

Supplementary Materials for
**Interstellar formation of glyceric acid [HOCH₂CH(OH)COOH]—The
simplest sugar acid**

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Tentative assignments of C₂H₄O₃ and C₃H₆O₃ isomers

The TPD profile of the ion signal at $m/z = 76$ for the irradiated CO₂–HOCH₂CH₂OH ice at 11.10 eV (fig. S7A) shows a broad sublimation event from 175 K to 320 K. The replacement of the CO₂–HOCH₂CH₂OH ice by ¹³CO₂–HO¹³CH₂¹³CH₂OH ice shifts the m/z by 2 amu from $m/z = 76$ to 78, indicating the presence of two carbon atoms. Therefore, the sublimation event peaking at 259 K can be clearly linked to a molecule of the formula C₂H₄O₃. Furthermore, the shift by 4 amu from $m/z = 76$ (C₂H₄O₃⁺) to 80 in the C¹⁸O₂–HOCH₂CH₂OH ice indicates the presence of two oxygen atoms and that one carbon dioxide participates in the formation of C₂H₄O₃ products. When lowering the photon energy to 8.77 eV, this sublimation event is absent (fig. S7B). Previous laboratory experiments revealed the formation of glycolic acid (**9**, IE = 10.00 – 10.54 eV) in irradiated carbon dioxide – methanol (**10**) ice with a sublimation event from 180 K to 310 K and a peak at 251 K (*12*). This result matches well with our TPD profile at $m/z = 76$, suggesting that the peak at 259 K in the irradiated CO₂–HOCH₂CH₂OH ice is likely associated with glycolic acid (**9**). Additionally, the TPD profile at $m/z = 90$ in the irradiated CO₂–HOCH₂CH₂OH ice at 11.10 eV shows a broad sublimation event after 180 K (fig. S8A). This TPD profile shifts the m/z by 3 amu from $m/z = 90$ to 93 in ¹³CO₂–HO¹³CH₂¹³CH₂OH ice and by 2 amu from $m/z = 90$ to 92 in C¹⁸O₂–HOCH₂CH₂OH ice, indicating the presence of three carbon atoms and at least one oxygen atom, respectively; hence, this sublimation event can be linked to a molecule of the formula C₃H₆O₃. Upon reducing the photon energy to 8.77 eV, a narrow peak from 205 K – 245 K remains and the high-temperature range (245 K – 320 K) of the TPD profile vanishes (fig. S8B). This absent sublimation event is linked to the C₃H₆O₃ isomers that have IEs between 8.77 eV and 11.10 eV and may be caused by glyceraldehyde (**5**, IE = 9.23 – 9.91 eV), 3-hydroxypropionic acid (**12**, IE = 9.11 – 10.50 eV) and/or lactic acid (**13**, IE = 9.82 – 10.18 eV) (Fig. 1). The remaining sublimation event at 8.77 eV can be correlated with other C₃H₆O₃ isomers.

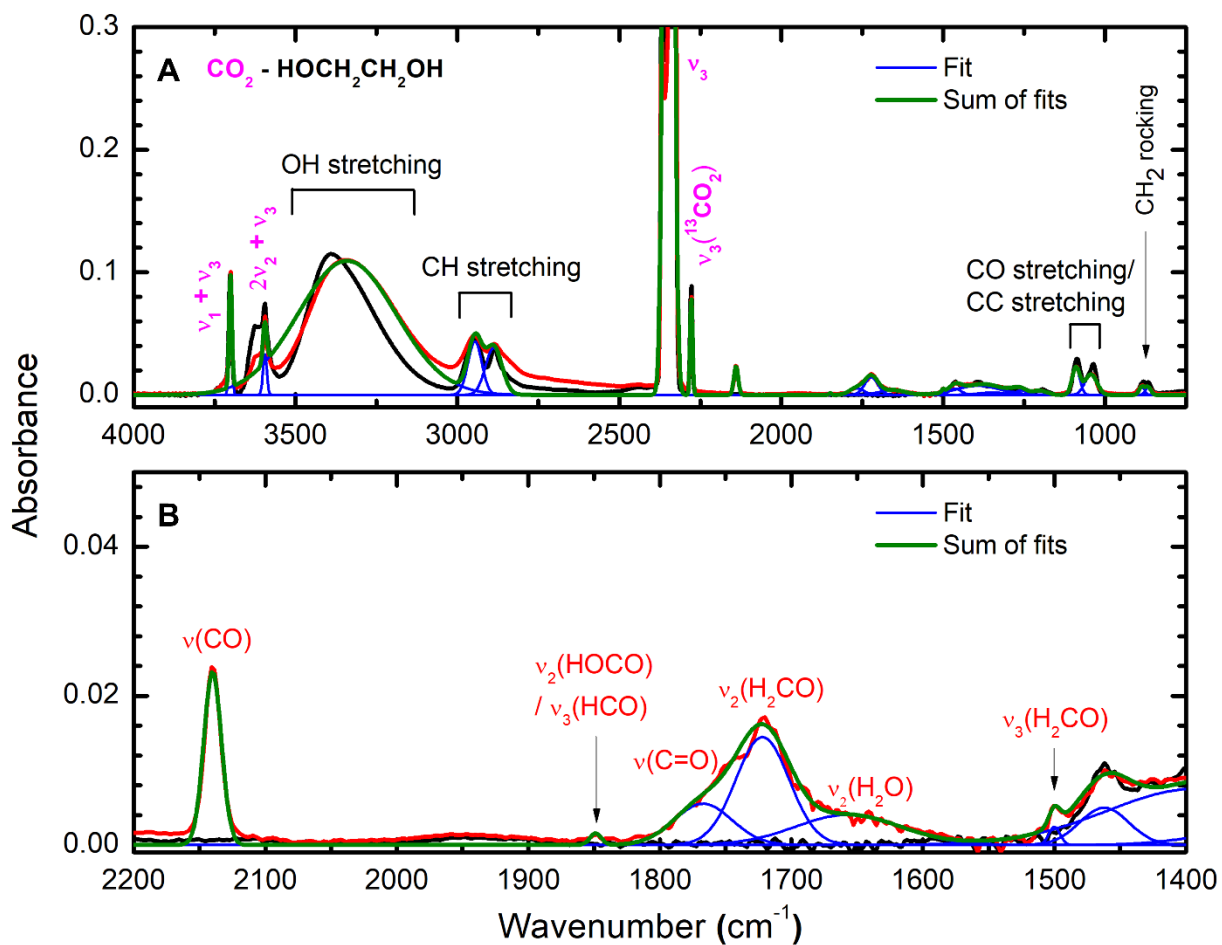


Fig. S1. Infrared spectra of (A) CO_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ ice before (black) and after (red) irradiation with (B) a magnified view and deconvolution of the region 2200 – 1400 cm^{-1} . Detailed assignments are compiled in table S1.

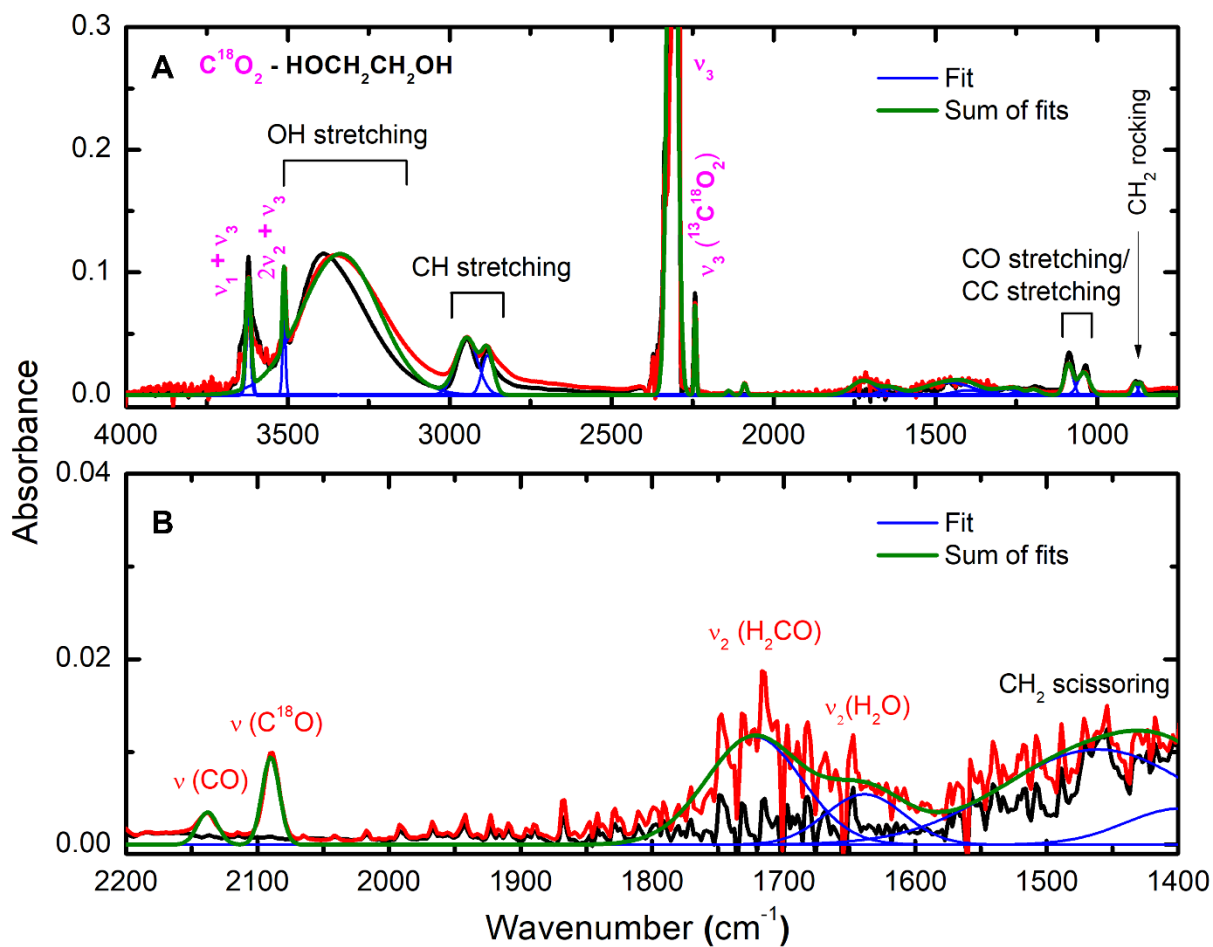


Fig. S2. Infrared spectra of (A) $C^{18}O_2$ - $HOCH_2CH_2OH$ ice before (black) and after (red) irradiation with (B) a magnified view and deconvolution of the region 2200–1400 cm^{-1} . Detailed assignments are compiled in table S2.

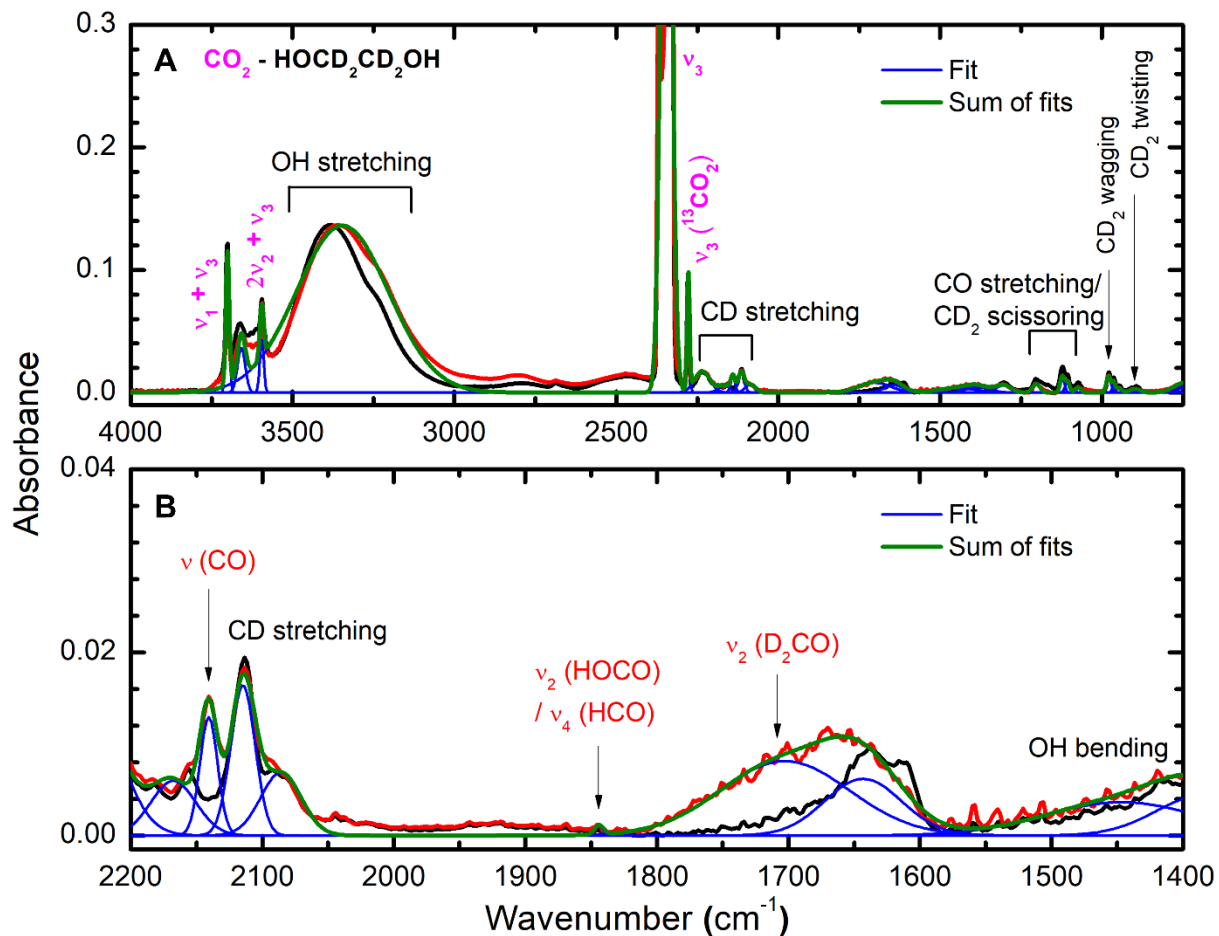


Fig. S3. Infrared spectra of (A) CO_2 - $\text{HOCD}_2\text{CD}_2\text{OH}$ ice before (black) and after (red) irradiation with (B) a magnified view and deconvolution of the region 2200 – 1400 cm^{-1} . Detailed assignments are compiled in table S3.

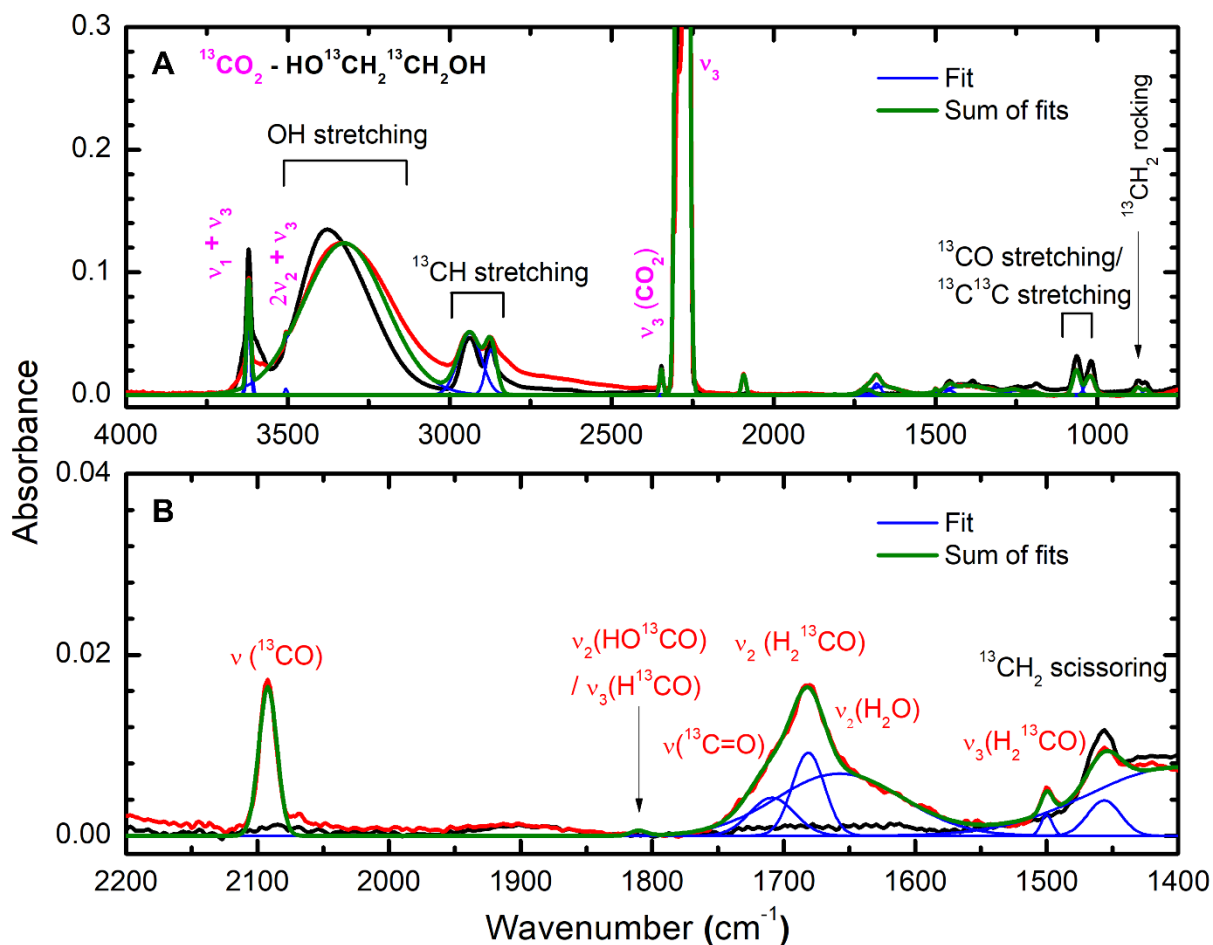


Fig. S4. Infrared spectra of (A) $^{13}\text{CO}_2$ - $\text{HO}^{13}\text{CH}_2^{13}\text{CH}_2\text{OH}$ ice before (black) and after (red) irradiation with (B) a magnified view and deconvolution of the region 2200–1400 cm^{-1} . Detailed assignments are compiled in table S4.

