Supporting Information:

Formation of Lactic Acid ($CH_3CH(OH)COOH$), a Metabolic Keystone for the Molecular Origins of Life, in Interstellar Ice Analogues

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Methods

Experimental. The experiments were conducted in an ultrahigh vacuum chamber evacuated by magnetically suspended turbomolecular pumps (Osaka, TG1300MUCWB and TG420MCAB) and an oil-free scroll pump (XDS35i, BOC Edwards) at pressures of a few 10^{-11} Torr.[1,2] A closed-cycle helium cryostat (Sumitomo Heavy Industries, RDK415E) was used to cool a polished silver substrate to temperatures as low as 5 K. The cryostat allows for vertical translation and horizontal rotation via an adjustable bellows (McAllister, BLT86) and a rotatable flange (Thermionics Vacuum Products, RNN-600/FA/MCO), respectively.[1] The carbon dioxide samples used in the experiment included carbon dioxide (CO_2, Airgas, 99.999%), carbon dioxide-^{13}C ($^{13}CO_2$, Sigma-Aldrich, 99 atom % ^{13}C), carbon dioxide-$^{18}O_2$ ($C^{18}O_2$, Sigma-Aldrich, 95 atom % ^{18}O), and carbon dioxide-^{13}C-$^{18}O_2$ ($^{13}C^{18}O_2$, Sigma-Aldrich, 99 atom % ^{13}C, 95 atom % ^{18}O). Isotopically labeled ethanol sample—ethanol-d_6 (CD_3CD_2OD; Cambridge Isotope Laboratories, 99 atom % D), ethanol-d_3 (CD_3CH_2OD; Sigma Aldrich, 99 atom % D), ethanol-d_2 (CH_3CD_2OD; CDN isotopes, 98.9 atom % D), or ethanol-$^{13}C_2$ ($^{13}CH_3{}^{13}CH_2OH$; Sigma Aldrich, 99 atom % ^{13}C)—was filled into a borosilicate vial interfaced with an ultrahigh vacuum chamber and subjected to several freeze-thaw cycles using liquid nitrogen to remove residual atmospheric gases. After the substrate was cooled to 4.9 ± 0.2 K, carbon dioxide gas and ethanol vapor were deposited separately onto the silver substrate via glass capillary arrays at partial pressures of 2×10^{-8} Torr for both carbon dioxide and ethanol. Although the temperature of 5 K is slightly below the typical 10–20 K range observed in cold molecular clouds, this lower temperature effectively immobilizes reactive species within the ice matrix, providing valuable mechanistic insights into the chemical processes occurring in such cold ices.[3] Laser interferometry was used to monitor the ice thickness during deposition; interference fringes between reflections of the helium-neon laser (CVI Melles-Griot, 25-LHP-230, 632.8 nm) from the silver substrate and the ice surface were recorded using a photodiode.[4] The thickness of the deposited CO_2−CD_3CD_2OD ice was determined to be 950 ± 50 nm (Table S12), based on an average index (n) of 1.24 ± 0.04, derived from the indices of carbon dioxide ice (n = 1.21)[5] at 10 K and that of ethanol ice (n = 1.26).[6] Infrared spectra of the ice mixtures were collected using a Fourier transform infrared (FTIR) spectrometer (Thermo Electron, Nicolet 6700) over the range of 6000−500 cm^{-1} with a resolution of 4 cm^{-1} (Figures S1−S4, Tables S1−S4). FTIR spectra of pure ethanol-d_3 (CD_3CH_2OH) ice and ethanol-d_2 (CH_3CD_2OH) ice were recorded at 5 K with a thickness of 380 ± 50 nm (Figures S10–S11, Tables S8−S9). Utilizing the

absorption bands of pure ethanol ices with known thickness, the thicknesses and column densities of ethanol-d_6, ethanol-d_3, ethanol-d_2, and ethanol-$^{13}C_2$ in the ice mixtures were determined using the integrated area of multiple absorption bands.[7] The ratio of carbon dioxide to ethanol in the CO_2–CD_3CD_2OD ice was estimated to be 1.6 ± 0.3:1 (Table S12). Densities of 0.98 g cm^{-3} and 0.584 g cm^{-3} were used for CO_2 and CH_3CH_2OH ices, respectively.[6,8] Variations in density were used based on the masses of isotopically labeled carbon dioxide and ethanol molecules.

After the deposition, the ice mixtures were irradiated with energetic electrons (SPECS, EQ PU-22, 5 keV), simulating the secondary electrons produced by galactic cosmic rays (GCRs) as they pass through the interstellar ices.[7] The CO_2–CD_3CD_2OD ice was processed at an incidence angle of 70° with a current of 22 nA for 5 minutes, corresponding to doses of 0.21 ± 0.04 eV per CO_2 molecule and 0.34 ± 0.06 eV per CD_3CD_2OD molecule, as calculated via Monte Carlo simulations using the CASINO software suite.[9] These doses simulate secondary electrons generated in the track of GCRs in cold molecular clouds over timescales up to 7×10^5 years.[10] The average penetration depth of electrons in CO_2–CD_3CD_2OD ice was determined to be 370 ± 40 nm. Approximately 99% of the electron energy was deposited within the top 570 ± 50 nm of the ice, well below the total ice thickness of 950 ± 50 nm, thereby preventing interactions between the substrate and electrons. Infrared spectra of the ices were recorded *in situ* before, during, and after irradiation using the FTIR spectrometer. Following irradiation, the ices were heated from 5 to 320 K at a rate of 0.5 K min^{-1} during the temperature-programmed desorption (TPD) phase. During TPD, molecules released into the gas phase were photoionized by pulsed (30 Hz) vacuum ultraviolet (VUV) light, generated via resonant four-wave mixing in a noble gas jet. VUV photons at 11.10 eV were produced through sum frequency generation ($2\omega_1 + \omega_2$), whereas 10.54 eV and 9.34 eV photons were generated via difference frequency generation ($2\omega_1 - \omega_2$). The fundamental laser beam (ω_1 or ω_2) was produced by a tunable dye laser (Sirah Lasertechnik, Cobra-Stretch) pumped by an Nd:YAG laser (Spectra-Physics Quanta Ray PRO 270-30 or 250-30). Detailed VUV generation parameters are listed in Table S13. The VUV light was spatially separated from the fundamental laser beams using a biconvex lithium fluoride lens (Korth Kristalle, R = 131 mm) in an off-axis geometry and was directed 2.0 ± 0.5 mm above the ice surface to ionize the subliming molecules in the gas phase. The VUV photon flux was monitored during TPD with a Faraday cup and used to correct for fluctuations in the TPD profiles. The resulting ions were mass-analyzed using a reflectron time-of-flight mass spectrometer (ReToF-MS, Jordan TOF Products) and

detected with a dual microchannel plate (MCP) detector. The ion signals were amplified, discriminated, and recorded with a multichannel scaler (FAST ComTec, MCS6A). Each mass spectrum featured an ion arrival time resolution of 3.2 ns and an accumulation time of 2 minutes with 3600 sweeps. Note that $C_2H_2O_4$ isomers (90 amu) may be formed via the recombination of two hydroxycarbonyl (HOĊO) radicals, whereas $C_4H_{10}O_2$ isomers (90 amu) can result from the recombination of radicals generated from ethanol (CH_3CH_2OH). To distinguish these species from $C_3H_6O_3$ isomers (90 amu), fully deuterated CO_2−CD_3CD_2OD ices were employed, facilitating clear mass spectrometric differentiation of the isomeric products. A gas phase mass spectrum of L-(+)-lactic acid ($C_3H_6O_3$, Sigma-Aldrich, ≥ 98%) was measured at a photon energy of 11.10 eV (Figure S8).

Computational. The energies and geometries of all the neutral and cationic states of conformers were calculated using the CBS-QB3 composite scheme, which provides accuracy of 4−8 kJ for relative energies, 0.01−0.02 Å for bond lengths, and 1−2° for bond angles. All calculations were performed in the GAUSSIAN 09 software package.[11] Three reaction products—lactic acid (**1**), monoethyl carbonate (**15**), and 3-hydroxypropanoic acid (**16**)—are evaluated for the computational study, reflecting their formation under low-dose irradiation conditions. Each backbone isomer has a number of conformational isomers arising from rotations around single bonds that differ in energies and ionization potentials. To obtain accurate ranges on ionization potentials, it was important to consider all possible conformational isomers, and we generated geometries of all possible conformers for each backbone isomer. Firstly, CBS-QB3 composite scheme calculations were carried out for neutral conformers, which includes geometry optimization and energy evaluation. Then the same procedure was applied for their cations, with their initial geometries taken from the corresponding neutral conformers. Among all considered isomers, monoethyl carbonate (**15**) has the lowest energy with 4 conformers and has the highest ionization potential (Table S6). In comparison with **15**, lactic acid (**1**) and 3-hydroxypropanoic acid (**16**) have slightly higher energies (by 12–56 kJ mol^{-1}), with 10 and 20 conformers identified, respectively (Tables S5 and S7). The Cartesian coordinates, harmonic vibrational frequencies, and infrared intensities of all computed structures are provided in Table S14.

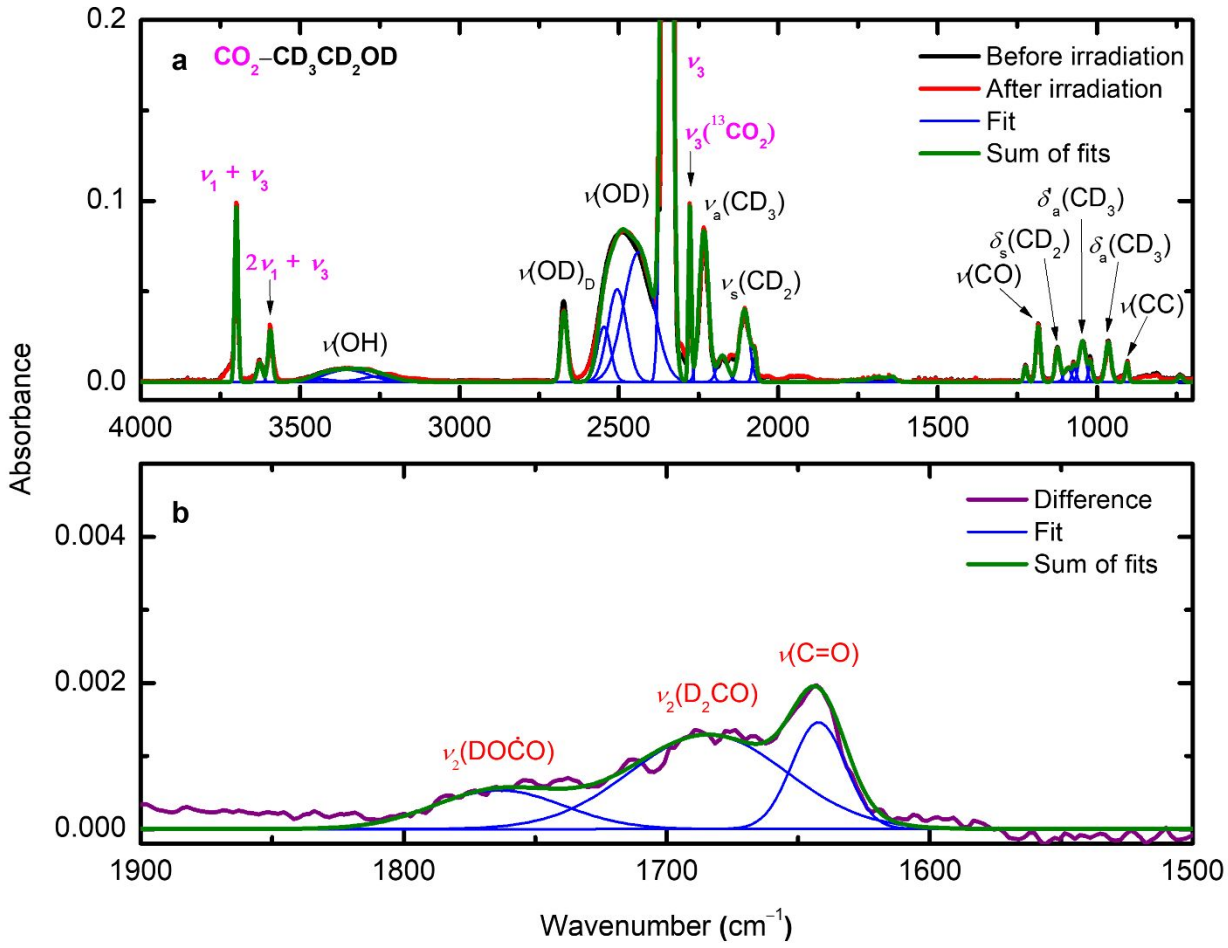


Figure S1. Infrared spectra of (**a**) CO_2–CD_3CD_2OD ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm^{-1} of the difference spectrum. The assignments of the absorptions of CO_2, CD_3CD_2OD, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S1.

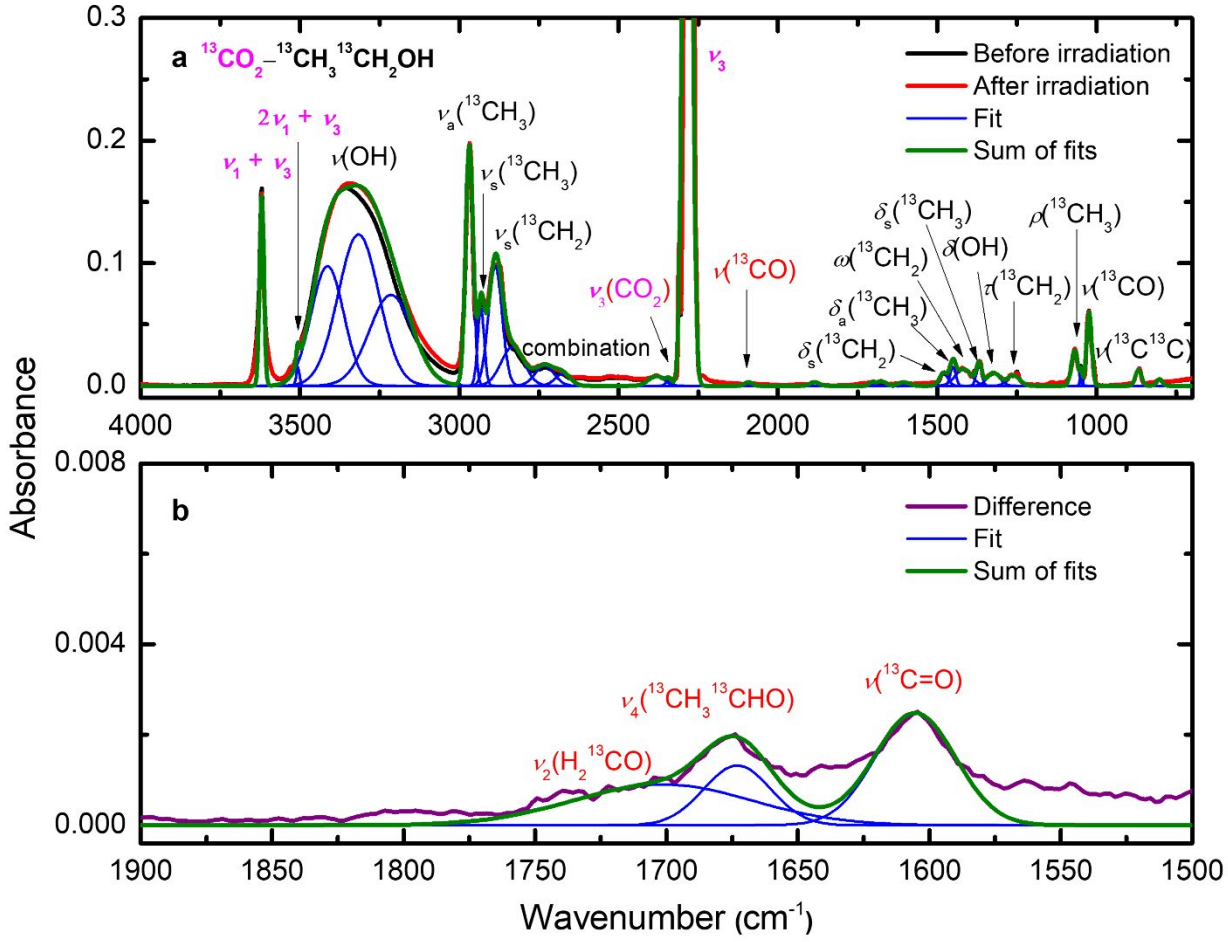


Figure S2. Infrared spectra of (**a**) $^{13}CO_2$–$^{13}CH_3{}^{13}CH_2OH$ ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm^{-1} of the difference spectrum. The assignments of the absorptions of $^{13}CO_2$, $^{13}CH_3{}^{13}CH_2OH$, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S2.

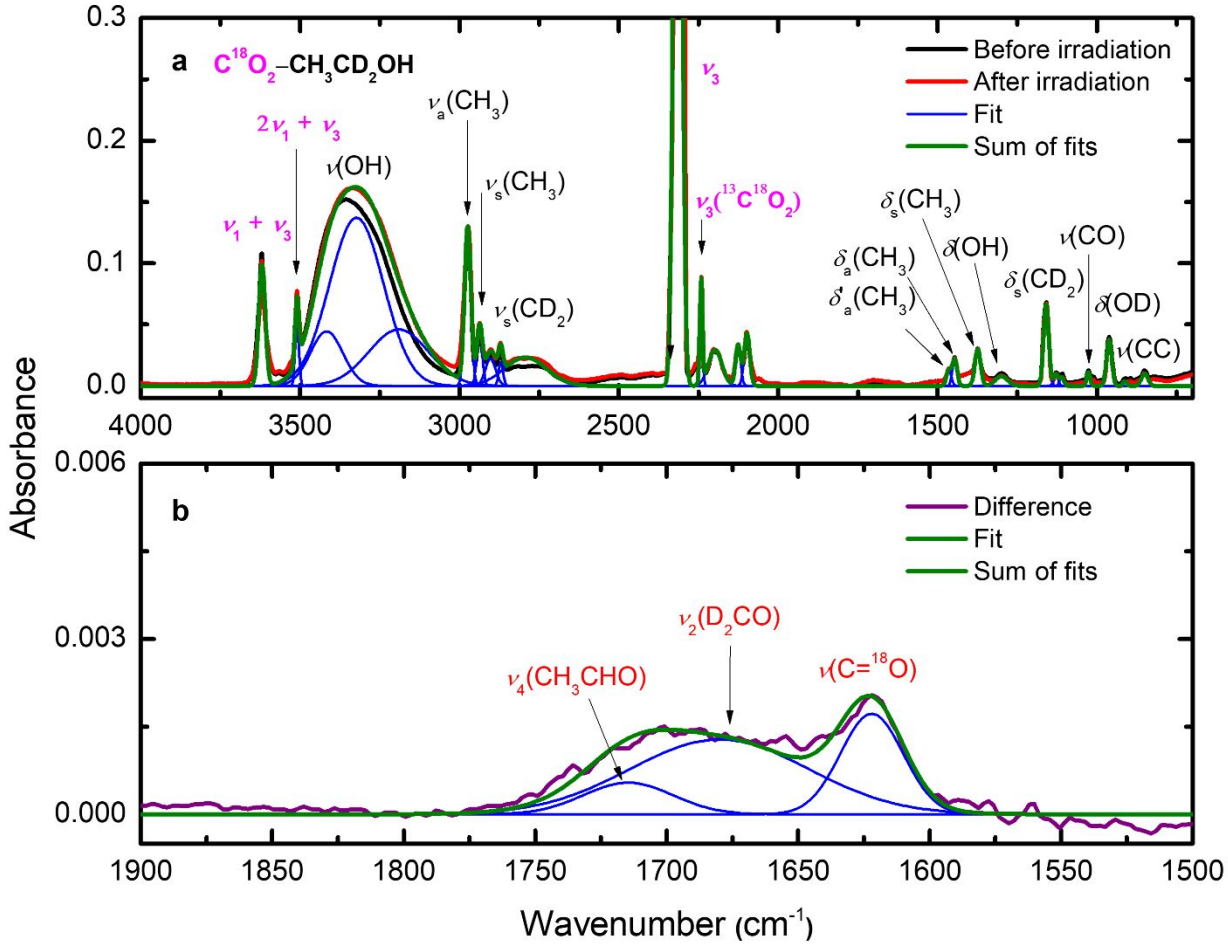


Figure S3. Infrared spectra of (**a**) $C^{18}O_2$–CH_3CD_2OH ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm^{-1} of the difference spectrum. The assignments of the absorptions of $C^{18}O_2$, CH_3CD_2OH, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S3.

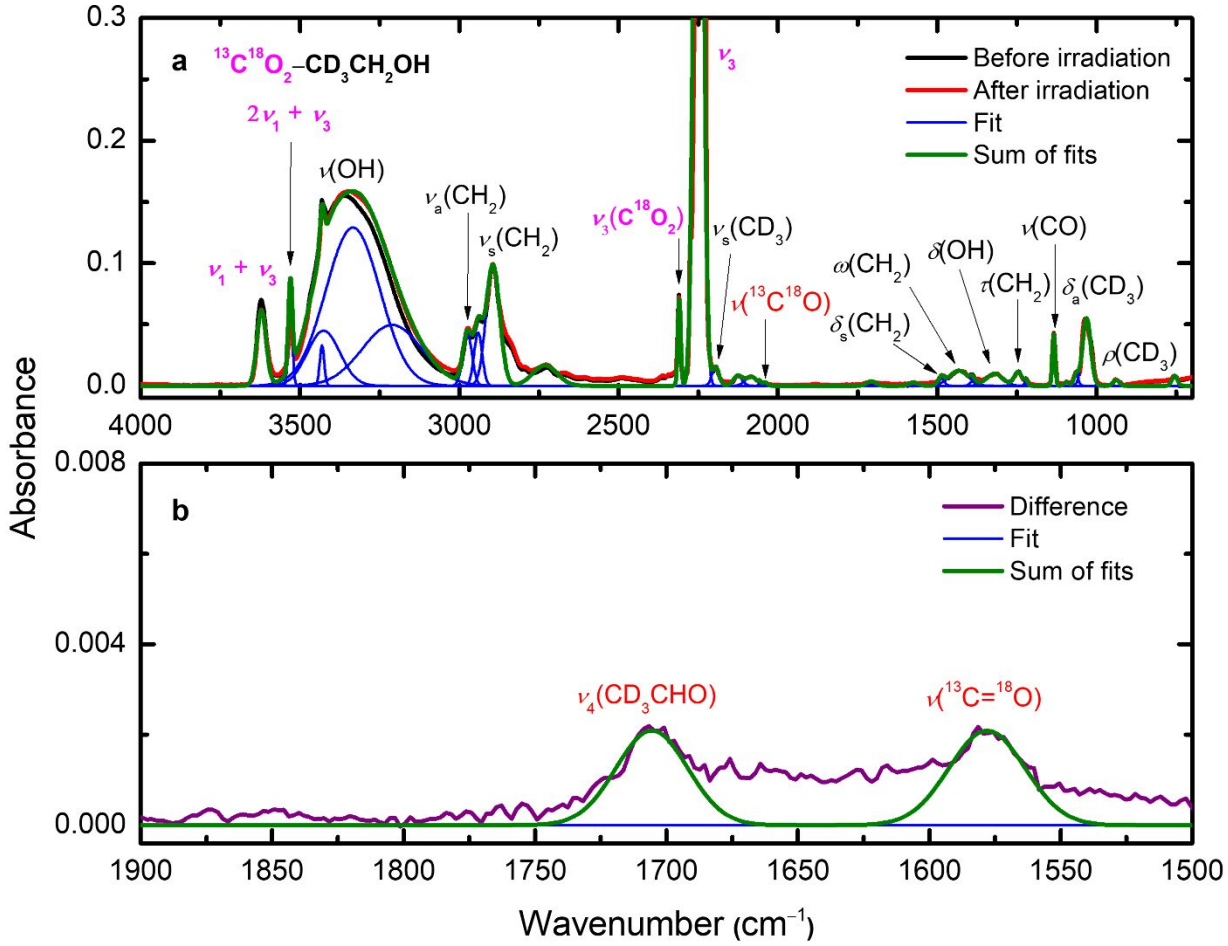


Figure S4. Infrared spectra of (**a**) $^{13}C^{18}O_2$–CD_3CH_2OH ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm^{-1} of the difference spectrum. The assignments of the absorptions of $^{13}C^{18}O_2$, CD_3CH_2OH, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S4.

