-hydroxy-4-(prop-1-en-2-yloxy)pentan-2-one (**15**, $C_8H_{14}O_3$) (Fig. S5). Since each of the above molecular formulae has multiple isomers, further work is needed to provide confidence in their identification and better analyze their formation pathways, which is beyond the scope of the present work.

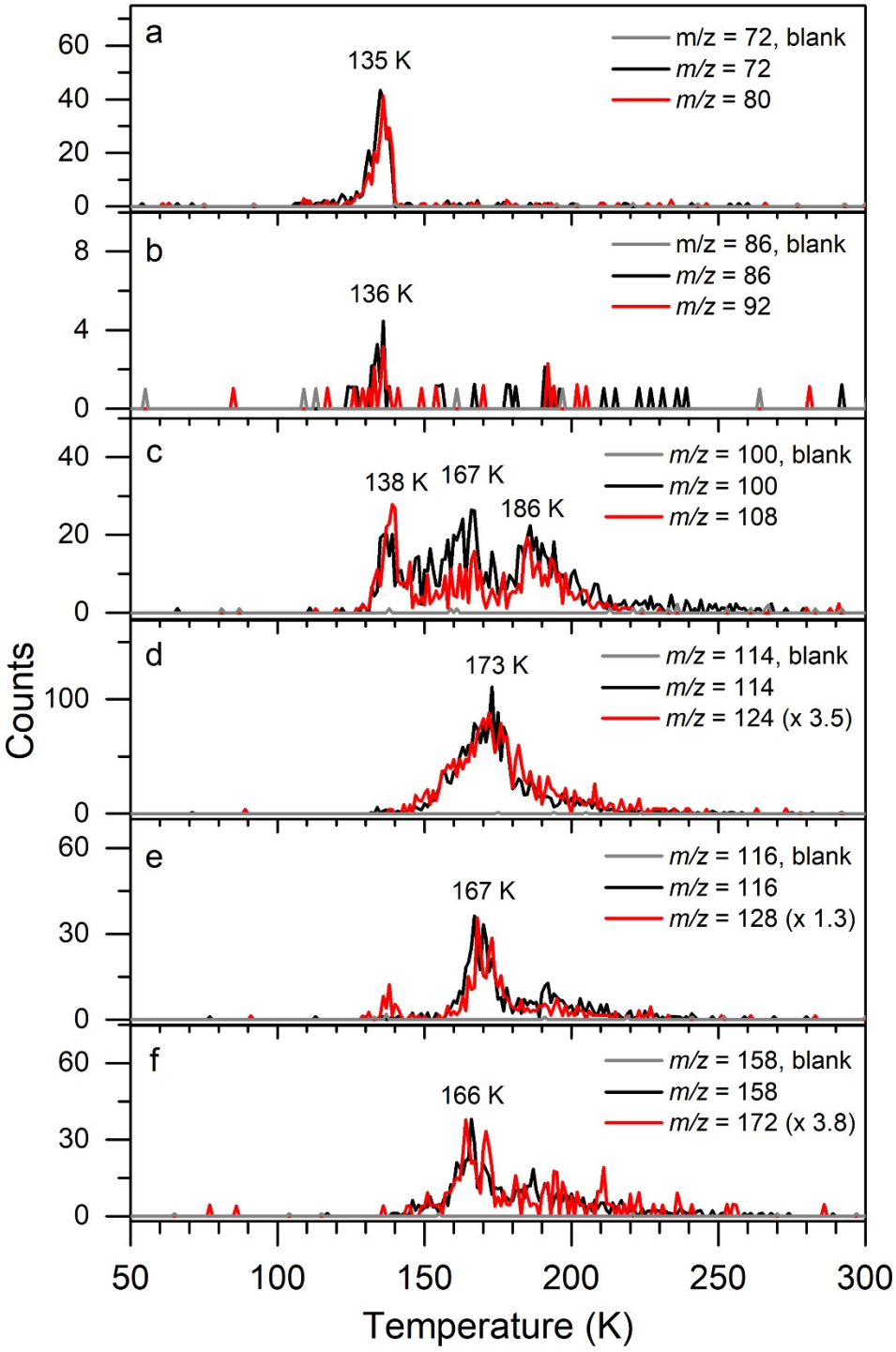



**Fig. S1** Temperature programmed desorption profiles of higher mass-to-charge ratios (*m/z*) recorded at 9.43 eV in blank or unirradiated acetone (gray), irradiated acetone (black), and irradiated acetone-$d_6$ (red) ices.

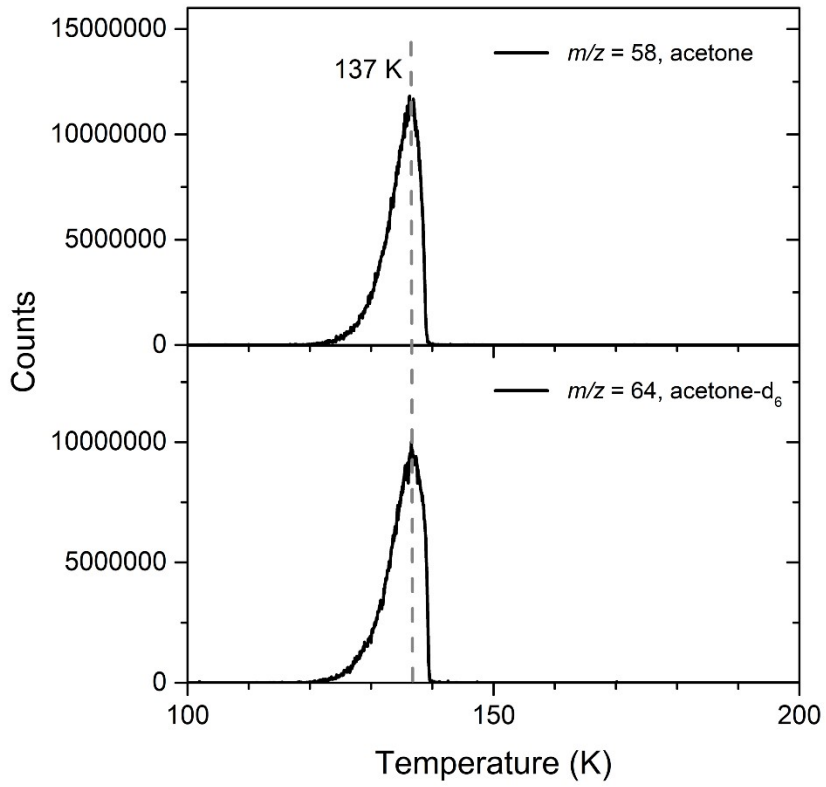



**Fig. S2** QMS TPD profiles of acetone (top) at *m/z* = 58 and acetone-$d_6$ (bottom) at *m/z* = 64. The dashed line indicates their peak sublimation temperature at 137 K.

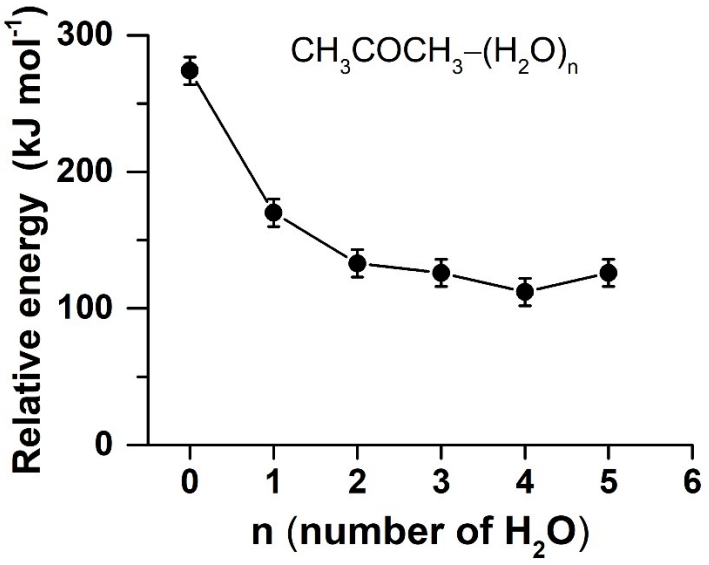



**Fig. S3** The reduction and leveling of the reaction barrier of systems $CH_3COCH_3 + n(H_2O)$ (n = 0 − 5) leading to the formation of propen-2-ol (**2**), as more water molecules are involved in the reaction. The anticipated accuracy of the reaction barriers is within 10 kJ $mol^{-1}$.

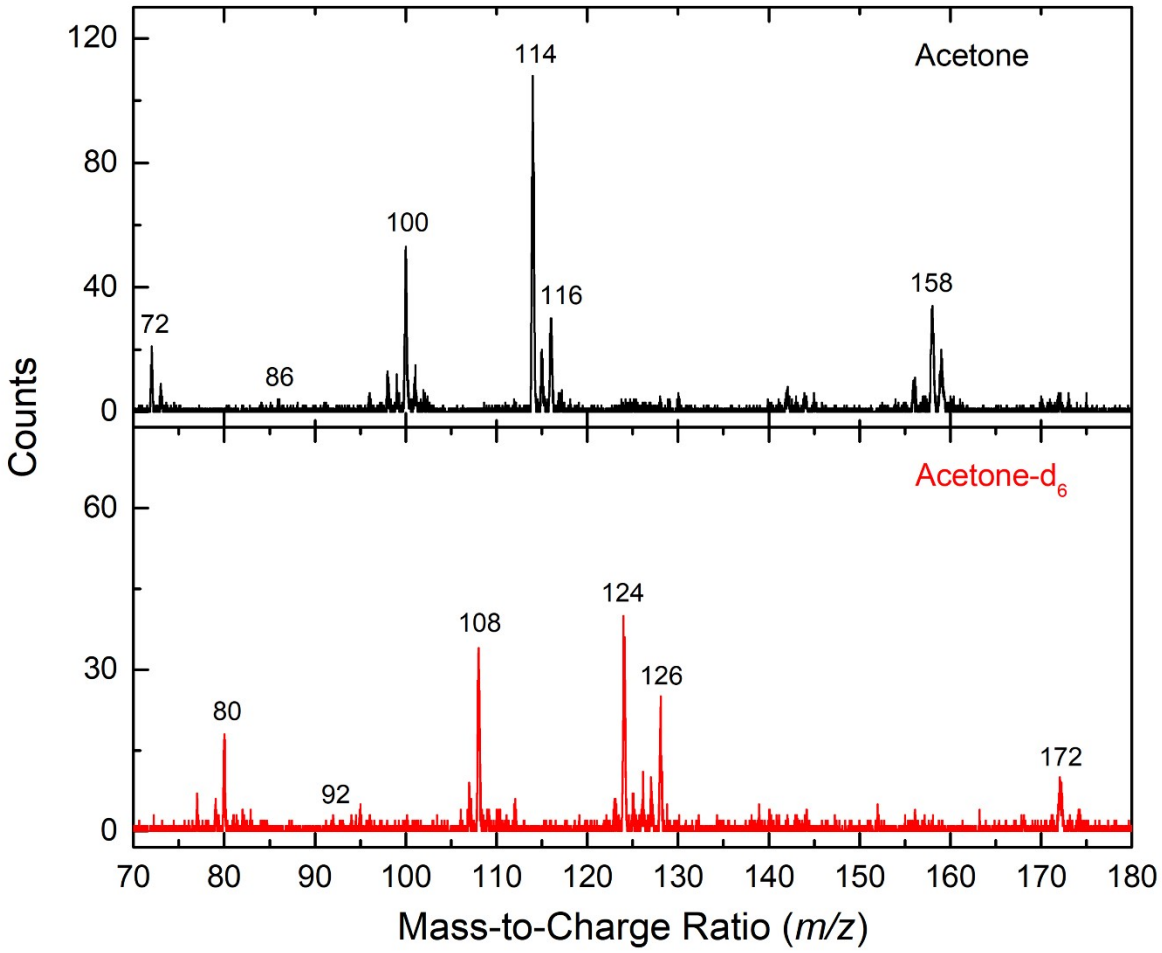



**Fig. S4** Mass spectra (integrated ion signals) of higher masses recorded at 9.43 eV in irradiated acetone (top) and acetone-$d_6$ (bottom) ices.