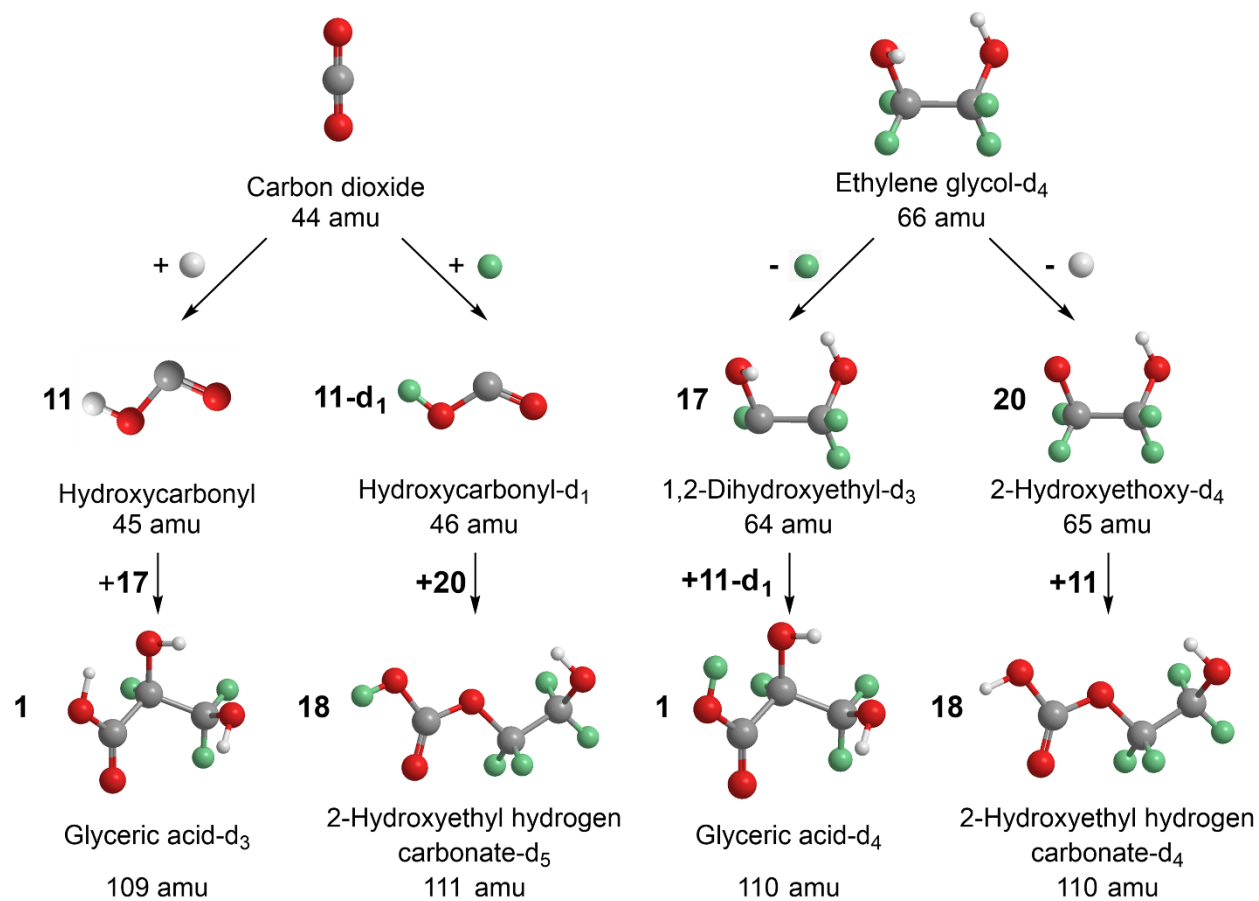


Fig. S5. Proposed formation pathways of isomers **1** ($m/z = 109$ and 110) and **18** ($m/z = 110$ and 111) via radical–radical reactions in carbon dioxide (CO₂)–ethylene glycol-d₄ (HOCD₂CD₂OH) ice after electron irradiation.

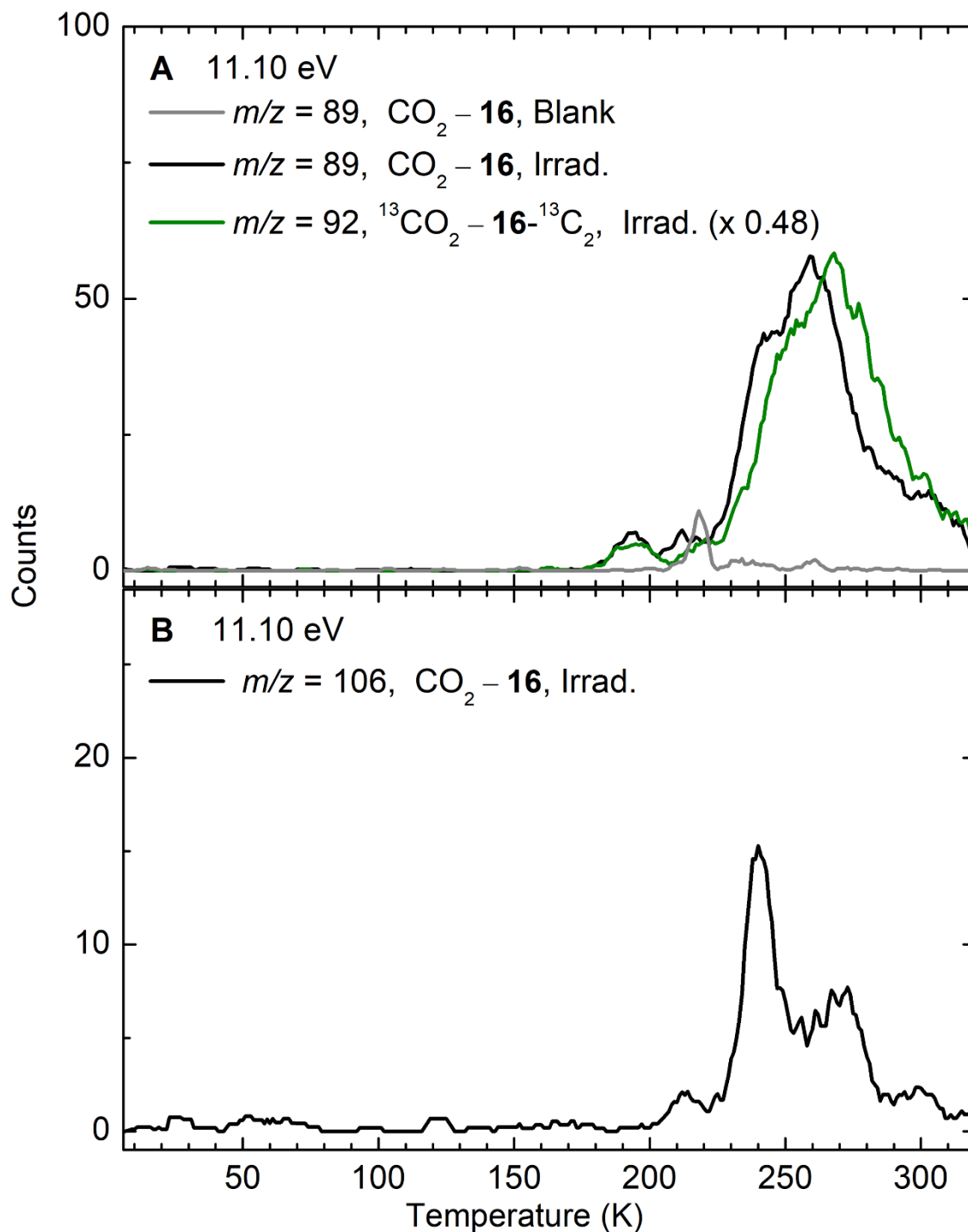


Fig. S6. TPD profiles of irradiated carbon dioxide-ethylene glycol ices. (A) TPD profiles measured at 11.10 eV with irradiated CO_2 -HOCH₂CH₂OH (**16**) ice ($m/z = 89$) and $^{13}\text{CO}_2$ -HO $^{13}\text{CH}_2$ $^{13}\text{CH}_2$ OH ice ($m/z = 92$), indicating the presence of three carbon atoms and confirming the formula C₃H₅O₃. (B) TPD profiles measured at 11.10 eV at $m/z = 106$ in irradiated CO_2 -HOCH₂CH₂OH ice.

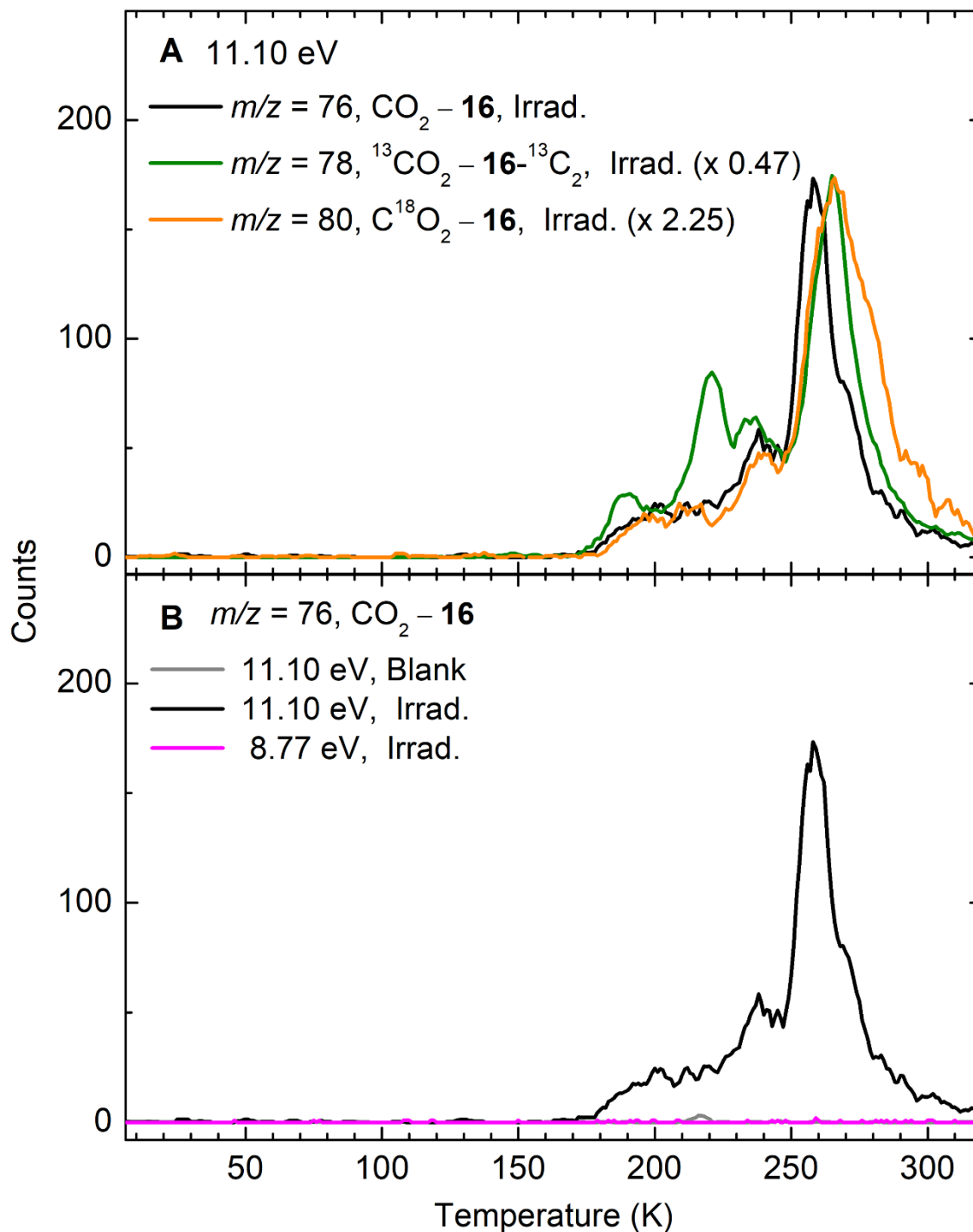


Fig. S7. TPD profiles of irradiated carbon dioxide-ethylene glycol ices. (A) TPD profiles measured at 11.10 eV with irradiated CO_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ (**16**) ice ($m/z = 76$), $^{13}\text{CO}_2$ - $\text{HO}^{13}\text{CH}_2^{13}\text{CH}_2\text{OH}$ ice ($m/z = 78$) and C^{18}O_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ ice ($m/z = 80$). (B) TPD profiles at $m/z = 76$ in irradiated CO_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ ice measured at 11.10 eV and 8.77 eV.

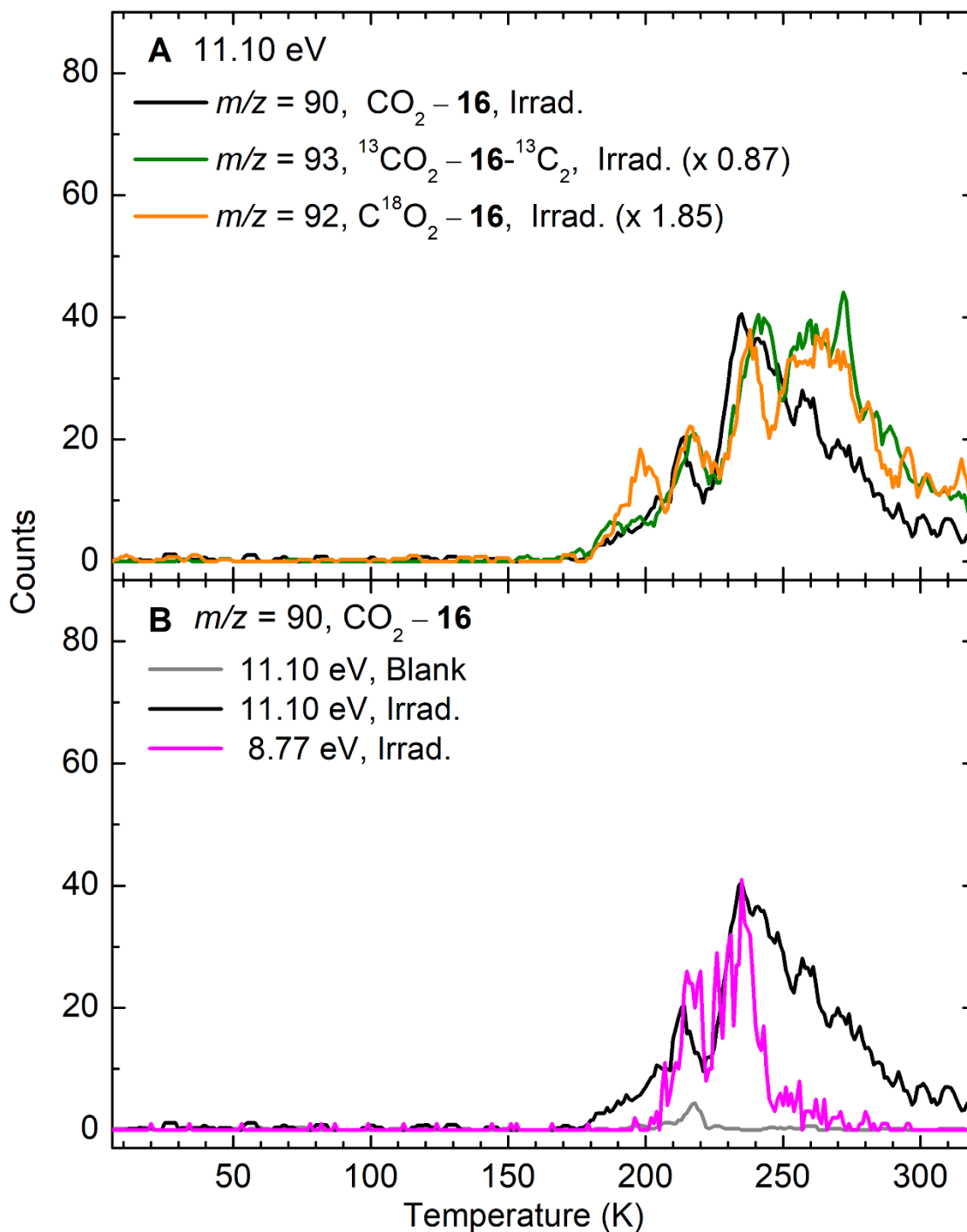


Fig. S8. TPD profiles of irradiated carbon dioxide-ethylene glycol ices. (A) TPD profiles measured at 11.10 eV with irradiated CO_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ (**16**) ice ($m/z = 90$), $^{13}\text{CO}_2$ - $\text{HO}^{13}\text{CH}_2^{13}\text{CH}_2\text{OH}$ ice ($m/z = 93$) and C^{18}O_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ ice ($m/z = 92$). (B) TPD profiles at $m/z = 90$ in irradiated CO_2 - $\text{HOCH}_2\text{CH}_2\text{OH}$ ice measured at 11.10 eV and 8.77 eV.