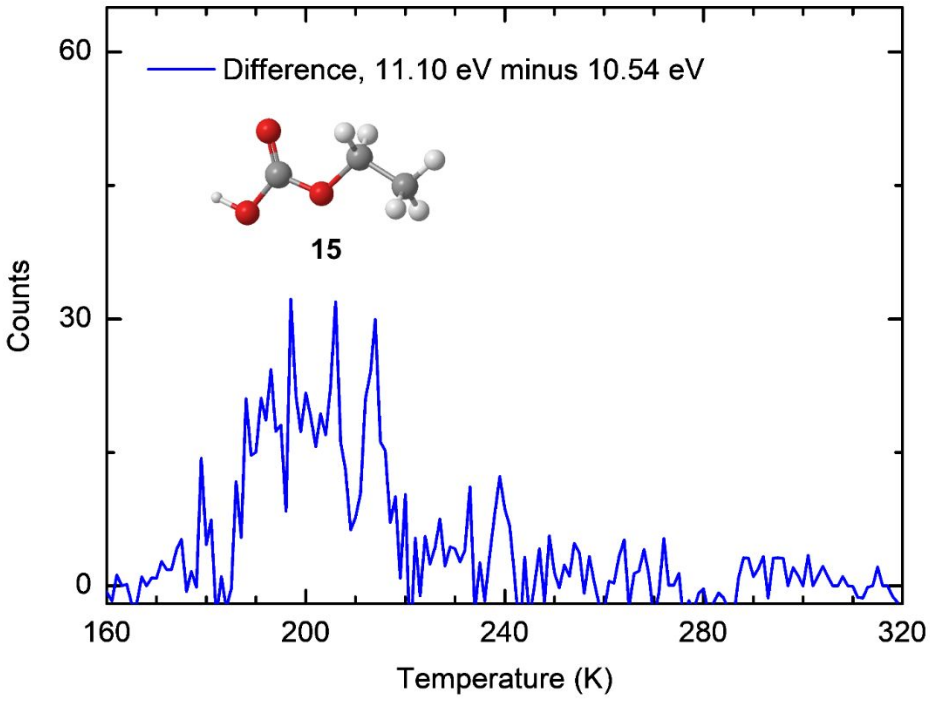


Figure S5. Difference in TPD profiles of *m/z* = 96 measured at photon energies of 11.10 eV and 10.54 eV from irradiated CO_2–CD_3CD_2OD ice.

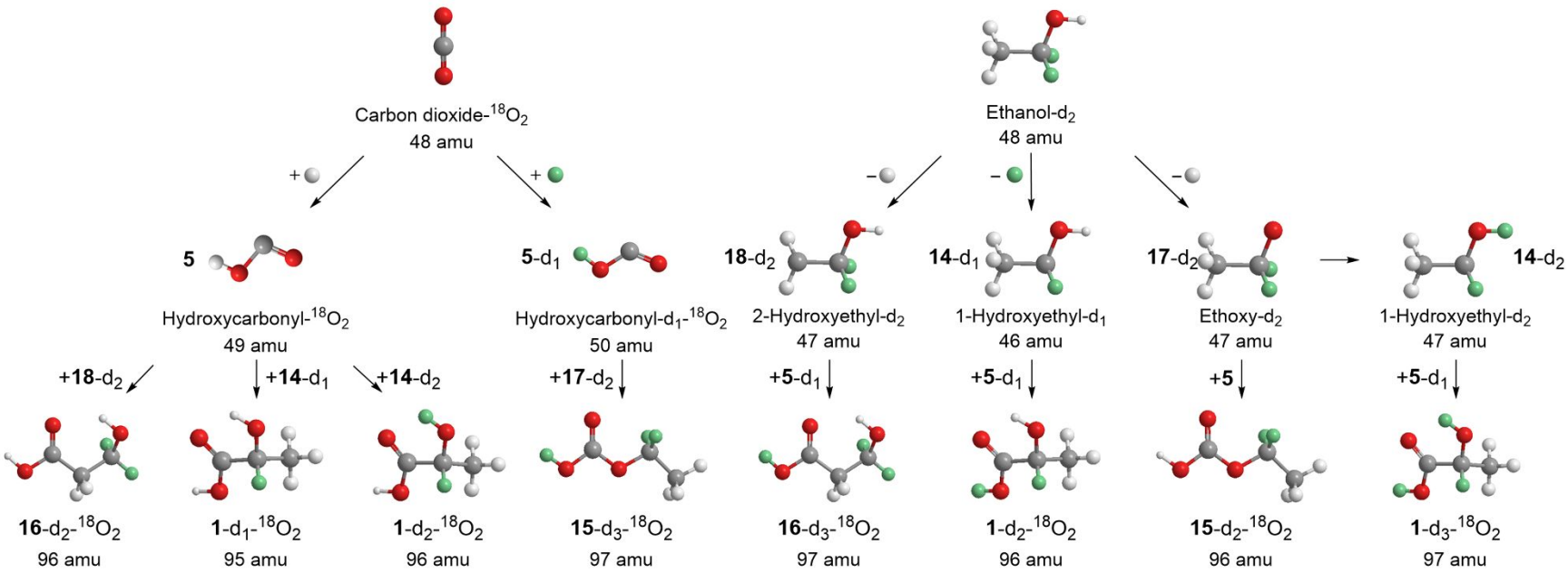


Figure. S6. Proposed formation pathways of isomers **1** (*m/z* = 95, 96, and 97), **15** (*m/z* = 96 and 97), and **16** (*m/z* = 96 and 97) via radical–radical reactions in carbon dioxide-$^{18}O_2$–ethanol-d_2 ($C^{18}O_2$–CH_3CD_2OH) ice after electron irradiation.

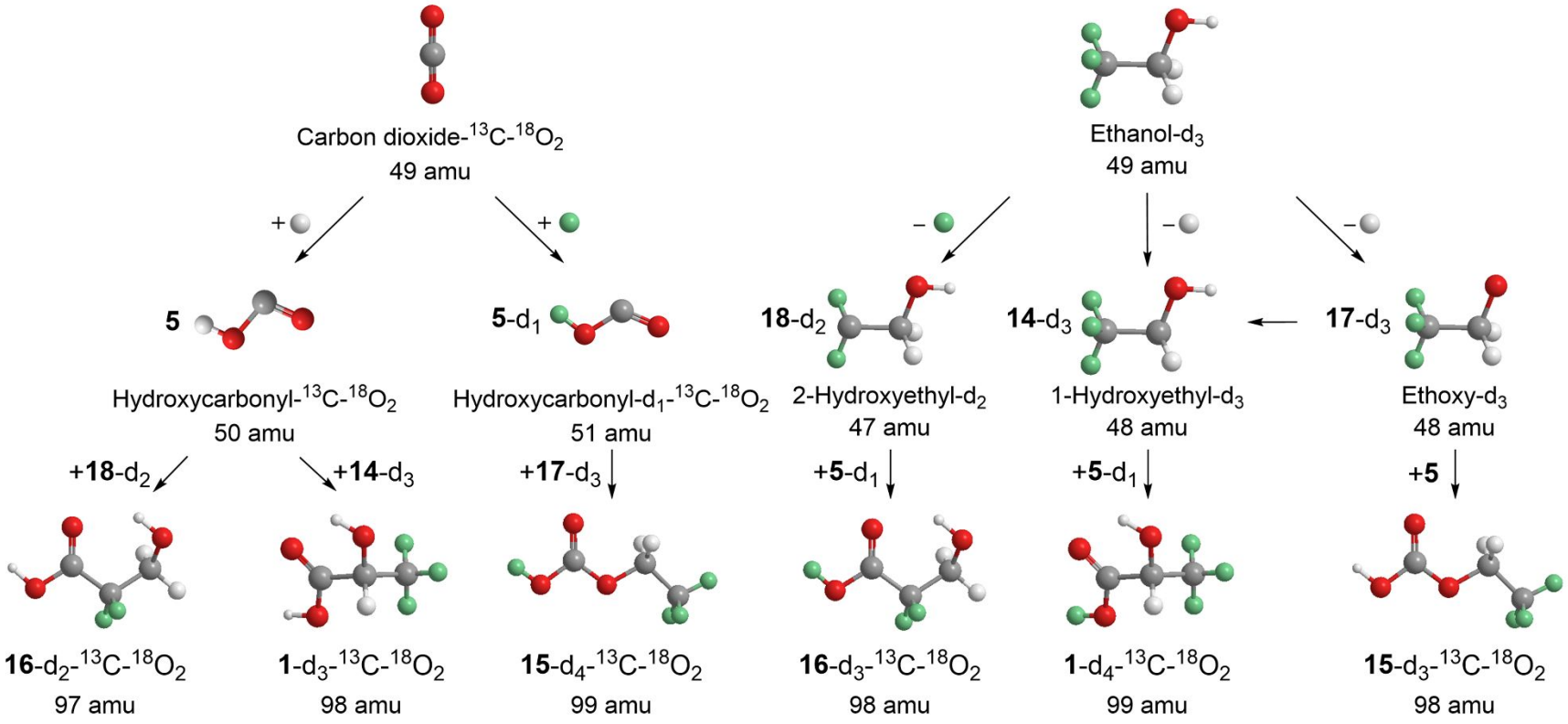


Figure. S7. Proposed formation pathways of isomers **1** (*m/z* = 98 and 99), **15** (*m/z* = 98 and 99), and **16** (*m/z* = 97 and 98) via radical–radical reactions in carbon dioxide-^{13}C-$^{18}O_2$–ethanol-d_3 ($^{13}C^{18}O_2$–CD_3CH_2OH) ice after electron irradiation.

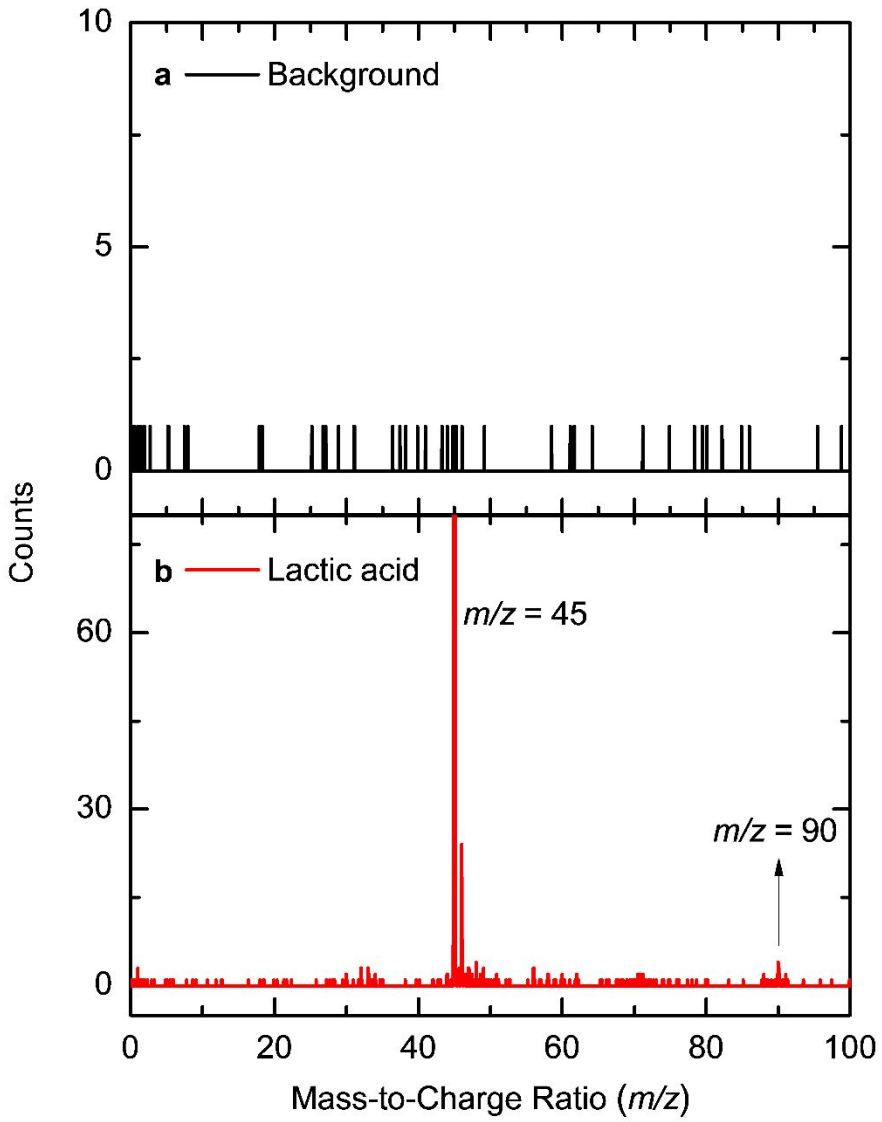


Figure S8. Gas phase mass spectra of lactic acid ($C_3H_6O_3$, m/z = 90) recorded at a VUV photon energy of 11.10 eV, showing a significant fragment signal of m/z = 45. Mass spectra were collected for background gases with 10800 laser pulses (a) and lactic acid at a pressure of 3 $\times 10^{-9}$ Torr with 30030 laser pulses (b).

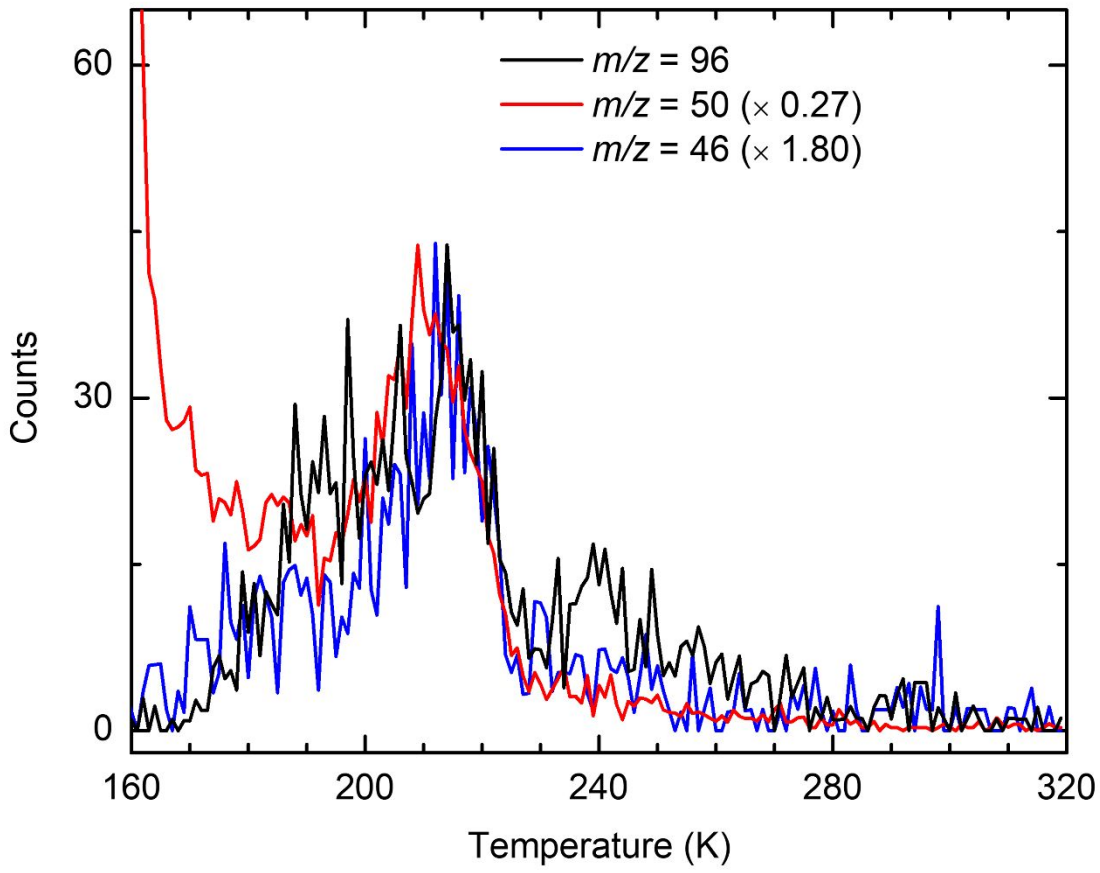


Figure S9. TPD profiles of *m/z* = 46, 50, and 96 in irradiated CO_2–CD_3CD_2OD ice measured at 11.10 eV.

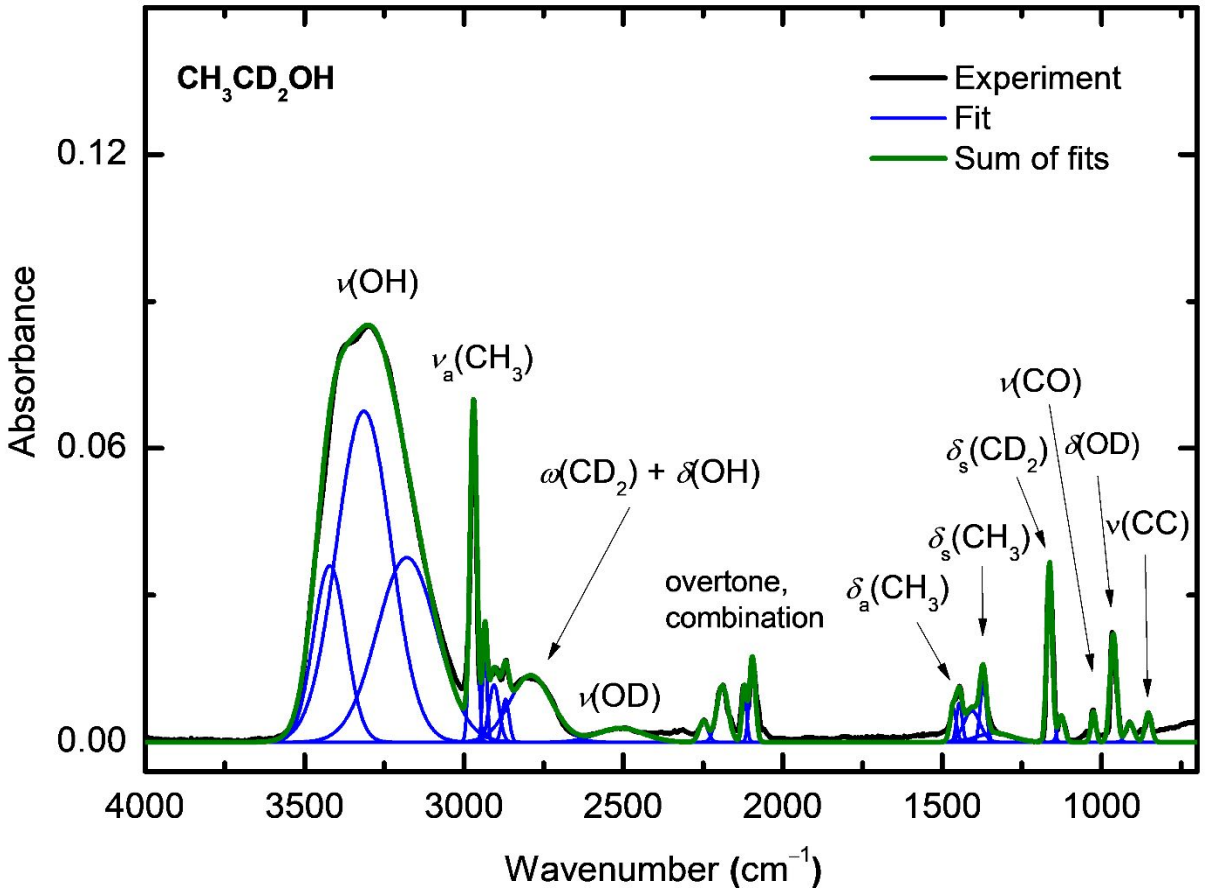


Figure S10. Infrared spectra of CH_3CD_2OH ice with a thickness of 380 ± 50 nm. The assignments of the absorptions are deconvoluted with Gaussian peaks and labeled in blue and green. Detailed assignments are compiled in Table S10.

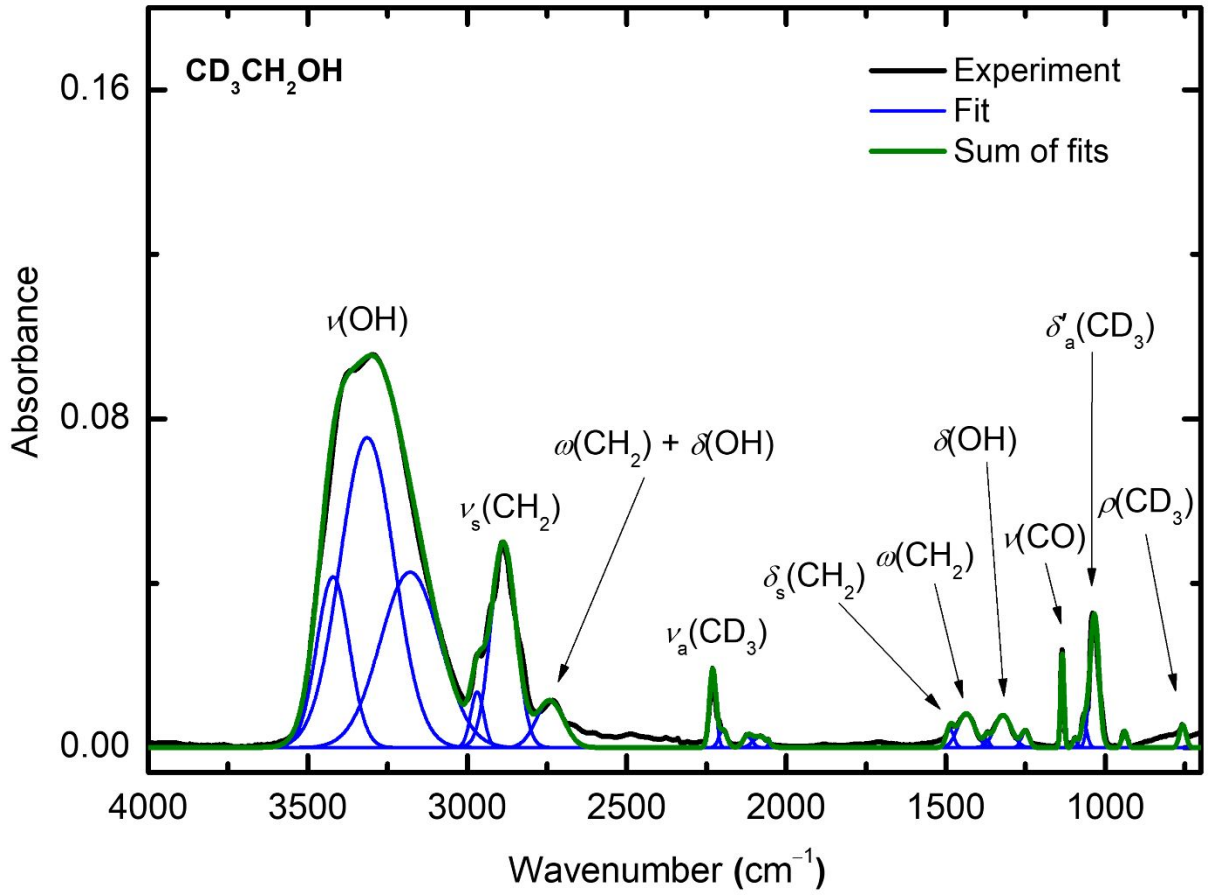


Figure S11. Infrared spectra of CD_3CH_2OH ice with a thickness of 380 ± 50 nm. The assignments of the absorptions are deconvoluted with Gaussian peaks and labeled in blue and green. Detailed assignments are compiled in Table S11.