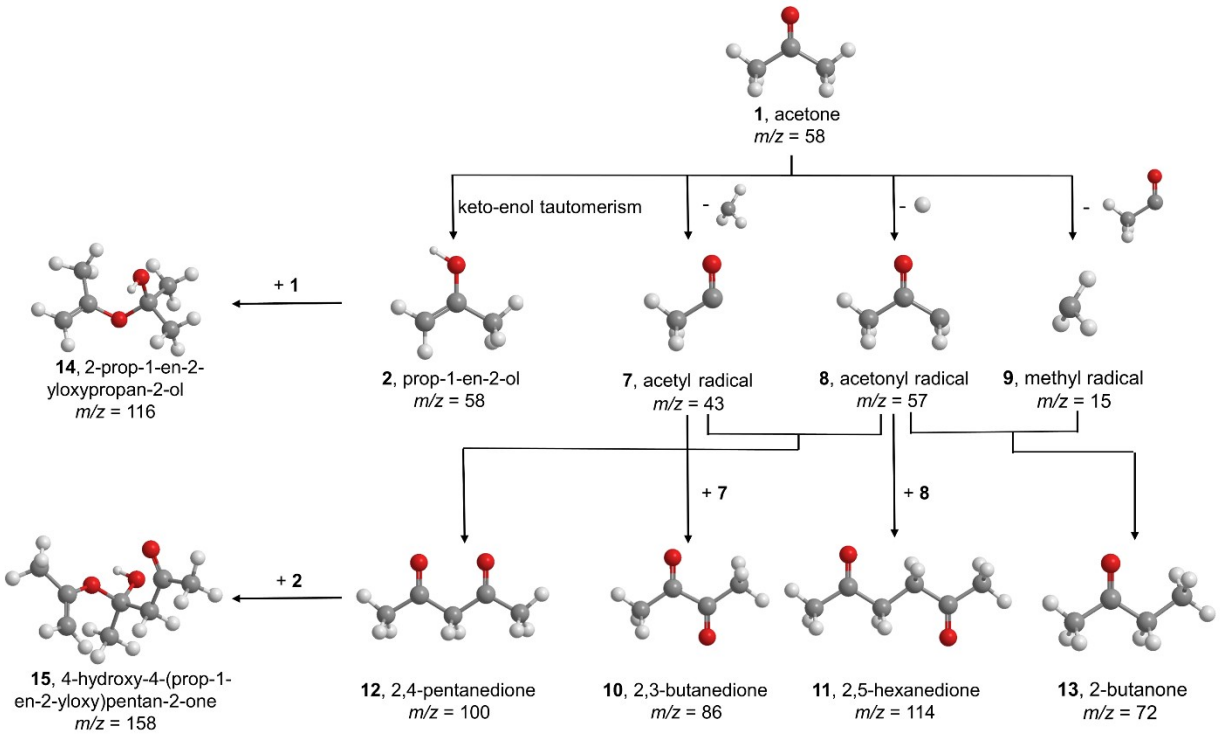



**Fig. S5** Proposed formation pathways for molecules **10** − **15** in irradiated acetone ice.

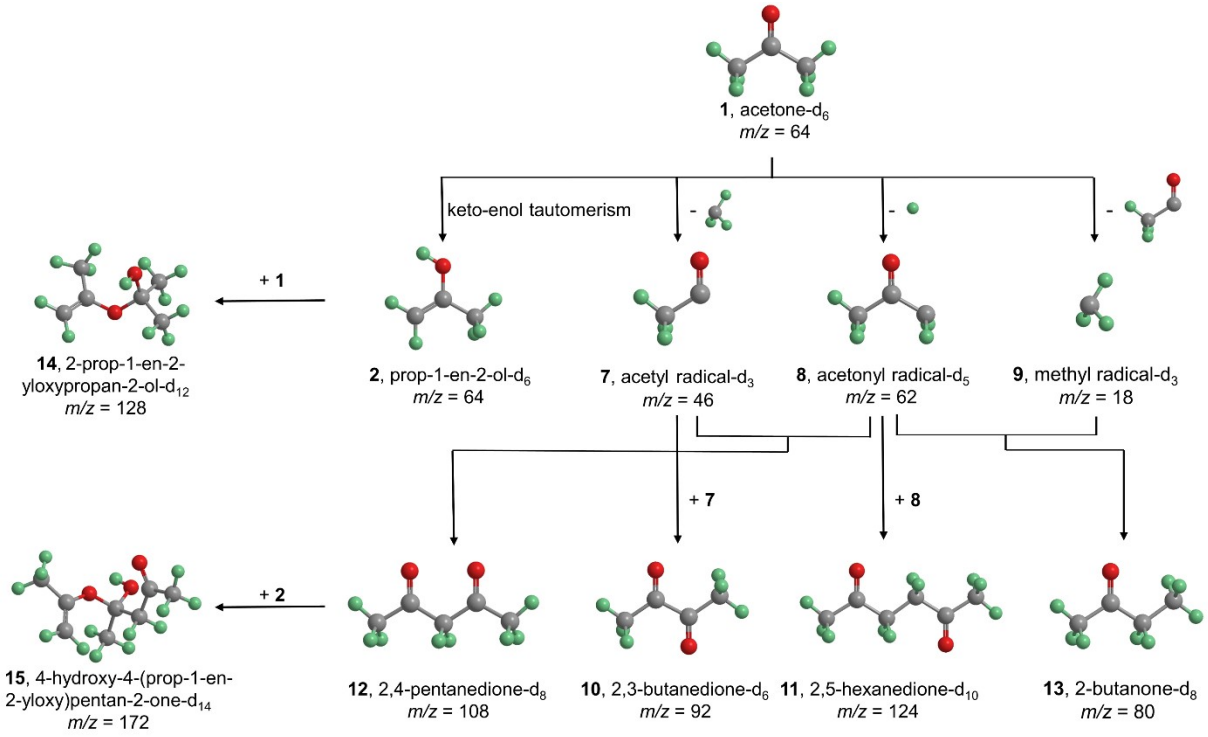



**Fig. S6** Proposed formation pathways for molecules **10** − **15** in irradiated acetone-$d_6$ ice.

**Table S1.** Conditions of ice studied in this work including the ice composition, thickness, irradiation parameters, and VUV photon energies.

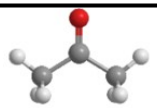
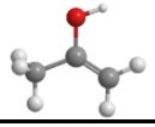
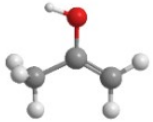
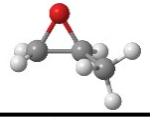
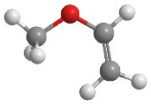
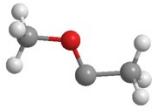
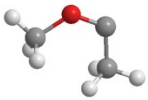
| Ice composition | Thickness (nm) | Current (nA) | Irradiation Time (s) | Dose (eV molecule$^{-1}$) | Photon energy (eV) |
|---|---|---|---|---|---|
| $CH_3COCH_3$ | 720 ± 50 | - | - | - | 9.43 |
| $CH_3COCH_3$ | 710 ± 30 | 21 ± 1 | 300 ± 10 | 0.34 ± 0.05 | 9.43 |
| $CD_3COCD_3$ | 710 ± 30 | 22 ± 2 | 300 ± 10 | 0.40 ± 0.06 | 9.43 |
| $CH_3COCH_3$ − $CD_3COCD_3$ (1.1 ± 0.2): 1 | 720 ± 50 | 15 ± 1 | 120 ± 10 | 0.10 ± 0.02 for $CH_3COCH_3$, 0.11 ± 0.02 for $CD_3COCD_3$ | 9.43 |
| $CH_3COCH_3$ | 710 ± 30 | 20 ± 2 | 300 ± 10 | 0.33 ± 0.05 | 8.90 |
| $CH_3COCH_3$ | 710 ± 30 | 20 ± 2 | 300 ± 10 | 0.33 ± 0.05 | 8.40 |

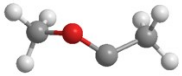
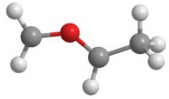
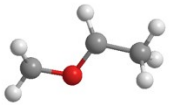
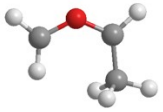
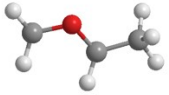
**Table S2.** Parameters for the generation of vacuum ultraviolet (VUV) light. The uncertainty for VUV photon energies is less than 0.001 eV.

| VUV photon energy (eV) | Nonlinear medium in four-wave mixing ($2\omega_1 - \omega_2$) | $\omega_1$ Dye laser wavelength (nm) | $\omega_1$ Dye | $\omega_2$ Dye laser wavelength (nm) | $\omega_2$ Dye |
|---|---|---|---|---|---|
| 9.43 | Krypton | 202.316 | Rhodamine 610 and 640 | 438.654 | Coumarin 440 |
| 8.90 | Xenon | 222.566 | Coumarin 450 | 553.180 | Pyrromethene 580 |
| 8.40 | Krypton | 202.316 | Rhodamine 610 and 640 | 321.497[a] | Rhodamine 640 |

[a] obtained from the second harmonic generation.

**Table S3.** Error analysis of adiabatic ionization energies (IE) of $C_3H_6O$ isomers **1** to **6**. The IEs were computed at the CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory including the zero-point vibrational energy (ZPVE) corrections. The IE ranges were corrected for the thermal and Stark effect by −0.03 eV and the combined error limits were determined to be -0.05/+0.03 eV.[2] The computed Cartesian coordinates and vibrational frequencies are shown in Table S8.

| Name | Isomer | Structure | Experimental IE (eV) [3] | Computed IE (eV) | IE range after error analysis (eV) | Corrected IE with electric field effect (eV) |
|---|---|---|---|---|---|---|
| acetone | **1** |  | 9.703 ± 0.006 | 9.70 | 9.697 – 9.709 | 9.667 – 9.679 |
| propen-2-ol | **2a** |  | – | 8.80 | 8.75 – 8.83 | 8.72 – 8.80 |
| | **2b** |  | – | 8.70 | 8.65 – 8.73 | 8.62 – 8.70 |
| propylene oxide | **3** |  | 10.22 ± 0.02 | 10.20 | 10.20 – 10.24 | 10.17 – 10.21 |
| methyl vinyl ether | **4** |  | 8.95 ± 0.01 | – | 8.94 – 8.96 | 8.91 – 8.93 |
| methoxy methyl carbene | **5a** |  | – | 7.72 | 7.67 – 7.75 | 7.64 – 7.72 |
| | **5b** |  | – | 7.54 | 7.49 – 7.57 | 7.46 – 7.54 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | **5t** (triplet) |  | – | 6.32 | 6.27 – 6.35 | 6.24 – 6.32 |
| | | | – | 11.02 [a] (q-state) | 11.97 – 11.05 | 11.94 – 11.02 |
| 1-methyleneoxyethyl | **6a** |  | – | 7.05 | 7.00 – 7.08 | 6.97 – 7.05 |
| | **6at** (triplet) |  | – | 6.53 | 6.48 – 6.56 | 6.45 – 6.53 |
| | | | – | 10.79 [a] (q-state) | 10.74 – 10.82 | 10.71 – 10.79 |
| | **6b** |  | – | 7.27 | 7.22 – 7.30 | 7.19 – 7.27 |
| | **6bt** (triplet) |  | – | 6.53 | 6.48 – 6.56 | 6.45 – 6.53 |
| | | | – | 10.76 [a] (q-state) | 10.71 – 10.79 | 10.68 – 10.76 |

[a] These isomers are not observable in these experiments because their IEs are much higher than the maximum photon energy (9.43 eV) used in the experiment.

**Table S4.** Absorption peaks observed in acetone ($CH_3COCH_3$) ice before and after electron irradiation at 5 K.

| Pristine acetone ice, before irradiation ($cm^{-1}$) | Assignment[4] | Approximate motion |
|---|---|---|
| 3002 | $\nu_1$, $\nu_{13}$ | $CH_3$ asym. stretch |
| 2967 | $\nu_9$, $\nu_{20}$ | $CH_3$ asym. stretch |
| 2921 | $\nu_2$, $\nu_{14}$ | $CH_3$ sym. stretch |
| 2854 | $2\nu_{21}$ | Overtone |
| 2781 | $\nu_3+\nu_6$ | Combination |
| 2581 | $\nu_3+\nu_7$ | Combination |
| 1708 | $\nu_3$ | C=O stretch |
| 1443 | $\nu_{21}$ | $CH_3$ asym. def |
| 1419 | $\nu_4$ | $CH_3$ asym. def |
| 1365 | $\nu_{16}$ | $CH_3$ sym. def |
| 1351 | $\nu_5$ | $CH_3$ sym. def |
| 1229 | $\nu_{17}$ | CCC asym. stretch |
| 1096 | $\nu_{22}$ | $CH_3$ rock |
| 1071 | $\nu_6$ | $CH_3$ rock |
| 899 | $\nu_{18}$ | $CH_3$ rock |
| 793 | $\nu_7$ | CCC sym. stretch |
| New absorption after irradiation ($cm^{-1}$) | Assignment[4] | |
| 2128 | $\nu$(CO)/ $\nu_2(H_2CCO)$ | CO stretch |

**Table S5.** Absorption peaks observed in acetone-$d_6$ ($CD_3COCD_3$) ice before and after electron irradiation at 5 K.

| Pristine acetone-$d_6$ ice, before irradiation ($cm^{-1}$) | Assignment[5] | Approximate motion |
|---|---|---|
| 2341 | $\nu_4+\nu_{15}$ | Combination |
| 2255 | $\nu_9$, $\nu_{20}$ | $CD_3$ asym. stretch |
| 2222 | $\nu_1$, $\nu_{13}$ | $CD_3$ asym. stretch |
| 2132 | $\nu_4+\nu_5$ | Combination |
| 2112 | $\nu_2$, $\nu_{14}$ | $CD_3$ sym. stretch |
| 1733 | $\nu_5+\nu_7$ | Combination |
| 1697 | $\nu_3$ | C=O stretch |
| 1662 | $\nu_5+\nu_8$ | Combination |
| 1253 | $\nu_{15}$ | $CD_3$ asym. def |
| 1092 | $\nu_4$ | $CD_3$ asym. def |
| 1031 | $\nu_{16}$ | $CD_3$ sym. def |
| 965 | $2\nu_{19}$ | $CD_3$ rock |
| 893 | $\nu_6$, $\nu_{22}$ | $CD_3$ rock |
| New absorption after irradiation ($cm^{-1}$) | Assignment[6] | |
| 2096 | $\nu_5$ (tentative) | $CD_3$ sym. stretch ($CD_3C(OD)CD_2$) |

**Table S6.** Integrated ion signals and relative signal strengths of the different isotopologues of propen-2-ol (**2**) in irradiated $CH_3COCH_3$−$CD_3COCD_3$ ice.

| *m/z* | Molecular formula | Integrated signal | Relative signal |
|---|---|---|---|
| 58 | $C_3H_6O$ | 329 ± 13 | 0.50 ± 0.03 |
| 59 | $C_3H_5DO$ | 638 ± 29 | 1 |
| 60 | $C_3H_4D_2O$ | 33 ± 12 | 0.05 ± 0.02 |
| 61 | $C_3H_3D_3O$ | 10 ± 9 | 0.02 ± 0.01 |
| 62 | $C_3H_2D_4O$ | 7 ± 5 | 0.01 ± 0.01 |
| 63 | $C_3HD_5O$ | 142 ± 37 | 0.22 ± 0.06 |
| 64 | $C_3D_6O$ | 312 ± 13 | 0.48 ± 0.03 |

**Table S7**. Detected mass-to-charge ratios in the irradiated acetone and acetone-$d_6$ ice and tentative assignments of molecules.