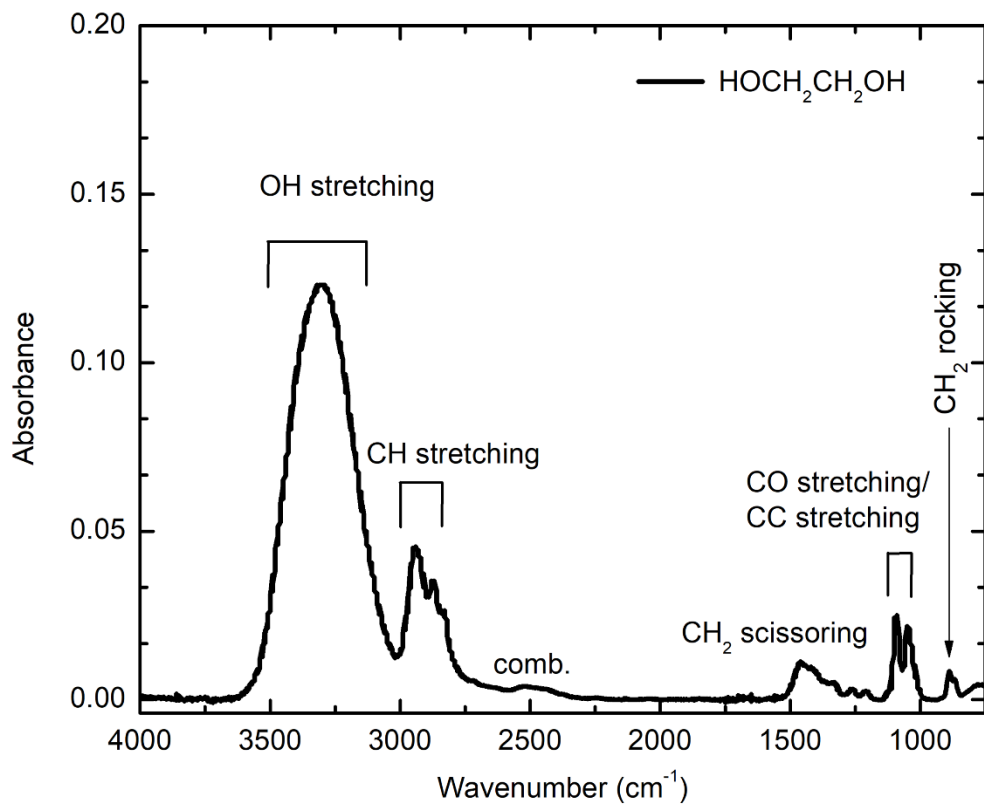


Fig. S9. Infrared spectrum of ethylene glycol (HOCH₂CH₂OH) ice with thickness of 470 ± 50 nm measured immediately after deposition at 5 K.

Table S1. Absorption peaks observed in CO₂-HOCH₂CH₂OH ice before and after electron irradiation (30 nA, 60 minutes) at 5 K.

Pristine ice, absorptions before irradiation	
(cm ⁻¹)	
CO₂	Assignment (27)
3701	combination (ν ₁ + ν ₃)
3595	combination (2ν ₂ + ν ₃)
2348	C-O asymmetric stretching (ν ₃)
2278	C-O asymmetric stretching (ν ₃ (¹³ CO ₂))
662	O-C-O bending (ν ₂)
HOCH₂CH₂OH	Assignment (57, 73)
3396	OH stretching
2946, 2888	CH stretching
1462	CH ₂ scissoring
1392, 1348	OH bending and CH ₂ wagging
1284, 1258, 1202	CH ₂ twisting
1090, 1043	CO stretching and CC stretching
886, 867	CH ₂ rocking
New absorptions after irradiation (cm ⁻¹)	
	Assignment (12, 27, 74, 75)
2140	ν (CO)
1849	ν ₂ (HO \dot{C} O) / ν ₃ (H \dot{C} O)
1767	C=O stretch
1722	ν ₂ (H ₂ CO)
1657	ν ₂ (H ₂ O)
1500	ν ₃ (H ₂ CO)

Table S2. Absorption peaks observed in C¹⁸O₂-HOCH₂CH₂OH ice before and after electron irradiation (30 nA, 60 minutes) at 5 K.

Pristine ice, absorptions before irradiation	
(cm ⁻¹)	
C¹⁸O₂	Assignment
3622	combination (ν ₁ + ν ₃)
3512	combination (2ν ₂ + ν ₃)
2313	C- ¹⁸ O asymmetric stretching (ν ₃)
2242	C- ¹⁸ O asymmetric stretching (ν ₃ (¹³ C ¹⁸ O ₂))
661	O-C-O bending (ν ₂)
HOCH₂CH₂OH	Assignment (57, 73)
3393	OH stretching
2947, 2883	CH stretching
1461	CH ₂ scissoring
1398	OH bending and CH ₂ wagging
1282, 1247, 1195	CH ₂ twisting
1089, 1042	CO stretching and CC stretching
884, 865	CH ₂ rocking
New absorptions after irradiation (cm⁻¹)	Assignment (12, 76)
2138	ν (CO)
2090	ν (C ¹⁸ O)
1722	ν ₂ (H ₂ CO)
1638	ν ₂ (H ₂ O)

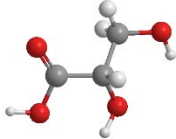
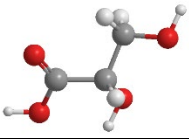
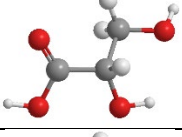
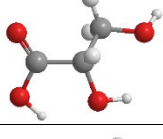
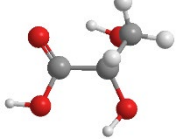
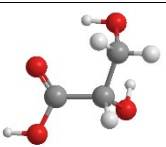
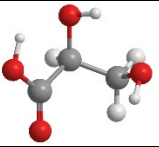
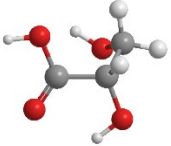
Table S3. Absorption peaks observed in CO₂-HOCD₂CD₂OH ice before and after electron irradiation (30 nA, 60 minutes) at 5 K.

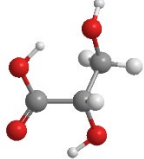
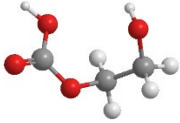
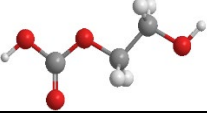
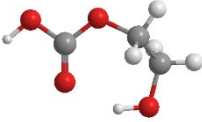
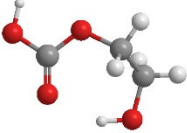
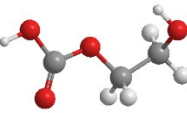
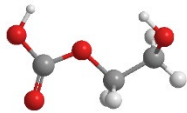
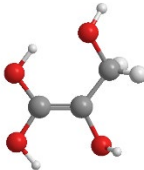
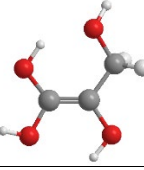
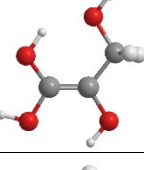
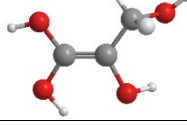
Pristine ice, absorptions before irradiation (cm ⁻¹)	
CO₂	Assignment (27)
3701	combination (ν ₁ + ν ₃)
3595	combination (2ν ₂ + ν ₃)
2346	C-O asymmetric stretching (ν ₃)
2278	C-O asymmetric stretching (ν ₃ (¹³ CO ₂))
662	O-C-O bending (ν ₂)
HOCD₂CD₂OH	Assignment (73)
3388	OH stretching
2235, 2168, 2115, 2086	CD stretching
1643	combination
1446, 1384, 1305	OH bending
1203, 1123, 1107, 1074	CO stretching and CD ₂ scissoring
979, 964	CD ₂ wagging
951, 898	CD ₂ twisting
740, 768	CD ₂ rocking
New absorptions after irradiation (cm ⁻¹)	
2141	ν (CO)
1844	ν ₂ (HOĊO) / ν ₄ (HĊO)
1703	ν ₂ (D ₂ CO)

Table S4. Absorption peaks observed in $^{13}\text{CO}_2\text{-HO}^{13}\text{CH}_2^{13}\text{CH}_2\text{OH}$ ice before and after electron irradiation (30 nA, 60 minutes) at 5 K.

Pristine ice, absorptions before irradiation	
(cm^{-1})	
$^{13}\text{CO}_2$	Assignment (27)
3621	combination ($\nu_1 + \nu_3$)
3506	combination ($2\nu_2 + \nu_3$)
2347	C-O asymmetric stretching (ν_3 (CO_2))
2282	$^{13}\text{C-O}$ asymmetric stretching (ν_3)
650	O- $^{13}\text{C-O}$ bending (ν_2)
$\text{HO}^{13}\text{CH}_2^{13}\text{CH}_2\text{OH}$	Assignment (57, 73)
3379	OH stretching
2938, 2872	^{13}CH stretching
1456	$^{13}\text{CH}_2$ scissoring
1399	OH bending and $^{13}\text{CH}_2$ wagging
1253, 1194	$^{13}\text{CH}_2$ twisting
1064, 1022	^{13}CO stretching and $^{13}\text{C}^{13}\text{C}$ stretching
875, 849	$^{13}\text{CH}_2$ rocking
New absorptions after irradiation (cm^{-1})	
2092	ν (^{13}CO)
1811	ν_2 ($\text{HO}^{13}\dot{\text{C}}\text{O}$) / ν_3 ($\text{H}^{13}\dot{\text{C}}\text{O}$)
1709	$^{13}\text{C=O}$ stretch
1681	ν_2 (H_2^{13}CO)
1658	ν_2 (H_2O)
1500	ν_3 (H_2^{13}CO)

Table S5. Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of distinct $C_3H_6O_4$ isomers **1**, **18**, and **19**; IEs and ΔE were computed at the CCSD(T)-F12b/cc-pVTZ-F12//B3LYP/aug-cc-pVTZ level of theory including the zero-point vibrational energy corrections. The computed Cartesian coordinates and harmonic frequencies of the neutrals and cations are listed in table S7. The IE ranges are corrected for the thermal and Stark effect by -0.03 eV and the combined error limits of $-0.05/+0.03$ eV (39).

Name	Isomer	Structure	ΔE (kJ mol ⁻¹)	Computed IE (eV)	Corrected IE ranges (eV)
Glyceric acid (2,3- Dihydroxypr opanoic acid)	1a		19.8	9.83	9.75 – 9.83
	1b		31.0	9.97	9.89 – 9.97
	1c		26.3	9.91	9.83 – 9.91
	1d		16.2	9.88	9.80 – 9.88
	1e		24.4	9.79	9.71 – 9.79
	1f		17.1	9.92	9.84 – 9.92
	1g		13.7	10.13	10.05 – 10.13
	1h		18.4	9.77	9.69 – 9.77

	1i		13.9	10.17	10.09 – 10.17
	18a		21.9	9.87	9.79 – 9.87
	18b		7.9	11.07	10.99 – 11.07
2-Hydroxyethyl hydrogen carbonate	18c		1.3	10.17	10.09 – 10.17
	18d		6.2	10.09	10.01 – 10.09
	18e		0.0	10.08	10.00 – 10.08
	18f		7.9	11.09	11.01 – 11.09
	19a		122.8	7.43	7.35 – 7.43
	Propene- 1,1,2,3-tetrol	19b		118.7	7.44
19c			118.7	7.32	7.24 – 7.32
19d			114.4	7.39	7.31 – 7.39

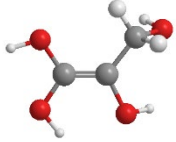
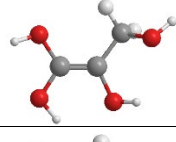
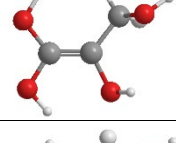
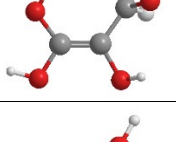
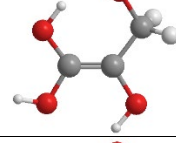
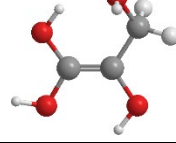
19e		111.8	7.42	7.34 – 7.42
19f		114.4	7.39	7.31 – 7.39
19g		126.2	7.53	7.45 – 7.53
19h		139.6	7.40	7.32 – 7.40
19i		118.7	7.32	7.24 – 7.32
19j		117.5	7.33	7.25 – 7.33

Table S6. Experimental conditions of ices including composition, ice thickness, irradiation parameters, and VUV photon energy.

Ice	Composition of carbon dioxide to ethylene glycol	Thickness (nm)	Current (nA)	Irradiation time (s)	Dose (eV/carbon dioxide)	Dose (eV/ethylene glycol)	Photon energy (eV)
CO ₂ -HOCH ₂ CH ₂ OH	2.1 ± 0.7 : 1	750 ± 80	-	-	-	-	11.10
CO ₂ -HOCH ₂ CH ₂ OH	3.1 ± 1.2 : 1	750 ± 80	31 ± 4	3600 ± 10	1.8 ± 0.3	3.1 ± 0.5	11.10
C ¹⁸ O ₂ -HOCH ₂ CH ₂ OH	1.5 ± 0.6 : 1	750 ± 80	29 ± 1	3600 ± 10	1.8 ± 0.3	2.9 ± 0.5	11.10
CO ₂ -HOCD ₂ CD ₂ OH	2.3 ± 0.5 : 1	770 ± 80	28 ± 2	3600 ± 10	1.6 ± 0.3	3.0 ± 0.5	11.10
¹³ CO ₂ -HO ¹³ CH ₂ ¹³ CH ₂ OH	1.4 ± 0.3 : 1	770 ± 80	32 ± 6	3600 ± 10	1.9 ± 0.3	3.3 ± 0.5	11.10
CO ₂ -HOCH ₂ CH ₂ OH	1.9 ± 0.5 : 1	750 ± 80	31 ± 2	3600 ± 10	1.8 ± 0.3	3.1 ± 0.5	8.77
CO ₂ -HOCH ₂ CH ₂ OH	3.1 ± 1.4 : 1	750 ± 80	104 ± 2	7200 ± 10	12 ± 2	21 ± 3	8.77

Table S7. Parameters for the generation of vacuum ultraviolet (VUV) light with an uncertainty below 0.001 eV for VUV photon energies.

VUV photon energy (eV)	Nonlinear medium in four-wave mixing	ω_1 laser wavelength (nm)	ω_1 Dye	ω_2 laser wavelength (nm)
11.10 ($2\omega_1 + \omega_2$)	Xenon	249.628	Coumarin 503	1064
8.77 ($2\omega_1 - \omega_2$)	Xenon	249.628	Coumarin 503	1064

Table S8. Differences in IEs and relative energies from B3LYP-based geometries for **1** and **18**. Isomer **1g** is the lowest relative energy conformer of glyceric acid (**1**); isomers **18e** and **18c** are the lowest and the next-lowest energy conformers of 2-hydroxyethyl hydrogen carbonate (**18**).

C ₃ H ₆ O ₄ isomers	Differences in IEs (eV)		Differences in relative energies (kJ mol ⁻¹)	
	PBE0 ^a	ω B97XD ^b	PBE0 ^a	ω B97XD ^b
1g	0.04	0.30	-0.03	-0.04
18c	0.04	-0.13	0.04	0.02
18e	0.00	0.00	0.00	0.00

^a calculated at the CCSD(T)-F12b/cc-pVTZ-F12//PBE0/aug-cc-pVTZ level of theory.