Table S1. Observed absorption peaks of CO_2−CD_3CD_2OD ice before and after irradiation at 5 K. Vibration mode: stretching (ν), bending (δ), wagging (ω), and rocking (ρ). Indication: asymmetric (a) and symmetric (s).

Pristine ice, absorptions before irradiation (cm^{-1})	
CO_2	Assignment[8]
3700	$\nu_1 + \nu_3$
3593	$2\nu_2 + \nu_3$
2349	C-O asymmetric stretching (ν_3)
2277	C-O asymmetric stretching (ν_3 ($^{13}CO_2$))
CD_3CD_2OD	Assignment[12]
3626	ν(OD) + $\nu_a(CD_3)$
3435, 3353, 3255	ν(OH)
2672	$\nu(OD)_D$
2547, 2505, 2438	ν(OD)
2233	$\nu_a(CD_3)$
2175	$\nu_s(CD_3)$
2106	$\nu_s(CD_2)$
2075	$2\nu_a(CD_3)$
1224	γ(OD) + $\rho(CD_3)$
1184	ν(CO)
1124	$\delta_s(CD_2)$
1092	$\omega(CD_2)$
1071, 1046	$\delta'_a(CD_3)$
1020, 967	$\delta_a(CD_3)$
906	ν(CC)
739	$\rho(CD_3)$
New absorptions after irradiation (cm^{-1})	Assignment[13-15]
1764	ν_2(DOĊO)
1684	$\nu_2(D_2CO)$
1642	C=O stretch

Table S2. Observed absorption peaks of $^{13}CO_2$–$^{13}CH_3{}^{13}CH_2OH$ ice before and after irradiation at 5 K. Vibration mode: stretching (ν), bending (δ), torsion (τ), wagging (ω), and rocking (ρ). Indication: asymmetric (*a*) and symmetric (*s*).

Pristine ice, absorptions before irradiation (cm^{-1})	
$^{13}CO_2$	Assignment[2]
3620	$\nu_1 + \nu_3$
3507	$2\nu_2 + \nu_3$
2343	C-O asymmetric stretching (ν_3 (CO_2))
2282	C-O asymmetric stretching (ν_3)
$^{13}CH_3{}^{13}CH_2OH$	Assignment[7]
3414, 3316, 3215	ν(OH)
2969	$\nu_a(^{13}CH_3)$
2932	$\nu_s(^{13}CH_3)$
2887, 2833	$\nu_s(^{13}CH_2)$
2733	$\omega(^{13}CH_2) + \delta$(OH)
2676	$\delta_s(^{13}CH_3) + \delta$(OH)
2382	δ(OH) + $\rho(^{13}CH_3)$
1885	$\nu(^{13}CO) + \nu(^{13}CC)$
1480	$\delta_s(^{13}CH_2)$
1451	$\delta_a(^{13}CH_3)$
1418	$\omega(^{13}CH_2)$
1369	$\delta_s(^{13}CH_3)$
1324	δ(OH)
1261	$\tau(^{13}CH_2)$
1069	$\rho(^{13}CH_3)$
1024	$\nu(^{13}CO)$
869	$\nu(^{13}C^{13}C)$
New absorptions after irradiation (cm^{-1})	Assignment[2,15,16]
2092	$\nu(^{13}CO)$
1702	$\nu_2(H_2{}^{13}CO)$
1673	$\nu_4(^{13}CH_3{}^{13}CHO)$
1605	^{13}C=O stretch

Table S3. Observed absorption peaks of $C^{18}O_2$−CH_3CD_2OH ice before and after irradiation at 5 K. Vibration mode: stretching (ν), bending (δ), torsion (τ), and wagging (ω). Indication: asymmetric (*a*) and symmetric (*s*).

Pristine ice, absorptions before irradiation (cm^{-1})	
$C^{18}O_2$	Assignment[2]
3620	$\nu_1 + \nu_3$
3510	$2\nu_2 + \nu_3$
2315	C-^{18}O asymmetric stretching (ν_3)
2242	C-^{18}O asymmetric stretching (ν_3 ($^{13}C^{18}O_2$))
CH_3CD_2OH	Assignment[12,17]
3417, 3323, 3191	ν(OH)
2974	$\nu_a(CH_3)$
2937	$\nu_s(CH_3)$
2903, 2870	$\nu_s(CD_2)$
2793	$\omega(CD_2) + \delta$(OH)
2242	$2\delta_s(CD_2)$
2198	$2\omega(CD_2)$
2126	δ(OD) + $\delta_s(CD_2)$
2098	ν(CO) + $\delta_s(CD_2)$
1465	$\delta'_a(CH_3)$
1446	$\delta_a(CH_3)$
1374	$\delta_s(CH_3)$
1300	δ(OH)
1160	$\delta_s(CD_2)$
1129	$\omega(CD_2)$
1027	ν(CO)
962	δ(OD)
912, 850	ν(CC)
New absorptions after irradiation (cm^{-1})	Assignment[13,18]
1715	$\nu_4(CH_3CHO)$
1680	$\nu_2(D_2CO)$
1622	C=^{18}O stretch

Table S4. Observed absorption peaks of $^{13}C^{18}O_2$–CD_3CH_2OH ice before and after irradiation at 5 K. Vibration mode: stretching (ν), bending (δ), torsion (τ), wagging (ω), and rocking (ρ). Indication: asymmetric (a) and symmetric (s).

Pristine ice, absorptions before irradiation (cm^{-1})	
$^{13}C^{18}O_2$	Assignment
3621	$\nu_1 + \nu_3$
3530	$2\nu_2 + \nu_3$
2310	C-^{18}O asymmetric stretching (ν_3 ($C^{18}O_2$))
2249	^{13}C-^{18}O asymmetric stretching (ν_3)
CD_3CH_2OH	Assignment[12,17]
3431	$\nu_s(CD_3) + \tau(CH_2)$
3426, 3334, 3211	ν(OH)
2975	$\nu_a(CH_2)$
2941	$2\delta_s(CH_2)$
2895	$\nu_s(CH_2)$
2731	$\omega(CH_2) + \delta$(OH)
2196	$\nu_s(CD_3)$
2126	$2\delta'_a(CD_3)$
2085	δ(OH) + $\rho(CD_3)$
1487	$\delta_s(CH_2)$
1433	$\omega(CH_2)$
1390	γ(OH) + $\rho(CD_3)$
1320	δ(OH)
1246	$\tau(CH_2)$
1135	ν(CO)
1065	$\delta'_a(CD_3)$
1031	$\delta_a(CD_3)$
939	$\rho'(CD_3)$
755	$\rho(CD_3)$
New absorptions after irradiation (cm^{-1})	Assignment[18,19]
2040	$\nu(^{13}C^{18}O)$
1706	$\nu_4(CD_3CHO)$
1578	^{13}C=^{18}O stretch

Table S5. Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of lactic acid (**1**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

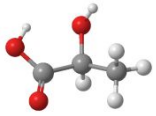
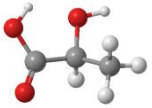
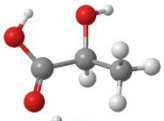
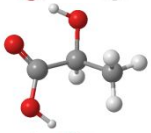
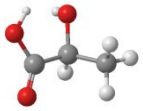
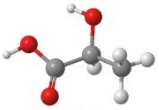
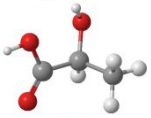
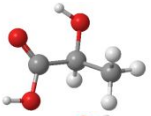
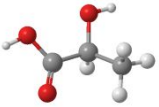
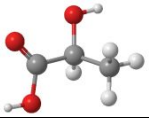
Conformer	Structure	ΔE (kJ mol^{-1})	Computed IE (eV)	Corrected IE ranges (eV)
1a		14	9.95	9.87–9.97
1b		12	9.97	9.89–9.99
1c		13	9.97	9.89–9.99
1d		20	9.90	9.82–9.92
1e		14	9.97	9.89–9.99
1f		10	10.04	9.96–10.06
1g		10	10.04	9.96–10.06
1h		0	10.16	10.08–10.18
1i		21	9.95	9.87–9.97
1j		20	9.96	9.88–9.98

Table S6. Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of monoethyl carbonate (**15**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

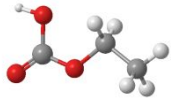
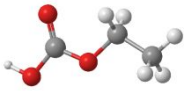
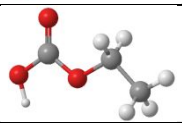
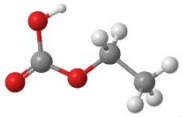
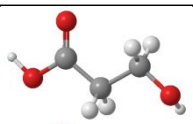
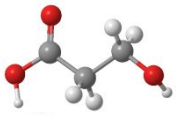
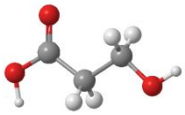
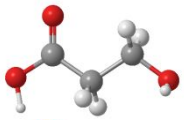
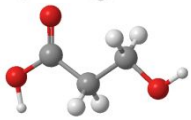
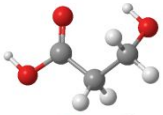
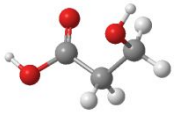
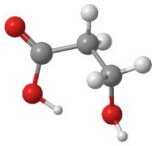
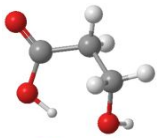
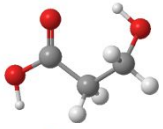
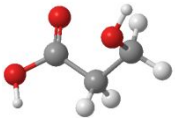
Conformer	Structure	ΔE (kJ mol^{-1})	Computed IE (eV)	Corrected IE ranges (eV)
15a		14	10.61	10.53–10.63
15b		0	10.76	10.68–10.78
15c		5	10.70	10.62–10.72
15d		42	10.53	10.45–10.55

Table S7. Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of 3-hydroxypropanoic acid (**16**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

Conformer	Structure	ΔE (kJ mol^{-1})	Computed IE (eV)	Corrected IE ranges (eV)
16a		12	9.27	9.19–9.29
16b		32	9.19	9.11–9.21
16c		28	9.23	9.15–9.25
16d		32	9.19	9.11–9.21
16e		28	9.23	9.15–9.25
16f		0	9.89	9.81–9.91
16g		8	9.99	9.91–10.01
16h		16	10.05	9.97–10.07
16i		19	10.08	10.00–10.10
16j		20	10.13	10.05–10.15
16k		28	10.04	9.96–10.06

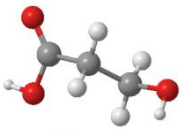
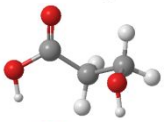
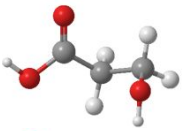
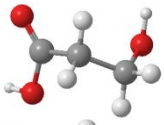
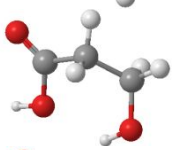
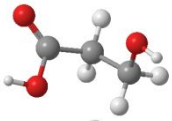
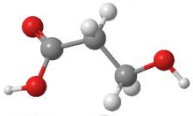
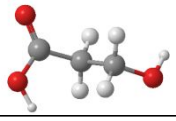
16l		16	10.22	10.14–10.24
16m		36	10.06	9.98–10.08
16n		13	10.31	10.23–10.33
16o		12	10.32	10.24–10.34
16p		9	10.48	10.40–10.50
16q		11	10.46	10.38–10.48
16r		14	10.44	10.36–10.46
16s		15	10.43	10.35–10.45
16t		37	10.43	10.35–10.45

Table S8. Error analysis of IEs and relative energies (ΔE) of prop-1-ene-1,1,2-triol ($CH_3C(OH)C(OH)_2$, **19**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

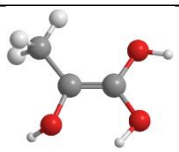
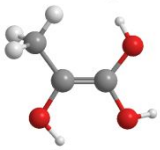
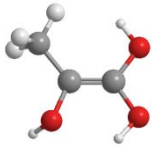
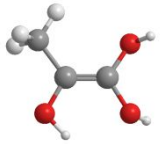
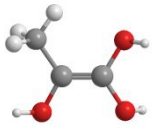
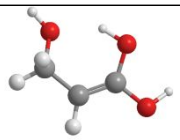
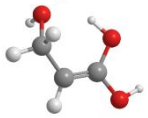
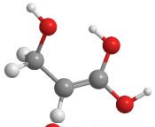
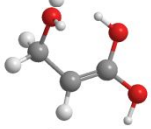
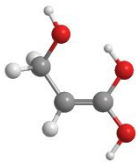
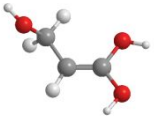
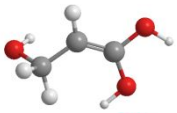
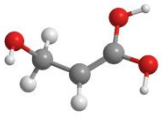
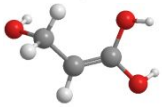
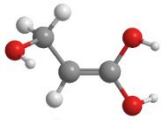
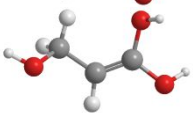
Conformer	Structure	ΔE (kJ mol^{-1})	Computed IE (eV)	Corrected IE ranges (eV)
19a		0	7.46	7.38–7.48
19b		8	7.54	7.46–7.56
19c		12	7.57	7.49–7.59
19d		3	7.69	7.61–7.71
19e		20	7.53	7.45–7.55

Table S9. Error analysis of IEs and relative energies (ΔE) of prop-1-ene-1,1,3-triol ($HOCH_2CHC(OH)_2$, **20**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

Conformer	Structure	ΔE (kJ mol^{-1})	Computed IE (eV)	Corrected IE ranges (eV)
20a		4	7.93	7.85–7.95
20b		0	7.98	7.90–8.00
20c		4	7.93	7.85–7.95
20d		8	8.08	8.00–8.10
20e		12	8.03	7.95–8.05
20f		17	8.27	8.19–8.29
20g		15	8.39	8.31–8.41
20h		18	8.40	8.32–8.42
20i		24	8.36	8.28–8.38
20j		24	8.35	8.27–8.37
20k		27	8.32	8.24–8.34

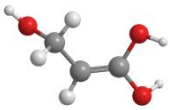
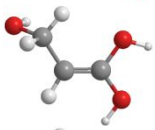
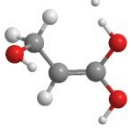
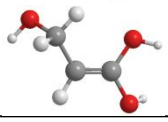
20l		28	8.31	8.23–8.33
20m		12	8.50	8.42–8.52
20n		21	8.46	8.38–8.48
20o		28	8.42	8.34–8.44

Table S10. Observed absorption peaks of ethanol-d_2 (CH_3CD_2OH) ice at 5 K. Vibration mode: stretching (ν), bending (δ), and wagging (ω). Indication: asymmetric (a) and symmetric (s).

Pristine ice, absorptions (cm^{-1})	
CH_3CD_2OH	Assignment[12,17]
3421, 3314, 3179	ν(OH)
2970	$\nu_a(CH_3)$
2935	$\nu_s(CH_3)$
2905, 2869	$\nu_s(CD_2)$
2791	$\omega(CD_2) + \delta$(OH)
2508	ν(OD)
2249	$2\delta_s(CD_2)$
2189	$2\omega(CD_2)$
2121	δ(OD) + $\delta_s(CD_2)$
2095	ν(CO) + $\delta_s(CD_2)$
1465	$\delta'_a(CH_3)$
1446	$\delta_a(CH_3)$
1371	$\delta_s(CH_3)$
1335	δ(OH)
1163	$\delta_s(CD_2)$
1126	$\omega(CD_2)$
1025	ν(CO)
963	δ(OD)
910, 853	ν(CC)

Table S11. Observed absorption peaks of ethanol-d_3 (CD_3CH_2OH) ice at 5 K. Vibration mode: stretching (ν), bending (δ), torsion (τ), wagging (ω), and rocking (ρ). Indication: asymmetric (a) and symmetric (s).

Pristine ice, absorptions (cm^{-1})	
CD_3CH_2OH	Assignment[12,17]
3421, 3314, 3179	ν(OH)
2969	$\nu_a(CH_2)$
2887	$\nu_s(CH_2)$
2741	$\omega(CH_2) + \delta$(OH)
2230	$\nu_a(CD_3)$
2199	$\nu_s(CD_3)$
2121	$2\delta'_a(CD_3)$
2082	δ(OH) + $\rho(CD_3)$
1486	$\delta_s(CH_2)$
1436	$\omega(CH_2)$
1372	γ(OH) + $\rho(CD_3)$
1320	δ(OH)
1251	$\tau(CH_2)$
1135	ν(CO)
1066	$\delta'_a(CD_3)$
939	$\rho'(CD_3)$
757	$\rho(CD_3)$

Table S12. Experimental conditions of carbon dioxide−ethanol ices including composition, ice thickness, irradiation current and time, and photon energy.

Ice	Composition of carbon dioxide to ethanol	Thickness (nm)	Current (nA)	Irradiation time (s)	Dose (eV/ carbon dioxide)	Dose (eV/ ethanol)	Photon energy (eV)
CO_2−CD_3CD_2OD	1.6 ± 0.3 : 1	950 ± 50	–	–	–	–	11.10
CO_2−CD_3CD_2OD	1.6 ± 0.2 : 1	920 ± 50	22 ± 1	300 ± 10	0.21 ± 0.04	0.34 ± 0.06	11.10
CO_2−CD_3CD_2OD	1.2 ± 0.4 : 1	900 ± 50	23 ± 1	300 ± 10	0.22 ± 0.04	0.35 ± 0.06	10.54
CO_2−CD_3CD_2OD	1.6 ± 0.3 : 1	950 ± 50	22 ± 1	300 ± 10	0.21 ± 0.04	0.34 ± 0.06	9.34
$^{13}CO_2$−$^{13}CH_3{}^{13}CH_2OH$	1.4 ± 0.6 : 1	920 ± 50	22 ± 1	300 ± 10	0.21 ± 0.04	0.31 ± 0.05	11.10
$C^{18}O_2$−CH_3CD_2OH	1.2 ± 0.3 : 1	920 ± 50	21 ± 1	300 ± 10	0.22 ± 0.04	0.31 ± 0.05	11.10
$^{13}C^{18}O_2$−CD_3CH_2OH	1.3 ± 0.2 : 1	920 ± 50	24 ± 1	300 ± 10	0.25 ± 0.04	0.32 ± 0.05	11.10

Table S13. Generation parameters of vacuum ultraviolet light with a photon energy uncertainty of less than 0.001 eV.

VUV photon energy (eV)	Nonlinear medium in four-wave mixing	Laser wavelength for ω_1 (nm)	Dye for ω_1	Laser wavelength for ω_2 (nm)	Dye for ω_2
11.10 ($2\omega_1 + \omega_2$)	Xenon	249.628	Coumarin 503	1064	–
10.54 ($2\omega_1 - \omega_2$)	Krypton	202.316	Rhodamine 610 and 640	722.321	LDS 722
9.34 ($2\omega_1 - \omega_2$)	Krypton	212.556	Stilbene 420	532	–

Table S14. Cartesian coordinates (Å), harmonic frequencies (cm^{-1}), and infrared intensities (km mol^{-1}) of isomers **1**, **15**, and **16** calculated at the composite CBS-QB3 level of theory.

1a				**1a$^+$**			
O	1.352704	-1.287671	-0.053042	O	1.208793	-1.400314	0.025094
C	0.839223	-0.203008	-0.054794	C	0.972003	-0.250520	-0.016663
C	-0.646416	0.023709	-0.399577	C	-0.798167	0.138838	-0.399115
C	-1.545208	-1.022119	0.242751	C	-1.687488	-0.922573	0.160130
O	1.515645	0.927208	0.210549	O	1.690232	0.808005	0.101149
O	-1.035049	1.371575	-0.083710	O	-0.929550	1.409334	0.028694
H	-0.716528	-0.048554	-1.489466	H	-0.623494	0.131619	-1.480529
H	-1.522008	-0.935492	1.334554	H	-1.694653	-0.925228	1.253933
H	-2.574686	-0.902676	-0.099909	H	-2.706294	-0.723617	-0.193717
H	-1.192389	-2.020496	-0.015105	H	-1.385673	-1.907604	-0.194268
H	0.870371	1.654278	0.147896	H	1.157373	1.625301	0.042790
H	-1.416757	1.372556	0.801374	H	-1.421147	1.468861	0.866189
Freq	Int			Freq	Int		
69.9431	6.0568			80.4994	2.5532		
232.4339	0.588			196.5917	7.4082		
265.2626	17.4379			227.6315	9.4784		
344.0584	55.0699			240.007	1.8404		
347.7646	55.7965			332.9677	3.9385		
416.5937	7.6255			385.9162	15.1718		
519.7772	1.8136			450.7592	8.2332		
566.8145	12.6245			531.0747	22.7863		
736.6324	11.5798			592.4454	77.2125		
761.7481	83.5524			623.454	85.5211		
816.8751	16.5803			684.2799	76.8671		
906.7986	8.8506			912.888	29.8742		
1054.9033	55.2255			994.041	22.6767		
1074.4069	22.6889			1057.035	60.0549		
1130.9969	40.8991			1154.4423	19.7098		
1198.0989	45.4032			1198.3688	73.0798		
1287.9706	2.6912			1226.7333	54.2224		
1335.8072	29.1977			1264.3899	396.3114		
1391.9398	328.4264			1330.5158	33.0178		
1398.9051	88.1789			1404.5641	11.4304		
1409.3302	35.6671			1434.0147	84.6565		
1493.0763	7.3148			1463.5124	10.5842		
1496.7878	10.4684			1475.2557	12.0677		
1858.2913	254.2846			1914.1239	133.0194		
3027.1448	12.1092			3023.6946	18.2214		
3051.8733	14.0676			3060.6557	18.3329		
3100.1344	23.7564			3091.773	5.9238		
3136.0255	5.5768			3144.923	2.1925		
3646.1715	146.2047			3633.8244	129.3304		
3811.7566	32.7884			3705.6502	209.1272		
1b				**1b$^+$**			
O	1.504635	-1.123274	-0.243350	O	1.208264	-1.400494	0.025202
C	0.851542	-0.129713	-0.081736	C	0.971533	-0.250586	-0.016697
C	-0.646477	-0.078804	-0.416412	C	-0.797701	0.138865	-0.398996
C	-1.417677	-1.092335	0.424605	C	-1.687713	-0.922189	0.160024
O	1.361749	1.008308	0.412530	O	1.690444	0.807516	0.101073

O	-1.086556	1.267954	-0.200031
H	-0.733123	-0.333656	-1.479348
H	-1.352874	-0.835756	1.484982
H	-2.471613	-1.115503	0.131657
H	-0.997319	-2.088009	0.278989
H	0.639142	1.658959	0.444842
H	-2.047170	1.295178	-0.173054

Freq	Int
48.6999	32.0876
141.145	103.5598
252.9766	4.7691
264.4809	8.4579
352.2804	15.023
411.0907	12.0168
527.4241	2.753
599.5752	13.7965
688.2346	82.3272
740.456	6.7591
813.0866	5.713
908.2761	9.105
1042.0318	8.0383
1100.8906	8.9875
1128.108	80.5541
1163.4718	94.4328
1267.3062	16.5554
1349.5133	59.1433
1388.122	104.3612
1401.4751	160.429
1408.4049	142.0337
1493.9863	5.9603
1499.462	11.3974
1861.1984	266.825
3022.4711	21.5874
3030.2754	18.0165
3096.2631	25.1755
3127.7055	7.761
3672.5448	150.2754
3850.3049	34.2519

O	-0.929056	1.409532	0.028731
H	-0.623464	0.131698	-1.480528
H	-1.694766	-0.925106	1.253830
H	-2.706403	-0.722559	-0.193707
H	-1.386449	-1.907327	-0.194562
H	1.158073	1.625142	0.042879
H	-1.420927	1.469173	0.866054

Freq	Int
80.6307	2.5526
196.8373	7.4324
227.7788	9.4796
240.1759	1.8337
333.1686	3.9273
386.1077	15.1756
450.7965	8.2203
531.156	22.7452
592.3952	77.4681
623.5354	85.7502
684.3993	76.5293
912.8525	29.8683
994.1565	22.6406
1056.9784	60.086
1154.4907	20.0346
1198.4259	73.5177
1226.6583	53.649
1264.5137	395.65
1330.3336	33.0518
1404.5753	11.4373
1433.9159	84.5367
1463.492	10.62
1475.2627	11.99
1913.2292	132.9816
3023.806	18.2132
3060.1743	18.4389
3091.8263	5.8747
3144.8612	2.1969
3633.8636	129.2023
3705.6857	209.3495