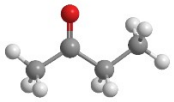
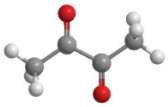
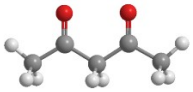
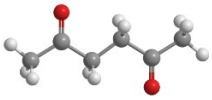
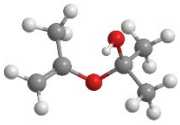
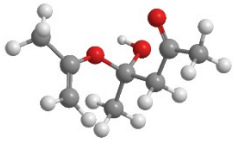
| Mass-to-charge ratio | | | | | |
|---|---|---|---|---|---|
| Acetone | Acetone-$d_6$ | Formula | Tentative assignment | IE (eV) | Corrected IE with electric field effect (eV) |
| 72 | 80 | $C_3H_8O$ | 2-butanone  | 9.52 ± 0.04[3] | 9.45 – 9.53 |
| 86 | 92 | $C_4H_6O_2$ | 2,3-butanedione  | 9.23 – 9.30[1] | 9.20 – 9.27 |
| 100 | 108 | $C_5H_8O_2$ | 2,4-pentanedione  | 8.85 ± 0.02[3] | 8.80 – 8.84 |
| 114 | 124 | $C_6H_{10}O_2$ | 2,5-hexanedione  | – | – |
| 116 | 128 | $C_6H_{12}O_2$ | 2-prop-1-en-2-yloxypropan-2-ol  | – | – |
| 158 | 172 | $C_8H_{14}O_3$ | 4-hydroxy-4-(prop-1-en-2-yloxy)pentan-2-one  | – | – |

**Table S8.** Cartesian coordinates for selected $C_3H_6O$ structures. B3LYP/cc-pVTZ optimized geometry (distances in Å), electronic energies (in hartree), zero-point vibrational energies (ZPVE), extrapolated CCSD(T)/CBS energies (in hartree) and adiabatic ionization energies (IE) at CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory.

**1**, Acetone ($C_{2v}$)

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.288092 | –0.620789 |
| C | –0.000000 | 0.000000 | 0.175466 |
| H | –0.876805 | 1.331963 | –1.270830 |
| H | 0.876805 | 1.331963 | –1.270830 |
| H | 0.000000 | 2.140897 | 0.052651 |
| C | –0.000000 | –1.288092 | –0.620789 |
| H | –0.876805 | –1.331963 | –1.270830 |
| H | –0.000000 | –2.140897 | 0.052651 |
| H | 0.876805 | –1.331963 | –1.270830 |
| O | –0.000000 | 0.000000 | 1.384697 |

E = –193.2331603
E[CCSD(T)/CBS] = –192.9201031
ZPVE = 52.2233 kcal $mol^{-1}$
IE = 9.70 eV

| Frequency | Intensity |
|---|---|
| 43.3611 | 0.0000 |
| 136.6537 | 0.0021 |
| 379.3676 | 1.4689 |
| 490.0400 | 0.3827 |
| 535.5428 | 14.7988 |
| 781.9256 | 1.8237 |
| 885.4521 | 9.9750 |
| 885.4690 | 0.0000 |
| 1085.1343 | 0.0258 |
| 1120.3492 | 2.5912 |
| 1233.9829 | 74.8958 |
| 1387.1958 | 18.7148 |
| 1387.8563 | 56.8165 |
| 1460.7372 | 0.6096 |
| 1466.3440 | 0.0000 |
| 1470.9001 | 27.9261 |
| 1488.3742 | 18.6373 |
| 1793.7782 | 175.0413 |
| 3025.4480 | 1.2215 |
| 3032.5185 | 7.1208 |
| 3077.3937 | 0.0000 |

| | |
|---|---|
| 3084.7486 | 19.7270 |
| 3138.5398 | 12.3851 |
| 3139.6114 | 7.4501 |

**1**$^{+}$, Acetone radical cation ($C_2$)

| | | | |
|---|---|---|---|
| C | –0.001471 | 1.326832 | –0.589947 |
| C | –0.000000 | –0.000000 | 0.152284 |
| H | –0.910702 | 1.338692 | –1.197145 |
| H | 0.872452 | 1.318096 | –1.245695 |
| H | 0.025010 | 2.163548 | 0.100767 |
| C | 0.001471 | –1.326832 | –0.589947 |
| H | –0.872452 | –1.318096 | –1.245695 |
| H | –0.025010 | –2.163548 | 0.100767 |
| H | 0.910702 | –1.338692 | –1.197145 |
| O | 0.000000 | 0.000000 | 1.356225 |

E = –192.8834063
E[CCSD(T)/CBS] = –192.5610784
ZPVE = 50.9363 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 47.8843 | 0.0023 |
| 141.5308 | 0.5411 |
| 334.7063 | 1.8206 |
| 363.4011 | 3.8903 |
| 476.8309 | 0.0008 |
| 692.1956 | 1.7829 |
| 897.1665 | 0.0092 |
| 900.9593 | 0.4029 |
| 1006.5598 | 0.3124 |
| 1064.8662 | 14.5513 |
| 1079.3092 | 1.2411 |
| 1301.7499 | 8.7149 |
| 1347.5160 | 0.2416 |
| 1422.0634 | 11.5468 |
| 1429.8093 | 22.1708 |
| 1438.8125 | 0.3620 |
| 1462.0548 | 36.5236 |
| 1619.3022 | 0.0004 |
| 3023.1233 | 47.9646 |
| 3030.4842 | 21.2369 |
| 3097.6561 | 0.0256 |
| 3104.4229 | 33.1251 |
| 3173.5431 | 0.3054 |

| | |
|---|---|
| 3174.5477 | 20.0913 |

**2a**, Acetone enol ($C_s$)

| | | | |
|---|---|---|---|
| C | 0.884998 | –1.113068 | 0.000000 |
| C | 0.009183 | 0.096873 | 0.000000 |
| H | 0.679520 | –1.727319 | –0.878845 |
| H | 0.679520 | –1.727319 | 0.878845 |
| H | 1.935803 | –0.834640 | 0.000000 |
| C | 0.436548 | 1.358491 | 0.000000 |
| H | –0.251272 | 2.194704 | 0.000000 |
| H | 1.491561 | 1.580920 | 0.000000 |
| O | –1.312053 | –0.260683 | 0.000000 |
| H | –1.855755 | 0.534703 | 0.000000 |

E = –193.2145068
E[CCSD(T)/CBS] = –192.9018861
ZPVE = 52.9908 kcal mol$^{-1}$
IE = 8.80 eV

| Frequency | Intensity |
|---|---|
| 187.3283 | 1.1643 |
| 411.6287 | 1.5652 |
| 441.6040 | 100.7564 |
| 483.3059 | 17.7674 |
| 509.1547 | 0.2782 |
| 726.7750 | 0.8548 |
| 817.2377 | 70.0750 |
| 861.8940 | 4.9361 |
| 983.3085 | 17.6640 |
| 1023.2629 | 32.8677 |
| 1075.2204 | 0.4398 |
| 1204.1578 | 144.1494 |
| 1362.5961 | 13.7729 |
| 1415.9614 | 26.6198 |
| 1455.3824 | 3.9278 |
| 1474.4121 | 7.5757 |
| 1492.9396 | 7.9098 |
| 1717.3330 | 153.5019 |
| 3032.4016 | 18.5007 |
| 3079.2851 | 13.7439 |
| 3130.5369 | 14.5274 |
| 3143.4238 | 4.8778 |
| 3239.7196 | 8.8899 |
| 3798.7554 | 29.4014 |

**2a**$^+$, Acetone enol radical cation ($C_s$)

| | | | |
|---|---|---|---|
| C | –0.116551 | –1.420121 | 0.000000 |
| C | 0.000000 | 0.047012 | 0.000000 |
| H | –1.154734 | –1.737476 | 0.000000 |
| H | 0.403462 | –1.826872 | 0.873819 |
| H | 0.403462 | –1.826872 | –0.873819 |
| C | 1.248164 | 0.721810 | 0.000000 |
| H | 1.305829 | 1.803517 | 0.000000 |
| H | 2.167529 | 0.153657 | 0.000000 |
| O | –1.112705 | 0.708045 | 0.000000 |
| H | –1.013584 | 1.677482 | 0.000000 |

E = –192.8980634
E[CCSD(T)/CBS] = –192.5766502
ZPVE = 52.2404 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 49.9316 | 2.1791 |
| 337.8396 | 0.0386 |
| 396.9033 | 0.8232 |
| 504.1019 | 10.0713 |
| 516.2239 | 13.5184 |
| 688.0623 | 101.4020 |
| 863.1349 | 6.5665 |
| 883.0662 | 52.6666 |
| 976.2592 | 4.0990 |
| 1031.4099 | 3.4012 |
| 1056.6947 | 3.8967 |
| 1177.8123 | 158.8569 |
| 1368.8930 | 92.0166 |
| 1433.7743 | 21.0690 |
| 1435.8196 | 17.5910 |
| 1460.3951 | 25.4498 |
| 1516.1887 | 73.0549 |
| 1540.7850 | 89.6238 |
| 3015.1288 | 50.1181 |
| 3057.4403 | 9.2174 |
| 3144.1412 | 21.5043 |
| 3161.6406 | 5.9289 |
| 3260.6477 | 10.8794 |
| 3666.3675 | 184.9125 |

**2b**, Acetone enol ($C_s$)

| | | | |
|---|---|---|---|
| C | 0.776425 | –1.166010 | 0.000000 |
| C | 0.013967 | 0.122323 | 0.000000 |
| H | 0.527893 | –1.763239 | –0.882473 |

| | | | |
|---|---|---|---|
| H | 0.527893 | –1.763239 | 0.882473 |
| H | 1.849012 | –0.988840 | 0.000000 |
| C | 0.560752 | 1.334031 | 0.000000 |
| H | –0.054609 | 2.221439 | 0.000000 |
| H | 1.632750 | 1.448615 | 0.000000 |
| O | –1.353680 | –0.003049 | 0.000000 |
| H | –1.593024 | –0.933782 | 0.000000 |

E = –193.2115300
E[CCSD(T)/CBS] = –192.8992280
ZPVE = 52.7952 kcal $mol^{-1}$
IE = 8.7 eV

| Frequency | Intensity |
|---|---|
| 202.8336 | 4.6008 |
| 249.9783 | 81.4330 |
| 413.3069 | 1.2100 |
| 472.7419 | 3.1359 |
| 503.2637 | 6.0558 |
| 740.5189 | 10.0632 |
| 847.6581 | 59.5270 |
| 853.3020 | 17.2559 |
| 979.5839 | 44.3935 |
| 1023.9128 | 2.2774 |
| 1074.0002 | 0.2970 |
| 1235.1715 | 35.8829 |
| 1327.2109 | 204.5558 |
| 1413.6977 | 7.4950 |
| 1440.9338 | 13.2862 |
| 1480.4724 | 7.2447 |
| 1491.1741 | 5.0486 |
| 1742.9148 | 93.7090 |
| 3008.2914 | 29.3854 |
| 3049.4967 | 19.9916 |
| 3125.5839 | 11.8057 |
| 3166.1677 | 0.2301 |
| 3255.5412 | 6.1575 |
| 3833.0242 | 55.4445 |

**2b**$^{+}$, Acetone enol radical cation ($C_s$)

| | | | |
|---|---|---|---|
| C | 0.170487 | –1.404240 | 0.000000 |
| C | 0.000000 | 0.062418 | 0.000000 |
| H | –0.777365 | –1.938630 | 0.000000 |
| H | 0.756572 | –1.703459 | 0.874699 |
| H | 0.756572 | –1.703459 | –0.874699 |
| C | 1.085928 | 0.969942 | 0.000000 |

| | | | |
|---|---|---|---|
| H | 0.895576 | 2.034655 | 0.000000 |
| H | 2.101816 | 0.602501 | 0.000000 |
| O | –1.170342 | 0.619379 | 0.000000 |
| H | –1.908927 | –0.015364 | 0.000000 |

E = –192.9000084
E[CCSD(T)/CBS] = –192.5784944
ZPVE = 52.3623 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 41.3179 | 0.7449 |
| 380.9711 | 0.1493 |
| 395.7799 | 0.6806 |
| 499.7314 | 13.4746 |
| 524.0014 | 3.8402 |
| 674.2079 | 116.3003 |
| 856.0381 | 6.4449 |
| 901.9067 | 6.1938 |
| 985.4888 | 10.7773 |
| 1033.9370 | 29.1984 |
| 1058.8680 | 17.0411 |
| 1176.9209 | 102.3452 |
| 1377.3590 | 44.9495 |
| 1434.7348 | 16.2037 |
| 1438.1265 | 138.5743 |
| 1453.5257 | 14.9907 |
| 1505.9555 | 85.7278 |
| 1562.2445 | 56.3008 |
| 3017.9836 | 40.4807 |
| 3065.6771 | 10.7328 |
| 3131.9248 | 2.3822 |
| 3157.1443 | 26.7637 |
| 3276.1903 | 15.3731 |
| 3677.9094 | 235.2477 |

**3**, Propylene oxide ($C_1$)

| | | | |
|---|---|---|---|
| O | 0.828151 | –0.788103 | –0.239678 |
| C | –0.151978 | –0.036276 | 0.485663 |
| C | 1.039391 | 0.616002 | –0.061056 |
| H | 0.949431 | 1.214820 | –0.962147 |
| H | 1.863181 | 0.881727 | 0.593531 |
| C | –1.507102 | 0.097896 | –0.148350 |
| H | –2.072435 | 0.904642 | 0.322842 |
| H | –2.078890 | –0.824440 | –0.033483 |
| H | –1.414651 | 0.312331 | –1.212823 |
| H | –0.153708 | –0.249991 | 1.551964 |

E = –193.1848099
E[CCSD(T)/CBS] = –192.8734273
ZPVE = 53.4227 kcal mol$^{-1}$
IE = 10.20 eV

| Frequency | Intensity |
|---|---|
| 206.8626 | 0.4530 |
| 366.6999 | 3.6260 |
| 410.5787 | 4.5829 |
| 771.9818 | 7.1502 |
| 845.3082 | 40.6571 |
| 908.1404 | 2.5280 |
| 974.1144 | 15.3056 |
| 1042.4171 | 8.6802 |
| 1130.4220 | 6.6258 |
| 1156.5150 | 1.0942 |
| 1165.4396 | 4.0121 |
| 1188.4077 | 0.6584 |
| 1294.6846 | 5.9149 |
| 1407.1784 | 3.4512 |
| 1440.1552 | 21.7397 |
| 1483.5629 | 5.0692 |
| 1497.8997 | 5.4985 |
| 1531.4050 | 5.0971 |
| 3027.9961 | 18.1314 |
| 3077.7230 | 29.2458 |
| 3085.1945 | 22.1969 |
| 3086.4761 | 9.1150 |
| 3109.3152 | 38.1208 |
| 3161.2533 | 31.8449 |