^b calculated at the CCSD(T)-F12b/cc-pVTZ-F12// ω B97XD/aug-cc-pVTZ level of theory.

Table S9. Cartesian coordinates, electronic energy (E at 0 K), zero-point vibrational energy (ZPVE), harmonic and anharmonic frequencies, and vibrational intensities of neutral C₃H₆O₄ isomers **1**, **18**, and **19** as well as their respective cations computed at the B3LYP/aug-cc-pVTZ theory level.

Isomer neutral and radical cation	Cartesian coordinates (Å), electronic energy (hartree), zero-point vibrational energy (hartree), harmonic frequencies (cm ⁻¹), and vibrational intensities (km mol ⁻¹)
	C,0.0678516674,0.0181723509,-0.0224145994
	O,-0.0686242938,0.0366442546,1.3855380182
	H,0.8140908454,0.0776473477,1.7694433037
	H,-0.9282301791,-0.0907349773,-0.4430007769
	C,0.9448958286,-1.1469042456,-0.4734271757
	C,0.9769522472,-1.2595710505,-1.9915448959
	O,2.197371701,-1.6254596476,-2.4503619466
	H,2.131408525,-1.7145558785,-3.4128781767
	O,0.0285214489,-1.0945877191,-2.7110586047
	O,2.2201800579,-0.9580452063,0.117026447
	H,2.8537684912,-1.5690341072,-0.2714149275
	H,0.4883343627,-2.078223925,-0.1110707985
	H,0.5026721354,0.9532262088,-0.3922305549
	E[B3LYP/cc-pVTZ] = -419.00366 Ha
	ZPVE[B3LYP/aug-cc-pVTZ] = 0.099668 Ha
	E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.41702 Ha
1a	Frequency and Intensity
	39.2007 2.3158
	113.712 6.109
	186.3786 0.5188
	208.2079 103.1659
	302.5181 29.6073
	352.1607 22.6043
	412.2852 86.9164
	430.2733 20.189
	498.1224 8.1999
	577.3281 53.7839
	629.8044 85.2859
	724.3623 38.3193
	877.1407 30.5601
	917.3253 19.8628
	1051.1345 33.0452
	1067.8603 156.7341

1110.7459	73.1226
1153.8215	222.0847
1192.6075	12.5366
1278.73	36.5415
1324.0883	41.767
1351.0803	28.2563
1367.2863	36.3355
1393.8242	17.7766
1424.9385	34.9397
1499.3447	2.5334
1812.2581	272.4256
2973.6225	13.8813
3005.2369	44.4279
3124.245	7.7394
3734.5755	78.0372
3795.7842	42.0865
3819.1512	60.3018

C,0.1116615768,0.2174075822,0.0202833794
 O,-0.0949431886,0.1889479843,1.3091853544
 H,0.6286757971,0.5661523745,1.8358333776
 H,-0.7736274079,0.0124954256,-0.5715741916
 C,1.0039643603,-1.5967633968,-0.4736534217
 C,0.9497394375,-1.4869715005,-1.9752774227
 O,2.1678733633,-1.2107694244,-2.4603664998
 H,2.1493058088,-1.1625297331,-3.4311076637
 O,-0.0679671273,-1.6206473749,-2.5878690386
 O,2.1627320325,-1.6614432965,0.1414364406
 H,2.8975295446,-1.4170210173,-0.4529610387
 H,0.2069608576,-2.1470308041,0.0142305669
 H,0.8872877829,0.8667465861,-0.3755545298

1a⁺

E[B3LYP/cc-pVTZ] = -418.65667 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.097911 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05418 Ha

Frequency and Intensity

60.7648	1.1256
87.6058	4.6582
117.1799	4.2345
146.068	15.0963
262.2871	2.9851
297.4251	11.078
324.506	9.8186
492.4744	65.6249
529.3906	49.5126

584.2005	56.9591
624.7429	122.4437
629.8858	64.7052
757.7553	2.9536
860.949	35.6673
874.2323	45.7856
1021.7085	25.3025
1112.8229	214.0791
1128.878	44.8863
1144.0673	91.5547
1213.5105	232.6861
1311.8473	262.5585
1330.2236	12.8108
1376.3925	24.1436
1391.1554	29.1954
1446.9789	112.3973
1530.1847	11.2332
1813.8639	198.3495
3085.4135	18.251
3168.1606	11.0409
3217.1936	5.5612
3628.3491	232.8804
3702.1135	336.0695
3705.786	150.1872

1b

C,0.0016233549,-0.081609762,-0.0206337578
O,0.0315689273,0.2411721348,1.3648144354
H,0.9308001873,0.1445355064,1.6888074752
H,0.5330259638,0.6638586672,-0.6145232624
C,-1.4536751091,-0.1079226892,-0.4548007141
C,-1.5789655197,0.0179282888,-1.9729870807
O,-2.6854066973,-0.612196642,-2.4333023195
H,-2.7309354645,-0.4565682462,-3.3881952729
O,-0.838854585,0.6391833845,-2.68850006
O,-2.0623940955,-1.2757367412,0.0582130474
H,-2.9558169288,-1.3489375786,-0.2916826541
H,-1.9330573283,0.7935374856,-0.0455934881
H,0.4381969258,-1.0673452592,-0.2090110362

E[B3LYP/cc-pVTZ] = -418.99919 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.09917 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.41225 Ha

Frequency and Intensity

39.3035	5.2823
97.5319	4.4414

168.0538	106.1945
210.6903	11.1637
236.7782	100.3747
308.0985	25.1109
374.836	1.9241
419.957	7.8715
494.2458	12.4118
569.0494	53.7658
629.2519	106.5711
725.0461	35.6024
893.6783	37.3216
921.8921	5.8915
1037.2612	65.0617
1069.5733	136.989
1129.6068	39.6494
1152.7673	231.5296
1211.2956	21.2991
1256.7689	28.9079
1300.3213	17.8066
1321.2935	31.7469
1368.5101	63.8003
1381.2488	8.9672
1462.3681	3.1225
1510.249	5.7195
1809.3156	271.1868
2963.1203	16.4236
3011.6895	35.2906
3067.3162	17.6082
3739.1082	79.0767
3815.8045	50.9888
3834.4221	43.3495

1b⁺

C,0.0177310245,-0.0365933914,-0.0900008181
O,0.1519147165,0.3483312238,1.2151190336
H,0.5761427564,-0.326999325,1.7657047007
H,0.3386699789,0.7837374322,-0.762976371
C,-1.5304991343,-0.1143857617,-0.4540134788
C,-1.5433056799,0.0195385436,-2.0397523283
O,-2.5438927246,-0.6464945338,-2.564166997
H,-2.5722762652,-0.523537117,-3.5308446577
O,-0.7333720376,0.7018407473,-2.5991905701
O,-2.0848537215,-1.2866450081,-0.054450744
H,-2.8624186177,-1.1714712039,0.5122950026
H,-2.0347277085,0.7736240712,-0.0636466466
H,0.5169970439,-0.9710471286,-0.3414708132

E[B3LYP/cc-pVTZ] = -418.65293 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.097703 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.04432 Ha

Frequency and Intensity

54.6378	1.093
139.2508	11.4385
188.6841	20.035
282.3398	18.6091
346.4333	42.8268
358.181	283.4157
375.5388	258.3933
414.7107	17.7863
485.9024	13.6174
551.1107	26.6042
637.2004	79.983
690.7568	52.6347
787.4881	184.4496
808.9879	45.3956
915.6868	94.4444
1114.4649	30.0221
1147.566	475.3706
1166.3851	35.6181
1196.4455	19.9471
1203.2035	6.1321
1255.3633	73.1064
1295.4771	6.8647
1342.9568	16.7083
1349.0077	11.6464
1414.1758	23.6798
1472.8277	12.5987
1745.8939	178.0887
2850.5034	88.7481
3056.9044	1.5913
3111.7253	3.4036
3665.6626	347.8235
3725.3773	415.4449
3735.9744	407.7516

1c

C,0.0086084523,-0.0446002199,-0.0716627845
O,0.0719985758,-0.0027788462,1.3548181115
H,0.9665102535,-0.2022116401,1.6426312413
H,0.5328133293,0.798542768,-0.5231580377
C,-1.477232938,0.0244683196,-0.4184658398
C,-1.6524228835,0.0414193272,-1.928019252
O,-2.5297937322,-0.8625511985,-2.3881224953
H,-2.5719770616,-0.745812953,-3.3494407271

O,-1.0606634669,0.8153747914,-2.6397387942
O,-2.1952398904,-1.0340517876,0.1735264312
H,-1.9104939928,-1.077164511,1.0944192644
H,-1.8561145284,0.9937092278,-0.0665799034
H,0.428528186,-0.9809388803,-0.4513867136

E[B3LYP/cc-pVTZ] = -419.00129 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.099757 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.4146 Ha

Frequency and Intensity

22.264	6.2809
121.245	3.4632
195.9051	8.4912
228.4077	98.1634
283.4787	12.259
352.7678	3.3464
402.1459	82.2791
446.8141	21.4695
517.7554	3.0472
586.9429	73.3848
645.9131	91.0394
736.9474	47.5051
872.3748	13.3642
927.4216	10.1369
1046.7684	35.5436
1071.2293	72.0416
1136.7814	86.7036
1172.317	335.0976
1222.2692	16.6808
1244.6499	24.1923
1268.2692	13.1846
1338.7685	42.256
1359.7506	39.7031
1431.0424	6.2975
1446.5662	12.9385
1511.3848	4.7533
1791.809	289.9112
2975.359	16.8157
3012.919	34.4996
3076.1772	19.8111
3728.9875	70.1391
3775.3724	56.284
3837.3754	56.5197

1c⁺ C,-0.0767265481,0.438208906,0.0779646895

O,0.2951828523,-0.7799313894,0.6380605545
H,1.1224942277,-1.1245004029,0.2761644156
H,-0.0664202807,1.2207518343,0.852140126
C,-1.5607988225,0.3197669695,-0.3253480801
C,-1.560952325,-0.6200834938,-1.6834266439
O,-2.3888872198,-0.119134836,-2.5594968251
H,-2.4471764187,-0.6783368927,-3.3574363037
O,-0.8819302368,-1.5982188822,-1.7223048333
O,-2.340236881,-0.3085360876,0.5866086672
H,-1.8503892202,-1.0328457902,1.0212192479
H,-2.0372415992,1.2543644276,-0.6185146504
H,0.547602775,0.7519000348,-0.7568098633

E[B3LYP/cc-pVTZ] = -418.65361 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.097796 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.04831 Ha

Frequency and Intensity

51.8043	2.0574
71.4035	2.499
208.7473	12.8593
218.8842	60.1752
266.4826	14.0664
330.6349	2.0958
348.056	3.3884
529.2172	46.1876
547.6894	67.2906
597.2936	79.0657
614.0764	120.4243
726.344	42.2635
745.2874	39.9662
830.2173	46.7546
946.0621	88.2435
1091.3717	102.9638
1133.1306	141.5876
1154.6119	258.4625
1171.4348	97.8679
1211.1668	61.7412
1243.5519	12.2889
1317.6652	27.955
1331.7143	34.6804
1373.9923	15.9451
1422.6802	23.7335
1465.5417	5.3741
1777.4407	212.1597

2954.6732	63.8804
3106.2853	4.6167
3107.7435	8.4108
3615.9237	147.4088
3645.7908	280.6035
3770.398	350.3388

C,-0.0013949239,-0.0551198328,-0.0594361375
 O,0.0450949597,-0.0388925805,1.3685417776
 H,0.9316565734,-0.2605417634,1.6656206982
 H,0.5797008423,0.7586257761,-0.4951806047
 C,-1.4693941109,0.1205447682,-0.4255290005
 C,-1.6522305981,0.0362010357,-1.940391542
 O,-2.4581459732,-0.9483041007,-2.3611314097
 H,-2.7781738726,-1.428789157,-1.5779745586
 O,-1.1048007315,0.7939490771,-2.693420032
 O,-2.2756289694,-0.8747451763,0.1936393793
 H,-1.9511204841,-0.9980663977,1.094339582
 H,-1.7943779891,1.1175420424,-0.11222125
 H,0.3670401553,-1.0097330534,-0.447548221

E[B3LYP/cc-pVTZ] = -419.00536 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.100113 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.41881 Ha

Frequency and Intensity

1d

61.5049	5.1396
122.6207	7.2736
190.9652	14.2641
246.9426	100.2623
313.068	10.2814
350.6197	7.1448
389.4884	102.0984
448.8388	34.6212
549.4275	5.7864
625.7985	20.9978
696.0967	73.8815
732.7868	10.9497
870.4301	24.4489
926.4128	7.6006
1044.5687	23.0294
1069.5633	76.9649
1117.3496	58.5302
1174.7583	111.1122
1225.4313	30.4831
1241.5933	8.2786

1273.482	9.9494
1346.8612	122.7893
1374.9539	261.3111
1401.1577	86.7806
1438.3924	2.836
1512.3676	5.3479
1835.3557	295.4636
3008.4557	21.0401
3025.2555	19.8668
3077.0262	17.7336
3649.8129	148.2491
3769.4418	72.0294
3833.4845	57.7111

C,0.0089398474,0.2924393122,0.0939744029
 O,0.0921444979,-0.9486601617,0.7638919695
 H,0.9135459703,-1.0357689935,1.2607494285
 H,0.1616735461,1.1408379247,0.7752071097
 C,-1.4210662476,0.3758898008,-0.3747006014
 C,-1.5748916916,-0.5257014227,-2.0265269904
 O,-2.6751932883,-1.1821739916,-2.1095758228
 H,-3.1901931348,-1.1572684132,-1.2795945709
 O,-0.6850493715,-0.3290757526,-2.7632865649
 O,-2.3064409408,-0.2510790865,0.3963929382
 H,-1.8072529036,-0.8762089539,0.9746935104
 H,-1.7873577478,1.3249322864,-0.7659331565
 H,0.7093663422,0.3845080891,-0.7359829711

1d⁺
 E[B3LYP/cc-pVTZ] = -418.65287 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.097907 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05337 Ha

Frequency and Intensity

65.0283	4.5995
85.6995	2.431
203.1326	1.978
225.5117	21.5793
258.5616	99.3513
285.9442	11.0357
356.0548	7.8286
409.676	11.5952
520.6429	39.4514
582.7646	46.2219
638.978	29.987
718.6071	9.5603
802.1986	105.7344

884.8218	34.6798
988.7578	37.2554
1080.2519	44.2443
1129.0845	37.5883
1175.7845	28.2907
1186.6828	107.7723
1212.7835	84.1777
1237.8524	26.5351
1251.6639	363.1405
1357.5347	47.0568
1419.5481	8.1892
1456.1942	83.2504
1489.6459	24.4549
1920.9916	131.4764
2982.3742	21.1952
3091.0068	2.7589
3101.0157	16.1384
3440.7729	300.7552
3609.6723	122.784
3806.8886	182.504

C,0.0930804354,0.0677607187,0.054985504
 O,-0.2803745082,-0.5745933549,1.2586538588
 H,0.2578150677,-0.2090891319,1.9691041287
 H,-0.6648936038,-0.1841886067,-0.6851051354
 C,1.4424307826,-0.3885064647,-0.5011341896
 C,2.5319488457,-0.2906146086,0.5603193529
 O,3.5641868663,-1.1240654537,0.3028713699
 H,4.2238712983,-1.0050982329,1.0023820141
 O,2.5154693992,0.4566721343,1.5047697326
 O,1.3136330985,-1.6867359714,-1.0455346682
 H,2.1874204231,-2.0719841595,-1.166618983
 H,1.7336609199,0.329067835,-1.2849876461
 H,0.1125992808,1.1542728369,0.1745298387

1e

E[B3LYP/cc-pVTZ] = -419.00162 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.099851 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.41545 Ha

Frequency and Intensity

45.9616	6.631
116.9548	2.4284
206.6363	1.7463
262.531	42.7448
290.1049	77.5102
343.9774	8.5039

435.7576	108.4879
448.9222	9.3964
538.0544	32.0557
572.0412	94.6877
653.6851	73.7405
743.9724	18.6563
858.8664	4.4926
900.157	11.783
980.3535	55.8432
1082.8489	46.3245
1112.8833	107.03
1152.5326	262.1854
1235.1544	60.4532
1247.9348	9.8228
1322.0663	29.1886
1359.8235	32.7656
1398.8594	7.8123
1403.3344	38.3491
1423.5975	31.1626
1486.3844	8.258
1801.8911	263.5019
2937.3474	27.7824
3026.7815	43.3603
3099.8938	13.3334
3735.1514	81.7195
3794.6858	40.5933
3810.2823	53.1408

1e⁺

C,-0.2042028813,-0.0784316714,0.2936983658
O,-0.0537919785,-0.4295642083,1.5276487923
H,0.2618056227,0.293645785,2.0993538126
H,-0.6345694389,-0.8366142953,-0.3478908275
C,1.8307096757,-0.2383474827,-0.8067738127
C,2.65549408,-0.2959686995,0.4358480189
O,3.3131205288,-1.4572817203,0.5077276368
H,3.8451251066,-1.5039537293,1.3196819358
O,2.6540520662,0.587929237,1.2502130847
O,1.7891189703,-1.2372710078,-1.6467058609
H,2.226598226,-2.0325037668,-1.287909457
H,1.6012546611,0.7283546475,-1.2353943604
H,-0.2538663333,0.9729044526,0.0347378493