1c

O	-1.401138	1.231547	-0.154400
C	-0.840239	0.174147	-0.069865
C	0.655048	0.012645	-0.387398
C	1.493582	1.065878	0.327730
O	-1.466424	-0.957841	0.285230
O	1.025084	-1.324652	-0.019416
H	0.741648	0.139059	-1.474488
H	1.444086	0.914602	1.408192
H	2.539028	1.004803	0.014241
H	1.113440	2.061075	0.094711
H	-0.797744	-1.664598	0.296068
H	1.849026	-1.563398	-0.452846

Freq	Int
65.9481	8.0013
167.9287	111.8085

1c^{+}

O	-1.594410	0.952605	-0.508711
C	-0.965988	0.061241	-0.065761
C	0.810014	0.148987	-0.452992
C	1.334712	1.075816	0.610897
O	-1.270700	-0.949699	0.667655
O	1.224508	-1.131061	-0.321653
H	0.785263	0.530789	-1.473769
H	1.247011	0.652379	1.613415
H	2.403147	1.213415	0.399428
H	0.839920	2.045291	0.563899
H	-0.502383	-1.535485	0.818004
H	1.279429	-1.597415	-1.172173

Freq	Int
80.5097	3.2469
189.7771	2.1852

227.6287	0.7263
269.5995	14.1287
354.6307	12.6752
421.3235	9.9187
527.2558	4.7713
577.2778	11.2069
689.0315	92.4331
741.8489	9.3684
813.2069	4.3965
909.5446	8.7067
1040.8966	6.7274
1114.7021	49.6263
1124.6876	24.6226
1165.107	110.2421
1246.5326	16.6965
1341.051	65.9424
1398.0193	160.833
1403.273	133.7078
1408.9481	104.016
1490.592	10.4879
1498.6116	6.5012
1860.5448	262.539
3008.6534	23.1724
3038.5033	17.0395
3105.3204	23.6895
3130.2986	8.5178
3668.868	153.9194
3855.9606	42.8241

227.48	2.2549
240.8399	7.4733
276.7111	15.464
429.657	4.0974
517.7526	15.9439
533.365	90.3077
567.5335	13.4022
632.5561	91.2734
693.7957	69.8941
899.3361	15.5883
995.3795	15.0088
1045.5469	37.6824
1133.7353	80.8436
1191.8328	61.546
1231.4733	6.6499
1266.77	297.7147
1291.4612	167.371
1396.9004	13.4262
1434.9093	0.6498
1462.6349	23.4228
1471.4518	14.2511
1887.3117	119.7307
3015.5625	33.7331
3097.7922	4.4367
3124.3585	3.8513
3152.1956	1.059
3625.7093	114.7971
3726.9211	262.1643

1d

O	1.228585	-1.158883	-0.419502
C	0.806200	-0.122744	0.018623
C	-0.666492	0.055328	0.402430
C	-1.342523	1.159880	-0.421151
O	1.619257	0.939619	0.192342
O	-1.342668	-1.164370	0.223828
H	-0.692197	0.333950	1.468158
H	-1.257288	0.939611	-1.487288
H	-2.401260	1.193249	-0.160839
H	-0.916344	2.150079	-0.230633
H	1.126089	1.684026	0.558446
H	-0.683501	-1.786637	-0.120596

Freq	Int
57.93	0.1886
226.0397	0.2091
260.8474	6.5649
321.4419	23.822
374.4772	96.9362
418.6081	2.1269
478.8067	102.9052
500.4001	2.7608
632.5042	9.5334
736.035	6.7715
810.6313	4.1348
927.3391	6.3779
1046.744	22.0229

1d^{+} (same as **1c**$^{+}$)

1104.3909	25.9986						
1157.5031	99.087						
1187.4501	32.3421						
1272.571	5.5196						
1313.0732	447.4691						
1361.046	2.7553						
1414.1214	6.455						
1432.6902	14.6437						
1487.3868	8.975						
1502.2578	10.0192						
1844.4282	241.4703						
2959.8171	40.699						
3029.2149	20.6176						
3098.3439	27.8267						
3123.0093	12.8762						
3707.5611	92.9871						
3804.767	45.7701						
1e				**1e$^+$**			
O	1.572706	-1.038825	-0.326625	O	1.594105	-0.952181	-0.508998
C	0.857209	-0.105892	-0.087399	C	0.965326	-0.061092	-0.065824
C	-0.648803	-0.112756	-0.407170	C	-0.809266	-0.149127	-0.452995
C	-1.373299	-1.133226	0.462778	C	-1.334191	-1.075794	0.611054
O	1.289438	1.021522	0.501571	O	1.270117	0.949480	0.668088
O	-1.214069	1.191209	-0.168881	O	-1.224243	1.130901	-0.321942
H	-0.746845	-0.387289	-1.461606	H	-0.784987	-0.531152	-1.473704
H	-1.308859	-0.843260	1.514330	H	-1.246380	-0.652288	1.613536
H	-2.426339	-1.184284	0.181511	H	-2.402642	-1.213182	0.399606
H	-0.916219	-2.116037	0.341759	H	-0.839518	-2.045335	0.564172
H	0.511431	1.603828	0.576617	H	0.501891	1.535412	0.818379
H	-1.308405	1.647030	-1.010389	H	-1.279410	1.597020	-1.172574
Freq	Int			Freq	Int		
44.0434	9.0884			80.4768	3.2533		
240.8132	6.7757			190.1762	2.1774		
256.7838	3.8196			227.654	2.2878		
271.7737	104.7923			241.2618	7.4639		
339.0585	3.3048			277.0	15.4293		
399.4174	8.8675			429.784	4.092		
521.9908	3.9666			517.8662	16.5078		
619.9666	8.5305			533.5893	89.9563		
731.1142	30.1784			567.6484	13.2728		
775.137	64.8699			632.7064	91.5433		
810.8387	7.5778			693.9117	69.7057		
909.6865	10.4696			899.3301	15.5347		
1047.9724	78.1279			995.5756	15.1477		
1064.6567	22.9348			1045.4696	37.7223		
1108.6014	23.6318			1133.8698	81.1545		
1217.3359	20.9846			1191.8373	61.357		
1262.0142	56.5224			1231.5776	6.4773		
1310.8896	9.9683			1266.9602	296.7187		
1383.4091	109.1592			1291.4084	167.7256		
1403.8057	296.4411			1396.9241	13.386		
1409.9797	9.244			1434.8662	0.6268		
1489.4055	12.1784			1462.5574	23.6522		
1498.6757	2.9124			1471.4363	14.0522		
1861.5749	264.9643			1886.6956	119.7669		

3043.2685	8.9435			3015.6569	33.6995		
3052.9235	16.3915			3097.8162	4.461		
3114.374	21.5537			3124.322	3.8344		
3131.7008	9.9421			3152.1864	1.066		
3637.5817	149.7653			3625.6223	114.663		
3847.3584	54.5177			3726.943	262.3839		
1f				**1f^{+}**			
O	1.236541	-1.346330	0.001668	O	1.092106	-1.429200	0.114128
C	0.773917	-0.238518	-0.054569	C	0.882165	-0.277634	-0.025621
C	-0.681209	0.106734	-0.374388	C	-0.776123	0.211882	-0.368290
C	-1.637860	-0.937019	0.181730	C	-1.732274	-0.857095	0.061193
O	1.525332	0.881503	0.101841	O	1.628546	0.786733	-0.027441
O	-1.068094	1.376480	0.121307	O	-0.939546	1.374127	0.287500
H	-0.734005	0.090880	-1.476709	H	-0.616832	0.323328	-1.453077
H	-1.607891	-0.926373	1.273185	H	-1.763055	-0.950397	1.148288
H	-2.654079	-0.704514	-0.139691	H	-2.729421	-0.567062	-0.284247
H	-1.364132	-1.931597	-0.169940	H	-1.463851	-1.815503	-0.382150
H	2.436742	0.592142	0.256922	H	2.571332	0.571845	0.117012
H	-0.355956	1.999061	-0.058934	H	-0.489636	2.121581	-0.143015
Freq	Int			Freq	Int		
45.2494	2.453			53.6989	0.8018		
221.8376	2.1871			207.9717	0.4809		
252.5671	3.1854			230.6029	0.5003		
312.6264	79.961			257.9016	1.0469		
344.0904	55.9702			351.1192	13.5851		
415.2072	10.9871			380.1238	1.6329		
510.0479	9.0744			461.4073	17.867		
539.483	37.4709			540.0419	95.6768		
621.1096	101.0646			550.1074	141.167		
732.3758	39.7934			580.2172	30.5971		
814.7579	8.6495			686.0805	68.9897		
929.4925	3.8703			915.4104	9.4755		
1047.6408	73.2254			1009.5326	1.8585		
1095.8044	23.6616			1051.4507	35.3456		
1157.1377	176.424			1119.1225	35.2446		
1160.9845	117.3203			1164.8378	200.3849		
1288.5285	57.3022			1223.6555	6.2472		
1328.4399	26.5026			1289.733	126.7942		
1368.1612	16.6277			1310.7526	43.2419		
1400.8174	41.9891			1400.6985	15.2304		
1425.9736	19.4609			1439.2015	18.5599		
1486.9301	10.8769			1462.4873	27.0175		
1501.916	1.1329			1474.8011	9.5432		
1836.2841	248.8197			1875.6106	183.8612		
2941.0812	39.3992			2979.0697	20.3457		
3050.7327	12.8123			3042.4791	14.6113		
3120.4747	20.0882			3113.4509	2.8641		
3138.2462	11.4637			3149.117	1.0325		
3761.6342	67.9706			3652.4837	265.4742		
3827.8001	46.1634			3710.7076	258.7139		
1g				**1g^{+}**			
O	1.598965	-0.951765	-0.453793	O	1.615865	-0.881212	-0.580525
C	0.811302	-0.105489	-0.125430	C	0.911640	-0.078320	-0.077409
C	-0.684856	-0.131167	-0.423942	C	-0.792284	-0.176700	-0.459038
C	-1.386033	-1.042710	0.593471	C	-1.380457	-0.962363	0.697522

O	1.152917	0.974794	0.621834
O	-1.261938	1.160482	-0.478362
H	-0.789559	-0.555324	-1.424096
H	-1.267361	-0.647723	1.606769
H	-2.451231	-1.081671	0.360467
H	-0.974495	-2.054094	0.563034
H	2.101819	0.904701	0.804137
H	-0.981210	1.642223	0.307655

Freq	Int
47.4076	3.0296
236.2908	0.8101
239.3583	6.9767
274.5577	45.6399
332.0285	78.9516
385.9409	8.8644
523.602	12.3416
589.5062	95.146
626.5779	59.4909
758.5712	30.8027
789.4758	16.0343
910.391	4.0378
1036.4575	102.2548
1086.4854	5.278
1116.9334	105.5424
1182.8507	177.5838
1297.3447	21.5886
1335.92	3.0639
1352.7294	30.4981
1399.6203	13.3752
1427.2423	68.667
1491.6947	15.0979
1497.0347	2.9457
1839.2984	267.5861
3031.738	12.9168
3084.0097	2.7514
3106.7076	30.4833
3121.229	14.5219
3760.7463	67.8748
3816.6997	39.7244

O	1.103301	0.900146	0.755156
O	-1.178695	1.099024	-0.632621
H	-0.771897	-0.678303	-1.424653
H	-1.297440	-0.432027	1.649108
H	-2.442481	-1.110148	0.467599
H	-0.908408	-1.941695	0.780586
H	2.042471	0.978272	1.014960
H	-1.379403	1.544532	0.209860

Freq	Int
52.3848	0.9203
201.4364	2.1724
220.0858	0.8906
242.8498	1.0971
290.6374	5.3612
428.3957	6.216
511.655	7.2928
538.2472	51.3856
553.8672	82.7844
587.5736	128.0064
688.5008	68.9727
881.0466	8.4883
1009.8063	51.3552
1043.1949	32.144
1127.5396	75.9415
1181.5133	101.2383
1226.1517	150.9636
1316.8346	21.5315
1324.5527	14.4697
1394.8389	7.2386
1435.2965	43.9326
1455.4031	9.952
1479.6904	9.7152
1859.4832	166.6335
3021.1625	22.262
3097.9608	8.3768
3137.2888	2.3327
3150.6062	2.8541
3654.205	269.1637
3693.1822	215.4715

1h

O	1.215795	-1.135122	-0.448492
C	0.777297	-0.117227	0.030797
C	-0.685226	0.069422	0.404068
C	-1.333188	1.186330	-0.422962
O	1.529608	0.968289	0.282790
O	-1.373316	-1.149928	0.230061
H	-0.710064	0.350314	1.465412
H	-1.281888	0.943491	-1.487142
H	-2.384458	1.266760	-0.142497
H	-0.842122	2.145580	-0.248678
H	2.434776	0.759751	0.006041
H	-0.746237	-1.762951	-0.179423

Freq	Int

1h$^+$

O	1.098054	1.400559	-0.166436
C	0.906772	0.249035	0.015408
C	-0.765407	-0.211087	0.373875
C	-1.714409	0.880626	-0.022410
O	1.656388	-0.803203	0.059788
O	-0.913112	-1.428671	-0.172824
H	-0.572154	-0.329893	1.449922
H	-1.761173	1.010556	-1.107252
H	-2.710708	0.610354	0.341906
H	-1.423078	1.828998	0.428472
H	2.598406	-0.580238	-0.076923
H	-1.423674	-1.400698	-1.001584

Freq	Int

45.4833	4.3853
234.4355	3.3193
245.9156	1.3898
311.7319	37.7257
328.434	45.4126
405.5578	12.2456
498.7558	14.2502
589.8354	58.2216
645.5296	42.6424
746.1787	53.4157
808.0324	27.5481
931.0226	0.8899
1050.9151	57.2936
1105.408	35.1253
1147.2173	253.5999
1191.1334	45.6343
1275.6557	35.3338
1348.5135	88.4542
1353.8127	5.867
1404.9757	12.2991
1444.102	12.8776
1494.303	12.5971
1501.3946	2.9736
1812.3839	288.3337
3003.7211	25.2259
3040.0118	15.0914
3112.893	23.4253
3123.9097	16.0012
3738.3239	83.679
3753.9788	66.0608

22.9075	2.7365
216.0463	2.1792
232.1739	2.9453
258.1062	1.0242
349.5498	14.3485
371.3766	5.204
448.0133	1.2217
540.9119	75.504
554.6236	38.4419
600.3557	202.5511
690.133	60.7537
912.138	22.0201
1012.726	14.4273
1044.1692	38.2716
1135.1633	39.8814
1169.371	146.4504
1217.9584	171.5996
1314.3047	21.6036
1328.1063	2.9786
1402.9407	17.231
1428.7104	57.6189
1467.6678	13.5962
1475.4154	7.2681
1870.573	205.5936
3011.1568	30.7733
3035.3266	8.0544
3101.8588	2.8476
3141.388	1.5547
3653.0861	276.0829
3693.8609	226.6369

1i

O	1.346387	-1.232027	-0.147985
C	0.804437	-0.156777	-0.076071
C	-0.677782	0.041515	-0.377451
C	-1.511042	-1.040605	0.312291
O	1.453394	0.975147	0.242233
O	-1.069830	1.351848	-0.003697
H	-0.755674	-0.089035	-1.468492
H	-1.467859	-0.910077	1.396000
H	-2.555638	-0.968683	-0.003589
H	-1.136699	-2.032798	0.058831
H	2.377482	0.719237	0.385647
H	-1.994898	1.456808	-0.245421

Freq	Int
15.3693	5.5472
234.4209	1.4372
246.7924	115.5861
262.3683	5.0277
325.7109	5.4424
417.7209	3.8396
515.3397	1.0098
549.6574	42.8176
645.9404	89.0502
748.1626	53.1484
812.0235	13.2807

1i^{+}

O	1.098904	-1.400558	0.164404
C	0.906794	-0.248854	-0.015486
C	-0.765521	0.210380	-0.373983
C	-1.714063	-0.881044	0.024270
O	1.655733	0.803959	-0.057819
O	-0.913544	1.428765	0.170806
H	-0.572711	0.327569	-1.450291
H	-1.760401	-1.009386	1.109328
H	-2.710579	-0.611624	-0.340065
H	-1.422546	-1.829984	-0.425296
H	2.597877	0.581287	0.078505
H	-1.423648	1.401919	0.999887

Freq	Int
23.1818	2.7474
216.1094	2.1837
232.2807	2.9373
258.2364	1.0227
349.587	14.3102
371.6573	5.2687
447.9918	1.2482
540.8614	74.7617
554.75	39.0917
600.4006	202.4518
690.0928	60.8916

918.5838	9.561
1047.7823	8.0948
1109.3905	20.0868
1150.3666	97.6893
1182.3585	318.1649
1249.6113	37.3398
1340.1586	15.7095
1364.7493	29.9116
1404.3828	14.5323
1440.7236	9.8616
1490.6803	7.8964
1503.633	9.1419
1816.8008	263.539
2964.6957	34.4743
3034.8907	19.0413
3100.1212	25.0496
3129.883	10.9183
3749.1736	56.6994
3836.7439	25.9264

1j			
O	-1.228199	-1.133874	0.549166
C	-0.790523	-0.170435	-0.012390
C	0.663533	0.083868	-0.389163
C	1.257653	1.192456	0.489759
O	-1.559158	0.884967	-0.390391
O	1.350035	-1.143631	-0.242197
H	0.661972	0.416520	-1.436923
H	1.253703	0.877574	1.535758
H	2.291999	1.389395	0.192907
H	0.691802	2.120331	0.390878
H	-2.462004	0.683303	-0.103437
H	2.277133	-0.982151	-0.441033

Freq	Int
50.3731	0.3512
230.6004	97.7175
241.5489	10.6217
246.5761	12.7919
309.7663	2.0212
395.9486	2.8331
500.4384	12.613
588.0815	72.9096
632.7467	63.4574
748.0431	38.7665
802.179	6.0785
920.715	14.6106
1047.57	6.5457
1100.7629	21.1585
1115.501	389.2365
1180.0659	16.1786
1250.4127	22.21
1323.2644	11.0117
1351.7282	17.2175
1401.7283	9.1429
1436.68	14.6366
1493.112	7.5569

912.1376	21.9977
1012.7663	14.4201
1044.1399	38.2246
1135.1132	39.7672
1169.4038	146.4155
1218.0498	171.7228
1314.3478	21.5659
1328.168	2.9828
1402.9707	17.1926
1428.7006	57.5803
1467.6657	13.618
1475.4324	7.2692
1870.4234	205.5061
3011.1259	30.7707
3035.3171	8.0561
3101.8348	2.8467
3141.3729	1.5617
3653.0732	276.0333
3693.8636	226.7221

1j$^+$			
O	-1.098304	1.400709	0.163919
C	-0.906352	0.248866	-0.015574
C	0.765098	-0.210254	-0.373978
C	1.713986	0.880721	0.024748
O	-1.655713	-0.803717	-0.057185
O	0.912956	-1.428952	0.170258
H	0.572385	-0.326800	-1.450440
H	1.759994	1.008948	1.109863
H	2.710532	0.611051	-0.339279
H	1.422924	1.829865	-0.424740
H	-2.597810	-0.580586	0.078738
H	1.424068	-1.402801	0.998745

Freq	Int
23.4401	2.7499
216.4268	2.2186
232.722	2.9324
258.8102	0.9945
349.7928	14.4488
371.9355	5.2942
448.0982	1.2694
540.9455	74.6101
554.7866	39.2895
600.3149	202.2711
690.2536	60.8857
912.2171	21.9375
1012.8972	14.3061
1044.1303	38.3036
1135.0844	39.7317
1169.5102	146.2553
1218.0375	171.8612
1314.4691	21.4711
1328.1165	2.9939
1402.9108	17.3863
1428.6601	57.3624
1467.7016	13.6459

1504.4819	16.8414			1475.4715	7.2471		
1857.8847	288.3523			1870.0389	205.4561		
2987.755	34.9601			3010.4364	30.861		
3031.3453	18.2431			3035.2583	8.0566		
3097.39	23.7643			3101.7586	2.8329		
3121.5608	15.5964			3141.1497	1.572		
3762.8917	62.1829			3653.0548	276.2319		
3839.3824	30.3308			3693.8199	227.1327		
15a				**15a$^+$**			
C	0.013406	0.062191	0.009561	C	0.047371	0.050209	0.027063
H	0.020461	0.110247	1.10024	H	0.03658	0.108986	1.115604
H	1.044795	0.111939	-0.34499	H	1.071268	0.116813	-0.341327
H	-0.410592	-0.899209	-0.29208	H	-0.352878	-0.928202	-0.262523
C	-0.810384	1.191097	-0.572974	C	-0.838367	1.083389	-0.596484
H	-0.819753	1.164082	-1.664757	H	-0.816521	1.102578	-1.684504
H	-1.843583	1.162426	-0.220147	H	-1.858525	1.094803	-0.217327
O	-0.195788	2.431549	-0.135984	O	-0.250459	2.464482	-0.171667
C	-0.709459	3.606649	-0.498748	C	-0.763019	3.549015	-0.529443
O	-0.244868	4.660694	-0.16849	O	-0.208533	4.645959	-0.130924
O	-1.812483	3.471921	-1.280919	O	-1.818909	3.625283	-1.277191
H	-2.10051	4.371223	-1.484224	H	-2.116766	4.531492	-1.484789
Freq	Int			Freq	Int		
72.7906	0.4366			30.6257	0.9732		
122.7401	2.4833			99.1629	12.9655		
213.5558	0.5525			164.409	0.6531		
259.381	1.2613			252.7019	1.7759		
375.5794	6.8468			323.2535	20.7168		
566.3121	11.2772			431.3816	11.2095		
568.8814	100.5894			452.5812	167.4061		
616.3792	27.8832			539.2138	55.9126		
786.8873	43.8483			720.1544	90.0695		
822.1073	0.101			752.0138	19.2369		
854.5933	0.5401			814.678	2.1822		
994.7282	3.3974			943.3224	89.1369		
1084.4135	102.4151			1056.6722	27.5512		
1125.9609	103.6852			1114.5301	0.323		
1177.4185	3.9981			1125.8106	8.7394		
1188.609	375.0637			1147.0662	161.5208		
1304.8713	0.6698			1277.3982	1.1794		
1365.6467	168.9206			1371.1755	105.0358		
1410.7081	45.2975			1410.1395	37.2784		
1434.9279	7.8665			1452.9881	229.9675		
1483.8696	7.3019			1456.6351	14.2957		
1501.7859	3.4432			1490.8014	2.1723		
1523.3724	1.0888			1498.9017	5.616		
1862.4073	606.9941			1654.4209	289.5051		
3040.0751	14.6909			3035.4788	23.2391		
3050.8591	20.0257			3097.9821	0.8435		
3090.3897	6.2652			3110.7084	11.4721		
3107.7105	25.5747			3141.0449	0.7792		
3120.7031	39.0277			3177.636	0.8096		
3806.3625	90.867			3676.9844	347.8997		
15b				**15b$^+$**			
C	0.032392	0.098542	0.023019	C	0.04573	0.087749	0.032522
H	0.039245	0.149755	1.113751	H	0.03636	0.158908	1.120534

H	1.063774	0.151534	-0.331688
H	-0.385672	-0.866633	-0.274488
C	-0.798842	1.218672	-0.564697
H	-0.812222	1.192331	-1.656657
H	-1.833562	1.190517	-0.215672
O	-0.199084	2.467839	-0.138068
C	-0.808821	3.571027	-0.568952
O	-1.790464	3.625534	-1.264925
O	-0.140441	4.639116	-0.094091
H	-0.611516	5.413473	-0.427228