**3**$^{+}$, Propylene oxide radical cation ($C_1$)

| | | | |
|---|---|---|---|
| O | –0.812977 | 0.825585 | –0.170935 |
| C | 0.176116 | –0.080792 | 0.488006 |
| C | –1.063539 | –0.603419 | –0.101799 |
| H | –1.122401 | –1.034899 | –1.100128 |
| H | –1.912728 | –0.827742 | 0.546067 |
| C | 1.520712 | –0.074656 | –0.171100 |
| H | 2.053903 | –0.946042 | 0.224208 |
| H | 2.088834 | 0.814749 | 0.097370 |
| H | 1.443780 | –0.162172 | –1.252650 |
| H | 0.152698 | 0.104636 | 1.561969 |

E = –192.8151624
E[CCSD(T)/CBS] = –192.4931845

ZPVE = 51.0130 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 171.0917 | 1.0275 |
| 265.0722 | 6.2472 |
| 337.4290 | 0.9421 |
| 399.6757 | 7.4099 |
| 637.9161 | 5.9540 |
| 741.1917 | 27.1708 |
| 909.9490 | 10.0678 |
| 928.8572 | 7.2026 |
| 1019.1844 | 26.9892 |
| 1100.6388 | 6.2430 |
| 1151.0243 | 22.8081 |
| 1172.3911 | 0.9912 |
| 1246.3029 | 8.3529 |
| 1344.6340 | 5.5320 |
| 1392.0829 | 28.4475 |
| 1425.9301 | 42.2753 |
| 1436.6627 | 9.7465 |
| 1483.7257 | 16.5636 |
| 3016.3457 | 35.4920 |
| 3037.1040 | 106.5865 |
| 3082.3838 | 11.5075 |
| 3103.1771 | 10.1779 |
| 3135.9039 | 35.4710 |
| 3145.4364 | 3.78350 |

**5a**, methoxy methyl carbene

| | | | |
|---|---|---|---|
| C | –1.834310 | 0.119978 | 0.000000 |
| C | –0.422597 | 0.613974 | 0.000000 |
| H | –2.336536 | 0.556213 | –0.868084 |
| H | –2.336536 | 0.556213 | 0.868084 |
| H | –1.951761 | –0.968260 | 0.000000 |
| O | 0.368176 | –0.422620 | 0.000000 |
| C | 1.787398 | –0.162473 | 0.000000 |
| H | 2.208044 | –0.626648 | –0.889807 |
| H | 2.208044 | –0.626648 | 0.889807 |
| H | 1.951377 | 0.912212 | 0.000000 |

E = –193.1294754
E[CCSD(T)/CBS] = –192.8259877
ZPVE = 51.6760 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 96.4397 | 3.7746 |
| 144.0836 | 4.5811 |

| | |
|---|---|
| 247.9529 | 5.2190 |
| 329.9715 | 13.3721 |
| 557.3315 | 10.2882 |
| 879.9765 | 9.6493 |
| 907.9582 | 1.8274 |
| 1013.4830 | 6.7496 |
| 1119.3066 | 11.3806 |
| 1178.7087 | 1.2988 |
| 1181.2616 | 69.8272 |
| 1315.1482 | 167.9477 |
| 1361.6062 | 12.8495 |
| 1448.2786 | 11.1378 |
| 1451.6717 | 5.2039 |
| 1475.3827 | 9.4937 |
| 1490.9292 | 4.4204 |
| 1500.0949 | 14.5144 |
| 2989.8054 | 25.9075 |
| 3045.4078 | 41.6049 |
| 3067.4877 | 2.9670 |
| 3074.0230 | 30.3611 |
| 3127.6556 | 17.3186 |
| 3143.9347 | 6.4613 |

**5a**$^{+}$, methoxy methyl carbene radical cation

| | | | |
|---|---|---|---|
| C | –1.345321 | –1.367745 | 0.000000 |
| C | –0.138649 | –0.562750 | 0.000000 |
| H | –1.318053 | –2.025454 | 0.875388 |
| H | –1.318053 | –2.025454 | –0.875388 |
| H | –2.242849 | –0.743855 | 0.000000 |
| O | 0.002157 | 0.649240 | 0.000000 |
| C | 1.344648 | 1.353676 | 0.000000 |
| H | 1.328187 | 1.957173 | 0.900051 |
| H | 1.328187 | 1.957173 | –0.900051 |
| H | 2.120983 | 0.597370 | 0.000000 |

E = –192.8538541
E[CCSD(T)/CBS] = –192.5424418
ZPVE = 51.7487 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 95.5055 | 1.7763 |
| 143.9092 | 0.2521 |
| 206.5568 | 6.3309 |
| 236.3693 | 10.4435 |
| 476.0835 | 8.4180 |
| 736.1612 | 70.5382 |
| 949.4676 | 15.3715 |

| | |
|---|---|
| 957.8452 | 5.7378 |
| 1106.3270 | 5.0296 |
| 1155.1684 | 0.1243 |
| 1181.1532 | 5.8559 |
| 1356.8490 | 67.9303 |
| 1395.1234 | 21.9253 |
| 1413.4977 | 63.6228 |
| 1438.3015 | 6.5435 |
| 1462.9248 | 15.5603 |
| 1477.7192 | 27.2187 |
| 1731.7704 | 312.9276 |
| 3001.8939 | 50.7238 |
| 3067.4975 | 23.9788 |
| 3087.3813 | 0.9066 |
| 3096.3889 | 18.3536 |
| 3210.1442 | 4.9045 |
| 3214.7029 | 4.3192 |

**5b**, methoxy methyl carbene

| | | | |
|---|---|---|---|
| C | –1.967297 | –0.009938 | 0.086807 |
| C | –0.561144 | –0.495334 | 0.303981 |
| H | –2.671119 | –0.757881 | 0.442718 |
| H | –2.112051 | 0.079274 | –0.998785 |
| H | –2.207301 | 0.961828 | 0.531498 |
| O | 0.358521 | 0.419037 | 0.199574 |
| C | 0.114972 | 1.839428 | –0.097230 |
| H | –0.448434 | 1.945139 | –1.021268 |
| H | 1.102252 | 2.275793 | –0.204388 |
| H | –0.415857 | 2.310772 | 0.726712 |

E = –193.1164876
E[CCSD(T)/CBS] = –192.8133171
ZPVE = 51.3223 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 56.8599 | 0.8443 |
| 169.0002 | 0.4241 |
| 340.8810 | 0.7486 |
| 378.9863 | 0.8921 |
| 573.2025 | 0.5111 |
| 783.7655 | 3.8064 |
| 810.9238 | 5.3502 |
| 948.1938 | 2.9040 |
| 1049.9960 | 33.8844 |
| 1118.7530 | 1.2926 |
| 1162.8999 | 0.2201 |
| 1308.7404 | 78.1168 |

| | |
|---|---|
| 1347.4503 | 45.1136 |
| 1435.7419 | 14.7232 |
| 1454.3453 | 0.2847 |
| 1481.0182 | 12.4335 |
| 1493.3063 | 3.9611 |
| 1500.1037 | 18.0625 |
| 2978.2132 | 5.8170 |
| 3033.9842 | 15.6102 |
| 3055.5562 | 14.4785 |
| 3120.2133 | 9.1297 |
| 3137.6556 | 15.8834 |
| 3160.6961 | 12.3819 |

**5b**$^{+}$, methoxy methyl carbene radical cation

| | | | |
|---|---|---|---|
| C | 1.631653 | 0.514275 | 0.218985 |
| C | 0.637480 | –0.518952 | –0.003520 |
| H | 2.375675 | 0.442195 | –0.581605 |
| H | 2.162138 | 0.276400 | 1.147145 |
| H | 1.204950 | 1.519691 | 0.262539 |
| O | –0.560365 | –0.602081 | –0.163446 |
| C | –1.606348 | 0.519368 | –0.191571 |
| H | –1.098455 | 1.464413 | –0.040025 |
| H | –2.285399 | 0.256745 | 0.610827 |
| H | –2.060513 | 0.421606 | –1.170382 |

E = –192.8480813
E[CCSD(T)/CBS] = –192.5364994
ZPVE = 51.5962 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 49.9728 | 1.0627 |
| 87.5585 | 3.2724 |
| 229.0026 | 1.7788 |
| 363.3434 | 0.6138 |
| 518.5413 | 21.4952 |
| 633.4510 | 40.5322 |
| 905.2366 | 0.7924 |
| 974.0019 | 5.9095 |
| 1089.1775 | 11.8098 |
| 1126.5234 | 2.7437 |
| 1130.2990 | 0.9726 |
| 1357.9320 | 66.2982 |
| 1397.7987 | 18.0950 |
| 1399.2409 | 51.4471 |
| 1438.8174 | 13.8859 |
| 1451.9227 | 15.1939 |
| 1476.1662 | 25.8152 |

| | |
|---|---|
| 1777.7934 | 252.7488 |
| 3002.1574 | 44.1903 |
| 3068.3113 | 27.3737 |
| 3088.6102 | 0.9446 |
| 3092.2211 | 19.2826 |
| 3215.2555 | 6.6177 |
| 3218.7121 | 1.9833 |

**5t**, methoxy methyl carbene, triplet

| | | | |
|---|---|---|---|
| C | 1.748119 | 0.462146 | 0.153742 |
| C | 0.562437 | –0.279832 | –0.340131 |
| H | 2.579779 | 0.338336 | –0.538175 |
| H | 2.067438 | 0.092314 | 1.137002 |
| H | 1.552263 | 1.539281 | 0.252384 |
| O | –0.600105 | –0.381062 | 0.297264 |
| C | –1.673696 | 0.476586 | –0.143586 |
| H | –1.382462 | 1.524951 | –0.060933 |
| H | –2.519120 | 0.272398 | 0.508413 |
| H | –1.933749 | 0.248314 | –1.176951 |

E = –193.0829400
E[CCSD(T)/CBS] = –192.7739003
ZPVE = 51.1986 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 87.1747 | 3.0628 |
| 137.4062 | 2.1173 |
| 147.6986 | 2.0881 |
| 406.6671 | 2.1171 |
| 428.4762 | 7.7781 |
| 846.6401 | 10.4910 |
| 970.5690 | 51.7888 |
| 1018.3177 | 1.6745 |
| 1079.7001 | 7.3052 |
| 1153.9042 | 1.7348 |
| 1185.8253 | 0.6120 |
| 1312.1986 | 139.1539 |
| 1382.2459 | 1.5666 |
| 1459.1392 | 4.4761 |
| 1462.3981 | 5.1591 |
| 1475.3775 | 0.4072 |
| 1487.8498 | 6.2098 |
| 1495.1653 | 10.6581 |
| 2943.5269 | 40.3305 |
| 2980.3417 | 32.0417 |
| 3024.7898 | 43.9049 |
| 3095.0809 | 31.1062 |

| | |
|---|---|
| 3100.7100 | 9.8808 |
| 3132.7414 | 19.4783 |

**5t**$^{+}$, methoxy methyl carbene radical cation, triplet

| | | | |
|---|---|---|---|
| C | 1.945377 | 0.183741 | 0.141902 |
| C | 0.551708 | 0.306333 | –0.242016 |
| H | 2.397015 | –0.611908 | –0.460243 |
| H | 2.048707 | –0.020281 | 1.210808 |
| H | 2.460999 | 1.108232 | –0.138672 |
| O | –0.463273 | 0.215825 | 0.429127 |
| C | –1.867438 | 0.369198 | –0.121224 |
| H | –2.285814 | 1.193983 | 0.443850 |
| H | –2.348404 | –0.573934 | 0.110688 |
| H | –1.791816 | 0.566850 | –1.184201 |

E = –192.8538544
E[CCSD(T)/CBS] = –192.5424418
ZPVE = 51.7478 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 94.9016 | 1.7488 |
| 143.6276 | 0.2799 |
| 206.4249 | 6.3210 |
| 236.4269 | 10.4320 |
| 476.1502 | 8.3877 |
| 736.4979 | 70.4535 |
| 949.1946 | 15.4197 |
| 957.8013 | 5.7183 |
| 1106.2516 | 5.1006 |
| 1155.2380 | 0.1252 |
| 1181.2397 | 5.8764 |
| 1356.6029 | 67.6154 |
| 1395.1081 | 21.9085 |
| 1413.4565 | 63.6970 |
| 1438.3149 | 6.5643 |
| 1462.9235 | 15.5514 |
| 1477.7484 | 27.2402 |
| 1731.5786 | 312.5163 |
| 3002.0938 | 50.5012 |
| 3068.3334 | 23.9973 |
| 3087.2200 | 0.9038 |
| 3096.4501 | 18.5285 |
| 3209.9194 | 4.9023 |
| 3214.5891 | 4.3213 |

**5t**$^{+}$, methoxy methyl carbene radical cation, triplet q-state

| | | | |
|---|---|---|---|
| C | 1.830365 | 0.248197 | 0.128868 |

| | | | |
|---|---|---|---|
| C | 0.599571 | –0.193367 | –0.507161 |
| H | 2.568755 | 0.405117 | –0.669147 |
| H | 2.218509 | –0.500966 | 0.827349 |
| H | 1.725570 | 1.218161 | 0.638283 |
| O | –0.601211 | –0.384942 | 0.314981 |
| C | –1.714160 | 0.345680 | –0.004757 |
| H | –1.442769 | 1.374410 | –0.325309 |
| H | –2.455732 | 0.273814 | 0.782626 |
| H | –2.081835 | –0.048064 | –0.995715 |

E = –192.6845330
E[CCSD(T)/CBS] = –192.3634925
ZPVE = 47.8669 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 70.2827 | 4.1422 |
| 107.2506 | 5.1729 |
| 134.9396 | 14.3491 |
| 332.7074 | 2.9236 |
| 392.0071 | 2.9162 |
| 678.9430 | 7.7607 |
| 817.2803 | 8.8738 |
| 901.4497 | 241.8780 |
| 997.2504 | 5.5268 |
| 1022.4438 | 39.3760 |
| 1133.9441 | 5.3261 |
| 1161.1857 | 7.8787 |
| 1228.8157 | 127.4985 |
| 1272.8334 | 46.9087 |
| 1328.5364 | 108.5492 |
| 1366.4682 | 15.2269 |
| 1412.4624 | 9.6033 |
| 1459.2887 | 3.7782 |
| 2664.4944 | 260.8535 |
| 2839.5885 | 164.8977 |
| 2937.5075 | 72.2139 |
| 2996.8683 | 69.3914 |
| 3041.5609 | 31.6849 |
| 3185.2598 | 12.4669 |