E[B3LYP/cc-pVTZ] = -418.65722 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.097603 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05325 Ha

Frequency and Intensity

53.7388	5.927
68.7929	2.4138
104.1322	3.0926
137.504	13.2683
262.3746	3.2863
295.4678	3.5475
307.3565	23.0825
463.5684	74.1843
515.0828	36.2238
566.3577	13.0707
615.2879	184.6674
632.149	57.6111
757.8171	2.9235
852.8389	45.8626
870.4381	52.5498
961.9636	22.9318
1060.3086	129.4022
1116.5849	66.434
1145.7799	174.9688
1214.3266	276.2916
1333.4357	217.3735
1346.0347	100.854
1393.2178	60.3045
1404.4435	21.0949
1467.1567	181.5384
1544.0125	19.8518
1792.0107	201.5983
3111.4291	29.0879
3195.6434	8.4379
3251.4966	5.9203
3634.4309	285.3147
3661.0593	189.6896
3706.3264	215.2292

1f

C,0.1647682934,0.2959648444,-0.0617741106
O,-0.4974492332,-0.5097919121,0.9022820185
H,0.098772277,-0.5938833608,1.6594980442
H,-0.5281772547,0.4170205314,-0.893453246
C,1.4309547185,-0.3888503982,-0.573688985
C,2.4898568243,-0.4672572371,0.5293448842
O,3.741529289,-0.4040039959,0.0480905251
H,4.3521208114,-0.5180639852,0.7930871992
O,2.2460045644,-0.6013972754,1.7070792222
O,1.1537933267,-1.708267005,-1.0182533463
H,0.4809421709,-2.0641566013,-0.4205822319
H,1.8434682623,0.1569527215,-1.421830985

H,0.404407383,1.2872525842,0.3365904502

E[B3LYP/cc-pVTZ] = -419.00515 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.100787 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.41915 Ha

Frequency and Intensity

35.4921	1.5716
151.7689	10.8165
209.6856	3.9798
256.5167	3.7313
320.6994	4.293
367.7132	4.0721
457.4428	58.7917
557.8023	27.4711
607.02	177.6591
627.6937	126.7858
737.9357	5.2096
776.1492	43.1966
837.0762	17.9791
916.3122	24.777
998.73	22.7664
1073.1019	48.9956
1096.718	79.3325
1158.9509	305.1182
1221.7838	25.0434
1255.3051	20.2154
1308.6593	5.1577
1377.861	3.4247
1405.7762	80.9979
1415.7554	37.898
1438.216	21.5277
1497.1136	5.7322
1780.4808	273.0681
3009.3646	40.3589
3079.1846	15.3939
3092.2288	19.3891
3716.2928	83.2286
3723.6243	58.4668
3731.8406	75.4313

1f⁺

C,-0.0552207122,0.2352036251,0.1706872511
O,-0.3467290908,-0.3876047403,1.2956095685
H,0.3044338129,-0.146713511,1.9908169608
H,-0.8044229574,0.0756306269,-0.5981687173
C,1.445400339,-0.5418819169,-0.5648982082

C,2.4916375167,-0.4346376805,0.5729375958
O,3.6723084349,-0.7581870934,0.0815068929
H,4.3588493096,-0.6957824216,0.7699163183
O,2.245487459,-0.0913701547,1.6979867904
O,1.1917500409,-1.8084690765,-0.8860897645
H,0.899440922,-1.9262140004,-1.8043393097
H,1.6145385428,0.14202713,-1.3983947048
H,0.3635178157,1.2395181238,0.2588187655

E[B3LYP/cc-pVTZ] = -418.65259 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.098044 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05186 Ha

Frequency and Intensity

36.4376	1.853
137.5004	13.4358
176.1447	7.1707
229.0428	4.8009
289.2031	4.4969
294.2923	12.896
395.7002	8.125
485.5707	81.165
544.3436	10.5984
591.2617	235.4553
593.1123	90.961
647.0063	42.3725
754.2759	52.6202
850.9355	33.6837
951.3181	65.8461
1041.4188	27.2502
1139.5617	87.0208
1169.3021	146.621
1215.3399	27.3931
1223.9667	49.5463
1257.5804	126.0647
1300.805	63.1182
1354.1263	57.6776
1409.8303	58.2579
1462.128	22.9741
1503.3431	0.0777
1798.0068	192.8427
3037.7567	10.7995
3073.4287	2.2974
3177.0268	1.0272
3515.6273	294.545

3672.4729	207.5565
3708.3684	263.995

C,0.0989062709,0.158130973,0.0170532325
O,-0.337411326,-0.9004917793,0.8696028091
H,0.0606215072,-0.789531079,1.7393417949
H,-0.6539868795,0.2497099149,-0.7644652419
C,1.4390578316,-0.1939123901,-0.6185658563
C,2.5843797091,-0.1255276553,0.4074901155
O,3.4643193491,-1.132336861,0.3240241511
H,3.1430728748,-1.7347440084,-0.3709713165
O,2.6917283648,0.7651767823,1.2069677954
O,1.3953371148,-1.4734879884,-1.244186946
H,0.7710192933,-2.0107033308,-0.7353521962
H,1.6718411991,0.5393584545,-1.394851368
H,0.1794895754,1.104243769,0.5508786731

E[B3LYP/cc-pVTZ] = -419.00637 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.100732 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42037 Ha

Frequency and Intensity

1g	60.5217	9.828
	98.7147	3.8958
	221.6969	6.4142
	275.6547	28.1196
	348.1174	28.8962
	368.3676	53.9829
	508.3707	78.9641
	519.8473	0.5337
	563.4584	46.0998
	599.4482	24.6854
	760.6493	46.7637
	772.6701	37.2787
	842.9535	19.25
	902.3606	9.0863
	991.0125	62.6407
	1058.0462	25.5203
	1100.7035	102.9352
	1191.6639	18.0081
	1203.0161	43.8358
	1251.327	2.4013
	1328.735	38.2661
	1366.4224	349.7207
	1383.7817	9.8565
	1399.4548	40.5013

1406.2745	76.7783
1492.7548	8.765
1828.5407	275.0059
3045.6801	6.0447
3063.6621	26.5395
3111.5483	9.5321
3624.4426	146.8699
3721.8634	71.3406
3804.4546	47.2818

Anharmonic Frequency and Intensity

48.346	10.44800276
84.48	2.91857779
135.265	38.68947835
210.583	6.79812471
267.853	35.26175182
404.61	100.5889543
476.925	13.33143087
509.057	1.54936264
573.819	12.488372
590.834	3.32500215
671.161	55.54683686
793.302	16.6907431
828.484	8.84881313
878.472	5.17960788
967	31.78783738
1030.429	16.13367772
1065.828	72.39330719
1146.681	29.53172434
1178.202	21.3205114
1215.076	2.91949586
1286.888	23.83752609
1327.749	59.8584282
1341.138	36.59124704
1369.015	30.47720358
1375.362	58.00066744
1451.119	6.04610777
1802.712	139.7046076
2906.739	8.38828706
2958.664	21.18544962
2963.766	12.2981964
3428.914	136.9111473
3543.418	39.27635749
3616.208	39.78149527

C,0.0156073416,-0.2214248002,0.2854502423
O,0.1637659593,0.4429844235,1.4999218774
H,0.2641475445,1.4028109647,1.3964646713
H,-0.3386100524,-1.2281927718,0.4923401566
C,1.3825256532,-0.2730884931,-0.4762029456
C,2.4416972819,-0.7699531511,0.587616789
O,3.2089877082,-1.7564038783,0.244956643
H,2.9552035938,-2.0875973498,-0.6398413493
O,2.4981763074,-0.1975914293,1.6524311361
O,1.362332164,-1.1558645667,-1.5329714448
H,1.5412703757,-0.7303678,-2.3825816792
H,1.6981007988,0.7337992892,-0.7620092716
H,-0.6848297912,0.2967743641,-0.3786091787

E[B3LYP/cc-pVTZ] = -418.65143 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.098876 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.04613 Ha

Frequency and Intensity

1g⁺

73.1479	4.7199
142.1559	3.3043
220.1875	4.5293
291.3475	24.2062
361.7205	8.9483
396.5752	32.2366
441.04	22.5132
455.1957	104.5528
527.619	11.6385
583.1153	25.5806
700.7276	19.5569
710.3321	99.8426
756.7362	20.3309
902.217	41.655
961.3012	97.7441
1047.5574	21.4248
1129.9583	6.3502
1157.2044	151.1964
1201.6621	20.5747
1245.8701	53.0107
1273.8214	38.2917
1299.4353	106.648
1330.5692	337.4893
1372.7378	2.6308
1419.987	13.2301
1479.306	3.2469

1663.1848	225.3328
3007.6541	16.443
3051.2082	0.4908
3135.5921	5.0651
3589.5446	156.7723
3712.2865	278.215
3760.6707	259.1421

C,0.1113363694,0.0801537835,0.0432359491
 O,-0.4937028507,-0.5039328906,1.1870979902
 H,-0.0536592055,-0.1828768106,1.9791635457
 H,-0.6416041429,0.0808540408,-0.743716039
 C,1.3119376679,-0.7181115925,-0.4892910098
 C,2.3293620569,-1.0039447291,0.600764565
 O,2.7594670926,0.1162649959,1.2187753949
 H,3.4139287073,-0.1492315061,1.8823760606
 O,2.7093283728,-2.1080326577,0.8930920476
 O,0.9083666341,-1.9196411036,-1.0957211374
 H,1.2894663908,-2.6501875644,-0.5900384368
 H,1.8112434581,-0.087434153,-1.2367870841
 H,0.4162775654,1.1118261232,0.2342935276

E[B3LYP/cc-pVTZ] = -419.00374 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.099538 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.4174 Ha

Frequency and Intensity

1h

38.4691	2.9622
100.2736	3.8905
195.0671	0.9286
243.5933	55.3507
274.9874	91.5356
312.9283	50.5478
352.0268	19.05
481.4897	14.1972
522.2775	7.2695
597.1376	37.1535
652.6574	87.6916
752.1748	26.6381
857.4608	4.0383
897.8432	12.7886
985.9826	57.3055
1081.8482	46.4384
1110.2681	260.1746
1158.2373	131.3666
1218.7227	27.3958

1271.4324	17.7249
1326.5731	4.7265
1334.3881	72.2891
1386.7202	16.945
1398.501	20.4093
1444.7381	5.7523
1486.9532	5.5985
1805.5229	303.6989
2983.0548	17.7495
3032.8711	43.4406
3097.4354	13.8801
3730.7715	81.9234
3737.7061	76.9851
3821.9587	32.6233

C,-0.0939082025,0.217413167,0.1836651304
 O,-0.7129927726,-0.585071011,1.00197575
 H,-0.4478879415,-0.4912826854,1.9318560322
 H,-0.5426106435,0.2653937927,-0.8004798358
 C,1.6086332571,-0.8435522965,-0.6348019873
 C,2.4076199458,-0.979895835,0.6316083035
 O,3.0768128498,0.1263529154,0.9294648316
 H,3.6195493978,-0.0082159658,1.7255698508
 O,2.3609554423,-2.0086545554,1.2535787605
 O,1.1141014148,-1.9510952739,-1.1068487699
 H,1.203322997,-2.6659438629,-0.4375869686
 H,1.8043820694,-0.0675499223,-1.3659422799
 H,0.4737703025,1.057807469,0.5711865561

1h⁺

E[B3LYP/cc-pVTZ] = -418.65942 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.097946 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05681 Ha

Frequency and Intensity

49.2298	2.6647
79.6581	3.1485
138.6471	5.5905
141.2843	2.9491
242.0367	10.9545
286.974	26.8187
364.0217	1.6729
463.4922	49.4206
517.2576	65.478
597.8325	51.5062
669.2457	25.3529
687.6709	121.7548

782.5209	10.3815
843.5493	33.1576
882.0675	69.4532
995.8909	15.5836
1087.4467	98.2025
1118.0016	25.2218
1166.2391	139.2439
1202.6964	246.1609
1309.4956	248.3236
1351.4586	111.6518
1388.9834	44.5083
1400.042	3.164
1482.6419	80.5872
1532.6639	11.7033
1795.8256	259.6591
3098.6165	20.1712
3173.1763	8.7325
3234.9273	6.0913
3517.2047	184.4332
3691.5047	169.7251
3701.1437	248.1256

ii C,0.0987413916,0.1978347484,0.0833984662
O,-0.0593502909,-0.8163464681,1.0894571047
H,0.7899998589,-1.0125613773,1.4943803414
H,0.6148325495,1.0733988142,0.4845252334
C,-1.3009998634,0.5838807032,-0.3952690317
C,-2.1460789815,1.2599223715,0.6912100034
O,-2.197057261,0.6500435992,1.8785933346
H,-1.553748087,-0.0867395958,1.8917502965
O,-2.7493690652,2.2770897862,0.4632267528
O,-1.1828810207,1.4323098902,-1.5061330385
H,-1.7921922978,2.1711034049,-1.3483866703
H,-1.8252284417,-0.3423545108,-0.6696777359
H,0.6612316103,-0.1861701166,-0.7686008551

E[B3LYP/cc-pVTZ] = -419.00648 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.100539 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42013 Ha

Frequency and Intensity

94.6304	1.5554
164.5226	6.7184
243.4286	4.9557
285.3381	78.4072
315.1857	42.6983

354.8	18.875
412.8491	14.418
470.7932	57.0166
535.6244	16.3425
622.6789	22.4307
738.6644	18.9583
756.0546	70.3866
823.3992	3.5213
1017.9817	3.273
1025.7162	54.4641
1071.0845	35.1243
1133.8496	165.0584
1220.2119	19.3872
1229.1239	17.8745
1242.0345	53.3227
1296.4418	31.8177
1344.5849	2.9502
1402.8089	314.0671
1434.505	8.0737
1449.6138	28.3868
1522.7418	3.1487
1816.657	319.6717
2968.8706	20.8711
3027.2539	33.5751
3077.7735	20.0825
3525.4716	343.6054
3675.074	115.3557
3831.5968	64.8912

1i⁺

C,0.3228313573,-0.1803872264,0.2220836931
O,0.7557172701,0.4998694847,1.2448014726
H,1.3475366468,1.2353164958,1.0144351507
H,0.8058540075,-0.0667994652,-0.7431361491
C,-1.4939743573,0.6875143384,-0.4967318145
C,-2.2059063041,0.9116159388,0.8269859515
O,-2.8600191516,-0.0893274967,1.394921117
H,-2.9917224463,-0.8611138207,0.8264487331
O,-2.1017137373,2.0050263128,1.3107781498
O,-1.1329072831,1.7942064525,-1.0877223513
H,-1.2703187054,2.535526859,-0.4481922467
H,-1.6869226063,-0.1433743889,-1.169383081
H,-0.1305545892,-1.1266622349,0.4931855764

E[B3LYP/cc-pVTZ] = -418.64576 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.097477 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.04319 Ha

Frequency and Intensity

28.8774	4.3523
96.8944	5.7832
121.905	6.6753
138.6738	1.3833
246.6996	10.2049
306.9689	29.6855
360.5369	29.9303
458.7608	22.9903
473.815	81.2769
518.751	74.848
690.184	15.8748
696.1607	4.8122
808.1041	9.7842
849.5396	74.1863
868.1924	6.6225
997.1415	19.3888
1100.2525	111.4224
1118.0244	22.7305
1163.6202	98.5745
1211.8316	54.4189
1291.6623	482.2456
1317.2259	245.0142
1374.9829	48.0672
1398.4211	0.9496
1462.0229	55.0157
1528.6143	12.3368
1816.8381	190.6775
3095.4606	19.8663
3142.0613	4.3501
3225.8289	2.7415
3425.8646	190.9718
3699.1013	250.7686
3754.3438	120.6292

18a	C,-0.1016600147,0.5629533565,-0.2199450546
	O,-0.69389474,0.3883580898,1.0560851349
	H,-0.8532806515,-0.5479882673,1.2114542879
	C,1.1583281086,-0.2549677188,-0.4336837437
	O,2.202506197,0.1346780402,0.4821047239
	C,2.3962880504,-0.4821604283,1.6455869656
	O,1.6106356036,-1.5795814467,1.8138752283
	H,1.8523943245,-1.9437879466,2.6752689934
	O,3.2067493164,-0.1165905194,2.4487190101
	H,0.9662646219,-1.3229675011,-0.3504755746
	H,1.5616181707,-0.0477268193,-1.4244023563

H,-0.8025631225,0.3155337515,-1.0275668229
H,0.1332867417,1.6242543796,-0.2938361453

E[B3LYP/cc-pVTZ] = -419.00644 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.100398 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = - 418.41694 Ha