Freq	Int
52.5628	0.0251
145.5979	4.6635
202.2006	2.7464
262.878	1.0219
376.8613	14.4595
524.787	26.3716
553.1964	105.4104
670.1639	6.4156
795.8568	37.4296
818.0571	2.6045
882.6792	4.1086
1003.4835	10.5899
1095.2664	47.3456
1138.0186	9.7657
1181.8678	4.752
1210.9117	611.8233
1301.0199	1.1606
1381.1386	117.0123
1416.2616	99.9355
1443.5308	60.6335
1485.3806	7.206
1501.7425	2.5023
1525.9457	9.9057
1827.4186	404.5025
3039.39	14.467
3052.1097	16.7688
3088.5713	4.615
3107.0254	25.641
3118.1422	40.2064
3811.715	95.3264

H	1.06883	0.160612	-0.337447
H	-0.345996	-0.895528	-0.24603
C	-0.843598	1.117639	-0.596043
H	-0.822467	1.123527	-1.684789
H	-1.863554	1.121841	-0.214577
O	-0.256727	2.493998	-0.178823
C	-0.742322	3.605856	-0.522165
O	-1.785902	3.680831	-1.261608
O	-0.160213	4.681696	-0.108964
H	-0.575351	5.514575	-0.402306

Freq	Int
14.1593	0.6444
109.9291	3.1331
142.3933	3.3533
252.984	0.0006
316.8162	21.0968
427.347	17.3012
429.6579	170.7509
471.8101	46.4851
740.9209	33.8991
742.5858	24.1142
814.2337	2.2404
952.7303	62.3307
1057.2462	7.5784
1123.7768	19.5376
1148.0855	10.6268
1155.208	243.3512
1291.8426	2.3062
1376.3348	101.119
1419.3084	53.5628
1448.5299	132.402
1472.9254	15.2769
1490.464	34.0314
1495.5346	10.0337
1522.2225	262.6514
3046.881	3.3162
3092.4803	0.8694
3115.9469	2.2598
3135.2482	0.5135
3169.9271	1.092
3686.4408	368.5102

15c

C	0.040844	0.110882	0.029871
H	0.045368	0.155181	1.121107
H	1.073116	0.158642	-0.323566
H	-0.381524	-0.850555	-0.272909
C	-0.784299	1.237869	-0.554431
H	-0.795364	1.216827	-1.646249
H	-1.819314	1.213392	-0.206899
O	-0.183333	2.485748	-0.123959
C	-0.795497	3.610684	-0.556982
O	-1.768612	3.662154	-1.249289
O	-0.147718	4.69314	-0.093289
H	0.601482	4.396396	0.439126

15c^{+}

C	0.038241	0.077651	0.027956
H	0.026618	0.128509	1.117174
H	1.063336	0.131966	-0.339943
H	-0.37441	-0.892069	-0.267941
C	-0.82813	1.134526	-0.585948
H	-0.803414	1.160561	-1.674155
H	-1.848148	1.157079	-0.205767
O	-0.213642	2.500906	-0.145514
C	-0.684743	3.62948	-0.477975
O	-1.73481	3.685748	-1.224852
O	-0.172909	4.744676	-0.111145
H	0.617157	4.631325	0.450643

Freq	Int
45.3211	3.6483
146.7002	3.3626
199.4101	7.3847
263.7023	0.8705
372.2927	9.0112
514.9501	115.9579
523.3273	1.5909
679.5141	2.0523
783.757	25.8704
815.4231	0.0766
879.2659	23.341
997.7569	21.6695
1084.3284	95.2886
1136.486	12.8289
1181.5802	3.8362
1201.2334	160.7526
1299.6069	1.0112
1334.3485	618.3359
1405.3004	62.2526
1432.6623	25.1481
1486.3472	7.5855
1501.5669	2.6118
1526.1299	10.0097
1881.3336	369.9797
3038.6557	14.3377
3055.4657	15.2313
3090.763	1.4086
3107.1559	25.0738
3117.4612	43.2871
3799.8308	68.3676

Freq	Int
30.3189	1.3512
122.5231	9.2727
149.5309	6.4266
256.3946	0.8983
320.3213	15.1893
440.8984	19.4494
462.9644	159.7791
499.6355	2.0679
724.9341	138.0399
743.3135	29.8746
816.2431	3.0346
949.3041	69.6814
1050.2691	42.5097
1121.3332	3.6326
1146.1705	8.8442
1151.6633	105.3411
1289.6933	2.0814
1371.0307	184.1181
1418.4859	39.7982
1473.5644	15.7406
1482.2032	154.9793
1494.0189	1.9332
1506.491	111.9256
1628.438	376.6739
3046.3535	3.1396
3094.4943	0.5616
3114.5087	2.3638
3135.5141	0.9553
3172.1919	0.6738
3683.3408	303.1918

15d

C	0.030253	0.039256	0.021751
H	0.03538	0.098751	1.111238
H	1.060112	0.098806	-0.333785
H	-0.387261	-0.926268	-0.274373
C	-0.797224	1.165694	-0.564911
H	-0.795986	1.107995	-1.660926
H	-1.831091	1.108591	-0.201342
O	-0.200209	2.405103	-0.141949
C	-0.709852	3.612203	-0.499899
O	-0.20683	4.627499	-0.137624
O	-1.81342	3.598709	-1.28635
H	-2.10474	2.706633	-1.50223

Freq	Int
37.9882	7.0918
86.6624	0.5013
214.8243	3.5162
252.4285	2.41
333.3518	88.1218
380.6752	1.7238
563.7395	8.5046
632.6114	3.4639
772.498	20.5577
846.4845	0.1657

15d$^+$

C	0.070841	0.027225	0.074454
H	0.094374	0.174292	1.154455
H	1.084061	0.044961	-0.327156
H	-0.358271	-0.960363	-0.124594
C	-0.80597	1.039076	-0.601537
H	-0.813412	0.947767	-1.688763
H	-1.813106	1.091994	-0.186146
O	-0.170891	2.418247	-0.336094
C	-0.765521	3.514558	-0.533689
O	-0.20571	4.550242	0.007214
O	-1.852322	3.761202	-1.177738
H	-2.184941	3.033773	-1.730805

Freq	Int
40.6046	1.401
74.8839	1.1378
159.8133	3.268
253.5763	1.1714
325.695	16.0907
358.1294	122.1826
456.9058	33.1134
562.6186	43.3024
717.0386	64.6304
768.1718	41.1457

853.4889	3.5461
987.6013	10.5737
1089.2576	81.8398
1118.505	142.4139
1176.7619	52.7172
1177.3452	5.8444
1304.2267	534.5612
1314.2852	0.3264
1406.0299	9.6422
1429.577	11.6964
1482.9106	7.6885
1503.308	6.0614
1526.1223	1.533
1899.3626	553.9267
2987.7411	35.7957
3030.1733	30.4834
3044.8856	12.4568
3114.046	18.8252
3125.1314	19.7996
3823.05	48.9353

827.1976	2.1506
949.3546	67.195
1056.8909	32.4956
1106.8199	183.0859
1117.8519	11.3136
1137.5819	11.4286
1291.6859	1.736
1371.5019	148.5259
1416.1228	38.7985
1465.8226	15.4125
1486.7215	13.5055
1496.6953	19.6843
1553.2503	130.2063
1611.7995	409.9319
3043.7766	8.4543
3067.0832	6.864
3114.5333	4.5851
3132.8368	1.286
3155.6495	1.6044
3725.7278	207.1692

16a

O	-1.332298	1.261361	-0.003308
C	-1.116488	0.076009	-0.006366
C	0.245907	-0.572730	-0.039864
C	1.391425	0.435683	0.050477
O	2.657400	-0.194552	-0.105522
O	-2.108220	-0.846524	0.014409
H	-2.942678	-0.353748	0.022637
H	0.295925	-1.304472	0.774222
H	0.331571	-1.148108	-0.967229
H	1.330029	0.994678	0.992049
H	1.309762	1.160761	-0.759215
H	2.815272	-0.745163	0.667419

Freq	Int
45.2737	3.5174
103.972	2.8616
179.6676	0.6522
317.0218	117.1227
376.0247	9.9739
454.8738	19.9961
529.7069	30.0226
640.5008	39.3607
670.2265	87.7637
805.8654	12.8743
895.3774	2.1406
1029.0065	109.6403
1068.2804	58.445
1070.5525	30.12
1150.5914	147.9177
1174.0911	74.923
1286.9344	31.5478
1311.014	7.039
1372.0127	39.3427
1404.4085	11.3266
1434.1185	74.468

16a$^+$

O	-0.866060	1.249532	0.296397
C	-0.944007	-0.001046	0.047452
C	0.203578	-0.933373	0.280944
C	1.495462	-0.203577	0.474434
O	2.025880	0.247394	-0.685865
O	-2.045897	-0.470996	-0.396386
H	-2.744073	0.204933	-0.497870
H	-0.055778	-1.525896	1.167532
H	0.232726	-1.636297	-0.562884
H	2.148643	-0.439776	1.305848
H	0.044167	1.458951	0.620870
H	2.932731	0.558624	-0.563635

Freq	Int
57.7313	1.0584
79.3883	2.0711
248.7354	5.2601
369.9162	9.5794
470.9708	167.227
501.1216	19.2823
525.2389	4.2655
579.9795	15.8991
680.2521	4.892
714.5204	229.0506
782.5784	12.499
868.7188	30.3231
916.2401	4.4812
1003.8034	3.4627
1183.4868	104.2571
1199.4979	126.4225
1216.1422	27.4917
1225.3864	127.6739
1301.4359	113.0261
1329.1105	9.7839
1399.9721	86.5131

1463.2955	12.3051			1452.2317	8.6393		
1513.6253	1.7742			1556.3363	230.2232		
1823.7767	283.7904			1646.6321	326.5821		
3013.1632	42.0338			3010.5975	10.6246		
3034.7422	10.2694			3058.0562	12.9379		
3069.1034	6.5284			3188.2554	1.5311		
3111.3452	23.0701			3410.1142	392.0055		
3752.1302	52.374			3662.9549	242.8382		
3827.7637	21.9883			3795.2339	171.3505		
16b				**16b$^+$**			
O	1.305726	1.297340	-0.024750	O	0.860568	1.293051	-0.242358
C	1.137469	0.111259	-0.006066	C	0.956204	0.040319	-0.046279
C	-0.224006	-0.565398	-0.013228	C	-0.185198	-0.894151	-0.351899
C	-1.384904	0.431495	0.015773	C	-1.490470	-0.175860	-0.483913
O	-2.641391	-0.230393	0.098487	O	-2.026262	0.163817	0.708351
O	2.207674	-0.729479	0.018103	O	2.095113	-0.343460	0.394849
H	1.911471	-1.646975	0.045603	H	2.145804	-1.301531	0.551935
H	-0.291248	-1.200067	-0.906870	H	0.072950	-1.403623	-1.289461
H	-0.304840	-1.236506	0.849519	H	-0.219870	-1.662800	0.434316
H	-1.328591	1.096953	-0.852509	H	-2.135493	-0.343088	-1.338093
H	-1.307877	1.055955	0.905865	H	-0.048254	1.498519	-0.566347
H	-2.826343	-0.633248	-0.755198	H	-2.933711	0.483409	0.613465
Freq	Int			Freq	Int		
52.8259	4.7065			60.8324	0.528		
104.114	8.7996			89.9052	2.4815		
180.9916	8.0541			251.9994	0.6213		
304.3559	123.6037			370.6058	14.4586		
371.0143	7.8405			471.655	170.8392		
453.3893	91.7407			506.8984	5.115		
459.7514	3.1692			527.6015	56.1753		
579.183	6.6388			587.7131	9.1862		
658.2543	8.9185			634.2612	33.7123		
810.25	4.912			684.163	7.3385		
890.1804	20.7985			790.5559	126.5338		
1030.1667	81.0063			874.4227	8.3648		
1060.2503	2.0254			921.903	9.4833		
1065.8671	88.2435			1005.8989	3.2936		
1141.6027	14.8834			1188.3062	179.6576		
1164.676	16.8248			1194.162	155.4093		
1275.3161	220.4752			1216.2317	49.5166		
1313.5311	53.5183			1224.7366	136.9813		
1343.4224	158.2326			1308.1237	107.2687		
1396.8376	9.4526			1328.235	12.8375		
1424.6224	58.3253			1406.546	56.9212		
1464.624	5.9802			1453.1719	20.1571		
1511.9739	1.6739			1544.8915	291.6276		
1856.9339	240.9457			1661.8688	203.5218		
3008.0468	14.4599			2990.7919	9.1005		
3027.5164	26.8298			3051.6773	11.481		
3051.1744	18.364			3189.1365	1.4972		
3112.0476	21.7135			3448.1478	364.9388		
3807.2658	43.3177			3724.7746	193.5987		
3829.8434	23.5338			3793.0556	183.0002		
16c				**16c$^+$** (same as **16b$^+$**)			
O	1.301950	-1.302733	0.000069				

C	1.133607	-0.116027	0.000037	
C	-0.223329	0.564240	0.000155	
C	-1.378267	-0.424298	-0.000137	
O	-2.574566	0.349968	0.000027	
O	2.203807	0.724413	-0.000113	
H	1.907443	1.642344	-0.000124	
H	-0.303355	1.215564	0.878220	
H	-0.303308	1.216039	-0.877563	
H	-1.310567	-1.067853	0.884908	
H	-1.310522	-1.067395	-0.885515	
H	-3.321282	-0.255379	-0.000111	
Freq	Int			
61.8857	6.8842			
104.216	6.0257			
183.9901	20.1196			
282.4981	126.24			
369.2556	2.2349			
456.1513	103.7754			
461.6236	1.6184			
581.5893	4.2291			
660.6699	15.9482			
827.0631	1.4873			
893.1604	24.7352			
1038.6539	2.7784			
1057.4403	125.3307			
1087.4211	4.806			
1143.2127	18.0763			
1216.0982	0.6771			
1254.4069	65.091			
1288.3771	253.3833			
1315.6366	0.144			
1367.8115	186.9582			
1460.6957	18.6858			
1475.7162	3.7428			
1528.2533	1.07			
1856.4393	241.4665			
3004.5559	32.6102			
3024.6359	19.3215			
3034.0167	18.5702			
3064.0553	33.5142			
3806.3897	44.6851			
3844.1331	31.7732			
16d				**16d**$^{+}$ (same as **16b**$^{+}$)
O	1.305745	-1.297341	-0.024759	
C	1.137470	-0.111263	-0.006072	
C	-0.224006	0.565385	-0.013256	
C	-1.384908	-0.431499	0.015797	
O	-2.641390	0.230403	0.098489	
O	2.207662	0.729494	0.018118	
H	1.911444	1.646986	0.045626	
H	-0.304826	1.236538	0.849460	
H	-0.291244	1.200015	-0.906926	
H	-1.307879	-1.055921	0.905916	
H	-1.328605	-1.096995	-0.852455	
H	-2.826363	0.633187	-0.755225	

Freq	Int
52.8307	4.7072
104.1111	8.8
180.9898	8.0541
304.3366	123.6069
371.0124	7.8362
453.3944	91.7338
459.755	3.1751
579.1839	6.6393
658.2543	8.9188
810.2503	4.9121
890.1853	20.7998
1030.167	81.0266
1060.248	2.031
1065.8668	88.2158
1141.6001	14.8891
1164.6758	16.8239
1275.3184	220.5015
1313.5341	53.4826
1343.4225	158.2336
1396.8365	9.4534
1424.6234	58.3267
1464.6262	5.9791
1511.974	1.674
1856.9375	240.9479
3008.0447	14.4586
3027.5236	26.822
3051.1669	18.3704
3112.0406	21.7153
3807.2588	43.3179
3829.8496	23.5351

16e

O	1.301977	1.302733	-0.000001
C	1.133608	0.116031	0.000000
C	-0.223330	-0.564222	-0.000001
C	-1.378273	0.424305	0.000002
O	-2.574566	-0.349972	0.000000
O	2.203789	-0.724434	0.000001
H	1.907407	-1.642360	0.000002
H	-0.303320	-1.215787	-0.877893
H	-0.303321	-1.215793	0.877886
H	-1.310558	1.067637	-0.885206
H	-1.310557	1.067632	0.885214
H	-3.321286	0.255369	-0.000006

Freq	Int
61.8915	6.8838
104.2103	6.0265
183.9862	20.1194
282.4961	126.2394
369.2548	2.235
456.1543	103.7747
461.6286	1.6182
581.5912	4.2299
660.6706	15.9487

16e$^+$ (same as **16b**$^+$)

827.0635	1.4874
893.1677	24.7362
1038.6587	2.7775
1057.4391	125.3263
1087.422	4.8059
1143.2109	18.0785
1216.0989	0.6771
1254.4079	65.0908
1288.3787	253.3992
1315.6373	0.144
1367.8181	186.9389
1460.6965	18.6879
1475.7204	3.743
1528.2544	1.0699
1856.4425	241.4693
3004.5586	32.6062
3024.6274	19.3264
3034.0146	18.5606
3064.0454	33.5242
3806.3825	44.6849
3844.135	31.773

16f

O	-0.683276	-1.268100	0.221658
C	-0.911660	-0.096765	0.020349
C	0.131359	0.985981	-0.113823
C	1.508593	0.525049	0.372768
O	2.017329	-0.553855	-0.388627
O	-2.166020	0.376545	-0.123736
H	-2.762909	-0.384155	-0.052222
H	0.184815	1.255540	-1.174457
H	-0.211823	1.875496	0.422836
H	1.453398	0.270546	1.440458
H	2.219032	1.347211	0.265426
H	1.403461	-1.286954	-0.252157

Freq	Int
56.7103	1.0441
173.435	4.663
249.69	2.6416
354.3725	1.3413
478.9865	9.9572
541.2484	17.6628
557.706	183.23
640.6157	47.3215
701.565	68.0509
815.5172	14.6858
885.2194	9.6003
971.9478	11.634
1073.7029	16.5576
1088.1831	68.8544
1157.4878	310.0834
1217.8273	3.7158
1256.1406	27.5997
1322.2002	1.7957
1398.9537	7.3165
1412.1427	93.8115

16f^{+}

O	-0.618019	-1.253680	-0.045563
C	-0.883741	-0.011359	-0.030021
C	0.161014	1.035245	-0.230812
C	1.577240	0.577289	0.198765
O	1.853266	-0.738876	-0.049422
O	-2.097053	0.371227	0.128308
H	-2.722126	-0.376275	0.206211
H	0.157276	1.250467	-1.308520
H	-0.146195	1.954687	0.270218
H	1.721956	0.685291	1.297175
H	2.362758	1.221255	-0.224872
H	0.393710	-1.371836	-0.134387

Freq	Int
108.1978	1.3137
164.5722	13.9654
304.7018	48.5252
394.1128	0.8417
498.6219	23.7831
533.5755	9.5079
665.5894	38.9897
740.1046	148.2047
742.0143	21.9155
862.2867	7.1914
909.2977	10.0388
969.9983	11.7184
1029.425	24.0121
1072.9678	74.4099
1155.2224	2.7487
1210.6803	150.2093
1241.0415	4.3524
1307.6708	9.345
1320.2067	45.5646
1336.0357	81.3392

1437.4013	27.1263			1406.173	13.6953		
1454.3786	46.3907			1439.8833	46.8623		
1510.8439	2.0619			1596.463	299.3792		
1800.7721	274.1737			1643.8069	430.9915		
2987.7315	58.3454			2806.5023	822.7702		
3038.3176	8.049			2865.3718	132.8041		
3080.4813	12.802			2989.3874	6.373		
3084.291	32.2829			3024.0454	21.9337		
3746.7434	65.6374			3115.1434	5.86		
3774.4661	66.9198			3657.1232	230.0933		
16g				**16g^{+}**			
O	1.000724	-1.268721	0.354912	O	0.445422	-1.222642	0.080752
C	0.943428	-0.091846	0.106381	C	0.857727	-0.061743	-0.007882
C	-0.198661	0.831537	0.475831	C	-0.104462	1.090885	-0.187551
C	-1.533707	0.107882	0.491788	C	-1.462437	0.620817	0.306761
O	-1.877382	-0.174546	-0.862632	O	-1.657680	-0.666669	-0.295676
O	1.944645	0.572813	-0.515170	O	2.124497	0.241789	0.029871
H	2.642163	-0.078067	-0.685959	H	2.689374	-0.549608	0.103925
H	0.022488	1.235468	1.470607	H	0.259438	1.980112	0.329491
H	-0.229496	1.674000	-0.217306	H	-0.120638	1.311541	-1.261473
H	-2.291820	0.747655	0.963167	H	-2.261855	1.276597	-0.062303
H	-1.434142	-0.811733	1.078330	H	-1.516365	0.555675	1.394433
H	-2.519452	-0.889124	-0.869723	H	-2.092830	-1.293897	0.308387
Freq	Int			Freq	Int		
48.1798	5.1772			121.1854	4.0935		
110.0392	2.5873			221.1529	1.7901		
189.1218	124.203			283.5012	5.8292		
255.8352	0.886			395.7932	2.0695		
373.2335	3.0927			480.2589	73.0932		
499.7988	26.0586			491.4993	13.1158		
535.4113	27.6175			555.1686	14.7684		
628.3404	35.2359			654.3852	50.7268		
693.7557	101.0696			712.9497	98.9711		
817.0497	7.5637			821.6045	8.7387		
898.5711	7.739			889.6073	7.1393		
999.0779	1.1988			934.3659	8.5182		
1054.9917	22.3764			1007.0941	48.9683		
1085.087	90.3579			1036.7408	6.3946		
1160.1878	210.4229			1154.4646	26.169		
1206.2301	74.9242			1211.3388	144.2173		
1275.5283	15.1876			1226.2529	103.7335		
1302.7631	47.1662			1269.0121	51.9105		
1322.8939	4.6365			1317.8365	28.0373		
1414.1498	54.4444			1402.383	42.0838		
1452.3186	15.9207			1427.5896	42.7798		
1455.9576	8.7236			1448.0043	34.2152		
1515.1389	9.4871			1471.1417	8.6504		
1829.0674	276.758			1591.4726	518.9463		
2988.4561	68.8978			3014.4045	37.9094		
3040.0853	10.166			3047.8313	8.3504		
3045.4401	25.6468			3110.8428	12.3237		
3103.8222	10.5271			3124.7347	5.1846		
3751.1444	51.5164			3686.4394	322.5247		
3852.6735	35.1677			3713.04	309.1186		
16h				**16h^{+}**			

O	2.209544	-0.327199	-0.151786	O	2.143956	-0.328940	-0.166645
C	1.073327	0.015780	0.025831	C	1.005952	0.105164	0.018854
C	-0.055908	-0.969417	0.337731	C	-0.021834	-1.033181	0.322419
C	-1.386593	-0.671521	-0.344038	C	-1.370720	-0.701108	-0.311671
O	-1.878855	0.574132	0.184786	O	-1.748960	0.596937	0.152137
O	0.715652	1.316311	-0.013641	O	0.649581	1.325314	0.005517
H	-0.245572	1.390433	0.140291	H	-0.361402	1.366637	0.115566
H	0.297323	-1.962312	0.058708	H	0.361033	-1.995437	-0.015670
H	-0.214405	-0.967151	1.422194	H	-0.066553	-1.034801	1.418937
H	-2.098899	-1.475752	-0.132206	H	-2.069136	-1.469257	0.047883
H	-1.254907	-0.600083	-1.430274	H	-1.337133	-0.742619	-1.404942
H	-2.639233	0.859855	-0.330730	H	-2.563808	0.903738	-0.267458
Freq	Int			Freq	Int		
84.4668	2.6922			109.5561	0.5556		
198.8063	9.8525			216.3661	5.3807		
265.4748	0.1668			280.3116	4.8979		
337.5662	73.7939			333.6081	28.5444		
393.7396	51.2419			402.5763	44.9597		
484.1924	9.4273			486.4673	22.7571		
574.1497	5.4761			510.1982	29.6513		
704.6569	22.3773			649.9464	74.9556		
781.4391	85.2673			685.095	14.9952		
825.6792	8.0996			861.6017	86.4235		
881.9218	24.1132			868.9954	22.5749		
960.3708	13.3019			959.9745	89.5617		
1048.5097	38.1028			1021.8751	55.2298		
1083.1761	9.4742			1052.6665	59.8923		
1170.7321	12.8083			1146.9439	26.7442		
1245.5863	36.2807			1209.3777	21.135		
1254.4496	92.7356			1219.6423	17.7652		
1307.5897	12.1667			1273.4661	62.5505		
1362.3342	1.0299			1324.2214	3.9937		
1434.4604	302.6523			1403.0869	12.853		
1444.5673	9.7154			1433.0072	29.2477		
1456.6236	10.6581			1466.2012	82.9099		
1526.5216	2.0794			1499.3033	179.2552		
1853.5881	342.1315			1613.9066	140.6014		
3008.2437	42.8266			2852.6087	256.0613		
3035.7038	8.7617			3000.8833	199.492		
3054.7154	40.0348			3036.4925	20.2341		
3117.5227	6.2152			3068.9735	8.5866		
3575.9004	339.6246			3140.7034	11.4474		
3841.7871	49.0847			3797.8811	235.8972		
16i				**16i**$^{+}$			
O	-2.222482	-0.321253	0.077176	O	-2.150336	-0.323652	0.112967
C	-1.075043	0.013669	-0.026618	C	-1.000989	0.103828	-0.025878
C	0.057460	-0.984469	-0.289704	C	0.007423	-1.038088	-0.311152
C	1.396667	-0.648810	0.368960	C	1.365338	-0.680298	0.350076
O	1.920224	0.615492	-0.081163	O	1.791503	0.615488	-0.056812
O	-0.708838	1.309034	0.054066	O	-0.644659	1.324610	0.026271
H	0.261144	1.383583	-0.038033	H	0.361391	1.381743	-0.068895
H	-0.296587	-1.961861	0.042685	H	-0.375049	-1.991974	0.055783
H	0.191233	-1.050079	-1.377207	H	0.059545	-1.084440	-1.405773
H	2.123197	-1.446272	0.186296	H	2.075624	-1.459585	0.055481
H	1.282338	-0.541466	1.448727	H	1.280710	-0.671674	1.436337