**6a**, 1-methyleneoxyethyl

| | | | |
|---|---|---|---|
| C | 1.849170 | –0.035737 | 0.000000 |
| C | 0.452807 | –0.532823 | 0.000000 |
| H | 2.410972 | –0.373173 | 0.878625 |
| H | 1.852544 | 1.053931 | 0.000000 |
| H | 2.410972 | –0.373173 | –0.878625 |
| O | –0.508597 | 0.338288 | 0.000000 |

| | | | |
|---|---|---|---|
| C | –1.811328 | 0.191523 | 0.000000 |
| H | –2.237102 | –0.799962 | 0.000000 |
| H | –2.369795 | 1.107463 | 0.000000 |
| H | 0.182808 | –1.581922 | 0.000000 |

E = –193.1132045
E[CCSD(T)/CBS] = –192.8057130
ZPVE = 50.7849 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 23.0379 | 0.5168 |
| 206.1886 | 0.0027 |
| 296.8997 | 2.7754 |
| 319.5769 | 112.0657 |
| 522.4038 | 6.4814 |
| 569.0577 | 7.8448 |
| 662.6667 | 16.1524 |
| 907.9233 | 31.4272 |
| 1037.5790 | 0.0740 |
| 1118.6766 | 4.6642 |
| 1172.6609 | 5.9020 |
| 1228.4298 | 71.3299 |
| 1375.5148 | 171.8412 |
| 1429.8952 | 23.3940 |
| 1453.1101 | 95.6229 |
| 1463.4629 | 6.2991 |
| 1489.1758 | 2.8655 |
| 1535.6161 | 44.6074 |
| 2980.4972 | 75.7292 |
| 3001.5530 | 30.1943 |
| 3099.6532 | 8.7135 |
| 3151.5320 | 14.0284 |
| 3159.2684 | 25.1375 |
| 3320.1775 | 5.3144 |

**6a**$^{+}$, 1-methyleneoxyethyl radical cation

| | | | |
|---|---|---|---|
| C | 0.986042 | –1.510508 | 0.000000 |
| C | –0.137066 | –0.589174 | 0.000000 |
| H | 0.905587 | –2.175329 | 0.870065 |
| H | 1.944137 | –0.998350 | 0.000000 |
| H | 0.905587 | –2.175329 | –0.870065 |
| O | 0.087084 | 0.688251 | 0.000000 |
| C | –0.845742 | 1.637396 | 0.000000 |
| H | –1.890539 | 1.356992 | 0.000000 |
| H | –0.456670 | 2.641833 | 0.000000 |
| H | –1.176518 | –0.911184 | 0.000000 |

E = –192.8628855
E[CCSD(T)/CBS] = –192.5471165
ZPVE = 51.1827 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 135.4274 | 0.3663 |
| 215.3904 | 4.4072 |
| 307.0168 | 9.2775 |
| 433.0774 | 9.2929 |
| 535.5964 | 1.7544 |
| 731.7787 | 34.1669 |
| 811.3312 | 12.8492 |
| 886.5432 | 81.7371 |
| 1032.2226 | 0.8920 |
| 1059.1482 | 123.0415 |
| 1151.2434 | 7.5950 |
| 1206.2477 | 4.3215 |
| 1293.6695 | 40.0952 |
| 1382.0509 | 70.9304 |
| 1425.0538 | 11.9950 |
| 1426.2041 | 19.3296 |
| 1473.0470 | 12.9586 |
| 1535.5679 | 17.3439 |
| 2992.5648 | 69.1800 |
| 3024.1071 | 11.1185 |
| 3132.7030 | 54.5609 |
| 3141.5258 | 20.4948 |
| 3154.4341 | 9.0617 |
| 3316.8403 | 19.0392 |

**6at**, 1-methyleneoxyethyl, triplet

| | | | |
|---|---|---|---|
| C | 1.348162 | –1.197781 | –0.025289 |
| C | –0.023091 | –0.663420 | –0.156249 |
| H | 1.668687 | –1.263467 | 1.024364 |
| H | 2.068070 | –0.554868 | –0.537200 |
| H | 1.406326 | –2.197519 | –0.454275 |
| O | –0.168010 | 0.650101 | 0.255816 |
| C | –1.398018 | 1.203719 | 0.021447 |
| H | –1.957378 | 0.841180 | –0.831931 |
| H | –1.488012 | 2.217129 | 0.378893 |
| H | –0.904745 | –1.285038 | –0.033110 |

E = –193.0948875
E[CCSD(T)/CBS] = –192.7848177
ZPVE = 49.8580 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|

| | |
|---|---|
| 89.0645 | 4.4431 |
| 173.5962 | 0.5584 |
| 222.3677 | 6.9915 |
| 295.1746 | 0.9084 |
| 481.7065 | 1.7534 |
| 591.7096 | 21.3715 |
| 614.7865 | 36.4555 |
| 889.7726 | 8.0580 |
| 1020.0611 | 3.2008 |
| 1113.5290 | 10.3183 |
| 1125.7160 | 5.4083 |
| 1204.7918 | 64.2019 |
| 1258.3356 | 237.3613 |
| 1366.8562 | 40.8209 |
| 1418.0871 | 34.8732 |
| 1461.4508 | 9.3651 |
| 1467.0128 | 0.4222 |
| 1486.3325 | 2.8857 |
| 2953.1110 | 34.8164 |
| 3042.0943 | 15.3439 |
| 3101.1092 | 4.1561 |
| 3111.3365 | 34.0937 |
| 3125.1575 | 37.4654 |
| 3263.0300 | 9.5003 |

**6at**$^{+}$, 1-methyleneoxyethyl radical cation, triplet

| | | | |
|---|---|---|---|
| C | 1.795666 | –0.167959 | 0.015016 |
| C | 0.460843 | 0.387478 | –0.127268 |
| H | 2.288311 | –0.175046 | –0.966119 |
| H | 1.786975 | –1.166332 | 0.443360 |
| H | 2.402886 | 0.508862 | 0.630264 |
| O | –0.564044 | –0.313641 | 0.246703 |
| C | –1.835103 | 0.073515 | 0.171895 |
| H | –2.071487 | 1.049807 | –0.229641 |
| H | –2.542411 | –0.653586 | 0.534302 |
| H | 0.263674 | 1.376195 | –0.536867 |

E = –192.8628850
E[CCSD(T)/CBS] = –192.5471210
ZPVE = 51.1804 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 134.3215 | 0.3604 |
| 215.2514 | 4.4114 |
| 306.8848 | 9.2799 |
| 433.1487 | 9.2761 |
| 535.4907 | 1.7536 |

| | |
|---|---|
| 731.7443 | 34.1972 |
| 811.3209 | 12.8303 |
| 886.4524 | 81.5571 |
| 1032.3252 | 0.8875 |
| 1059.1238 | 123.0695 |
| 1151.2328 | 7.5629 |
| 1206.1469 | 4.3320 |
| 1293.8439 | 40.0900 |
| 1381.9560 | 70.7666 |
| 1424.9917 | 11.9919 |
| 1426.2279 | 19.3214 |
| 1472.9701 | 12.9515 |
| 1535.5729 | 17.2960 |
| 2992.8886 | 69.1229 |
| 3024.7181 | 11.1333 |
| 3132.3987 | 53.9471 |
| 3141.3007 | 21.0942 |
| 3154.1824 | 9.0451 |
| 3316.7098 | 19.0546 |

**6at**$^{+}$, 1-methyleneoxyethyl radical cation, triplet, q-state

| | | | |
|---|---|---|---|
| C | 1.655344 | –0.241697 | 0.056224 |
| C | 0.488344 | 0.730186 | –0.032778 |
| H | 1.984342 | –0.541490 | –0.942748 |
| H | 1.356033 | –1.119184 | 0.629306 |
| H | 2.453184 | 0.299133 | 0.563071 |
| O | –0.639845 | 0.232933 | –0.639218 |
| C | –1.796790 | –0.045843 | 0.041246 |
| H | –2.419444 | 0.819198 | 0.273452 |
| H | –1.785316 | –0.962323 | 0.632305 |
| H | 0.689460 | 1.748378 | –0.399214 |

E = –192.7087577
E[CCSD(T)/CBS] = –192.3844963
ZPVE = 47.5123 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 144.8821 | 3.4012 |
| 164.0218 | 2.2568 |
| 286.6558 | 6.9277 |
| 363.4720 | 45.6959 |
| 469.8462 | 6.5272 |
| 491.4564 | 10.4745 |
| 636.2938 | 144.3598 |
| 794.7816 | 91.8971 |
| 857.4964 | 13.9691 |

| | |
|---|---|
| 950.0922 | 5.8398 |
| 976.3812 | 0.8635 |
| 989.2137 | 4.9183 |
| 1034.1449 | 4.5591 |
| 1172.0870 | 24.7049 |
| 1310.4139 | 39.9024 |
| 1358.0011 | 14.1113 |
| 1425.5162 | 32.1606 |
| 1443.9948 | 14.6361 |
| 2952.8459 | 205.7888 |
| 3011.7653 | 172.4843 |
| 3016.3455 | 20.8433 |
| 3099.2695 | 7.5398 |
| 3132.3481 | 11.0413 |
| 3153.9932 | 63.8612 |

**6b**, 1-methyleneoxyethyl

| | | | |
|---|---|---|---|
| C | 1.429739 | –0.644198 | 0.000000 |
| C | 0.659138 | 0.606942 | 0.000000 |
| H | 2.498036 | –0.440438 | 0.000000 |
| H | 1.192188 | –1.266160 | –0.877668 |
| H | 1.192188 | –1.266160 | 0.877668 |
| O | –0.641995 | 0.574564 | 0.000000 |
| C | –1.437441 | –0.470696 | 0.000000 |
| H | –1.031561 | –1.467043 | 0.000000 |
| H | –2.484274 | –0.233590 | 0.000000 |
| H | 1.065801 | 1.602739 | 0.000000 |

E = –193.1194698
E[CCSD(T)/CBS] = –192.8136406
ZPVE = 51.3465 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 230.2630 | 4.4944 |
| 279.2240 | 0.1121 |
| 301.5178 | 24.1596 |
| 398.6635 | 55.4454 |
| 548.3303 | 52.3548 |
| 592.1802 | 4.1683 |
| 645.6668 | 2.1549 |
| 937.8283 | 8.4751 |
| 1027.1509 | 0.1573 |
| 1120.9249 | 44.2542 |
| 1156.8990 | 7.4211 |
| 1213.0137 | 33.1919 |
| 1390.2059 | 38.1856 |
| 1429.6286 | 135.3225 |

| | |
|---|---|
| 1449.2262 | 38.5075 |
| 1454.0217 | 9.7268 |
| 1480.7322 | 12.2494 |
| 1514.1884 | 4.7781 |
| 2930.2562 | 38.9185 |
| 2942.2856 | 42.7964 |
| 3118.6876 | 9.6412 |
| 3181.2097 | 7.7450 |
| 3246.7160 | 4.8384 |
| 3328.5677 | 5.1193 |

**6b**$^{+}$, 1-methyleneoxyethyl radical cation

| | | | |
|---|---|---|---|
| C | –1.441133 | 0.534417 | 0.000000 |
| C | –0.021174 | 0.868893 | 0.000000 |
| H | –2.040008 | 1.440573 | 0.000000 |
| H | –1.702257 | –0.066963 | 0.880685 |
| H | –1.702257 | –0.066963 | –0.880685 |
| O | 0.939901 | –0.016308 | 0.000000 |
| C | 0.800786 | –1.330033 | 0.000000 |
| H | –0.180900 | –1.779945 | 0.000000 |
| H | 1.733253 | –1.871240 | 0.000000 |
| H | 0.375108 | 1.876108 | 0.000000 |

E = –192.8609005
E[CCSD(T)/CBS] = –192.5464685
ZPVE = 51.4455 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 121.0535 | 1.8860 |
| 273.7486 | 4.6257 |
| 293.8845 | 2.4211 |
| 504.9968 | 12.3757 |
| 585.8411 | 6.1165 |
| 703.1492 | 15.2404 |
| 786.9320 | 35.1146 |
| 931.8280 | 13.5264 |
| 1040.6974 | 0.0051 |
| 1057.3183 | 117.8034 |
| 1117.1836 | 7.0607 |
| 1195.0183 | 3.1213 |
| 1275.9854 | 35.2110 |
| 1369.7773 | 19.0440 |
| 1446.8448 | 19.7408 |
| 1453.4462 | 13.8444 |
| 1472.1198 | 43.6517 |
| 1519.8502 | 9.6546 |
| 2987.1359 | 25.6550 |

| | |
|---|---|
| 3026.4026 | 3.8506 |
| 3149.9394 | 7.9123 |
| 3151.5561 | 54.8239 |
| 3205.7604 | 29.6204 |
| 3316.1890 | 14.6591 |

**6bt**, 1-methyleneoxyethyl, triplet

| | | | |
|---|---|---|---|
| C | –1.712029 | 0.824489 | 0.327697 |
| C | –0.427147 | 0.332181 | –0.209490 |
| H | –2.132179 | 1.582897 | –0.331823 |
| H | –1.597240 | 1.271541 | 1.325845 |
| H | –2.433312 | 0.009885 | 0.426540 |
| O | 0.150043 | –0.692382 | 0.522823 |
| C | 1.229807 | –1.273945 | –0.086384 |
| H | 1.650324 | –2.098976 | 0.464947 |
| H | 1.817632 | –0.670900 | –0.765656 |
| H | 0.272569 | 0.978957 | –0.730592 |

E = –193.0941805
E[CCSD(T)/CBS] = –192.7846289
ZPVE = 49.7378 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 93.2074 | 3.4117 |
| 170.4327 | 0.5613 |
| 206.0163 | 3.3482 |
| 298.2683 | 3.0813 |
| 480.2045 | 0.2452 |
| 525.0949 | 31.9584 |
| 578.8678 | 36.2038 |
| 894.5851 | 9.1964 |
| 1016.9600 | 3.8095 |
| 1112.9386 | 7.1655 |
| 1128.7505 | 5.4925 |
| 1208.7387 | 63.6849 |
| 1261.4890 | 240.5474 |
| 1368.7635 | 40.4161 |
| 1419.2883 | 38.3129 |
| 1461.7983 | 7.5836 |
| 1472.2464 | 1.8357 |
| 1486.8298 | 3.3653 |
| 2950.9580 | 34.8010 |
| 3041.8042 | 15.5088 |
| 3101.2670 | 4.2814 |
| 3119.2037 | 24.2336 |
| 3123.1627 | 40.5538 |
| 3271.2485 | 10.3874 |