Frequency and Intensity

71.6806	5.8018
73.7774	0.1924
137.0217	6.9098
265.8617	124.5922
276.6772	15.7713
358.7754	13.6951
497.4868	35.9203
553.1216	75.7513
589.1328	18.3974
594.7031	8.6547
777.9106	34.3804
826.5635	1.1788
886.9769	22.0611
951.9555	6.4745
1062.272	59.9832
1093.3956	72.1279
1107.8866	83.2333
1155.8026	316.0247
1241.9012	66.1163
1308.5187	3.0307
1354.0977	120.2636
1370.6792	10.9456
1422.3427	50.3058
1426.4097	24.9742
1495.6856	2.1728
1500.3155	12.177
1831.732	657.9739
2981.598	54.1727
3065.2262	29.1125
3085.6648	9.483
3116.3501	15.655
3781.9203	101.0431
3806.2327	28.1909

18a⁺ C,-0.25809609,0.127204279,-0.3614343678
O,-0.9932866263,0.8855091084,0.4334476933
H,-1.2231543334,1.7484229457,0.0512343713
C,1.564071161,0.3684384778,0.0321083519

O,1.8008124488,0.0766800008,1.3071677626
C,1.9816530362,-1.2963422381,1.6278526769
O,2.4002481086,-1.3235318042,2.864332329
H,2.537574351,-2.2417397316,3.1499076638
O,1.7466250825,-2.161255739,0.8473087673
H,1.9379082166,-0.3395539799,-0.7054087842
H,1.6709903802,1.431521731,-0.1529958974
H,-0.2984477313,-0.9246643747,-0.0907004054
H,-0.2302253978,0.379318295,-1.4196355146

E[B3LYP/cc-pVTZ] = -418.65471 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.098285 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.0523 Ha

Frequency and Intensity

62.4464	2.8005
71.743	2.4303
136.5594	11.077
192.1664	1.5521
312.9461	5.6818
370.3205	2.3975
411.8712	14.5909
485.2462	124.9159
549.3518	35.0379
582.9387	95.3979
642.201	19.0734
767.5657	41.2048
789.0437	232.4132
844.9104	42.2584
916.022	17.9447
1117.5042	44.9062
1138.7882	36.6811
1173.8432	440.0703
1213.8762	39.5744
1250.4608	61.4936
1276.7799	173.8397
1299.1074	84.6823
1361.9886	86.3794
1378.4008	40.8473
1471.5454	16.2583
1515.0605	1.4836
1877.1348	353.4668
3059.1472	15.9932
3071.9796	7.5176
3177.1305	3.6766

3199.512	10.5979
3702.7112	348.9103
3721.9224	224.6871

C,-0.006164302,0.,-0.0395576606
 O,-0.0170352184,0.,1.3834621598
 H,0.8874692432,0.,1.7069073655
 C,-1.4576061267,0.,-0.4739158132
 O,-1.4506147251,0.,-1.9158735744
 C,-2.6472956743,0.,-2.4994743053
 O,-2.467687129,0.,-3.8331189934
 H,-3.348532208,0.,-4.2285589205
 O,-3.7162049311,0.,-1.9459174219
 H,-1.9773011796,-0.8844673418,-0.1085002399
 H,-1.9773011796,0.8844673418,-0.1085002399
 H,0.4971081762,0.8872227258,-0.4359217609
 H,0.4971081762,-0.8872227258,-0.4359217609

E[B3LYP/cc-pVTZ] = -419.01177 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.100292 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42215 Ha

Frequency and Intensity

18b	53.1185	2.0853
	78.0362	6.0332
	142.381	0.6316
	178.2904	32.6224
	219.0554	85.0272
	333.6368	18.0511
	365.8674	2.5922
	545.0377	99.7775
	577.2325	56.79
	668.6063	0.8406
	796.6952	29.3189
	826.1846	4.1629
	954.1761	21.683
	1032.2457	29.7667
	1069.1261	63.4914
	1106.2319	28.7172
	1157.4564	0.0047
	1201.1272	603.7866
	1233.2073	3.0697
	1245.905	24.0558
1303.8299	0.6398	
1364.1239	85.4153	
1413.7446	196.3447	

1468.1567	10.9637
1516.2047	4.6643
1531.0769	5.3199
1802.6057	438.2057
2999.8011	42.4387
3032.8274	28.6247
3064.4671	15.8406
3115.2124	18.9945
3791.0817	106.2625
3836.2647	48.5341

C,-0.0616386699,0.0808701097,0.0159706388
 O,0.1194905969,-0.3343920561,1.3232152594
 H,0.9175035384,0.0496366444,1.7218670786
 C,-1.5124855311,-0.085359349,-0.3832309376
 O,-1.4879572709,-0.3527088364,-1.8167403179
 C,-2.5702100641,0.0166498244,-2.4555469781
 O,-2.5363194246,-0.2659998931,-3.7268316128
 H,-3.3461691539,0.0215843913,-4.1815792552
 O,-3.5117026515,0.5783134543,-1.8846194681
 H,-1.9723092491,-0.9312762037,0.1249756674
 H,-2.1030785381,0.8185141232,-0.1909961699
 H,0.3530250191,1.0788883767,-0.1689606827
 H,0.5144246786,-0.5965898601,-0.6672750443

E[B3LYP/cc-pVTZ] = -418.63892 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.096618 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.01174 Ha

18b⁺

Frequency and Intensity

56.7516	1.3885
93.9418	3.5905
120.2958	18.8275
199.893	21.1255
307.21	41.1442
339.0999	63.3164
385.5181	0.8135
528.7813	132.3405
547.1556	43.4773
617.3765	54.9437
728.2074	93.2602
781.6366	26.1017
942.8583	82.1031
981.9964	507.2253
1006.2516	111.094
1097.1561	46.6472

1101.3784	60.57
1160.3191	144.9533
1191.1134	182.1091
1222.4675	13.8034
1249.7742	27.9369
1291.0887	745.4329
1339.5513	51.2096
1422.641	153.8845
1425.8725	3.9803
1484.0133	23.3896
1550.6985	1671.7467
2731.0742	286.4592
2977.4129	3.4764
3001.5208	22.561
3113.2167	1.7168
3702.4312	1693.8458
3711.7307	103.5215

C,-0.0664267656,0.3392242048,-0.0831251629
 O,-0.9468944923,-0.4399692272,0.6997153466
 H,-0.4431084442,-0.8040475204,1.4417880627
 C,1.2852607041,-0.3055638245,-0.3553344797
 O,2.3106942705,-0.001017282,0.6342812136
 C,2.2047225721,-0.5515674646,1.8327794927
 O,3.2999322295,-0.2521076161,2.5453585401
 H,3.1824400396,-0.6469969902,3.4192314248
 O,1.2840713628,-1.2189843774,2.2508466414
 H,1.1858068317,-1.387529237,-0.4384985231
 H,1.7162882928,0.092540841,-1.270457681
 H,-0.5617257595,0.4868409231,-1.0447116375
 H,0.0978082537,1.332583228,0.3542764173

18c

E[B3LYP/cc-pVTZ] = -419.01454 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.101139 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42552 Ha

Frequency and Intensity

63.5601	2.1028
114.4674	3.6088
173.3234	3.3
251.3718	10.2395
344.6763	5.6124
462.4225	6.4194
539.547	34.287
543.3745	57.5745
557.6757	138.1641

670.4657	3.1157
803.6318	29.1668
807.0015	11.681
932.7939	27.0814
954.9604	13.5546
1084.5899	14.7488
1095.7704	34.3184
1112.693	65.1362
1209.8017	494.6331
1246.7527	16.1138
1306.333	31.5925
1373.4564	44.6913
1389.1505	65.8453
1432.1095	156.944
1455.4304	58.901
1485.9237	36.1202
1496.1526	4.6631
1770.9527	401.4381
2978.6062	47.7388
3055.6962	11.7023
3070.1602	32.9075
3127.2217	13.0026
3701.3035	226.4714
3783.6694	105.2552

Anharmonic Frequency and Intensity

38.869	2.56221634
127.203	2.01417808
161.305	1.52367418
249.891	8.00907845
340.391	4.99487461
414.969	27.75313035
460.347	7.66141339
513.993	141.829828
607.439	34.97693785
660.401	1.9237081
791.323	2.94472132
793.011	69.13256653
907.86	12.96740542
934.044	24.31217063
1058.793	33.89929923
1062.802	25.90428958
1085.448	34.97326302
1170.094	405.0360022
1220.069	9.49374437

1277.235	33.58811945
1312.499	88.98585736
1355.014	0.33170023
1403.785	102.3476237
1417.98	25.95105265
1438.872	50.1414606
1460.439	11.51315354
1738.288	301.6064121
2836.938	20.71517583
2911.568	13.06562589
2969.157	16.31391183
2988.912	16.73759365
3512.128	201.9094159
3607.256	94.72739694

C,-0.0681590024,-0.1970337395,-0.1828673659
 O,-0.508825452,0.0068755248,1.1517999128
 H,-0.5703646622,0.9502819645,1.3831495145
 C,1.4391875366,0.0513763793,-0.3065610667
 O,2.1903979824,-0.8581743536,0.5222572233
 C,2.1470301927,-0.7146707257,1.8222752701
 O,3.0600376456,-1.4127249042,2.4301810155
 H,2.9696082736,-1.362468166,3.3970254905
 O,1.329590412,0.0112714653,2.4152239259
 H,1.7567283097,-0.174637281,-1.3205810481
 H,1.7004171226,1.0754282512,-0.0423590711
 H,-0.3154415385,-1.2268129692,-0.426540337
 H,-0.5813377248,0.4946942114,-0.8568538085

18c⁺

E[B3LYP/cc-pVTZ] = -418.65893 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.100065 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05061 Ha

Frequency and Intensity

102.4668	3.0956
144.1457	6.7594
231.3278	5.0706
292.2362	5.4713
342.5256	3.433
468.3978	1.8845
509.2891	41.0471
550.0293	92.4115
572.3507	48.295
652.5263	9.9262
782.4093	21.4506
840.2072	2.6763

910.2421	21.0161
929.4703	11.4772
954.725	9.8916
1047.7311	40.3608
1089.4612	14.6902
1174.1643	43.9403
1189.2308	173.7044
1289.2318	41.983
1321.9822	47.9705
1341.1008	103.3433
1379.3658	0.4301
1462.9439	29.9035
1483.5071	37.4802
1495.8527	52.5477
1569.8784	785.1408
3034.3281	10.7506
3076.8249	2.9176
3138.9039	5.9152
3156.3429	2.4956
3683.034	287.8703
3707.0289	325.7141

C,-0.007767967,-0.0035606987,0.0053130498
 O,0.0027971277,-0.0081958265,1.4164103502
 H,0.9257918402,0.0049860818,1.7087122966
 C,0.9643071268,-0.9799506169,-0.6426274303
 O,2.2860713783,-0.4259099058,-0.9146992225
 C,3.0938263367,-0.1726702377,0.1243488052
 O,4.3037887616,0.2165089521,-0.2969256187
 H,4.3259200103,0.2065415267,-1.2627256464
 O,2.813201821,-0.2640440129,1.2898481826
 H,1.0790283468,-1.8724893567,-0.028297808
 H,0.6159721028,-1.2607080666,-1.6335710313
 H,-1.0167234861,-0.2944248855,-0.2934985971
 H,0.175110096,0.999685996,-0.4019007224

18d

E[B3LYP/cc-pVTZ] = -419.01263 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.100946 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42347 Ha

Frequency and Intensity

63.5818	0.6258
115.4298	2.7074
174.0078	7.0916
247.8428	16.7907
344.789	2.2324

460.7752	1.8908
530.1701	85.9515
540.6291	5.8492
550.355	113.2571
676.0721	0.3851
794.95	27.7925
804.1121	12.3082
932.0717	67.8903
951.6084	14.4004
1076.8964	52.611
1089.3325	21.3441
1113.3827	55.3408
1207.0123	78.2409
1246.0778	18.7146
1304.3829	49.5258
1332.9311	576.3723
1385.9917	48.3168
1409.4983	63.5956
1455.2718	56.182
1482.4333	20.7928
1495.2114	3.625
1823.9691	362.4154
2974.8287	49.7021
3055.106	12.166
3070.4165	31.671
3126.0936	12.9498
3698.185	216.8476
3776.6071	86.383

18d⁺

C,-0.0970638106,-0.0213547225,0.0834255767
O,0.1136104125,-0.1900426346,1.3942234462
H,0.9936311198,0.1886077465,1.6652518524
C,1.0434420235,-1.0112525151,-0.73859989
O,2.2396076929,-0.3668263508,-0.9332752461
C,3.0792700607,-0.0757825177,0.1353461824
O,4.3073254712,0.1111854841,-0.2424446299
H,4.4429246225,-0.0284500014,-1.1934857121
O,2.6753552097,0.0380957714,1.2612540993
H,1.1129835402,-1.9124170773,-0.1345927363
H,0.5668884901,-1.1361978081,-1.7078181397
H,-1.0669326344,-0.4165710752,-0.2057729485
H,0.150281297,0.9667746499,-0.3131252468

E[B3LYP/cc-pVTZ] = -418.6533 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.097662 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.04947 Ha

Frequency and Intensity

84.6969	4.3029
116.1131	0.8771
141.8076	1.5005
258.5542	10.7275
302.7457	9.7826
388.2573	61.4841
407.9928	0.1808
529.2691	105.2868
537.0621	96.976
553.2703	4.0644
672.7806	16.7036
778.7884	23.9984
845.8527	38.6055
912.4366	15.6666
965.8978	127.7008
1033.4743	41.3062
1166.7098	66.4494
1188.6513	136.7863
1204.1016	22.3185
1244.9551	37.4999
1273.8511	75.7467
1294.685	69.6509
1333.5651	487.0206
1420.226	63.1394
1476.8085	35.5797
1500.8067	1.0246
1819.7225	346.5156
3025.7865	9.3195
3074.4861	12.0727
3156.3001	2.2607
3174.339	9.1203
3262.031	240.265
3722.4656	233.0295

18e

C,0.0338377188,-0.0725951405,0.017414645
O,-0.0957610366,0.7999348663,1.1285949898
H,0.5060104376,0.503804293,1.8193034752
C,1.4180347336,-0.0512288677,-0.5884104385
O,2.3200453004,-0.5798514495,0.41422951
C,3.6055238188,-0.638858202,0.0691666342
O,4.301813494,-1.1247281442,1.1128333635
H,5.2262838909,-1.1601913143,0.8353208731
O,4.0784566737,-0.3192371043,-0.9905848663
H,1.4705008388,-0.6737169197,-1.4819446378
H,1.7267448904,0.9624950844,-0.8396385235

H,-0.2354093402,-1.0989926569,0.2886938443
H,-0.677573603,0.2744686977,-0.7321350585

E[B3LYP/cc-pVTZ] = -419.01498 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.10066 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42554 Ha

Frequency and Intensity

43.7875	1.0794
93.6203	1.8866
166.7388	2.3826
216.4572	7.4923
302.2381	23.4436
358.8402	113.313
482.2617	39.7617
535.6145	11.4292
548.9012	97.3898
667.3171	3.961
799.0923	32.2558
847.8042	3.8323
895.9431	23.5157
1004.0468	9.4516
1063.2201	110.7056
1102.8983	30.2853
1114.0242	3.3353
1195.5039	558.5987
1229.8723	36.5615
1272.006	14.2203
1370.1055	129.8861
1382.254	28.3556
1419.236	75.2184
1430.1946	77.085
1494.2698	3.4292
1498.8067	10.7494
1802.5462	440.4508
3005.2729	40.3355
3055.1629	9.5025
3085.0224	23.8186
3109.3388	17.2104
3786.6847	106.7002
3805.7439	36.7216

Anharmonic Frequency and Intensity

12.53	0.34039071
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78.207	1.81217929
157.839	3.4684581
188.824	66.25652468
210.83	19.64340905
408.307	21.07724681
425.721	95.33123495
476.255	42.12343077
540.137	15.44006866
658.498	2.78016289
784.668	20.22237491
832.824	4.1689617
878.14	17.14431
978.243	8.69166262
1033.498	82.56439104
1072.718	14.96594032
1091.568	1.87060908
1145.661	459.1695847
1200.717	21.90223791
1246.838	8.5562846
1333.719	61.4024783
1339.808	12.73930781
1389.671	26.89093451
1405.964	114.4640241
1449.007	2.58887402
1466.62	10.97565058
1768.437	381.571903
2853.057	21.97654286
2885.722	3.05643748
2956.964	18.09692251
2975.315	14.58963081
3588.554	86.7350644
3630.632	30.60762037

18e⁺

C,0.1508196114,-0.2699133987,0.0877464848
O,-0.2595871462,0.4557288999,1.1138866751
H,0.1225687302,0.1845122755,1.9647842471
C,1.6746268001,0.5224562581,-0.6624082779
O,2.708552354,0.4048645255,0.1705764639
C,3.4635635471,-0.7985359375,0.0858826814
O,4.5309542193,-0.6013263458,0.8134144459
H,5.0970702079,-1.3905770546,0.7955592158
O,3.0864934655,-1.7379286302,-0.535506617
H,1.7122563116,-0.0860389273,-1.5636614637
H,1.3291768286,1.5483036454,-0.7239412246
H,0.5569837822,-1.2602762773,0.2843916845
H,-0.4949708943,-0.1499658908,-0.7778805047