H	2.252946	0.507578	-0.978923	H	2.395075	0.581710	-0.810621
Freq	Int			Freq	Int		
86.4022	4.5708			113.1962	1.6754		
201.963	5.2852			193.0504	1.2679		
264.6892	9.9699			274.0414	5.2155		
362.3792	27.4332			343.2804	41.0294		
403.0263	76.5197			376.3551	22.1148		
498.3759	25.9268			467.1263	4.3204		
572.9192	2.7972			511.5833	10.7558		
697.8666	8.4125			678.0174	5.8466		
816.5877	10.8057			703.8587	19.1504		
839.4267	88.0223			855.532	4.7825		
877.4312	13.9553			868.4959	24.747		
959.1756	13.7485			966.1456	96.5964		
1024.8052	75.2936			988.3364	171.0818		
1058.8981	5.7239			1057.4434	74.1783		
1163.8037	38.6175			1139.7582	45.8369		
1218.8627	63.4935			1182.2305	58.3097		
1279.9028	17.142			1217.6002	19.5482		
1350.4672	3.9958			1308.2226	6.4485		
1381.2515	4.7423			1357.7034	8.3245		
1410.826	11.5268			1378.8234	32.1171		
1425.0855	322.3299			1433.4849	165.6243		
1461.1489	7.2495			1443.1716	92.4356		
1513.6587	3.2414			1484.7165	2.4328		
1852.6759	341.5712			1617.2105	149.4007		
3019.2977	9.6672			2940.1132	186.4299		
3039.7138	41.5709			3041.2057	15.6995		
3099.3772	10.6869			3045.4886	45.1198		
3106.0291	16.5845			3121.1316	9.1549		
3554.7251	355.2947			3132.7135	16.9295		
3818.2	37.5996			3796.4048	235.6828		
16j				**16j**$^{+}$			
O	0.632204	-1.299013	-0.256584	O	0.394841	-1.245183	-0.084533
C	0.918775	-0.150743	-0.039964	C	0.868172	-0.107808	0.004210
C	-0.095116	0.978039	0.060119	C	-0.068765	1.077418	0.191271
C	-1.495579	0.533105	-0.376972	C	-1.440642	0.652756	-0.309447
O	-2.009875	-0.494466	0.445349	O	-1.679041	-0.620375	0.300146
O	2.215514	0.194117	0.147231	O	2.161328	0.035931	-0.044666
H	2.289058	1.142890	0.305558	H	2.445717	0.960773	0.021503
H	-0.127305	1.309939	1.104728	H	-0.088506	1.286806	1.267760
H	0.244800	1.829638	-0.542383	H	0.302574	1.967557	-0.322215
H	-1.465085	0.227751	-1.431584	H	-1.484771	0.584270	-1.397391
H	-2.182667	1.377702	-0.293808	H	-2.215615	1.342460	0.047643
H	-1.430021	-1.255430	0.310418	H	-2.129018	-1.239045	-0.301081
Freq	Int			Freq	Int		
61.2171	1.5486			118.233	3.5366		
173.9129	12.1289			223.0542	6.4472		
251.8915	9.7759			284.9212	9.6222		
356.1376	5.6171			393.7614	19.4123		
459.8511	69.2784			475.1767	13.7272		
503.4651	27.4837			486.7065	66.873		
565.5611	107.1483			538.163	67.1185		
579.4293	60.8381			591.6171	37.9925		

670.6433	2.359
821.6684	15.2579
892.4952	2.8459
964.9583	16.6428
1068.471	23.674
1088.6495	76.9018
1145.168	53.3275
1219.3486	9.3846
1256.9092	66.2822
1295.1113	304.3147
1382.1475	122.9141
1404.0385	9.6236
1435.4643	23.4817
1451.9324	40.5121
1508.4333	2.5849
1835.4619	224.884
2995.0994	48.8862
3014.3233	15.3534
3056.004	19.5192
3084.2226	32.6573
3770.8481	73.9515
3806.5212	49.9646

695.2891	12.9832
820.9407	18.7091
899.3724	10.9333
934.9927	15.5257
1010.6379	52.3919
1039.2592	5.6513
1159.652	35.5142
1204.4531	134.3578
1226.1339	42.3167
1278.0475	52.7464
1319.4588	2.6991
1388.0372	208.4681
1406.3568	108.1389
1446.8283	24.7147
1476.6775	8.0653
1612.8196	400.416
3021.9946	25.5471
3040.7128	7.0368
3102.4156	4.7493
3115.1826	8.5023
3718.3583	381.8269
3755.8719	181.8237

16k

O	-1.013206	-1.342603	-0.133530
C	-0.961050	-0.147003	-0.081211
C	0.181711	0.677561	-0.669307
C	1.519267	-0.022906	-0.498703
O	1.860139	0.060444	0.882745
O	-1.976808	0.559422	0.477090
H	-1.758969	1.498316	0.484083
H	-0.035666	0.816927	-1.734471
H	0.240028	1.670967	-0.212865
H	2.279056	0.469528	-1.119863
H	1.412075	-1.062300	-0.824742
H	2.462915	-0.657453	1.092736

Freq	Int
33.574	9.4615
105.5612	11.8064
174.0944	117.8147
262.9485	6.6197
379.0495	10.6515
467.183	108.4238
507.0244	1.7044
583.4526	4.3149
658.7527	4.1148
823.409	14.3576
896.2751	9.5004
997.7226	2.2892
1047.6039	2.1646
1081.0279	95.4768
1147.5279	22.0675
1205.874	17.4475
1274.0718	14.6106
1294.0681	279.7979
1311.3172	157.5428

16k^{+} (same as **16j**$^{+}$)

1392.1263	62.6333
1447.9634	3.1213
1451.1652	12.1628
1514.4648	8.858
1860.1662	236.0088
2991.8213	67.819
3028.6879	10.1936
3054.1009	15.0331
3072.6839	26.6214
3817.6972	43.7617
3855.4744	40.391

16l

O	-1.967056	-0.966976	-0.263957
C	-1.155948	-0.147204	0.078145
C	0.267184	-0.422498	0.501453
C	1.307586	0.227237	-0.428952
O	2.632999	-0.112672	-0.050250
O	-1.433732	1.183210	0.109096
H	-2.350945	1.279650	-0.188251
H	0.403677	-0.030402	1.515505
H	0.412322	-1.501894	0.522035
H	1.157414	1.312473	-0.455253
H	1.182325	-0.153439	-1.444725
H	2.824592	0.319910	0.787707

Freq	Int
34.5973	1.4665
102.3957	2.7133
188.8871	0.9701
316.4491	99.2126
373.8055	34.2389
432.7574	3.4647
582.8643	57.6453
627.8127	66.8469
725.4751	49.1914
806.8776	1.1784
890.3605	10.2147
1022.1676	6.3014
1036.4931	126.5356
1066.4423	89.2509
1145.5873	59.7811
1217.7962	180.4108
1292.6402	1.7035
1307.0799	9.1005
1362.4386	45.0609
1397.1364	0.8407
1424.0902	41.1474
1477.2936	8.9643
1520.5757	1.4412
1834.489	325.4355
3020.3094	38.0129
3034.4828	9.6898
3086.8001	22.9575
3128.1094	12.7677
3754.3896	57.321
3825.4134	24.6286

16l$^+$

O	-2.048214	-0.922392	0.104619
C	-1.170985	-0.097277	-0.011374
C	0.245274	-0.650283	-0.134919
C	1.350835	0.475078	0.173054
O	2.549546	-0.136571	-0.141953
O	-1.310584	1.201375	-0.069649
H	-2.247204	1.466909	-0.015032
H	0.363995	-1.488564	0.551568
H	0.373683	-1.013640	-1.157862
H	1.278112	0.793506	1.213440
H	1.190708	1.292651	-0.528256
H	2.963977	-0.555262	0.631441

Freq	Int
41.3048	5.6023
111.5052	4.243
195.2909	2.0915
330.2296	1.2211
405.6422	103.0508
430.8461	57.4349
544.8759	40.8555
590.1395	48.9881
689.6824	117.2867
785.5791	96.536
818.8298	13.7128
831.4571	18.9822
1020.7822	77.5514
1108.119	60.3647
1136.8506	32.1724
1197.5826	249.862
1212.3434	37.7255
1264.679	7.6884
1322.6752	1.9415
1361.3741	14.8539
1369.9475	68.5439
1450.8561	15.2752
1503.0589	78.1446
1700.4422	394.4259
3070.9496	4.669
3079.9236	7.9441
3136.5211	3.173
3161.0142	10.1264
3688.8589	438.1202
3717.1649	504.6471

16m				**16m$^+$**			
O	1.082880	1.330617	0.068878	O	0.407728	1.249310	-0.031152
C	0.977338	0.145694	-0.060526	C	0.870606	0.105018	0.012817
C	-0.190199	-0.521107	-0.785252	C	-0.072271	-1.068351	0.240478
C	-1.520624	0.163625	-0.465857	C	-1.452829	-0.670346	-0.278785
O	-1.924010	-0.046958	0.880399	O	-1.716037	0.701107	0.032648
O	1.946984	-0.685138	0.404502	O	2.159050	-0.052522	-0.086025
H	1.701380	-1.602566	0.242085	H	2.436265	-0.981036	-0.046290
H	0.017300	-0.435863	-1.858945	H	0.292544	-1.978566	-0.242308
H	-0.254318	-1.591802	-0.556946	H	-0.073108	-1.248585	1.323372
H	-2.289105	-0.171918	-1.173729	H	-2.235506	-1.296302	0.166353
H	-1.393140	1.240369	-0.578754	H	-1.514349	-0.732556	-1.363370
H	-2.228039	-0.955657	0.965864	H	-1.784799	0.855954	0.991417
Freq	Int			Freq	Int		
37.6867	2.8274			117.3927	1.6455		
112.2652	1.4424			187.0058	2.2076		
237.9567	7.0288			297.568	1.1668		
319.5413	133.2968			398.6167	7.0438		
381.6637	10.9106			480.0793	39.2238		
457.2796	90.23			531.0449	58.6158		
509.0764	11.3467			552.4188	29.0247		
580.1713	3.1938			595.3077	34.089		
665.3979	5.1039			702.6367	6.8439		
816.7533	16.8745			821.0414	22.1275		
884.7128	4.9484			886.3787	9.0886		
991.2077	4.6242			934.8574	13.4013		
1025.084	41.5793			1015.8171	7.3401		
1082.5475	63.5842			1029.4628	45.5483		
1126.5966	45.2402			1141.1437	43.1229		
1201.7726	23.36			1199.9273	148.7956		
1254.304	11.1442			1233.7647	58.7457		
1291.0444	389.3959			1292.3464	50.9598		
1387.6084	65.5128			1319.4677	4.3879		
1393.4492	6.1989			1388.5314	244.0028		
1417.3528	30.6421			1414.2179	28.2239		
1457.6515	9.3881			1456.3675	23.7904		
1503.4728	6.8258			1483.3693	5.1122		
1864.0821	234.2302			1609.8467	392.9909		
3001.5923	53.7288			3028.221	3.9577		
3014.2772	31.003			3032.8218	16.3485		
3052.1591	17.4111			3097.0021	1.1904		
3113.3784	11.0575			3148.381	5.8115		
3821.3289	37.3191			3702.4296	227.8348		
3827.6362	24.5084			3756.1618	208.7284		
16n				**16n$^+$**			
O	-1.210483	-1.189749	0.451098	O	-2.021860	-0.586444	-0.466007
C	-0.951170	-0.137835	-0.072649	C	-1.048231	-0.033352	0.001907
C	0.239322	0.111131	-0.974531	C	0.131765	-0.933617	0.336731
C	1.541884	-0.353131	-0.317445	C	1.490797	-0.109547	0.505940
O	1.843885	0.381296	0.861296	O	1.992222	0.390217	-0.668838
O	-1.721093	0.965570	0.076552	O	-0.933163	1.237576	0.275780
H	-2.454262	0.712011	0.658101	H	-1.742811	1.733723	0.053553
H	0.074086	-0.463130	-1.893111	H	-0.082813	-1.436348	1.285036
H	0.288318	1.167764	-1.247731	H	0.229775	-1.695912	-0.436933
H	2.359606	-0.296545	-1.047866	H	2.145996	-0.884691	0.941178

H	1.434998	-1.391786	-0.002986
H	2.018566	1.293757	0.609774

Freq	Int
33.6882	1.0952
115.3301	0.677
225.5867	6.9015
336.5804	123.7876
399.2177	6.1306
472.7994	30.7424
557.2958	37.0878
640.6048	49.2858
722.8211	74.3063
815.039	8.8755
889.6637	4.6106
997.2836	0.7016
1031.7602	44.0561
1082.5483	52.2847
1136.6311	205.7927
1208.7077	134.8318
1255.9268	12.9915
1318.9639	2.2251
1386.9554	7.0982
1409.1151	50.7283
1420.4591	44.7607
1471.2833	10.6611
1508.6917	5.8529
1832.4255	278.0592
2997.917	64.5235
3039.0476	11.8375
3085.9512	5.768
3110.412	22.4516
3746.5655	52.0817
3822.305	21.8783

H	1.337412	0.719178	1.191424
H	2.368855	-0.307640	-1.229212

Freq	Int
39.3821	4.6165
113.0038	0.8288
241.7359	5.2751
336.6058	5.1276
367.9943	80.1298
477.444	32.197
528.8049	24.2895
569.8266	52.5159
687.0491	120.6756
748.4678	7.3899
821.8501	8.6414
890.6157	4.8642
960.9972	110.2444
1083.4231	160.6323
1137.8538	6.6144
1199.5161	225.6035
1220.9653	17.8979
1267.4971	7.659
1299.6069	86.4418
1364.5788	30.4404
1380.372	72.6282
1443.0523	19.6995
1475.3421	23.9601
1672.5464	337.9342
2929.3098	45.4434
3068.9839	8.2612
3132.5212	5.1964
3169.7265	5.6706
3686.8547	375.7365
3727.0787	404.4143

16o

O	-1.606132	-1.100952	-0.061272
C	-0.967325	-0.099372	0.128635
C	0.249473	0.016120	1.019279
C	1.506211	0.438004	0.247459
O	1.784293	-0.418996	-0.850278
O	-1.274169	1.086838	-0.450602
H	-2.037649	0.924533	-1.024224
H	0.044167	0.755605	1.800710
H	0.391222	-0.955085	1.498339
H	2.353886	0.490894	0.943919
H	1.360072	1.429540	-0.181980
H	1.926211	-1.309126	-0.511792

Freq	Int
53.9816	2.614
105.7986	1.1486
222.6736	10.4036
335.2712	124.0126
408.4297	6.9151
465.9247	12.8007
563.634	40.2923

16o^{+} (same as **16n**$^{+}$)

617.1296	82.6733
715.8849	45.7274
813.8894	6.6675
888.0333	5.8361
992.4156	8.9366
1021.8117	58.0599
1085.2154	68.2102
1125.6766	159.1377
1230.7343	113.0018
1251.5199	17.0544
1345.3376	22.4456
1361.1485	11.4152
1395.1453	20.216
1428.3393	35.5837
1470.6631	11.3354
1512.2737	2.3738
1834.9589	310.4812
2992.7526	68.2904
3042.593	11.6315
3090.4615	1.4928
3111.4795	28.3265
3760.4851	59.7628
3819.2599	23.4027

16p

O	-2.184080	-0.409400	-0.131044
C	-1.047974	-0.062329	0.046060
C	0.128917	-0.964969	0.333800
C	1.436076	-0.580149	-0.379136
O	2.050951	0.574665	0.160040
O	-0.687168	1.256499	0.010858
H	-1.492376	1.761586	-0.178802
H	0.310317	-0.940821	1.414165
H	-0.180806	-1.977567	0.069145
H	1.254405	-0.474930	-1.458528
H	2.151608	-1.394048	-0.247111
H	1.417118	1.296346	0.077947

Freq	Int
36.6378	3.4645
177.9176	5.2451
243.6372	0.3015
357.9599	2.381
467.6925	19.9431
486.3943	112.2377
555.6177	47.3613
614.3966	82.5704
722.0601	44.4726
801.1551	13.9502
880.6849	12.9088
948.4013	13.9135
1071.9142	11.3333
1079.6461	47.7499
1160.6509	318.7988
1213.1566	11.2376
1255.3485	15.1584
1326.6606	13.2084

16p$^+$

O	-2.146856	-0.451643	0.272554
C	-1.056353	-0.004366	0.005470
C	0.097607	-1.003692	-0.049341
C	1.458930	-0.333237	-0.475888
O	2.025500	0.350428	0.573156
O	-0.768377	1.251502	-0.244465
H	-1.560963	1.816386	-0.184761
H	0.194645	-1.456669	0.939766
H	-0.156758	-1.790622	-0.762599
H	1.377882	0.243500	-1.396095
H	2.064719	-1.247263	-0.642685
H	2.197234	1.280148	0.354975

Freq	Int
38.5931	2.5035
122.87	2.1324
241.1445	4.4617
261.9363	133.2633
337.5002	2.7295
474.6164	25.3124
534.3037	34.2132
576.2036	42.8967
692.2605	132.7766
792.3435	7.2273
822.5816	17.3626
888.2551	28.7304
926.1011	131.4468
1109.0435	4.2448
1145.255	98.0243
1197.8482	245.6733
1232.4381	59.7351
1258.3619	7.3246

1363.5828	8.0594
1404.4456	8.2769
1441.3297	57.2517
1453.951	34.2117
1513.8939	0.9723
1841.4511	316.7948
2980.3362	61.3339
3040.4025	7.251
3084.7432	30.2377
3105.9157	10.6788
3751.594	72.6747
3805.2831	58.6528

16q			
O	1.814475	-0.754752	-0.570771
C	0.993784	-0.120956	0.037641
C	-0.223589	-0.693303	0.732407
C	-1.506079	0.087023	0.480952
O	-1.774355	0.021972	-0.916326
O	1.092673	1.222156	0.210539
H	1.893329	1.497363	-0.259836
H	-0.331652	-1.724545	0.395431
H	-0.016149	-0.705914	1.808311
H	-1.377497	1.122772	0.815056
H	-2.320020	-0.367342	1.062618
H	-2.495054	0.626072	-1.115106

Freq	Int
57.8446	0.0137
109.1057	1.05
228.6485	77.0209
267.3529	44.4603
387.7204	4.3075
484.3555	1.6162
554.1351	44.4075
607.7851	75.9408
696.4849	69.9316
813.1239	5.2633
896.3467	9.2695
984.7267	10.1427
1044.6628	56.8538
1088.9448	87.0627
1167.6084	114.018
1219.2501	111.8195
1265.6436	10.5152
1299.864	38.8208
1348.7534	22.7615
1381.7163	23.4001
1455.0945	4.2064
1458.8335	13.8585
1521.9413	4.499
1838.6722	315.9549
2983.9873	69.5249
3035.0253	34.339
3044.1668	10.6241
3117.8304	10.189
3761.1411	57.2431

1289.5218	35.4062
1344.8363	19.0005
1355.8132	18.8352
1434.6855	15.9027
1458.7757	35.8915
1693.0955	264.2842
2880.3477	132.4259
3079.9783	9.4587
3129.1266	15.6289
3137.024	8.3839
3687.5057	313.0469
3741.9739	513.6532

16q^{+} (same as **16p**$^{+}$)

3844.818	32.2356						
16r				**16r$^+$**			
O	-2.059073	-0.896397	-0.253089	O	-2.048116	-0.922436	-0.104920
C	-1.164309	-0.147577	0.040002	C	-1.170970	-0.097278	0.011415
C	0.259342	-0.547796	0.343580	C	0.245288	-0.650194	0.135322
C	1.317190	0.335149	-0.311959	C	1.350816	0.474932	-0.173584
O	2.580745	-0.190091	0.082431	O	2.549534	-0.136377	0.142061
O	-1.350600	1.194293	0.152203	O	-1.310672	1.201354	0.069876
H	-2.285854	1.356305	-0.042883	H	-2.247297	1.466832	0.015089
H	0.399556	-0.503447	1.429112	H	0.373706	-1.012718	1.158566
H	0.386994	-1.585081	0.035034	H	0.364009	-1.489018	-0.550494
H	1.190349	1.372214	0.018026	H	1.190597	1.293122	0.526985
H	1.199504	0.307583	-1.404502	H	1.278160	0.792431	-1.214260
H	3.267534	0.351328	-0.316889	H	2.964054	-0.555726	-0.630929
Freq	Int			Freq	Int		
41.1242	2.3896			41.372	5.6063		
104.6043	3.9059			111.4875	4.2436		
195.5527	2.1354			195.2966	2.0913		
267.2772	120.2783			330.2283	1.2227		
367.3173	5.6108			405.639	102.9662		
440.6275	4.395			430.8127	57.5102		
571.6538	49.4105			544.8923	40.8741		
629.6428	76.2465			590.1832	49.0395		
709.7771	70.0374			689.6785	117.2335		
819.3406	2.5239			785.5894	96.5535		
884.1657	15.8281			818.8151	13.7206		
1027.2019	37.0506			831.4831	18.9996		
1060.6825	35.9818			1020.775	77.5993		
1074.9214	75.6505			1108.121	60.3317		
1186.2945	159.0209			1136.8214	32.1972		
1232.4438	7.7983			1197.5697	249.8093		
1253.9872	84.9106			1212.3535	37.7826		
1307.1051	7.5351			1264.686	7.6862		
1331.2958	3.1151			1322.6845	1.9474		
1365.244	67.6417			1361.3771	14.8627		
1463.7507	5.1696			1369.953	68.5326		
1477.7956	7.6215			1450.8532	15.2788		
1532.2679	2.0234			1503.0612	78.1562		
1834.8671	330.1346			1700.4367	394.4859		
2980.8354	54.05			3070.9349	4.6787		
3033.7959	31.9183			3079.8889	7.9406		
3046.653	13.2737			3136.5294	3.1681		
3122.6911	10.0526			3161.0151	10.141		
3753.7859	56.6708			3688.8651	438.1699		
3841.3204	29.8011			3717.1614	504.6206		
16s				**16s$^+$** (same as **16r$^+$**)			
O	1.984259	-0.956633	-0.276817				
C	1.157867	-0.152119	0.067039				
C	-0.266618	-0.456061	0.466237				
C	-1.310297	0.281456	-0.389191				
O	-2.632802	0.015453	0.053628				
O	1.418874	1.178879	0.128854				
H	2.341207	1.291690	-0.145868				
H	-0.398968	-1.537008	0.391397				
H	-0.412196	-0.160793	1.509520				