**6bt**$^{+}$, 1-methyleneoxyethyl radical cation, triplet

| | | | |
|---|---|---|---|
| C | –1.792090 | –0.155763 | –0.017984 |
| C | –0.462371 | 0.401340 | 0.160652 |
| H | –2.385249 | 0.523491 | –0.644161 |
| H | –2.308996 | –0.169283 | 0.950563 |
| H | –1.770813 | –1.151726 | –0.451426 |
| O | 0.572937 | –0.295949 | –0.191072 |
| C | 1.840954 | 0.093056 | –0.082249 |
| H | 2.558527 | –0.630777 | –0.430747 |
| H | 2.065305 | 1.067598 | 0.330290 |
| H | –0.277499 | 1.388229 | 0.580271 |

E = –192.8628850
E[CCSD(T)/CBS] = –192.5471204
ZPVE = 51.1808 kcal mol$^{-1}$

| Frequency | Intensity |
|---|---|
| 134.5331 | 0.3617 |
| 215.2243 | 4.4110 |
| 306.8729 | 9.2794 |
| 433.1392 | 9.2753 |
| 535.4984 | 1.7543 |
| 731.7369 | 34.1983 |
| 811.3300 | 12.8339 |
| 886.4867 | 81.5601 |
| 1032.2995 | 0.8894 |
| 1059.2040 | 123.0845 |
| 1151.2528 | 7.5691 |
| 1206.1949 | 4.3354 |
| 1293.8731 | 40.0825 |
| 1381.9692 | 70.8260 |
| 1425.0049 | 11.9942 |
| 1426.1870 | 19.3227 |
| 1472.9845 | 12.9505 |
| 1535.6029 | 17.2930 |
| 2992.7875 | 69.1332 |
| 3024.5317 | 11.1320 |
| 3132.4055 | 54.0330 |
| 3141.3171 | 20.9868 |
| 3154.3051 | 9.0527 |
| 3316.7234 | 19.0544 |

**6bt**$^{+}$, 1-methyleneoxyethyl radical cation, triplet, q-state

| | | | |
|---|---|---|---|
| C | –1.683433 | –0.221780 | –0.066425 |
| C | –0.537255 | 0.768439 | 0.058490 |
| H | –2.515086 | 0.339181 | –0.490030 |
| H | –1.962307 | –0.616952 | 0.914511 |

| | | | |
|---|---|---|---|
| H | –1.389898 | –1.036797 | –0.727878 |
| O | 0.626258 | 0.254657 | 0.578141 |
| C | 1.738999 | 0.064491 | –0.203512 |
| H | 1.951717 | –0.990466 | –0.399330 |
| H | 2.552303 | 0.754064 | 0.040910 |
| H | –0.740595 | 1.755381 | 0.499260 |

E = –192.7104871
E[CCSD(T)/CBS] = –192.3862877
ZPVE = 47.8024 kcal $mol^{-1}$

| Frequency | Intensity |
|---|---|
| 143.9840 | 2.5162 |
| 163.7291 | 2.3738 |
| 300.1649 | 5.7358 |
| 434.6810 | 16.4097 |
| 449.0680 | 24.5153 |
| 595.9410 | 177.6518 |
| 692.4751 | 59.2398 |
| 787.9562 | 103.4722 |
| 861.4352 | 4.9904 |
| 943.7548 | 1.5430 |
| 971.4944 | 1.2630 |
| 1004.6999 | 4.6518 |
| 1051.4545 | 6.8810 |
| 1179.3041 | 15.9405 |
| 1315.6496 | 43.9413 |
| 1360.3642 | 19.6637 |
| 1427.1415 | 32.1179 |
| 1444.7458 | 12.4923 |
| 2958.2485 | 301.8091 |
| 2993.1606 | 141.3534 |
| 3016.1739 | 9.9116 |
| 3099.2120 | 6.4473 |
| 3110.1069 | 65.1820 |
| 3133.3235 | 9.8122 |

**Table S9.** The ωB97X-D/6-311G(d,p) optimized geometries and harmonic frequencies of the reactants, transition states, and products depicted in Fig. 5.

| | | | |
|---|---|---|---|
| **R0**, Acetone, $CH_3C(O)CH_3$ | | | |
| C | 0.000000 | 1.285376 | 0.612598 |
| C | 0.000000 | 0.000000 | -0.187852 |
| O | 0.000000 | 0.000000 | -1.392832 |
| C | 0.000000 | -1.285376 | 0.612598 |
| H | 0.943971 | 1.377015 | 1.159027 |
| H | -0.802116 | 1.278292 | 1.356041 |
| H | -0.116116 | 2.137148 | -0.055773 |
| H | 0.116116 | -2.137148 | -0.055773 |
| H | -0.943971 | -1.377015 | 1.159027 |
| H | 0.802116 | -1.278292 | 1.356041 |
| | | | |
| Frequencies | | | |
| 53.4499 | | 133.5866 | 383.5578 |
| 492.7647 | | 541.1902 | 795.5710 |
| 884.8346 | | 894.6565 | 1086.0112 |
| 1122.8809 | | 1244.2777 | 1387.7351 |
| 1397.4726 | | 1463.9048 | 1468.6523 |
| 1473.9393 | | 1491.5856 | 1852.1136 |
| 3043.4252 | | 3048.6544 | 3112.8430 |
| 3118.9099 | | 3165.8703 | 3167.3884 |
| **P0**, propen-2-ol, $CH_3C(OH)CH_2$ | | | |
| C | -0.980498 | -1.033274 | 0.000000 |
| C | -0.085172 | -0.046750 | 0.000000 |
| O | -0.406360 | 1.275492 | 0.000000 |
| C | 1.397703 | -0.231494 | 0.000000 |
| H | -2.048070 | -0.838031 | 0.000000 |
| H | -0.659492 | -2.065263 | 0.000000 |
| H | -1.361527 | 1.363465 | 0.000001 |
| H | 1.832950 | 0.246697 | -0.881555 |
| H | 1.661868 | -1.288384 | -0.000004 |
| H | 1.832948 | 0.246689 | 0.881560 |
| | | | |
| Frequencies | | | |
| 181.8918 | | 419.4738 | 443.1288 |
| 494.3902 | | 512.8506 | 734.1046 |
| 823.6144 | | 877.8479 | 991.3134 |
| 1032.9915 | | 1078.5027 | 1228.4877 |
| 1381.6810 | | 1425.3841 | 1464.6694 |
| 1476.6993 | | 1497.6885 | 1750.3240 |
| 3052.1622 | | 3117.6329 | 3158.2009 |
| 3159.0225 | | 3259.8322 | 3902.2729 |
| **TS0** | | | |
| C | 1.462468 | 0.264308 | -0.018764 |

| | | | |
|---|---|---|---|
| C | 0.002851 | -0.024197 | -0.007499 |
| O | -0.430997 | -1.226760 | 0.012078 |
| C | -1.106807 | 0.861681 | 0.044471 |
| H | 1.681870 | 1.004276 | 0.755286 |
| H | 1.737588 | 0.714953 | -0.975914 |
| H | 2.047885 | -0.637303 | 0.154511 |
| H | -1.460330 | -0.560291 | 0.289328 |
| H | -1.699207 | 0.813470 | -0.871004 |
| H | -1.010895 | 1.868228 | 0.441923 |

Frequencies

| | | |
|---|---|---|
| -2183.3396 | 111.1829 | 372.6432 |
| 423.8953 | 565.8434 | 671.0433 |
| 773.4529 | 906.3437 | 990.2182 |
| 1027.8534 | 1111.6509 | 1190.2282 |
| 1344.1638 | 1408.1479 | 1459.7540 |
| 1476.4764 | 1501.9741 | 1576.2689 |
| 1975.9951 | 3064.1761 | 3109.0196 |
| 3133.9494 | 3174.7429 | 3195.0570 |

**R1**, $CH_3C(O)CH_3 \cdot H_2O$

| | | | |
|---|---|---|---|
| C | -0.233169 | 1.335134 | -0.033484 |
| C | -0.723346 | -0.092043 | -0.024373 |
| O | 0.033734 | -1.035326 | -0.099271 |
| C | -2.214958 | -0.300450 | 0.078235 |
| H | -0.709838 | 1.910779 | 0.764527 |
| H | -0.523495 | 1.800900 | -0.980954 |
| H | 0.852145 | 1.360855 | 0.061755 |
| H | -2.457239 | -1.351287 | -0.071462 |
| H | -2.740871 | 0.318618 | -0.653544 |
| H | -2.556025 | 0.015010 | 1.069345 |
| O | 2.749788 | -0.075538 | -0.029128 |
| H | 2.964601 | -0.253201 | 0.886700 |
| H | 1.931389 | -0.570613 | -0.171449 |

Frequencies

| | | |
|---|---|---|
| 44.8599 | 96.9296 | 127.4351 |
| 134.5612 | 166.8138 | 223.5359 |
| 318.3338 | 398.4345 | 498.1665 |
| 559.9697 | 654.0177 | 805.8163 |
| 891.1885 | 913.3768 | 1097.5411 |
| 1129.2106 | 1264.4333 | 1394.3161 |
| 1405.1294 | 1465.7502 | 1472.1872 |
| 1477.8583 | 1501.4934 | 1674.7694 |
| 1825.5976 | 3041.7677 | 3049.2668 |
| 3113.7875 | 3120.5699 | 3161.5391 |
| 3169.4080 | 3763.7976 | 3957.4475 |

**P1**, $CH_3C(OH)CH_2 \cdot H_2O$

| | | | |
|---|---|---|---|
| C | -0.328959 | 1.348812 | -0.162279 |
| C | -0.757938 | 0.085023 | -0.083547 |
| O | 0.012088 | -1.002449 | -0.311123 |
| C | -2.159883 | -0.308327 | 0.261524 |
| H | -1.006138 | 2.167098 | 0.039699 |
| H | 0.680263 | 1.590222 | -0.476284 |
| H | 2.308818 | 0.484931 | 0.859912 |
| H | -2.163285 | -0.943714 | 1.151420 |
| H | -2.589365 | -0.892233 | -0.557237 |
| H | -2.785677 | 0.565587 | 0.440807 |
| O | 2.597832 | -0.038029 | 0.108381 |
| H | 3.218003 | -0.676350 | 0.463240 |
| H | 0.938695 | -0.724764 | -0.393811 |

Frequencies

| | | |
|---|---|---|
| 35.8064 | 106.0116 | 153.5592 |
| 183.1496 | 204.0923 | 286.2667 |
| 362.1544 | 428.4540 | 518.0219 |
| 539.8549 | 716.7164 | 786.4634 |
| 835.6364 | 884.9228 | 1000.6809 |
| 1038.2082 | 1077.0688 | 1304.2188 |
| 1411.9283 | 1428.5300 | 1476.0123 |
| 1494.1734 | 1505.9885 | 1632.6027 |
| 1736.9915 | 3049.5509 | 3114.3444 |
| 3154.4317 | 3166.6708 | 3260.5593 |
| 3688.8976 | 3875.7821 | 3983.3154 |

**TS1**

| | | | |
|---|---|---|---|
| C | 0.040877 | 1.272258 | -0.197644 |
| C | -0.589685 | 0.009702 | -0.150292 |
| O | 0.054750 | -1.054115 | -0.428403 |
| C | -2.002503 | -0.160158 | 0.327468 |
| H | -0.522693 | 2.127830 | 0.156786 |
| H | 0.628187 | 1.469462 | -1.094496 |
| H | 1.288482 | 0.754934 | 0.343588 |
| H | -2.121745 | -1.117524 | 0.835300 |
| H | -2.662691 | -0.152244 | -0.545676 |
| H | -2.304717 | 0.661338 | 0.978492 |
| O | 2.121703 | -0.104932 | 0.245962 |
| H | 2.357307 | -0.455360 | 1.107835 |
| H | 1.234113 | -0.746864 | -0.199501 |

Frequencies

| | | |
|---|---|---|
| -1894.9220 | 118.4046 | 124.7542 |
| 373.9518 | 465.3423 | 501.2940 |
| 559.3909 | 587.7429 | 619.6087 |

| | | |
|---|---|---|
| 721.9188 | 764.2422 | 829.0781 |
| 882.6548 | 1002.5008 | 1042.7039 |
| 1096.9712 | 1168.9084 | 1327.9344 |
| 1382.5812 | 1420.0360 | 1466.2941 |
| 1480.7788 | 1499.4627 | 1530.0218 |
| 1591.4864 | 1679.9564 | 1933.1042 |
| 3056.9981 | 3123.1253 | 3131.4291 |
| 3165.6345 | 3220.4339 | 3909.4875 |

**R2**, $CH_3C(O)CH_3 \cdot (H_2O)_2$

| | | | |
|---|---|---|---|
| O | -2.263614 | 1.412655 | -0.427760 |
| H | -2.327652 | 1.435391 | -1.382350 |
| C | 0.535345 | 0.773541 | 1.020602 |
| C | 1.248155 | -0.139752 | 0.061082 |
| O | 0.753577 | -1.185828 | -0.310675 |
| C | 2.593685 | 0.301968 | -0.450684 |
| H | 0.065325 | 0.183935 | 1.809544 |
| H | 1.197512 | 1.522522 | 1.456281 |
| H | 2.959203 | -0.391841 | -1.205826 |
| H | 3.301153 | 0.353400 | 0.382795 |
| H | 2.518566 | 1.311344 | -0.865966 |
| H | -0.275730 | 1.275074 | 0.474465 |
| O | -2.007728 | -1.312214 | 0.092698 |
| H | -2.187220 | -1.677763 | 0.958365 |
| H | -2.323144 | 0.467063 | -0.209370 |
| H | -1.049003 | -1.410571 | -0.038049 |

Frequencies

| | | |
|---|---|---|
| 30.0781 | 58.8940 | 85.7965 |
| 123.9783 | 148.7993 | 182.6117 |
| 195.5879 | 200.1645 | 234.7920 |
| 262.1524 | 367.0018 | 398.5877 |
| 463.5375 | 513.0912 | 550.6592 |
| 664.6726 | 806.0459 | 838.7264 |
| 896.0110 | 944.6303 | 1090.2869 |
| 1121.6400 | 1263.3110 | 1394.6422 |
| 1412.9517 | 1465.1046 | 1476.2672 |
| 1487.1753 | 1500.6418 | 1666.1749 |
| 1687.2565 | 1809.3342 | 3011.2794 |
| 3046.6576 | 3111.3427 | 3116.2511 |
| 3155.6562 | 3170.2891 | 3636.5479 |
| 3690.6747 | 3957.9040 | 3967.6404 |