E[B3LYP/cc-pVTZ] = -418.65495 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.098301 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.05268 Ha

Frequency and Intensity

52.9848	5.2318
79.4984	1.9634
130.9227	6.6836
193.6464	4.3581
319.0976	14.3298
373.5584	8.9914
414.721	34.1211
481.3192	56.9914
542.7814	58.4177
586.5026	105.3095
638.4748	6.2624
771.4441	43.8469
788.7656	235.9443
855.6527	52.2136
913.5388	22.026
1116.5012	54.0975
1132.6744	71.8942
1173.1878	425.3151
1217.1484	21.8185
1252.648	68.3075
1274.2178	170.3725
1287.2313	86.0409
1360.0492	97.5117
1381.7215	24.491
1471.4133	16.3738
1511.7657	1.5249
1881.2054	354.5599
3061.9721	17.5159
3075.6549	7.9595
3181.0488	5.5031
3204.7604	13.0702
3702.8562	217.3882
3720.3011	261.4083

18f

C,-0.0156387263,-0.0064300262,-0.0014466382
O,-0.0592507005,-0.0058245677,1.417496163
H,0.842335982,-0.0093375239,1.7533287982
C,0.6419025617,1.2258687235,-0.576732872
O,2.0416502118,1.1838417416,-0.1991533844
C,2.7963667699,2.2179968719,-0.629888612
O,4.0683077032,2.0740393198,-0.2214770838

H,4.1551250777,1.2559868048,0.2839489483
O,2.413760337,3.1410997888,-1.2852575926
H,0.5695075572,1.2411027048,-1.6643189273
H,0.1991047928,2.1365079467,-0.17654001
H,0.4826221462,-0.9053175236,-0.3804422799
H,-1.0519231815,-0.0315836282,-0.3386152903

E[B3LYP/cc-pVTZ] = -419.0118 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.100329 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.42219 Ha

Frequency and Intensity

39.3025	8.0127
95.5518	3.7559
164.9278	3.9774
215.3963	8.7818
292.4931	56.686
332.4837	71.7629
480.6505	12.0959
505.0596	108.4302
529.7575	2.6012
677.5157	2.8231
789.2127	20.1093
844.5804	25.3391
893.948	22.2224
998.6028	28.6937
1051.915	130.4246
1097.4693	57.5143
1112.0196	3.6633
1188.6353	148.1349
1225.6538	10.2881
1272.1337	13.9216
1318.3316	616.8222
1378.4896	8.6864
1405.951	63.7049
1425.8387	25.7904
1494.0128	4.2453
1498.5272	11.4133
1854.4453	403.6506
3003.6177	41.3757
3057.6654	8.2524
3086.1136	22.2191
3112.3107	15.0411
3782.5627	66.6049
3814.0566	32.1774

C,-0.0331679394,0.0488420552,-0.0131612799
O,0.0513586452,0.0294068509,1.3852012579
H,0.6848007673,-0.6317947021,1.705415635
C,0.6268376954,1.3610124761,-0.4770512979
O,2.0185055231,1.3292198715,0.0326015767
C,2.8403436802,2.0337706505,-0.7016876101
O,4.0765475436,2.1381071111,-0.3372528013
H,4.2628213407,1.689226333,0.5046164763
O,2.4315766779,2.5890569459,-1.7400561124
H,0.6353908754,1.4020402343,-1.5693449622
H,0.141555515,2.2293957958,-0.041387865
H,0.4356922442,-0.8183239434,-0.4737693785
H,-1.0883920374,0.1179909536,-0.2932224195

E[B3LYP/cc-pVTZ] = -418.63557 Ha
ZPVE[B3LYP/aug-cc-pVTZ]= 0.097693 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.01188 Ha

Frequency and Intensity

18f⁺

49.7794	4.0952
93.4756	8.948
152.276	2.6292
197.9748	18.8691
253.293	25.5092
297.1794	5.3303
461.6431	128.6232
465.2492	51.1017
499.7979	163.6094
619.7799	1.8738
778.56	31.8332
839.8522	44.8066
878.3459	368.2333
929.2098	179.4749
976.4645	160.4375
1037.3322	178.0044
1079.2107	13.9436
1155.5836	408.2366
1183.0379	39.3455
1252.4354	61.7581
1292.2883	111.7297
1319.4181	39.6767
1356.283	40.131
1420.1382	57.5449
1475.1625	115.3743
1485.6586	104.7497

1586.1739	1699.2474
3014.2817	33.8692
3032.4883	11.7702
3117.9294	29.5831
3153.634	2.4343
3703.6514	253.9953
3724.6724	702.3125

C,0.0003495777,0.027582951,-0.087977302
 C,-0.0013449174,-0.0339754809,1.4061751621
 C,1.06161619,0.0449631465,2.223530919
 O,2.3481866598,0.1206106254,1.8532336779
 H,2.3757714292,-0.0134867526,0.8891724645
 O,0.9503530711,0.0653720112,3.5663937271
 H,0.0054059295,0.1061168951,3.7685213369
 O,-1.2721208929,-0.0121758164,2.0050743591
 H,-1.6915881038,-0.8757435967,1.9099044375
 O,1.3017765897,-0.330082163,-0.5882041779
 H,1.3946500012,-0.0065583746,-1.4882014216
 H,-0.7507344282,-0.6692162604,-0.4808806265
 H,-0.2697228109,1.0298560779,-0.4455925656

E[B3LYP/cc-pVTZ] = -418.96649 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.099403 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37752 Ha

19a

Frequency and Intensity

65.6064	1.3869
178.0032	19.4681
240.5933	4.338
265.4142	67.766
285.459	25.7737
311.8092	4.7016
347.988	87.5903
431.4706	14.2479
516.6648	6.9682
539.1165	56.2511
624.9588	1.9169
662.3486	80.9262
679.8138	63.8238
764.7966	27.5902
1011.6786	19.36
1033.3005	71.0105
1086.4353	114.3937
1185.6293	20.5017
1207.6679	82.452

1227.9289	169.5157
1250.1123	53.9123
1282.2894	75.866
1382.9111	129.4311
1426.4469	19.4407
1478.2645	59.8894
1519.1856	3.4866
1766.2357	305.5412
2959.0539	91.398
2976.5355	51.1021
3604.8442	248.0832
3738.6297	24.9478
3750.1951	70.7246
3831.6749	40.8806

C,-0.0050458179,-0.0779277313,-0.0678728024
C,-0.0175877108,-0.0519250134,1.4297836668
C,1.1316739761,-0.0064121022,2.2731219219
O,2.3380971056,0.0366656832,1.8264777827
H,2.3293960069,0.058272664,0.8348213557
O,1.0316053021,-0.0067499562,3.5678890739
H,0.109842068,-0.0443745714,3.8724624284
O,-1.1669631814,-0.0934260588,2.0941561607
H,-1.9551407225,-0.1078983909,1.5310145456
O,1.3238103686,0.118279809,-0.5193427147
H,1.4074891481,-0.0427853033,-1.4660719893
H,-0.4060685789,-1.0422771799,-0.4060490103
H,-0.6685096691,0.7138214138,-0.4392404286

19a⁺

E[B3LYP/cc-pVTZ] = -418.70214 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.099883 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.10508 Ha

Frequency and Intensity

61.1959	18.6393
137.5635	12.2223
207.0927	102.5446
281.8419	4.0628
331.6384	13.0616
344.0334	3.7171
411.4627	113.5251
438.0703	10.4684
538.807	8.3917
571.7206	88.8065
614.8638	3.613
682.4329	8.1873

772.6643	12.2831
830.4617	112.2261
987.4262	2.3402
1074.1002	11.7672
1105.013	190.3785
1180.8911	39.2609
1217.5742	33.7162
1253.9577	22.5354
1295.2646	276.8626
1366.1488	76.2629
1405.3055	112.6367
1466.6594	158.5586
1491.9465	23.8856
1609.488	140.4878
1638.232	230.9796
2976.488	14.1856
3006.5529	0.8396
3296.8142	586.616
3706.255	173.0243
3738.3216	236.1741
3803.4824	161.9274

19b

C,0.0256825188,0.0110448039,-0.1737710759
C,-0.0326930385,-0.0848022652,1.3154207503
C,0.9986521993,0.028221858,2.154097319
O,2.3074041738,0.2009480207,1.8350458739
H,2.3871964657,0.060103933,0.8741866403
O,0.7879500905,-0.0123215619,3.5017422134
H,1.6215260211,-0.2405168671,3.929577619
O,-1.3291300979,-0.2854227497,1.7636445182
H,-1.3203947625,-0.2921644648,2.7273963864
O,1.3623913405,-0.2673774057,-0.6300773225
H,1.4602524721,0.0523525511,-1.530779732
H,-0.6758810838,-0.7175876431,-0.5909652258
H,-0.2816422107,1.0060813,-0.5181499502

E[B3LYP/cc-pVTZ] = -418.96732 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.098789 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37847 Ha

Frequency and Intensity

61.5472	0.544
170.2034	9.8946
225.7071	103.4816
251.455	25.1984
260.2974	103.659

290.8044	21.9459
321.5185	37.8139
352.794	34.2561
431.7133	0.6695
505.43	21.6154
611.0841	9.9845
621.5463	77.1235
625.9872	29.6881
752.5718	8.3911
1003.9397	49.1659
1036.4418	93.7847
1075.9113	70.5792
1168.2625	148.5155
1210.4713	68.7119
1226.3018	40.4472
1263.7867	87.3023
1282.0986	107.3319
1383.6282	96.9724
1414.9667	118.5594
1470.3249	60.2846
1516.9235	1.6577
1817.812	110.5087
2974.3939	77.7005
3020.4302	31.1626
3593.2059	256.18
3792.0572	93.4651
3796.6935	55.863
3833.1651	40.5755

19b⁺

C,-0.0017841256,-0.076799549,-0.0495725066
C,-0.0044095104,-0.0569638441,1.4512492985
C,1.1642268636,-0.0194189845,2.2615087335
O,2.3671129297,0.0224293278,1.7834453233
H,2.3348351189,0.053512934,0.7891354064
O,1.0145192993,-0.0294951083,3.5519883348
H,1.8700265869,0.0067127299,4.0140391401
O,-1.1463212389,-0.0977019933,2.108910281
H,-1.9269458186,-0.1073179722,1.5346532305
O,1.3197788389,0.1338837044,-0.522810182
H,1.3921456664,-0.0375308167,-1.4685867257
H,-0.3967673344,-1.0433883053,-0.3865203674
H,-0.6751031875,0.7106373863,-0.4100719523

E[B3LYP/cc-pVTZ] = -418.70402 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.099847 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.10627 Ha

Frequency and Intensity

65.9794	15.9497
131.0328	5.2998
210.2062	108.0216
290.4569	21.6572
337.2311	4.5835
351.6595	5.7228
436.3015	8.614
456.0211	117.0132
528.692	3.6766
557.61	112.3061
612.4365	13.608
680.5174	41.3981
757.0692	5.1374
829.3443	67.1333
991.2352	3.6546
1065.3462	28.3236
1100.4246	171.3142
1179.539	244.1043
1215.6165	1.3375
1259.0595	0.202
1314.7423	94.6911
1373.2051	92.4569
1411.0385	68.7113
1461.8603	219.2159
1493.3555	16.0233
1576.7236	204.6511
1681.3214	163.2952
2983.2124	13.0069
3015.0859	0.8818
3232.581	620.1706
3692.2802	320.6784
3732.4273	189.1525
3803.9368	159.0803

19c

C,-0.0163906687,-0.0561049692,-0.0032941012
C,0.0409057619,-0.0079520491,1.4882489846
C,1.1403125077,-0.0964985276,2.23879199
O,2.425784193,-0.1963045861,1.8119127569
H,2.4214460672,-0.0236062569,0.8529233703
O,1.036941505,-0.1071453564,3.5993594154
H,1.890173487,0.1502422553,3.9677900532
O,-1.2232079802,0.1163549474,2.0436653334
H,-1.1375781837,0.0938413956,3.0033955152
O,1.2653955837,0.2987977488,-0.5541756629
H,1.3049686823,0.0106148704,-1.4698455526

H,-0.3057059316,-1.0537938945,-0.3554774994
H,-0.7811429925,0.6507216263,-0.3390354703

E[B3LYP/cc-pVTZ] = -418.96732 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.098791 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37847 Ha

Frequency and Intensity

61.5511	0.5468
170.5025	9.5493
225.7814	102.4799
251.7321	24.2577
260.2037	105.8509
290.8103	22.0608
321.4692	37.9441
352.788	34.2894
431.7174	0.6648
505.5031	21.571
611.0356	9.5066
621.9046	76.5856
626.0435	30.7184
752.5926	8.3717
1003.9887	49.0253
1036.5303	93.7566
1075.9955	70.7151
1168.2159	148.5403
1210.4754	69.1422
1226.366	40.0018
1263.8987	87.4575
1282.0516	107.2236
1383.539	97.0133
1415.0687	118.3545
1470.3059	60.2479
1516.9167	1.6587
1817.7797	110.4189
2974.4911	77.6804
3020.317	31.1636
3592.8831	256.1104
3791.7404	93.1841
3796.8167	55.8501
3833.198	40.654

19c⁺

C,-0.019734196,-0.0371338722,-0.0177291841
C,0.0096795186,-0.0211473701,1.4787273128
C,1.1915389252,-0.0010741596,2.2612856716
O,2.3912758593,0.0108341269,1.781885184

H,2.346070436,0.0138483748,0.7836175816
O,1.0373676635,0.0046887737,3.5620621576
H,1.8864505819,0.0215302669,4.0361856635
O,-1.1750251047,-0.0326640399,2.0472587767
H,-1.135386601,-0.0281003154,3.018410209
O,1.3149829612,0.0383650663,-0.5022165053
H,1.3541692013,-0.0447559852,-1.4612237632
H,-0.5181655191,-0.9566454548,-0.3436599903
H,-0.6213216948,0.8114217926,-0.3603439814

E[B3LYP/cc-pVTZ] = -418.70826 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.099773 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.11059 Ha

Frequency and Intensity

34.7255	41.4985
144.0555	7.4803
177.4702	100.9906
283.8428	11.9533
337.7056	18.6025
355.179	6.1311
437.0811	0.6735
516.9363	138.1818
530.4896	15.1343
561.5152	121.5563
616.686	21.1436
664.8052	8.6085
757.7282	4.4931
842.0471	65.586
993.5531	2.3434
1054.2289	82.6996
1111.8259	49.8345
1168.4269	149.5467
1213.188	148.8882
1243.6807	2.8095
1312.4779	3.0392
1397.6526	177.0964
1413.4644	164.3883
1467.2267	157.1437
1489.0664	20.2317
1577.0705	193.5387
1674.3443	112.4134
3004.8694	8.1525
3039.7588	0.0409
3172.865	663.3323

	3691.649	135.3462
	3698.2372	355.6704
	3811.3565	164.653
	C,0.335629612,-0.3111331233,-0.0469964811	
	C,0.1769705956,-0.0364631152,1.3970121345	
	C,1.0645633956,-0.2919909759,2.3615163442	
	O,2.246819058,-0.9142096556,2.1543344136	
	H,2.7672055663,-0.8424219201,2.9626888165	
	O,0.8478581298,0.0012076818,3.6677070419	
	H,-0.0056694204,0.4558223868,3.719974265	
	O,-1.0411731361,0.5113995927,1.811657169	
	H,-1.2501552995,1.2316376099,1.2044098535	
	O,0.1141396604,0.9332157818,-0.7490981377	
	H,-0.0634795219,0.7408286891,-1.674326926	
	H,1.3346183574,-0.7012543078,-0.2467190046	
	H,-0.4061296838,-1.0453066949,-0.3834847424	
	E[B3LYP/cc-pVTZ] = -418.96933 Ha	
	ZPVE[B3LYP/aug-cc-pVTZ] = 0.098679 Ha	
	E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37999 Ha	
	Frequency and Intensity	
19d	86.9865	11.6456
	125.4319	51.7463
	176.9289	26.6517
	229.8036	18.8517
	255.9697	46.075
	267.5305	82.6722
	358.4206	5.2588
	413.2726	88.7258
	433.3636	4.9453
	522.5518	110.4299
	538.5818	12.7321
	595.1433	20.0033
	659.158	13.965
	780.6497	41.8742
	972.9184	178.1615
	983.4921	36.8413
	1071.4048	107.2412
	1189.2703	111.5441
	1205.9508	153.5314
	1233.1879	30.0541
	1260.3911	29.8081
	1270.5095	90.4732
	1354.1765	186.7029

1399.3949	80.8007
1443.2648	6.5253
1503.3781	5.8133
1820.264	234.7349
2979.6591	61.9201
3065.8418	19.0369
3731.2901	81.1316
3766.6578	78.7985
3801.9129	116.1601
3818.2782	23.2235