H	-1.181369	0.017176	-1.447585
H	-1.169156	1.357883	-0.294683
H	-2.827881	-0.910194	-0.122609

Freq	Int
41.0124	3.3491
105.2769	5.1514
188.7995	0.5563
323.2975	102.8239
376.697	38.2759
434.5899	3.5096
580.0485	57.2849
628.7731	65.6806
719.037	47.59
808.4729	5.9919
891.3242	8.25
1016.3885	12.7907
1051.6793	55.5088
1070.8352	122.1026
1135.2873	137.6477
1225.6427	109.7492
1278.8146	14.0696
1325.919	4.2131
1359.7432	65.2532
1401.2235	2.4268
1422.5842	33.6352
1475.9482	9.5289
1519.8703	1.3008
1831.5503	320.8124
2992.286	52.0681
3051.2832	9.7075
3097.6893	0.6098
3119.2434	27.1736
3755.4181	58.8695
3826.2289	24.7074

16t

O	1.822357	-1.090813	-0.228253
C	1.171316	-0.138773	0.092845
C	-0.252936	-0.209874	0.620635
C	-1.286251	0.082521	-0.484514
O	-2.611659	0.086884	0.019257
O	1.676452	1.118514	-0.060613
H	1.056263	1.773518	0.279954
H	-0.404021	-1.218181	1.009763
H	-0.409599	0.500368	1.438898
H	-1.161901	-0.639311	-1.301208
H	-1.124946	1.079533	-0.901190
H	-2.845769	-0.815846	0.256862

Freq	Int
31.1767	11.0109
99.029	10.5142
183.8782	8.1193
318.1501	104.2394
371.423	31.1148
444.8668	5.0003

16t$^+$

O	1.910438	-1.011128	-0.227058
C	1.182490	-0.080029	0.047873
C	-0.256261	-0.491231	0.411497
C	-1.329199	0.278208	-0.464945
O	-2.537904	0.015328	0.169020
O	1.588717	1.155790	0.061147
H	0.925261	1.782305	0.388838
H	-0.370047	-1.563258	0.255361
H	-0.392694	-0.274370	1.477792
H	-1.288836	-0.060759	-1.501152
H	-1.163444	1.355481	-0.404618
H	-2.982422	-0.761008	-0.207651

Freq	Int
69.822	16.1676
94.9879	12.2126
190.2001	7.3018
335.4523	0.5476
391.635	27.1754
402.6738	124.1582

478.2287	102.5032	503.5349	91.4391
622.6317	10.3837	580.7161	19.3905
722.1334	2.4826	674.5682	10.1554
807.5079	1.7092	771.748	2.1961
888.336	23.6779	817.2851	26.5706
1009.6933	7.4899	851.5185	145.5155
1034.7081	17.3934	1018.7643	113.9463
1066.5281	153.6458	1103.0769	41.5322
1126.0218	27.2611	1125.0225	7.9929
1218.5874	7.3693	1188.2949	81.1363
1270.021	65.6787	1223.746	81.5626
1314.1065	298.74	1273.6789	86.4656
1319.5708	57.4694	1318.183	165.7656
1397.4469	2.2418	1356.0446	19.7222
1421.6627	41.1803	1379.3534	56.3518
1490.8671	5.7193	1453.4969	18.0951
1518.4046	1.9119	1498.3356	115.5542
1861.1378	273.7221	1678.2835	512.4095
3008.5801	31.9287	3044.5448	10.2502
3040.424	21.0065	3059.3346	1.5139
3073.1288	14.3011	3122.262	4.1487
3106.8603	25.9312	3144.7671	6.2417
3812.7074	40.1542	3735.479	582.5647
3826.9073	28.9326	3759.1346	95.8892

Table S15. Cartesian coordinates (Å), harmonic frequencies (cm^{-1}), and infrared intensities (km mol^{-1}) of isomers **19** and **20** calculated at the composite CBS-QB3 level of theory.

19a				**19a$^+$**			
C	0.681483	0.082383	-0.019335	C	0.730155	0.084119	-0.000007
C	-0.650823	-0.037925	-0.001249	C	-0.678314	-0.085024	-0.000041
C	-1.644621	1.072264	0.031456	C	-1.667781	1.015570	0.000011
O	1.332289	1.268999	-0.060474	O	1.224113	1.287266	-0.000007
O	1.527998	-0.982402	0.005682	O	1.570291	-0.913776	0.000020
O	-1.125491	-1.362338	0.074889	O	-1.023973	-1.369567	0.000003
H	-2.290745	1.070759	-0.857198	H	-2.310792	0.946904	-0.885420
H	-2.296954	0.986534	0.907909	H	-2.309493	0.947978	0.886479
H	-1.137008	2.036875	0.068598	H	-1.178486	1.987396	-0.000907
H	2.232615	1.113032	0.248186	H	2.197371	1.280996	-0.000019
H	0.964368	-1.763658	0.110349	H	1.116923	-1.775344	0.000010
H	-1.666884	-1.537947	-0.703858	H	-1.983336	-1.507297	-0.000037
Freq	Int			Freq	Int		
164.6687	33.765			87.7016	0.2207		
187.0643	3.2522			138.599	6.9651		
224.1833	43.961			250.4838	3.4392		
248.3891	96.9759			370.0027	3.1167		
312.4876	48.0179			380.4793	1.1761		
337.4646	23.1645			472.5104	165.1561		
374.2697	39.3614			524.2405	204.1398		
502.4752	18.124			526.0497	23.0463		
545.0153	98.8816			560.9293	4.4118		
571.2006	1.0275			571.9142	41.3146		
631.4436	18.1613			666.8208	14.2633		
755.5825	20.5616			780.6896	22.68		
965.9878	38.9748			1004.5063	10.5915		
1056.7926	7.9462			1017.3074	5.9086		
1092.0845	202.0577			1102.3273	245.2796		
1218.5028	184.0757			1160.8317	42.1762		
1232.2153	27.0266			1216.0695	123.1204		
1247.4573	41.5866			1360.9495	374.1941		
1346.872	174.7293			1400.5995	57.8318		
1399.6755	71.1006			1426.493	93.7645		
1429.0271	23.7996			1463.5712	16.4846		
1478.1794	9.4765			1472.9802	39.5575		
1495.147	15.1481			1571.4475	121.8658		
1826.8472	160.5766			1683.1082	120.1398		
2987.8526	65.6679			3016.3635	6.4694		
3034.2102	36.7916			3066.6573	0.498		
3117.247	9.7678			3155.7214	1.8975		
3743.1323	71.6401			3700.6385	199.5554		
3769.8378	18.6807			3715.4986	345.0243		
3812.5724	90.9969			3763.966	232.3404		
19b				**19b$^+$**			
C	-0.667160	0.087133	-0.014155	C	-0.711284	0.111534	-0.003068
C	0.655572	-0.100314	0.008564	C	0.682994	-0.142363	-0.008979
C	1.692205	0.971085	-0.051462	C	1.722186	0.918091	-0.004337
O	-1.342628	1.286484	-0.016185	O	-1.281654	1.288631	0.005702
O	-1.511321	-0.989116	-0.112645	O	-1.509260	-0.927111	-0.006271
O	1.193371	-1.370846	0.071172	O	1.109239	-1.384927	0.005978

H	2.281146	1.007560	0.871502
H	2.387421	0.767376	-0.872056
H	1.250528	1.953859	-0.225522
H	-0.876948	1.905507	0.553725
H	-2.297608	-0.799802	0.413499
H	0.456386	-1.994101	0.062444

Freq	Int
157.9648	2.3814
177.504	30.8925
206.4083	31.4884
246.2416	17.2486
301.8298	102.4223
339.7061	39.5174
377.6748	21.056
447.0006	122.6987
509.93	27.6786
549.4837	8.2238
584.4764	8.4561
755.8899	3.2859
975.1193	40.3477
1062.1295	8.8523
1082.809	109.2661
1175.8108	233.9118
1214.7377	74.3714
1281.8043	169.8802
1350.5557	93.9297
1386.1874	85.1427
1436.6417	5.7555
1471.5063	6.4136
1498.5477	1.9906
1817.1874	28.6089
3016.7022	38.259
3061.7015	21.6079
3106.6161	23.9224
3792.111	58.5395
3795.836	42.8125
3847.9116	45.9517

H	1.945135	1.235435	1.021875
H	2.641255	0.518481	-0.434073
H	1.427528	1.796439	-0.584503
H	-0.659741	2.032242	0.023407
H	-2.450692	-0.682254	0.001441
H	0.386540	-2.036653	0.026878

Freq	Int
47.7865	0.2756
132.2359	5.7838
245.1603	7.6761
361.2496	0.0137
390.0169	2.1467
432.116	245.8254
507.9481	43.0166
517.4435	16.7799
567.2759	33.1604
602.2999	143.0154
639.1106	0.6211
779.7679	8.3965
996.9087	25.0776
1024.4081	4.7348
1108.0267	159.9695
1168.2611	16.4714
1183.6106	196.3563
1364.5741	438.8807
1407.2185	23.0565
1437.1367	33.4762
1464.6301	53.2426
1476.6146	52.9717
1550.3657	116.9264
1668.9897	54.789
3019.6069	8.7367
3085.5132	2.7002
3133.0601	3.1787
3696.7499	158.7332
3722.0486	367.0635
3758.8759	144.3745

19c

C	0.710263	-0.086957	0.012539
C	-0.625939	0.055355	0.014695
C	-1.665525	-1.016677	-0.035874
O	1.412098	-1.244314	0.015313
O	1.557486	0.960738	-0.018671
O	-1.083770	1.387635	-0.068125
H	-1.232816	-2.018080	-0.123269
H	-2.302727	-1.021920	0.858849
H	-2.321965	-0.873603	-0.901328
H	0.804857	-1.975766	0.160356
H	0.993074	1.740819	-0.124482
H	-1.539731	1.605751	0.753583

Freq	Int
112.2209	10.5809
163.5555	4.1665
251.87	11.3911

19c$^+$

C	0.753426	-0.100338	0.002496
C	-0.658281	0.098626	0.009764
C	-1.696666	-0.962687	0.005668
O	1.342767	-1.259628	-0.006935
O	1.586355	0.893372	0.007322
O	-0.974972	1.391304	-0.013951
H	-1.308095	-1.942035	0.289072
H	-2.489568	-0.717100	0.719408
H	-2.153034	-1.054062	-0.987810
H	0.731118	-2.008799	-0.035004
H	1.125025	1.749769	0.018066
H	-1.929513	1.558243	-0.002782

Freq	Int
50.1339	0.0907
119.5164	0.0734
263.1864	6.5617

279.4284	60.4748			358.0828	12.6143		
302.4454	23.7552			393.8565	3.7928		
345.5917	43.707			431.661	1.6477		
384.2304	42.8725			453.8404	158.9689		
511.3917	7.396			532.2709	7.9518		
570.7031	20.4317			564.4982	8.2661		
575.8682	125.0109			597.1706	214.2409		
647.3832	27.7439			667.8879	7.1955		
762.2602	13.699			791.2607	2.3702		
962.7571	22.4743			996.9119	10.8962		
1050.3315	4.7994			1011.8306	8.8094		
1105.5138	54.0174			1107.4676	77.5916		
1184.9273	409.9411			1161.5337	269.6902		
1230.9596	10.6064			1187.6034	131.2714		
1253.6737	21.1163			1365.8334	248.275		
1358.5924	174.6688			1397.0539	133.787		
1418.9317	23.2428			1419.9441	89.3567		
1451.5432	10.4678			1458.3663	23.7426		
1464.3439	8.9084			1479.9274	31.8671		
1500.2042	10.499			1592.6415	79.6804		
1783.1079	238.832			1637.101	186.2562		
2987.3498	58.4176			3015.7481	5.4682		
3034.853	31.7461			3075.9077	1.2276		
3071.188	36.8539			3116.5623	1.3546		
3748.3939	75.8365			3712.0319	197.9138		
3764.797	18.5326			3764.4624	271.9995		
3856.8933	43.0652			3789.2615	133.748		
19d				**19d**$^{+}$			
C	-0.657607	0.096002	-0.003262	C	-0.708579	0.106534	0.000012
C	0.664358	-0.091922	0.000654	C	0.689706	-0.122890	-0.000015
C	1.690039	0.989084	-0.011855	C	1.705363	0.951998	0.000226
O	-1.265134	1.320839	0.103934	O	-1.148254	1.340890	-0.000554
O	-1.508743	-0.994425	-0.099786	O	-1.481305	-0.964421	0.000636
O	1.199160	-1.357368	0.018064	O	1.136188	-1.357565	-0.000259
H	1.218286	1.969677	-0.043068	H	1.255054	1.941267	0.000691
H	2.317008	0.926612	0.883311	H	2.348002	0.840853	0.879945
H	2.348764	0.875803	-0.878961	H	2.347673	0.841569	-0.879826
H	-1.808531	1.459824	-0.683112	H	-2.111706	1.445796	0.002117
H	-2.117218	-0.966439	0.650472	H	-2.437981	-0.811761	-0.002390
H	0.458686	-1.976826	-0.019565	H	0.426982	-2.022809	-0.000458
Freq	Int			Freq	Int		
173.0071	2.4806			48.0028	2.9469		
192.1546	3.3544			56.7234	0.3176		
240.8935	0.3113			175.3973	2.3218		
303.3549	70.0448			261.0908	0.1559		
345.2955	28.9323			374.4948	196.5718		
362.7556	13.9467			391.4842	104.3003		
420.5048	96.2761			393.8872	7.867		
517.7722	109.3578			525.5268	4.0784		
548.8302	120.8503			568.0707	23.3391		
553.4332	14.2675			596.1559	132.6495		
579.8808	12.6878			627.3323	5.6272		
753.7407	3.3865			780.4058	2.4116		
979.8368	45.6139			1020.5408	20.7064		
1066.9955	20.3443			1021.2111	2.2359		

1077.8531	78.2898
1203.5916	269.8182
1250.2246	97.5902
1270.2906	138.0377
1300.9238	32.5643
1380.8796	40.7623
1433.6394	7.3037
1477.9766	7.8261
1491.5078	2.6997
1817.3631	10.3264
3024.133	34.4026
3067.7129	22.1956
3140.8944	9.5184
3744.9401	33.2532
3755.6985	25.8434
3779.9764	42.3938

19e			
C	-0.679045	0.035002	-0.019539
C	0.650752	-0.090473	-0.007654
C	1.604244	1.062018	-0.028410
O	-1.287654	1.261600	0.122014
O	-1.531552	-1.028367	-0.138401
O	1.194902	-1.356088	0.108324
H	2.195084	1.093670	0.893833
H	2.311082	0.966447	-0.864202
H	1.075371	2.007404	-0.135467
H	-1.975078	1.321729	-0.553701
H	-2.081201	-1.068351	0.655031
H	2.013463	-1.377339	-0.397365

Freq	Int
171.0555	55.092
186.2443	31.0732
203.3017	43.7568
224.5807	152.5407
261.8248	17.2876
364.7144	9.3236
370.7134	3.5372
425.4438	71.1352
539.6637	103.9025
559.0913	19.1594
578.6189	10.6488
752.2737	2.573
976.193	62.4397
1056.6165	25.718
1086.1929	188.4963
1223.9435	117.7238
1233.6485	240.3367
1268.9038	56.8749
1308.6052	32.6162
1338.3948	33.3666
1415.6378	5.8713
1482.3041	7.7642
1489.8181	7.6462
1829.2632	24.624
2991.6728	56.1437

1089.2157	147.2223
1121.0614	210.7384
1165.1912	251.0876
1370.2275	177.5618
1400.7887	26.7779
1456.0053	158.5058
1456.3433	18.3208
1474.9466	18.5554
1515.9953	148.4357
1676.1753	12.0188
3032.6443	12.1239
3082.2966	2.0634
3169.098	1.3282
3709.0965	147.2746
3759.6595	63.2723
3774.2277	508.156

19e$^+$			
C	-0.727197	0.061911	0.000000
C	0.680624	-0.113194	0.000001
C	1.651995	1.008597	-0.000026
O	-1.183738	1.293770	0.000057
O	-1.482477	-1.005640	-0.000054
O	1.063563	-1.373681	0.000030
H	2.295262	0.945412	0.885338
H	2.295283	0.945352	-0.885371
H	1.155820	1.976034	-0.000063
H	-2.148809	1.379794	-0.000191
H	-2.437855	-0.843657	0.000160
H	2.028980	-1.462411	0.000020

Freq	Int
73.6269	0.394
103.7965	1.5541
226.5707	0.0082
267.5746	5.7806
382.3218	64.0675
394.9178	3.1731
432.1317	233.8189
521.7637	120.9906
531.8053	9.2758
554.1265	10.3215
649.8539	8.9785
781.4855	4.564
1008.1062	31.5914
1023.1714	5.7279
1078.6592	242.4286
1130.3424	257.6276
1175.2037	93.8659
1366.9451	129.8781
1405.3403	34.5778
1437.9248	216.6231
1468.4071	15.9386
1477.4303	7.3551
1522.6228	167.8061
1691.7591	33.6743
3019.7133	5.2821

3041.2944	30.8305			3069.753	0.299		
3138.1698	7.3282			3162.6973	1.2352		
3756.9538	33.0391			3755.9497	375.9073		
3769.2084	31.6257			3759.6408	64.3965		
3819.666	34.8997			3773.4256	338.5215		
20a				**20a**$^{+}$			
C	0.883519	0.072634	-0.024509	C	0.912386	0.007689	-0.000030
C	-0.079030	1.005823	0.033597	C	-0.098843	1.013945	0.000038
C	-1.520198	0.691175	-0.215440	C	-1.549904	0.725110	-0.000267
O	-1.839064	-0.616638	0.336997	O	-1.768097	-0.678933	0.000686
O	0.681120	-1.251435	-0.206482	O	0.675146	-1.257582	-0.000313
O	2.194266	0.369040	0.102678	O	2.147760	0.402129	0.000166
H	0.207028	2.023963	0.253403	H	0.233238	2.044994	0.000171
H	-1.761480	0.676948	-1.289680	H	-2.001479	1.205488	-0.883938
H	-2.152594	1.450306	0.257214	H	-2.002170	1.206694	0.882376
H	-2.680916	-0.902049	-0.032068	H	-2.704767	-0.906083	-0.001209
H	-0.271227	-1.408908	-0.039488	H	-0.316151	-1.409137	-0.000283
H	2.662863	-0.465791	0.223193	H	2.771027	-0.347333	0.000122
Freq	Int			Freq	Int		
95.3861	2.5641			74.1931	49.7643		
204.542	12.9593			161.656	46.9193		
265.939	4.2996			234.396	87.1698		
343.641	147.546			304.569	23.3519		
363.128	43.3387			394.642	1.0142		
412.861	52.6734			528.488	13.6483		
524.211	19.9209			570.453	98.501		
649.556	10.8029			664.041	39.0903		
681.882	25.486			689.023	3.848		
721.48	49.4741			723.165	71.8832		
754.705	70.1516			875.322	73.8225		
877.7	19.8399			877.824	48.1965		
958.209	30.3094			926.972	5.2905		
1037.67	16.5029			1012.14	4.7928		
1088.11	66.858			1139.75	68.2794		
1205.09	22.4337			1192.23	136.637		
1217.9	189.458			1215.13	82.7747		
1253.09	30.8957			1225.71	0.0143		
1280.35	108.552			1323.09	54.8641		
1405.68	142.082			1406.31	43.3167		
1418.09	6.9835			1427.18	55.1069		
1475.39	136.016			1461.33	33.331		
1519.36	1.3244			1585.22	283.359		
1765.66	352.391			1642.28	324.316		
2949.74	95.5193			2954.53	10.5234		
3029.57	51.7531			2976.8	0.0389		
3215.82	2.7895			3135.5	660.118		
3518.81	307.03			3212.4	18.237		
3808.84	91.932			3694.96	295.87		
3828.17	19.6721			3836.31	179.243		
20b				**20b**$^{+}$ (same as **20a**$^{+}$)			
C	-0.877722	-0.083839	-0.025794				
C	0.096175	-1.008603	0.029786				
C	1.513790	-0.641149	-0.295080				
O	1.908426	0.632157	0.291984				
O	-0.675861	1.231848	-0.263541				

O	-2.181224	-0.370524	0.158196	
H	-0.165695	-2.028819	0.270522	
H	1.678731	-0.482135	-1.365788	
H	2.201495	-1.428616	0.027383	
H	1.851308	0.525682	1.249470	
H	0.283398	1.398789	-0.149967	
H	-2.653419	0.468799	0.221790	
Freq	Int			
134.809	5.2994			
205.547	3.0505			
249.233	8.7629			
348.935	125.869			
392.691	66.2563			
469.443	76.6833			
532.063	58.7522			
658.94	6.2514			
684.717	22.6421			
723.539	38.2105			
820.091	56.9325			
873.092	15.5385			
940.318	81.0921			
1007.9	32.2087			
1071.86	25.5119			
1194.13	67.9843			
1218.12	115.691			
1253.57	96.877			
1352.37	1.1935			
1394.47	112.888			
1397.81	55.3401			
1455.34	164.12			
1512.21	0.1309			
1751.02	357.751			
3023.2	65.6654			
3056.85	33.6478			
3213.82	3.5639			
3506.11	274.549			
3790.19	22.3719			
3806.72	96.172			
20c				**20c**$^{+}$ (same as **20a**$^{+}$)
C	-0.883537	-0.072628	0.024518	
C	0.079035	-1.005793	-0.033611	
C	1.520182	-0.691124	0.215543	
O	1.839152	0.616570	-0.337112	
O	-0.681173	1.251435	0.206550	
O	-2.194271	-0.369060	-0.102718	
H	-0.206997	-2.023918	-0.253508	
H	2.152599	-1.450377	-0.256879	
H	1.761354	-0.676675	1.289807	
H	2.681015	0.901978	0.031932	
H	0.271163	1.408946	0.039521	
H	-2.662873	0.465755	-0.223336	
Freq	Int			
95.4209	2.5652			
204.543	12.9707			

265.851	4.2883
343.676	147.544
363.173	43.2899
412.87	52.7202
524.211	19.927
649.553	10.8039
681.867	25.479
721.487	49.4546
754.715	70.1758
877.695	19.8384
958.211	30.3316
1037.68	16.5048
1088.12	66.8392
1205.1	22.4628
1217.91	189.458
1253.1	30.9205
1280.35	108.525
1405.68	142.044
1418.09	6.9978
1475.38	136.023
1519.36	1.3222
1765.64	352.395
2949.72	95.5129
3029.6	51.751
3215.83	2.7905
3518.85	306.87
3808.83	91.9221
3828.15	19.6604

20d

C	0.887918	-0.016281	-0.027440
C	-0.054976	-0.981536	0.017387
C	-1.486923	-0.668587	-0.307261
O	-1.938735	0.571225	0.303156
O	0.638018	1.279425	-0.253029
O	2.212053	-0.192564	0.164725
H	0.224101	-1.998337	0.263809
H	-2.139493	-1.494213	-0.006865
H	-1.651700	-0.494080	-1.375478
H	-1.866275	0.455400	1.258510
H	-0.325985	1.402982	-0.141323
H	2.392558	-1.138014	0.186415

Freq	Int
136.233	6.2588
203.439	3.5893
246.688	2.9045
384.43	70.6292
396.098	8.7983
468.135	155.712
543.324	6.9176
640.04	56.6364
684.515	35.8604
710.467	25.421
814.082	79.1181
880.256	20.8858
948.623	81.459

20d$^+$

C	0.925096	0.036088	0.000017
C	-0.067619	-0.997237	-0.000026
C	-1.529031	-0.751948	0.000158
O	-1.793590	0.640088	-0.000421
O	0.638549	1.284641	0.000174
O	2.201084	-0.209129	-0.000071
H	0.261279	-2.030655	-0.000108
H	-1.963793	-1.249270	0.883498
H	-1.964179	-1.250013	-0.882563
H	-2.737224	0.837038	0.000862
H	-0.354378	1.399798	0.000128
H	2.419274	-1.153113	-0.000171