**P2**, $CH_3C(OH)CH_2 \cdot (H_2O)_2$

| | | | |
|---|---|---|---|
| O | -1.653957 | 1.577689 | -0.423159 |
| H | -1.394947 | 1.602955 | -1.345823 |
| C | 0.632589 | 0.319045 | 1.320780 |
| C | 1.107670 | -0.173235 | 0.165437 |

| | | | |
|---|---|---|---|
| O | 0.444110 | -1.013502 | -0.642898 |
| C | 2.459360 | 0.159880 | -0.385169 |
| H | -0.327893 | 0.006138 | 1.712355 |
| H | 1.240953 | 0.977215 | 1.925347 |
| H | 2.361643 | 0.586471 | -1.387075 |
| H | 3.048849 | -0.755821 | -0.479550 |
| H | 2.991460 | 0.862003 | 0.255983 |
| H | -0.817437 | 1.534451 | 0.062968 |
| O | -2.170715 | -1.075058 | 0.075925 |
| H | -2.561412 | -1.254956 | 0.930482 |
| H | -2.240045 | -0.112548 | -0.063174 |
| H | -0.454390 | -1.193077 | -0.296745 |

Frequencies

| | | |
|---|---|---|
| 39.0128 | 77.2780 | 131.0755 |
| 158.4091 | 181.0715 | 214.5886 |
| 235.3113 | 245.8895 | 293.5566 |
| 309.5852 | 430.8060 | 493.6229 |
| 523.4601 | 537.9877 | 547.8276 |
| 747.1400 | 792.5144 | 831.0555 |
| 884.3404 | 981.0690 | 1001.7590 |
| 1041.8680 | 1076.6585 | 1307.2852 |
| 1410.2061 | 1430.5352 | 1475.4661 |
| 1490.5588 | 1498.4115 | 1653.3251 |
| 1659.6700 | 1716.3100 | 3052.4545 |
| 3118.5595 | 3157.0709 | 3172.0934 |
| 3266.9438 | 3506.2836 | 3624.5507 |
| 3739.9379 | 3946.4957 | 3968.8197 |

**TS2**

| | | | |
|---|---|---|---|
| O | -1.699005 | 1.267331 | -0.489782 |
| H | -1.587741 | 1.418717 | -1.430842 |
| C | 0.472480 | 0.914578 | 0.929730 |
| C | 1.044866 | -0.125316 | 0.177047 |
| O | 0.475472 | -1.233074 | -0.062514 |
| C | 2.394853 | 0.065883 | -0.468978 |
| H | -0.216019 | 0.614201 | 1.718662 |
| H | 1.106914 | 1.757669 | 1.182113 |
| H | 2.379779 | -0.332782 | -1.484748 |
| H | 3.129227 | -0.512119 | 0.099908 |
| H | 2.708717 | 1.110274 | -0.475342 |
| H | -0.679208 | 1.291457 | 0.022687 |
| O | -1.928135 | -1.054162 | 0.032183 |
| H | -2.325906 | -1.212767 | 0.888822 |
| H | -1.940668 | 0.125642 | -0.267686 |
| H | -0.834948 | -1.231919 | 0.080527 |

Frequencies

| | | |
|---|---|---|
| -1563.4525 | 69.2758 | 102.3644 |
| 106.3293 | 173.4542 | 376.1070 |
| 395.6707 | 418.1767 | 496.5235 |
| 528.5967 | 562.0996 | 615.0470 |
| 633.7429 | 643.8013 | 706.8317 |
| 767.4122 | 849.1832 | 871.3277 |
| 999.1052 | 1047.2176 | 1089.8015 |
| 1172.9196 | 1313.7276 | 1362.4772 |
| 1397.2215 | 1435.1531 | 1467.2191 |
| 1481.6594 | 1508.2975 | 1541.5129 |
| 1589.1343 | 1660.3841 | 1710.9307 |
| 1779.0309 | 1843.5946 | 3059.1341 |
| 3123.1621 | 3134.0731 | 3158.6736 |
| 3212.5358 | 3914.8460 | 3946.4875 |

**R3**, $CH_3C(O)CH_3 \cdot (H_2O)_3$

| | | | |
|---|---|---|---|
| O | 0.132863 | 2.040051 | -0.505067 |
| H | 0.081234 | 1.912367 | -1.452584 |
| H | 0.986379 | 0.661928 | 1.877864 |
| C | 0.624698 | -0.261499 | 1.426789 |
| C | 1.255081 | -0.497987 | 0.077023 |
| O | 0.706158 | -1.171432 | -0.774422 |
| C | 2.618478 | 0.087925 | -0.151346 |
| H | -0.458176 | -0.222048 | 1.324398 |
| H | 0.893675 | -1.100301 | 2.078641 |
| H | 3.039165 | -0.281397 | -1.085408 |
| H | 3.282752 | -0.144226 | 0.685956 |
| H | 2.496570 | 1.173393 | -0.193048 |
| O | -1.982535 | -1.579839 | -0.383045 |
| H | -2.084322 | -2.310109 | 0.226315 |
| H | -1.029292 | -1.547285 | -0.595160 |
| H | -2.382439 | 0.106888 | -0.009487 |
| O | -2.383358 | 1.063085 | 0.187746 |
| H | -2.842542 | 1.162058 | 1.020540 |
| H | -0.757570 | 1.803188 | -0.194522 |

Frequencies

| | | |
|---|---|---|
| 41.1800 | 65.7447 | 76.2892 |
| 97.0629 | 108.6944 | 118.9635 |
| 148.9966 | 169.1855 | 197.5638 |
| 206.7886 | 228.1717 | 246.4648 |
| 252.8162 | 276.4639 | 368.4378 |
| 400.6943 | 447.6077 | 491.0581 |
| 546.8672 | 562.6565 | 680.4393 |
| 754.6271 | 806.4284 | 877.6061 |
| 906.5640 | 940.7528 | 1094.8088 |

| | | |
|---|---|---|
| 1123.6783 | 1266.8688 | 1387.8148 |
| 1405.0098 | 1466.2002 | 1471.5532 |
| 1482.2599 | 1498.4477 | 1670.8468 |
| 1687.3373 | 1697.6131 | 1806.9347 |
| 3048.6062 | 3052.1206 | 3130.3434 |
| 3139.9165 | 3169.1433 | 3184.4865 |
| 3545.4079 | 3613.3910 | 3680.4300 |
| 3952.7815 | 3967.8299 | 3973.9560 |

**P3**, $CH_3C(OH)CH_2\cdot(H_2O)_3$

| | | | |
|---|---|---|---|
| O | -0.684412 | 1.868316 | -0.593280 |
| H | -0.320740 | 1.296997 | -1.277276 |
| H | -0.091490 | 1.700105 | 0.149661 |
| C | 0.873794 | -0.135687 | 1.396447 |
| C | 1.484630 | -0.210304 | 0.205837 |
| O | 0.889967 | -0.647207 | -0.923676 |
| C | 2.893244 | 0.225567 | -0.047589 |
| H | -0.150120 | -0.468498 | 1.515933 |
| H | 1.412888 | 0.207735 | 2.268591 |
| H | 2.908804 | 1.004617 | -0.815143 |
| H | 3.476005 | -0.616742 | -0.428896 |
| H | 3.363007 | 0.607765 | 0.858315 |
| O | -1.489363 | -1.738148 | -0.352745 |
| H | -1.548190 | -2.451630 | 0.281571 |
| H | 0.031821 | -1.083289 | -0.712619 |
| H | -2.107269 | -1.040271 | -0.052226 |
| O | -2.870815 | 0.478564 | 0.330955 |
| H | -3.037029 | 0.772603 | 1.226088 |
| H | -2.210714 | 1.100945 | -0.032197 |

Frequencies

| | | |
|---|---|---|
| 34.6909 | 56.2036 | 60.0889 |
| 100.5997 | 130.5001 | 180.8361 |
| 183.2893 | 224.3933 | 242.8117 |
| 256.7564 | 259.2569 | 277.1800 |
| 290.3716 | 365.9861 | 428.6054 |
| 497.9260 | 528.4641 | 540.9207 |
| 560.4671 | 624.3563 | 725.9231 |
| 751.7994 | 820.2907 | 855.2427 |
| 885.1849 | 1000.2483 | 1033.9505 |
| 1053.4576 | 1079.1137 | 1314.7901 |
| 1411.8355 | 1422.2280 | 1476.2327 |
| 1491.7317 | 1503.9942 | 1677.8933 |
| 1684.5655 | 1703.1489 | 1722.0918 |
| 3050.9458 | 3117.3434 | 3156.0753 |
| 3171.9182 | 3268.4103 | 3389.6866 |
| 3529.1923 | 3597.5796 | 3806.5648 |

| | | | |
|---|---|---|---|
| 3891.5462 | 3966.0377 | 3970.5331 | |
| **TS3** | | | |
| O | 0.836883 | 1.951816 | 0.209325 |
| H | 0.477792 | 2.150469 | 1.076955 |
| H | 0.064821 | 1.422862 | -0.345816 |
| C | -0.854219 | 0.432919 | -1.205677 |
| C | -1.425887 | -0.237689 | -0.120313 |
| O | -0.877037 | -1.170285 | 0.538884 |
| C | -2.773244 | 0.215119 | 0.399369 |
| H | -0.036051 | -0.057613 | -1.729382 |
| H | -1.490267 | 1.064945 | -1.816110 |
| H | -2.710568 | 0.378487 | 1.477824 |
| H | -3.495704 | -0.589598 | 0.238214 |
| H | -3.135685 | 1.118323 | -0.093426 |
| O | 1.413401 | -1.761654 | -0.090679 |
| H | 1.411594 | -2.136595 | -0.971316 |
| H | 0.393268 | -1.549325 | 0.166646 |
| H | 2.113517 | -0.648147 | 0.081114 |
| O | 2.587546 | 0.321342 | 0.286756 |
| H | 3.273367 | 0.505662 | -0.355877 |
| H | 1.767672 | 1.148680 | 0.276615 |
| | | | |
| Frequencies | | | |
| -1101.1789 | 41.8804 | 78.0259 | |
| 93.3127 | 112.7206 | 136.7226 | |
| 156.1908 | 325.3637 | 362.9665 | |
| 387.3985 | 402.9528 | 471.2057 | |
| 484.2237 | 547.4066 | 564.4771 | |
| 594.8418 | 633.2741 | 655.7461 | |
| 687.0627 | 702.5376 | 800.5369 | |
| 858.8160 | 873.3081 | 1004.9825 | |
| 1056.3676 | 1088.7940 | 1121.2025 | |
| 1235.0970 | 1296.1367 | 1361.3028 | |
| 1406.3400 | 1475.4764 | 1484.5599 | |
| 1492.4828 | 1545.2745 | 1561.5631 | |
| 1619.2598 | 1679.6432 | 1727.3953 | |
| 1773.2438 | 1830.7405 | 1898.9257 | |
| 2095.9545 | 3057.2735 | 3121.4497 | |
| 3130.1715 | 3154.0591 | 3212.7055 | |
| 3915.6591 | 3946.6844 | 3950.9369 | |
| **R4**, $CH_3C(O)CH_3 \cdot (H_2O)_4$ | | | |
| O | 0.093465 | 1.838235 | 1.213973 |
| H | 0.017188 | 2.709998 | 1.601186 |
| H | 0.931909 | -0.405856 | 1.841861 |
| C | 1.239194 | -1.223550 | 1.181342 |
| C | 1.376098 | -0.627852 | -0.189899 |

| | | | |
|---|---|---|---|
| O | 0.578295 | -0.870615 | -1.080790 |
| C | 2.496394 | 0.348716 | -0.404860 |
| H | 0.480359 | -2.004481 | 1.196340 |
| H | 2.197257 | -1.603783 | 1.542700 |
| H | 2.546599 | 0.648998 | -1.450358 |
| H | 3.450655 | -0.075843 | -0.083856 |
| H | 2.287913 | 1.219845 | 0.223813 |
| O | -1.662612 | -2.126443 | -0.050770 |
| H | -2.201089 | -2.658732 | -0.635799 |
| H | -0.906387 | -1.817075 | -0.578470 |
| O | -2.409590 | 0.511138 | 0.496099 |
| H | -1.728003 | 0.800560 | 1.114522 |
| H | -2.287693 | -0.448969 | 0.416721 |
| H | -0.102842 | 1.955096 | 0.260363 |
| O | -0.784930 | 1.703482 | -1.367311 |
| H | -0.313427 | 0.948089 | -1.731695 |
| H | -1.559577 | 1.301889 | -0.926431 |

Frequencies

| | | |
|---|---|---|
| 36.6384 | 52.5336 | 71.3077 |
| 95.4330 | 105.5281 | 110.6062 |
| 145.9467 | 150.0704 | 156.9933 |
| 178.6942 | 201.1180 | 219.7177 |
| 230.8657 | 256.5956 | 266.9663 |
| 281.9999 | 401.7244 | 410.2301 |
| 413.4460 | 451.2319 | 500.0349 |
| 556.1242 | 564.3747 | 582.5914 |
| 603.4230 | 661.7375 | 768.2035 |
| 819.8193 | 857.8502 | 886.3902 |
| 929.2765 | 1045.1527 | 1105.1158 |
| 1134.9303 | 1275.8934 | 1394.1418 |
| 1403.6386 | 1468.2343 | 1473.1791 |
| 1483.8306 | 1496.5961 | 1657.7996 |
| 1673.3370 | 1691.0281 | 1707.0452 |
| 1793.0343 | 3047.2824 | 3052.6609 |
| 3124.4442 | 3131.3136 | 3168.7571 |
| 3171.7043 | 3483.0001 | 3588.3273 |
| 3643.4194 | 3707.0849 | 3830.1673 |
| 3877.7119 | 3960.5077 | 3966.0009 |