Freq	Int
60.8382	43.5403
149.715	34.5074
229.583	102.265
307.604	5.4114
395.531	10.5292
497.183	88.1542
542.783	9.127
629.241	22.9628
697.555	30.4424
697.806	12.446
873.539	118.221
885.816	9.141
919.261	7.8158

1016.96	20.7222
1079.25	40.133
1201.6	18.2535
1209.77	186.673
1247.28	133.496
1352.72	0.8999
1396.55	48.2543
1417.28	73.0567
1486.97	48.7247
1511.75	0.1358
1707.87	480.015
3022.37	65.6303
3054.71	32.9718
3181.2	12.0096
3542.14	257.415
3790.5	22.624
3842.7	62.8375

20e			
C	-0.893599	-0.006525	0.024240
C	0.037496	-0.980162	-0.023922
C	1.485972	-0.712537	0.243520
O	1.868556	0.549922	-0.367279
O	-0.637086	1.293553	0.212457
O	-2.224576	-0.185412	-0.127080
H	-0.259909	-1.991697	-0.268436
H	2.095569	-1.521859	-0.172308
H	1.701628	-0.650465	1.321319
H	2.716262	0.817927	0.002130
H	0.317749	1.407754	0.034889
H	-2.405668	-1.130823	-0.125410

Freq	Int
100.78	4.642
203.055	24.8704
261.322	0.5232
369.465	31.2931
380.878	107.617
417.588	13.7753
534.005	10.8193
634.304	74.3312
680.954	36.4662
705.465	14.2173
756.877	105.547
885.814	24.4832
965.201	29.1435
1045.92	13.8601
1090.99	78.2915
1207.17	121.276
1222.01	55.6817
1245.87	127.859
1278.58	89.0948
1422.42	5.9418
1429.07	89.3491
1499.67	41.3584
1518.61	0.8026
1721.35	475.048

1022.85	21.0047
1149.22	76.0127
1182.01	115.499
1211.24	18.1304
1226.51	0.0025
1315.65	207.866
1406.07	59.0462
1431.78	24.5136
1457.98	22.9018
1586.94	384.082
1625.64	204.461
2949.2	14.6443
2970.19	0.0404
3182.03	593.325
3192.75	65.1447
3773.83	224.222
3834.4	182.507

20e^{+} (same as **20d**$^{+}$)

2951.77	91.3148						
3030.2	51.4953						
3184.9	10.8627						
3550.14	288.783						
3823.71	17.7762						
3844.4	59.8396						
20f				**20f$^+$**			
C	-0.963652	-0.042680	0.040900	C	-1.056533	-0.050805	0.000012
C	0.229036	-0.575767	0.323480	C	0.279003	-0.506651	-0.000149
C	1.483576	0.216577	0.457909	C	1.435100	0.403549	-0.000299
O	2.406733	-0.203222	-0.561171	O	2.604064	-0.349780	0.000388
O	-1.186962	1.285244	-0.066615	O	-1.288705	1.226884	0.000139
O	-2.123937	-0.734670	-0.145761	O	-2.108413	-0.821726	0.000027
H	0.303362	-1.652499	0.428167	H	0.469194	-1.575331	-0.000319
H	1.928972	0.050090	1.450333	H	1.351465	1.082272	0.874407
H	1.254805	1.284495	0.366415	H	1.351855	1.081186	-0.875928
H	3.249841	0.222410	-0.375995	H	3.373944	0.230189	-0.000123
H	-2.071146	1.404567	-0.432697	H	-2.240970	1.433422	0.000203
H	-1.926275	-1.676663	-0.181582	H	-1.906478	-1.771323	-0.000057
Freq	Int			Freq	Int		
66.0198	3.9619			61.3277	28.8052		
136.974	59.5302			162.353	12.6564		
224.642	67.0641			176.415	3.452		
261.38	72.3877			302.422	104.777		
291.492	111.673			382.724	0.7403		
368.634	13.7845			478.8	8.7283		
428.349	22.5475			501.572	136.629		
529.038	30.3051			567.333	172.25		
576.789	18.5275			592.661	0.8204		
647.577	5.3001			615.728	41.7243		
763.396	59.5215			692.351	28.9548		
889.775	64.0673			898.382	12.2943		
1006.35	103.384			978.852	11.26		
1023.51	43.4645			1081.72	92.5384		
1113.36	33.0548			1122.52	168.352		
1188.42	176.979			1169.39	150.585		
1206.98	54.5787			1196.59	0.9216		
1244.53	73.8269			1207.04	161.106		
1270.38	34.2395			1238.2	53.5862		
1347.24	145.624			1316.35	99.759		
1418.05	81.914			1373.97	168.067		
1476.39	17.8529			1450.92	62.0628		
1516.29	1.0082			1569.75	171.617		
1777.76	354.961			1615	500.128		
2959.42	85.0643			2871.74	0.1602		
3029.25	32.827			2878.88	96.3265		
3166.39	15.7191			3185.65	18.0067		
3817.21	72.3512			3698.55	365.662		
3818.08	39.7227			3745.36	260.932		
3836.25	59.6379			3827.23	198.601		
20g				**20g$^+$**			
C	0.965019	-0.074656	-0.041976	C	1.064225	-0.053923	-0.003262
C	-0.229310	-0.605130	-0.342660	C	-0.277382	-0.498742	0.077464
C	-1.495934	0.171273	-0.493442	C	-1.458438	0.382763	0.184023
O	-2.474578	-0.138129	0.503604	O	-2.581932	-0.335667	-0.218916

O	1.263387	1.244523	0.113379
O	2.064015	-0.831132	0.150654
H	-0.274604	-1.681766	-0.443751
H	-1.984792	-0.051258	-1.445692
H	-1.299845	1.259649	-0.501308
H	-2.002205	-0.214986	1.339290
H	0.485068	1.775379	-0.091827
H	2.815140	-0.238032	0.270665

Freq	Int
75.6885	0.5182
119.978	32.5561
252.611	117.459
265.458	47.5224
339.876	98.8831
396.936	42.0654
433.387	11.8239
530.615	28.9811
573.783	13.8563
655.771	2.7299
783.757	28.5356
871.17	26.0967
987.375	110.824
1018.61	113.926
1117.8	13.0533
1169.09	160.447
1216.92	45.7564
1229.52	109.087
1322.23	12.4717
1354.61	55.4921
1412.89	101.926
1439.59	148.821
1516.67	5.1028
1763.83	349.655
2895.94	118.862
3056.24	39.5756
3195.24	3.1212
3806.81	31.1001
3814.02	17.4288
3817.61	127.423

O	1.465925	1.185737	-0.078556
O	1.996867	-0.951797	0.004798
H	-0.431240	-1.572292	0.089769
H	-1.321205	1.310441	-0.406896
H	-1.519927	0.711524	1.243818
H	-3.385984	0.111743	0.068715
H	0.751013	1.838606	-0.137868
H	2.890034	-0.566797	-0.065497

Freq	Int
54.7237	20.2499
139.813	2.5495
187.06	1.5421
295.181	126.97
380.093	9.5299
482.448	13.849
499.959	186.59
567.163	58.8588
598.566	18.8799
634.975	18.454
705.182	43.4281
888.01	30.3164
976.669	19.8689
1092.97	95.7781
1111.74	179.541
1159.35	162.464
1196.24	129.55
1208.76	56.3796
1269.19	45.9385
1323.36	26.504
1404.75	54.8371
1458.7	17.0113
1546.57	249.461
1620.17	327.942
2863.91	42.5992
2887.79	37.9453
3199.8	26.6609
3689.33	373.598
3747.21	115.173
3824.06	176.04

20h

C	0.939771	-0.043400	-0.037305
C	-0.209784	-0.674340	-0.310497
C	-1.507505	0.034654	-0.548573
O	-2.365239	0.103743	0.602348
O	1.062725	1.297602	-0.004683
O	2.138289	-0.637533	0.221738
H	-0.201134	-1.760137	-0.320382
H	-2.040782	-0.443928	-1.381943
H	-1.322167	1.072023	-0.826886
H	-2.466137	-0.792817	0.936481
H	1.979781	1.507204	0.207004
H	2.029351	-1.594328	0.208749

Freq	Int
50.4388	4.9511

20h$^+$

C	0.929719	-0.029613	-0.055433
C	-0.262434	-0.716289	-0.389798
C	-1.549556	0.008006	-0.605188
O	-2.005478	0.128874	0.752455
O	0.938984	1.264882	-0.071140
O	2.060917	-0.603903	0.247540
H	-0.261424	-1.797755	-0.308045
H	-2.238870	-0.549321	-1.238885
H	-1.414967	1.012958	-0.997634
H	-2.575343	-0.619574	0.978418
H	1.806354	1.635600	0.173034
H	2.022502	-1.573350	0.264790

Freq	Int
69.7109	2.0256

112.394	57.2789
208.629	41.245
229.88	147.999
279.391	83.0025
370.26	11.65
436.897	11.6047
544.306	18.7456
582.564	14.7742
655.191	6.0159
749.286	82.7081
873.047	49.321
992.271	159.923
1018.63	43.8611
1090.65	26.1881
1186.5	93.5783
1198.49	103.484
1227.51	80.836
1347.96	154.016
1360.1	5.3239
1413.83	82.8927
1459.06	58.983
1504.13	0.6896
1761.5	375.942
2978.76	86.4858
3105.29	10.219
3147.77	21.6023
3822.1	120.274
3824.32	9.6413
3837.84	61.9115

20i			
C	-0.946906	-0.073842	-0.027046
C	0.234864	-0.646779	-0.253802
C	1.500271	0.103725	-0.532333
O	2.484746	-0.076145	0.494063
O	-1.115374	1.279272	0.101289
O	-2.099998	-0.797236	0.090885
H	0.276122	-1.727963	-0.205789
H	1.280480	1.165834	-0.686819
H	1.975634	-0.277628	-1.439939
H	2.071746	0.186548	1.323072
H	-1.878153	1.543856	-0.428776
H	-2.610188	-0.436405	0.827434

Freq	Int
69.1274	0.3004
157.48	1.7572
242.691	17.7983
279.079	137.942
350.81	136.051
417.64	2.596
493.514	109.478
544.252	66.8222
566.354	23.8459
605.393	18.4343
829.193	12.7425
877.135	40.3871

110.207	4.4501
255.688	6.7885
358.398	56.3068
375.071	96.7854
506.51	112.505
519.926	91.2871
579.103	102.178
593.175	34.5287
665.426	8.0539
776.822	48.6876
873.931	25.3479
972.715	32.6333
1037.85	23.5075
1106.2	35.5254
1165.92	111.096
1182.31	98.8964
1210.24	115.821
1347.95	17.7132
1359.64	59.0608
1390.86	76.331
1503.85	18.4595
1571.06	247.105
1600.53	383.356
3094.74	7.6156
3161.45	0.773
3190.14	6.2729
3699.62	349.702
3750.93	235.799
3776.9	191.342

20i$^+$			
C	-1.054665	-0.059835	-0.000011
C	0.281200	-0.506669	0.000001
C	1.436731	0.402693	0.000068
O	2.606280	-0.350053	-0.000042
O	-1.284427	1.227783	-0.000033
O	-1.994587	-0.964356	0.000004
H	0.444935	-1.578522	0.000054
H	1.353426	1.080379	0.875558
H	1.353405	1.080723	-0.875131
H	3.375093	0.231008	-0.000231
H	-2.216267	1.498762	0.000014
H	-2.908310	-0.636470	-0.000049

Freq	Int
58.9862	14.9689
168.515	17.4399
177.374	1.4424
296.503	127.934
352.962	3.8074
383.8	0.1082
483.089	3.3684
506.86	284.278
575.776	7.9111
620.064	33.6512
675.763	20.2177
913.968	9.3162

982.328	158.741
1025.19	74.8415
1114.66	5.6158
1177.34	87.5388
1216.82	37.1253
1242.77	24.2181
1286.13	187.226
1346.74	73.719
1388.77	27.36
1429.79	66.583
1507.71	0.3304
1777.31	185.298
3021.08	47.0593
3067.64	33.0624
3190.57	5.1852
3771.81	38.7052
3777.5	51.6556
3818.3	14.5783

20j			
C	0.956890	-0.071175	-0.047049
C	-0.253131	-0.542615	-0.345323
C	-1.493387	0.291888	-0.427108
O	-2.535916	-0.204930	0.421421
O	1.235959	1.265259	0.048919
O	2.027718	-0.888445	0.188642
H	-0.344253	-1.608650	-0.513724
H	-1.917451	0.256920	-1.434403
H	-1.258314	1.338472	-0.201991
H	-2.168184	-0.266861	1.308927
H	1.822831	1.396015	0.804888
H	2.781050	-0.559546	-0.318677

Freq	Int
84.1013	0.6025
159.389	1.9384
236.409	11.7888
283.728	154.526
360.081	100.853
423.308	18.1543
500.582	82.3924
515.359	88.7868
573.327	45.6566
606.127	8.2397
823.482	23.5012
894.315	33.0851
984.417	149.533
1024.33	80.7936
1116.64	7.6233
1172.69	82.1637
1215.12	22.0635
1243.01	32.6136
1291.25	174.618
1334.05	105.267
1386.02	27.267
1429.39	60.9951
1510.2	0.573

969.189	44.7553
1067.65	254.825
1119.36	214.192
1134.89	152.457
1179.06	107.987
1200.16	0.8895
1241.66	32.9069
1313.89	102.755
1378.17	86.7778
1456.1	30.7248
1530.26	264.649
1629.49	301.555
2872.51	0.5448
2879.6	89.9212
3203.89	27.2193
3735.72	66.749
3749.31	556.527
3829.28	184.082

20j^{+} (same as **20i**$^{+}$)

1780.65	180.442			
3018.09	41.7357			
3063.24	32.9431			
3190.45	4.6731			
3769.95	38.6513			
3776.72	49.5714			
3818.26	14.7325			
20k				**20k**$^+$ (same as **20i**$^+$)
C	0.963732	-0.071301	-0.041114	
C	-0.240912	-0.559931	-0.323979	
C	-1.480712	0.263278	-0.422509	
O	-2.436083	-0.242138	0.521987	
O	1.231718	1.270262	0.033968	
O	2.045063	-0.873960	0.192652	
H	-0.327626	-1.629486	-0.466156	
H	-1.889678	0.192322	-1.441781	
H	-1.244174	1.315143	-0.226276	
H	-3.277995	0.184194	0.335234	
H	1.761776	1.425849	0.826529	
H	2.799460	-0.513603	-0.290787	
Freq	Int			
68.7843	1.9499			
164.046	6.4639			
234.972	74.5905			
263.149	28.1597			
287.972	167.04			
420.96	18.5178			
494.921	52.8516			
515.1	120.953			
573.641	51.8843			
605.072	6.7475			
823.582	27.2365			
892.377	48.957			
1001.72	48.3242			
1023.6	84.6678			
1113.5	26.6263			
1188.19	94.3588			
1236.76	100.121			
1245.58	19.6409			
1266.45	40.6322			
1302.11	199.21			
1357.84	52.4889			
1463.13	16.0737			
1517.46	1.0801			
1791.88	189.122			
2960.76	74.9998			
3030.02	35.4582			
3196.77	4.7589			
3769.95	38.8339			
3776.08	45.7255			
3825.86	10.9461			
20l				**20l**$^+$ (same as **20i**$^+$)
C	0.956241	-0.067471	0.022647	
C	-0.228512	-0.628881	0.250621	
C	-1.486369	0.131589	0.503440	

O	-2.402499	-0.127759	-0.570954
O	1.137381	1.279976	-0.130569
O	2.107542	-0.801917	-0.062629
H	-0.278200	-1.709882	0.227699
H	-1.262898	1.201226	0.581994
H	-1.926498	-0.199139	1.456537
H	-3.245966	0.267619	-0.330081
H	1.930103	1.533526	0.358982
H	2.595916	-0.507167	-0.842168

Freq	Int
66.0344	1.0528
159.94	16.5067
234.767	76.2336
262.367	117.448
281.416	64.5594
416.206	5.8372
488.224	101.943
540.918	93.0936
567.081	36.6815
606.893	18.2656
828.845	19.655
879.571	54.0424
1000.39	70.2548
1025.49	71.4398
1116.03	21.4323
1183.87	101.668
1235.32	92.3566
1254.01	19.5232
1267.71	51.7075
1300.7	187.454
1363.46	54.1768
1464.75	15.9067
1515.46	0.8485
1790.2	196.037
2958.74	81.1241
3032.91	35.8399
3196.56	5.2323
3771.74	39.6278
3780.87	49.6351
3823.1	9.9693

20m

C	0.953237	-0.045891	0.038187
C	-0.234328	-0.601951	0.308655
C	-1.498886	0.174600	0.501885
O	-2.493709	-0.124900	-0.488107
O	1.153735	1.286566	-0.054998
O	2.122005	-0.714775	-0.171595
H	-0.295455	-1.684145	0.357044
H	-1.276637	1.247579	0.524740
H	-1.973050	-0.085182	1.452032
H	-2.079306	0.017573	-1.345380
H	2.084179	1.430754	-0.262881
H	1.963885	-1.662263	-0.100319

Freq	Int

20m$^+$

C	0.927947	-0.031282	0.047059
C	-0.253282	-0.764662	0.294960
C	-1.561174	-0.111387	0.603397
O	-2.080546	0.057976	-0.724615
O	0.908173	1.264000	0.153270
O	2.081768	-0.554805	-0.260292
H	-0.236576	-1.829963	0.094032
H	-1.463882	0.829326	1.144567
H	-2.227942	-0.782008	1.139971
H	-1.879816	0.948400	-1.044892
H	1.781766	1.663038	-0.011260
H	2.070334	-1.522176	-0.341821

Freq	Int

62.0036	25.7869
123.585	47.982
212.87	85.6518
254.023	55.2099
353.887	93.8875
373.035	18.8469
429.572	27.1174
535.964	4.6505
574.672	11.042
650.167	1.6486
763.058	73.7536
880.293	36.47
989.327	191.635
1022.47	53.806
1115.22	22.5183
1183.61	149.98
1201.21	52.8402
1216.63	37.9498
1326.17	97.8827
1375.34	71.1344
1412.61	113.25
1455.96	43.3594
1509.38	0.3221
1766.45	342.5
3018.87	42.3421
3064.71	36.8311
3160.27	15.8582
3816.49	12.7181
3821.49	114.092
3835.92	63.1195

44.6112	7.0402
114.547	6.891
246.219	13.4073
333.28	8.7434
374.064	127.803
507.955	77.4998
526.544	136.86
578.3	97.4836
592.078	28.0344
665.162	7.7145
780.663	42.7841
878.874	17.3758
965.746	46.7713
1034.31	32.5874
1109.33	35.9527
1168.06	92.7941
1185.41	57.4801
1209.71	172.178
1350.01	41.0106
1364.04	28.7078
1384.98	73.3841
1501.61	25.1227
1565.64	184.95
1600.97	459.597
3095.04	6.1304
3161.23	0.9045
3195.5	9.9872
3698.39	331.3
3744.55	266.597
3777.97	142.988

20n

C	0.984382	-0.030035	-0.033025
C	-0.202150	-0.591084	-0.335640
C	-1.488627	0.150505	-0.502464
O	-2.460243	-0.158940	0.501569
O	1.245692	1.284113	0.113871
O	2.135913	-0.702178	0.169971
H	-0.246066	-1.671348	-0.426364
H	-1.972887	-0.106613	-1.448090
H	-1.316696	1.241522	-0.538346
H	-1.996090	-0.159199	1.345406
H	0.443705	1.780279	-0.083595
H	1.955504	-1.644918	0.094474

Freq	Int
74.9743	5.5805
130.527	0.8217
265.12	29.4003
296.447	17.729
358.816	63.2247
434.746	14.0598
451.47	210.79
540.374	0.5888
585.95	10.4509
666.376	0.6294
746.484	56.8668

20n$^+$

C	1.083033	-0.034397	-0.007265
C	-0.262475	-0.487276	0.056024
C	-1.448698	0.390123	0.155559
O	-2.573993	-0.359434	-0.178572
O	1.451739	1.208889	-0.065350
O	2.101715	-0.835778	-0.004172
H	-0.445825	-1.557628	0.058841
H	-1.332449	1.283428	-0.490898
H	-1.486568	0.777283	1.196557
H	-3.377511	0.114351	0.065428
H	0.715678	1.835844	-0.125541
H	1.859828	-1.773387	0.054459

Freq	Int
51.8759	33.7928
126.491	4.075
185.319	8.2957
297.524	115.953
379.777	8.1065
457.668	1.5287
483.84	8.3042
544.849	69.3126
607.641	198.968
638.576	20.3738
689.339	1.9533

875.98	28.8502
998.22	122.208
1020.59	72.486
1120.34	7.8177
1170.46	327.024
1210.61	32.683
1233.75	14.2361
1329.82	8.3294
1362.9	105.321
1423.54	63.6462
1468.34	40.1503
1517.54	1.1607
1721.91	451.979
2907.75	107.428
3059.21	38.1688
3158.65	12.7533
3812.7	13.6504
3821.4	45.3837
3843.51	71.1496

20o			
C	0.944447	-0.070682	0.024714
C	-0.223445	-0.665791	0.262405
C	-1.500992	0.064546	0.544072
O	-2.408412	0.085515	-0.567154
O	1.085804	1.282556	-0.094139
O	2.110383	-0.774103	-0.102360
H	-0.232086	-1.749332	0.224544
H	-1.293118	1.110493	0.766832
H	-1.993857	-0.378152	1.421665
H	-2.575608	-0.827858	-0.819471
H	1.878190	1.548215	0.389886
H	2.594211	-0.423552	-0.861384

Freq	Int
61.1978	5.3055
153.789	2.0464
224.157	60.1751
268.333	106.401
305.007	140.823
417.743	3.6602
493.62	105.99
547.112	92.9322
577.75	12.399
608.225	15.029
824.744	25.0516
873.211	45.0728
1001.98	163.031
1006.49	40.7601
1090.49	6.6426
1171.41	54.5924
1225.86	98.2171
1243.91	26.5495
1295.45	221.242
1360.07	22.779
1380.04	38.0176
1431.98	56.7103

887.732	14.3821
979.962	13.1063
1098.45	37.8398
1114.26	141.555
1161.37	329.628
1184.89	29.9274
1205.53	45.2164
1262.29	66.4238
1328.71	16.0744
1400.46	119.338
1457.95	42.9653
1560.05	411.922
1596.43	185.886
2862.93	43.6861
2885.06	34.9423
3178.93	16.726
3758.34	323.182
3768.28	58.1012
3823.26	181.116

20o$^+$			
C	0.923343	-0.041305	0.061378
C	-0.266655	-0.729537	0.387845
C	-1.558291	-0.016294	0.601740
O	-1.981937	0.163584	-0.760844
O	0.926467	1.261140	0.104313
O	1.968852	-0.758375	-0.245432
H	-0.232485	-1.808202	0.292569
H	-1.440939	0.972188	1.039077
H	-2.262052	-0.601963	1.192421
H	-2.504952	-0.598836	-1.045388
H	1.750607	1.699305	-0.161057
H	2.792388	-0.270476	-0.407697

Freq	Int
75.5296	6.4966
114.669	4.8206
254.589	21.3302
347.436	18.7089
372.389	18.1823
387.612	103.083
514.527	204.909
526.006	158.577
594.174	11.5432
635.808	7.9656
801.52	35.733
872.616	6.0743
972.597	35.8647
1034.61	40.0532
1097.75	55.3362
1129.93	175.637
1172.24	214.096
1197.47	28.0886
1346.63	9.2922
1361.38	46.2727
1390.64	28.3142
1505.31	41.4269

1503.98	0.3828	1544.48	240.749
1780.22	203.206	1608.45	260.677
2973.81	84.2379	3095.13	8.8178
3111.58	12.7123	3160.9	0.9675
3174.43	8.3447	3208.29	12.0981
3771.56	38.6471	3734.31	89.0477
3778.95	52.8691	3749.85	512.507
3823.79	18.2348	3778.27	145.954

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