**P4**, $CH_3C(OH)CH_2 \cdot (H_2O)_4$

| | | | |
|---|---|---|---|
| O | -0.638637 | 2.902178 | -0.409758 |
| H | -1.310321 | 3.205439 | 0.202616 |
| H | -0.995542 | 2.089167 | -0.789713 |
| C | -0.735729 | -0.159586 | -1.226819 |
| C | -1.339227 | -0.510548 | -0.076108 |
| O | -0.788308 | -0.380538 | 1.139441 |
| C | -2.698757 | -1.134204 | -0.008208 |

| | | | |
|---|---|---|---|
| H | 0.274116 | 0.234593 | -1.230366 |
| H | -1.241055 | -0.299173 | -2.173069 |
| H | -3.359334 | -0.517601 | 0.606593 |
| H | -2.628575 | -2.111674 | 0.476838 |
| H | -3.135960 | -1.258423 | -0.998607 |
| O | 1.269864 | -2.307107 | 0.072253 |
| H | 0.592347 | -2.143866 | -0.592647 |
| H | 0.834706 | -2.032082 | 0.885440 |
| O | 2.905363 | -0.128673 | -0.468383 |
| H | 3.140974 | -0.114120 | -1.394976 |
| H | 2.474870 | -0.988459 | -0.308325 |
| H | 0.756447 | 2.070858 | 0.551700 |
| O | 1.169719 | 1.344335 | 1.044106 |
| H | -0.003813 | 0.240317 | 1.116687 |
| H | 1.899412 | 1.009476 | 0.493370 |

Frequencies

| | | |
|---|---|---|
| 39.0847 | 58.5108 | 64.1985 |
| 72.5896 | 91.4771 | 131.6118 |
| 146.7840 | 175.6413 | 181.2073 |
| 194.8942 | 218.7389 | 222.0621 |
| 229.0549 | 241.9050 | 255.6430 |
| 269.2900 | 309.3426 | 359.9764 |
| 435.5946 | 478.5246 | 491.5743 |
| 536.8032 | 557.1292 | 574.3137 |
| 659.3219 | 713.5709 | 755.1933 |
| 767.5362 | 839.8882 | 858.8399 |
| 887.7069 | 1007.2441 | 1041.0440 |
| 1073.2514 | 1161.5568 | 1334.9533 |
| 1420.3957 | 1429.1917 | 1475.1501 |
| 1492.6574 | 1525.1660 | 1642.0457 |
| 1674.7969 | 1675.6713 | 1692.7426 |
| 1705.2612 | 3052.6233 | 3095.1296 |
| 3119.2647 | 3156.7811 | 3165.1752 |
| 3263.5659 | 3603.0242 | 3657.3639 |
| 3721.8960 | 3788.2795 | 3836.4065 |
| 3903.8896 | 3955.8399 | 3975.1935 |

**TS4**

| | | | |
|---|---|---|---|
| O | 0.218480 | 2.285063 | 0.552848 |
| H | 0.895680 | 2.889629 | 0.242121 |
| H | 0.707267 | 1.348193 | 0.931576 |
| C | 1.100301 | -0.093681 | 1.317702 |
| C | 1.493442 | -0.494188 | 0.034519 |
| O | 0.682968 | -0.833511 | -0.882492 |
| C | 2.954173 | -0.438960 | -0.353680 |
| H | 0.104819 | -0.395901 | 1.638095 |

| | | | |
|---|---|---|---|
| H | 1.853715 | -0.025245 | 2.095922 |
| H | 3.061561 | 0.116546 | -1.288371 |
| H | 3.296291 | -1.459092 | -0.548396 |
| H | 3.584476 | 0.003287 | 0.419156 |
| O | -1.458937 | -2.086450 | 0.199327 |
| H | -1.137761 | -2.627285 | 0.919807 |
| H | -0.656162 | -1.727378 | -0.241939 |
| O | -2.996356 | 0.101209 | 0.172089 |
| H | -3.096375 | 0.454764 | 1.056144 |
| H | -2.583493 | -0.783135 | 0.281193 |
| H | -0.420712 | 1.837893 | -0.340132 |
| O | -1.020197 | 1.192821 | -1.181787 |
| H | -0.446193 | 0.391768 | -1.277182 |
| H | -1.858287 | 0.863872 | -0.759111 |

Frequencies

| | | |
|---|---|---|
| -1151.5063 | 24.1463 | 48.3123 |
| 75.2119 | 81.4212 | 108.8189 |
| 121.4316 | 138.2970 | 198.0650 |
| 226.1843 | 262.7775 | 293.4725 |
| 319.5084 | 331.2552 | 417.7887 |
| 452.4439 | 473.8235 | 512.3051 |
| 541.5494 | 554.4991 | 576.2654 |
| 617.4626 | 643.9794 | 683.3142 |
| 741.4538 | 825.8465 | 855.7029 |
| 868.4678 | 893.1177 | 949.7393 |
| 997.6621 | 1033.5744 | 1056.9173 |
| 1089.1840 | 1238.1733 | 1330.9252 |
| 1399.5378 | 1471.3381 | 1483.6717 |
| 1491.6583 | 1512.9082 | 1583.8613 |
| 1659.0255 | 1676.2361 | 1693.7332 |
| 1702.1649 | 1753.8708 | 1810.7023 |
| 3058.4548 | 3125.9694 | 3131.9185 |
| 3154.2571 | 3219.5527 | 3249.2962 |
| 3357.8431 | 3431.0681 | 3513.6859 |
| 3917.6492 | 3956.3965 | 3967.8667 |

**R5**, $CH_3C(O)CH_3 \cdot (H_2O)_5$

| | | | |
|---|---|---|---|
| O | 0.699002 | 1.108780 | 1.658158 |
| H | 0.712289 | 1.643453 | 2.451858 |
| H | 1.117183 | -2.610708 | 1.165651 |
| C | 0.513621 | -2.048926 | 0.453545 |
| C | 1.316475 | -1.036440 | -0.306344 |
| O | 0.836873 | -0.449894 | -1.267916 |
| C | 2.710486 | -0.743104 | 0.155583 |
| H | -0.283206 | -1.523632 | 0.994982 |
| H | 0.024817 | -2.731272 | -0.245504 |

| | | | |
|---|---|---|---|
| H | 3.183846 | -0.001713 | -0.486623 |
| H | 3.299134 | -1.664713 | 0.170591 |
| H | 2.646188 | -0.364534 | 1.178833 |
| O | 0.928420 | 2.412051 | -0.731888 |
| H | -0.038476 | 2.460417 | -0.649979 |
| H | 1.069962 | 1.607256 | -1.243915 |
| H | 0.994310 | 1.692407 | 0.930695 |
| O | -1.658573 | 1.675750 | 0.150774 |
| H | -1.856545 | 0.982791 | -0.495499 |
| H | -1.043423 | 1.262096 | 0.775188 |
| O | -2.531325 | -1.048596 | 1.212224 |
| H | -2.736363 | -0.120807 | 1.348520 |
| H | -2.504704 | -1.126319 | 0.250452 |
| O | -1.865901 | -0.602029 | -1.518438 |
| H | -0.891162 | -0.646558 | -1.574221 |
| H | -2.205303 | -0.655840 | -2.411048 |

Frequencies

| | | |
|---|---|---|
| 45.6764 | 62.1323 | 64.1537 |
| 70.0399 | 84.4352 | 112.7429 |
| 118.2946 | 120.6913 | 153.0717 |
| 159.1789 | 173.5995 | 182.6938 |
| 190.0953 | 208.5263 | 218.5322 |
| 226.6573 | 253.3835 | 260.3037 |
| 302.7774 | 330.0075 | 376.6258 |
| 396.3333 | 406.8030 | 431.0414 |
| 443.0437 | 513.9710 | 556.1186 |
| 571.6776 | 599.1736 | 652.1645 |
| 697.4227 | 701.5776 | 759.4539 |
| 816.4975 | 858.0422 | 892.0539 |
| 960.9949 | 1026.3506 | 1093.5940 |
| 1122.9064 | 1276.9979 | 1394.2733 |
| 1400.3853 | 1465.5775 | 1479.5976 |
| 1488.3037 | 1496.2573 | 1645.3269 |
| 1661.3854 | 1681.9865 | 1696.4318 |
| 1709.3965 | 1776.3535 | 3031.6569 |
| 3053.4431 | 3115.2110 | 3133.5302 |
| 3160.9795 | 3169.4706 | 3534.7974 |
| 3548.2581 | 3688.8516 | 3726.9481 |
| 3773.2782 | 3812.3599 | 3844.6824 |
| 3925.6529 | 3960.4761 | 3971.0234 |

**P5**, $CH_3C(OH)CH_2\cdot(H_2O)_5$

| | | | |
|---|---|---|---|
| O | -0.002421 | 0.679273 | 1.995030 |
| H | 0.699512 | 0.040204 | 1.837780 |
| H | -0.817338 | 0.158940 | 1.905737 |
| C | 2.043482 | -1.619305 | 0.323343 |

| | | | |
|---|---|---|---|
| C | 1.962047 | -0.423399 | -0.261433 |
| O | 0.955231 | -0.150360 | -1.136921 |
| C | 2.939783 | 0.694984 | -0.065403 |
| H | 1.292675 | -2.378326 | 0.137800 |
| H | 2.879780 | -1.866281 | 0.962928 |
| H | 2.426650 | 1.591826 | 0.293285 |
| H | 3.404348 | 0.949342 | -1.021892 |
| H | 3.716397 | 0.421635 | 0.648630 |
| O | -0.126668 | 2.085964 | -0.404095 |
| H | -1.058341 | 1.937244 | -0.649988 |
| H | 0.627094 | 0.787585 | -0.996114 |
| H | -0.093609 | 1.819871 | 0.533772 |
| O | -2.648888 | 0.999881 | -0.858279 |
| H | -2.388217 | 0.197685 | -1.326580 |
| H | -2.833925 | 0.661647 | 0.026615 |
| O | -2.251217 | -0.817233 | 1.301527 |
| H | -2.765244 | -1.418156 | 1.839458 |
| H | -1.943884 | -1.312885 | 0.518944 |
| O | -1.312803 | -1.555154 | -1.122905 |
| H | -0.428882 | -1.126204 | -1.183106 |
| H | -1.294755 | -2.316774 | -1.701167 |

Frequencies

| | | |
|---|---|---|
| 47.2793 | 58.6488 | 70.9944 |
| 77.9094 | 86.1108 | 110.0908 |
| 124.1502 | 136.2118 | 185.0378 |
| 191.0531 | 212.4202 | 223.1347 |
| 236.3456 | 254.4180 | 261.8796 |
| 271.6734 | 290.2139 | 303.2576 |
| 374.0229 | 398.7539 | 433.5280 |
| 456.4866 | 498.1277 | 512.7807 |
| 525.7724 | 546.7404 | 580.6189 |
| 595.2620 | 708.8419 | 743.3143 |
| 753.7058 | 772.6844 | 807.8863 |
| 852.7766 | 860.7753 | 874.8648 |
| 921.0295 | 996.1346 | 1036.2430 |
| 1068.0675 | 1081.9568 | 1326.1928 |
| 1416.4239 | 1435.5513 | 1477.9524 |
| 1494.0987 | 1557.5817 | 1656.2637 |
| 1674.9898 | 1691.4012 | 1717.0852 |
| 1745.2861 | 1759.0985 | 3043.5535 |
| 3051.1913 | 3118.0066 | 3154.5310 |
| 3168.7625 | 3265.6897 | 3420.8369 |
| 3598.7869 | 3624.0456 | 3641.6743 |
| 3715.7035 | 3808.9162 | 3859.9934 |
| 3873.2800 | 3970.3900 | 3973.6327 |

**TS5**

| | | | |
|---|---|---|---|
| O | 1.707122 | 1.471142 | 1.197264 |
| H | 2.639454 | 1.495471 | 1.424401 |
| H | 1.342957 | 0.469017 | 1.327410 |
| C | 0.620391 | -1.028466 | 1.355149 |
| C | 0.949504 | -1.140912 | 0.023416 |
| O | 0.295260 | -0.558457 | -0.929759 |
| C | 2.198524 | -1.876149 | -0.405797 |
| H | -0.368545 | -0.662141 | 1.626788 |
| H | 1.148626 | -1.633381 | 2.084310 |
| H | 2.856707 | -1.199639 | -0.960175 |
| H | 1.914833 | -2.673309 | -1.097674 |
| H | 2.744783 | -2.309517 | 0.432922 |
| O | 1.189733 | 1.899110 | -1.118960 |
| H | 0.271626 | 2.239772 | -1.088198 |
| H | 1.021503 | 0.949496 | -1.358039 |
| H | 1.511030 | 1.747871 | 0.101382 |
| O | -1.383394 | 1.613857 | -0.536964 |
| H | -2.176660 | 1.458751 | -1.054788 |
| H | -0.954321 | 0.735209 | -0.515313 |
| O | -2.614338 | 0.000416 | 1.614144 |
| H | -2.307262 | 0.856755 | 1.304716 |
| H | -2.667061 | -0.507632 | 0.792085 |
| O | -2.381630 | -1.119069 | -1.042437 |
| H | -1.409219 | -1.137540 | -1.114338 |
| H | -2.680991 | -2.012016 | -1.208387 |

Frequencies

| | | |
|---|---|---|
| -697.4828 | 34.0930 | 58.8356 |
| 69.5737 | 84.3632 | 102.3268 |
| 120.6561 | 134.7412 | 141.9633 |
| 148.7912 | 159.6099 | 201.0831 |
| 211.7111 | 238.0609 | 243.8180 |
| 328.6209 | 346.0354 | 390.4713 |
| 444.4603 | 450.9147 | 457.4393 |
| 471.5250 | 498.7321 | 538.2455 |
| 555.4317 | 588.6384 | 606.6579 |
| 626.5804 | 652.7140 | 717.1667 |
| 745.1388 | 772.4652 | 820.8103 |
| 869.0879 | 880.4048 | 923.7360 |
| 1005.2029 | 1022.0099 | 1063.8746 |
| 1081.3406 | 1164.8635 | 1361.8641 |
| 1420.4017 | 1462.8478 | 1478.6261 |
| 1491.0553 | 1549.9714 | 1601.9385 |
| 1656.8424 | 1690.8107 | 1705.0719 |
| 1731.4117 | 1753.1977 | 1789.9450 |

| | | |
|---|---|---|
| 2032.1046 | 3051.3712 | 3121.2586 |
| 3124.9671 | 3153.3115 | 3231.7892 |
| 3312.3412 | 3543.1700 | 3589.8244 |
| 3623.9568 | 3771.4198 | 3901.8088 |
| 3917.8042 | 3925.4816 | 3969.1528 |

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