C,0.4505407432,-0.1623755784,-0.0535276457
 C,0.2666300548,0.1700769456,1.3959704299
 C,1.0430570791,-0.349246223,2.4489289916
 O,2.0027085073,-1.184433403,2.1626148412
 H,2.4797376081,-1.4851499543,2.95513771
 O,0.8586067797,-0.0434871238,3.7044171255
 H,0.1269540963,0.5842016164,3.8355628635
 O,-0.6825130849,1.0054314441,1.7468670131
 H,-1.1533322577,1.2995707986,0.9353694273
 O,-0.535677708,0.5949121425,-0.715803373
 H,-0.5296308785,0.4415587878,-1.6664517033
 H,1.4675550003,0.1019054478,-0.3671909067
 H,0.3265613736,-1.2416329511,-0.2032200272

E[B3LYP/cc-pVTZ] = -418.70744 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.099499 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.10917 Ha

19d⁺

Frequency and Intensity

26.0617	73.6313
133.3039	50.8257
162.8539	35.94
180.2873	7.8334
332.9702	5.2096
362.8593	0.1049
396.5215	10.2124
504.1711	224.5244
534.544	1.4375
559.8354	35.9887
626.9353	39.6767
657.2783	0.0268
716.5475	81.5618
814.1186	6.5791
992.3689	0.2687
1055.8555	152.2811

1112.2981	36.5713
1154.4484	165.1577
1203.3216	182.483
1209.6542	5.6226
1227.8906	0.342
1379.019	440.8586
1431.0868	44.2416
1436.836	67.397
1490.1832	38.9935
1554.6976	114.1054
1697.3999	112.654
2991.3646	19.7378
3019.2102	0.1327
3507.2267	387.28
3686.5148	206.757
3697.0521	298.4123
3820.3287	173.2847

C,0.2491520029,-0.3184728082,0.0113085129
 C,0.1561239891,-0.0545990846,1.4660641293
 C,1.0707679811,-0.3439983759,2.3969451352
 O,2.2383654875,-0.9759899423,2.1384202176
 H,2.7001433032,-1.1035819401,2.9747787733
 O,0.9095418848,-0.061336128,3.7133912647
 H,0.0555368899,0.3850587026,3.8091910961
 O,-1.0211524787,0.5393842245,1.934426059
 H,-1.2660539988,1.2341399813,1.311516441
 O,0.1172519891,0.8996151397,-0.7543742474
 H,0.8984740469,1.4389978314,-0.5915673807
 H,1.1794590573,-0.8362533565,-0.2246816088
 H,-0.5859129906,-0.9356621362,-0.3253742497

19e

E[B3LYP/cc-pVTZ] = -418.97052 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.098826 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.38113 Ha

Frequency and Intensity

76.7675	39.7586
110.3734	36.9284
164.6118	37.0605
219.9849	1.7893
266.1641	26.5228
333.4741	55.2841
364.8813	32.2266
421.1968	132.0518
439.5102	13.9183

511.0316	96.2497
531.9473	6.4038
601.2207	4.9722
661.8079	9.1027
787.5336	35.9893
945.7213	35.29
969.3185	195.0361
1054.3484	164.5539
1184.4023	18.7295
1205.3444	150.6259
1226.516	16.9364
1261.4125	127.43
1330.7986	89.9867
1367.3871	107.1263
1393.5639	110.1809
1422.6285	19.456
1492.7857	5.4995
1813.7422	224.823
3037.1628	32.1605
3082.1151	17.2421
3732.9099	82.9908
3768.7325	78.8424
3793.742	22.0926
3806.6635	125.5892

19e⁺

C,0.5706911502,-0.1315592893,0.0747817755
C,0.3038122069,0.1795951925,1.5160007676
C,1.0110186264,-0.3644929902,2.604669719
O,1.976943373,-1.206167555,2.3621700524
H,2.4026061399,-1.5251043331,3.1765514325
O,0.7564694026,-0.0752892043,3.851767763
H,0.0242316297,0.5577303916,3.9495543151
O,-0.655861929,1.0199225277,1.8236269005
H,-1.0748387635,1.3314179273,0.9906357973
O,-0.3738078107,0.6384363342,-0.632185831
H,-0.2979567904,0.5167651998,-1.5844764193
H,1.6049402059,0.1341237159,-0.1748093105
H,0.4534497228,-1.2080758094,-0.0982428194

E[B3LYP/cc-pVTZ] = -418.70744 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.099509 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.10917 Ha

Frequency and Intensity

28.8361	71.7558
133.7946	49.0827

164.1703	39.9086
180.2512	7.763
332.7763	5.1888
362.7136	0.0922
396.4837	10.2135
504.4369	225.3969
534.5759	1.4315
559.631	35.1603
626.9553	39.6974
657.1682	0.0328
715.4736	81.3705
814.2356	6.5814
992.3116	0.2619
1055.7829	151.9768
1112.2627	36.5568
1154.5174	165.1531
1203.3168	182.8671
1209.7737	5.8435
1227.7157	0.0257
1379.0009	440.6206
1431.1751	43.8207
1436.9181	67.7152
1490.2495	39.1279
1554.9764	114.2937
1697.377	112.7419
2991.388	19.7674
3019.1395	0.1319
3509.0054	387.1755
3686.9094	208.1451
3696.7493	296.9417
3819.4739	173.3671

19f

C,0.0081909047,0.2197130646,-0.0508931132
C,0.0237668658,0.1917042674,1.4273316319
C,1.0761327946,-0.0563938318,2.2110488186
O,2.3299871214,-0.2624194626,1.7488989551
H,2.8695303406,-0.5798801575,2.4820890883
O,1.0066331801,-0.0750627612,3.5652749527
H,0.0784722612,0.0624215493,3.8049985802
O,-1.1735145677,0.4955311251,2.0831459661
H,-1.8728576498,-0.0029615237,1.643159615
O,-1.0177767208,-0.6997533495,-0.4882970701
H,-1.2437102507,-0.5023032074,-1.4018309871
H,-0.2371047828,1.2246995966,-0.4146794855
H,0.9852288025,-0.0684411932,-0.4413968355

E[B3LYP/cc-pVTZ] = -418.96933 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.098686 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.38 Ha

Frequency and Intensity

87.1485	10.6742
126.7299	50.7468
177.9479	27.3087
230.6278	19.7397
255.9566	46.5165
267.3793	82.9523
358.4182	5.2027
413.4712	88.3841
433.0157	5.2166
522.1392	111.1964
538.9155	12.3292
595.0959	20.0129
658.8592	14.0906
780.6895	41.6667
973.5759	177.4051
983.9021	38.1304
1071.3636	106.5923
1189.2912	111.66
1205.9376	154.6171
1233.4907	30.1109
1260.3995	28.7421
1270.5125	91.2977
1353.9795	186.7532
1399.2202	80.2686
1443.2843	6.3506
1503.4199	5.8638
1820.3638	233.8738
2979.3755	61.94
3065.5126	19.0743
3731.7704	80.9912
3766.736	79.0718
3801.2209	115.1469
3818.5154	23.252

19f⁺

C,0.0275831147,0.0094600847,-0.0481123885
C,-0.0244835609,-0.0136089525,1.4492053052
C,1.098701,0.0071139231,2.2973610026
O,2.2854478188,0.0495401855,1.7587498369
H,2.9937846222,0.0607621862,2.4252789455
O,1.0237005805,-0.0139658924,3.6002649694
H,0.1068637611,-0.0451652562,3.9241333761
O,-1.190384152,-0.056286707,2.0497112991

H,-1.89339333,-0.0662437591,1.3625440508
O,-1.3231642018,-0.0148145693,-0.4475931756
H,-1.4155859304,-0.0233980983,-1.4061232765
H,0.5520681317,0.9114690576,-0.3855394095
H,0.5918404453,-0.8580080859,-0.4110304189

E[B3LYP/cc-pVTZ] = -418.70744 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.099507 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.10917 Ha

Frequency and Intensity

28.1419	72.208
133.6618	49.328
163.8672	39.0282
180.2368	7.8097
332.7953	5.2037
362.7203	0.0954
396.496	10.2127
504.4618	225.3314
534.5764	1.4315
559.6698	35.1998
626.98	39.6891
657.193	0.0299
715.8135	81.448
814.2412	6.5815
992.3096	0.268
1055.8519	151.996
1112.3288	36.5624
1154.5514	165.2634
1203.3375	182.9574
1209.7344	5.4646
1227.8478	0.2508
1379.1032	440.5279
1431.1468	43.9374
1436.9371	67.7091
1490.2585	39.1307
1554.993	114.2595
1697.4172	112.7101
2991.3262	19.7522
3019.0705	0.1335
3508.4538	387.2572
3686.8746	208.078
3696.7393	297.0078
3819.5928	173.3925

19g C,-0.0242143923,0.2715049644,-0.0620529429

C,0.0115541477,0.1873596419,1.4121302636
C,1.0546681598,-0.1328535307,2.1949490776
O,2.3099101562,-0.447042627,1.8102040115
H,2.3407212163,-0.5576498445,0.8551382055
O,0.97904725,-0.1434377095,3.5361784044
H,0.0729138795,0.1112319229,3.763785235
O,-1.1726511077,0.5262484221,2.0835421439
H,-1.8776540909,-0.0383724384,1.7452055296
O,-0.9498690171,-0.7185176119,-0.557539146
H,-1.224773914,-0.4734005198,-1.4465384103
H,-0.3624398463,1.2668255527,-0.371746146
H,0.9687939532,0.1107228909,-0.4972793789

E[B3LYP/cc-pVTZ] = -418.96516 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.098895 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37572 Ha

Frequency and Intensity

73.7847	5.3589
121.443	3.9594
228.3557	18.3132
245.7063	2.0389
281.3837	100.6185
308.4578	36.6917
368.3674	17.8797
399.6078	89.035
450.3711	5.8086
533.0807	6.4537
562.1598	130.7984
610.8298	23.3364
679.0822	8.7992
782.2065	44.9075
963.9926	72.3969
979.4288	102.4733
1080.7941	24.8754
1173.0843	381.9166
1201.7442	60.5008
1234.0265	53.2004
1257.0022	32.2044
1271.3138	5.9681
1352.1109	202.0915
1421.6084	15.6538
1442.3387	30.7188
1505.7365	1.6595
1764.3065	333.2061

2977.3688	57.7235
3005.6831	54.3921
3732.6281	87.9282
3767.6487	55.9257
3806.4401	19.9521
3827.826	49.0297
C,-0.010189507,0.0079617206,-0.078897134	
C,-0.0184706569,-0.0125802057,1.4244403518	
C,1.1171513334,0.0110928391,2.2663480185	
O,2.3538133958,0.0552720959,1.8528331157	
H,2.4624633895,0.0731664286,0.8920422412	
O,1.0201877383,-0.0103089899,3.5608083834	
H,0.0967114836,-0.0431971494,3.8633383421	
O,-1.1745160641,-0.0569847067,2.047653733	
H,-1.8951560606,-0.0687934517,1.3802198582	
O,-1.36820302,-0.0178196107,-0.4429750773	
H,-1.4879663025,-0.0249764025,-1.3989808913	
H,0.4947658257,0.9147479693,-0.4386622371	
H,0.5354148394,-0.8649614237,-0.4621918571	
E[B3LYP/cc-pVTZ] = -418.69722 Ha	
ZPVE[B3LYP/aug-cc-pVTZ] = 0.099384 Ha	
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.09943 Ha	

19g⁺

Frequency and Intensity

55.2046	76.8813
118.037	5.7839
176.7243	63.7432
187.2825	12.0686
342.1905	4.1943
356.1221	23.2519
403.6382	10.5785
412.7134	36.6911
530.8847	14.4344
588.7888	184.0173
648.6346	3.1248
664.5268	31.3519
708.6857	57.6779
813.794	7.719
995.2898	0.0164
1063.8591	95.8988
1115.5868	37.1508
1156.4219	146.5571
1175.3069	206.2415
1217.7829	151.811

1246.9574	0.3519
1378.7861	283.8988
1420.2017	188.1066
1435.1571	35.4161
1496.7283	19.6577
1574.0334	78.5441
1653.0613	151.1255
2969.2897	20.0775
2996.3976	1.2182
3513.3562	366.5588
3696.0937	200.7747
3769.3298	144.7806
3812.3127	180.0014

C,-0.0151522331,0.2748922271,-0.0442068879
 C,-0.0028727831,0.2414924984,1.4388095838
 C,1.0680928024,-0.0194572126,2.1995992476
 O,2.3232565788,-0.3325155459,1.7561661148
 H,2.2885110136,-0.6433342252,0.8463495894
 O,1.0343922932,0.0590826149,3.5442896058
 H,1.8705838017,-0.2808538444,3.8834441598
 O,-1.1972721983,0.5760075373,2.0587290474
 H,-1.887650389,0.0164233954,1.6846851118
 O,-0.9038416577,-0.7574100578,-0.5185825326
 H,-1.1961459616,-0.5349112307,-1.4076966587
 H,-0.3822429766,1.2508934775,-0.3805289874
 H,0.9851084261,0.1363807613,-0.4686344588

19h
 E[B3LYP/cc-pVTZ] = -418.95936 Ha
 ZPVE[B3LYP/aug-cc-pVTZ] = 0.098015 Ha
 E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.36971 Ha

Frequency and Intensity

63.0183	5.5846
97.1185	22.4885
197.0581	63.353
249.8645	16.2503
267.0201	25.8126
281.6838	58.8297
314.0712	48.0394
343.1755	179.7573
389.5296	14.7233
454.6638	16.4726
521.707	6.0181
594.615	28.6398
657.0003	7.9289

779.301	31.325
971.0463	127.6462
986.0028	73.8961
1067.7996	60.7487
1173.1873	220.4452
1198.5281	129.4657
1228.3453	142.1718
1260.4317	61.1396
1268.1522	15.1309
1349.6145	28.1515
1375.1892	161.6933
1428.469	39.0821
1508.8001	1.557
1800.7109	201.8375
2981.9941	55.5152
3010.8747	54.0599
3773.5991	59.8788
3797.9584	107.3607
3810.3036	26.1549
3822.6086	47.6143

19h⁺

C,-0.0055251291,0.0081963308,-0.059216923
C,-0.0169080843,-0.0163163477,1.4473039692
C,1.142630382,0.0070782165,2.251314537
O,2.3731323991,0.0539080696,1.7916818921
H,2.4562767252,0.0741108652,0.8278793856
O,1.0091752608,-0.0191522258,3.5431698431
H,1.8656909531,0.0003569406,4.0038475683
O,-1.1641827772,-0.0626000398,2.0656542857
H,-1.8814528382,-0.0730741462,1.39500337
O,-1.3602516943,-0.0164825475,-0.4301477203
H,-1.4749079021,-0.0214742194,-1.3866120955
H,0.5001727518,0.9164447432,-0.4147431463
H,0.5409166695,-0.8643052441,-0.4427120309

E[B3LYP/cc-pVTZ] = -418.69747 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.099184 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.09899 Ha

Frequency and Intensity

69.6799	68.2281
107.625	0.003
178.3623	80.5601
192.0594	1.6107
342.0298	14.5813
358.1689	18.9687

394.9457	154.335
408.174	6.5968
522.3888	9.8979
536.3821	76.8795
626.3026	21.5101
653.0619	0.0344
733.0716	88.3374
808.9595	12.5136
998.7314	0.0883
1054.3571	123.1894
1112.9953	35.9551
1154.7416	154.2432
1184.9505	216.8777
1213.6513	166.8584
1254.4696	0.2232
1388.2595	91.8521
1422.5483	260.3585
1437.7685	44.5296
1496.464	5.9228
1534.9148	144.9682
1695.0002	92.3607
2967.5943	20.8752
2996.1931	1.9946
3516.043	372.0127
3695.4613	311.6534
3757.0389	135.3367
3814.4944	174.7833

19i

C,-0.344070257,0.364535156,0.0929976785
C,-0.0337713391,0.3690218256,1.5539505465
C,1.0087935327,-0.2214834099,2.1406341305
O,1.9667827072,-0.9823932724,1.5508643923
H,1.6670128855,-1.1632181676,0.6415391905
O,1.2061814864,-0.0770521988,3.4832160591
H,1.774014352,-0.7966902897,3.7826116572
O,-0.9647044579,1.1040553951,2.2711708529
H,-0.6957384533,1.1161001182,3.1966078308
O,0.307553451,-0.7502756844,-0.5425729256
H,0.3334775638,-0.600651029,-1.4912481077
H,-1.4290316511,0.2865666463,-0.0255435381
H,-0.0225744008,1.2995732546,-0.3819202093

E[B3LYP/cc-pVTZ] = -418.96732 Ha
ZPVE[B3LYP/aug-cc-pVTZ] = 0.098787 Ha
E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37847 Ha

Frequency and Intensity

60.7249	0.5472
170.1599	9.8699
225.5403	104.5732
251.2572	22.3942
259.7643	105.2877
290.748	22.0449
321.3751	38.0983
352.6747	34.066
431.6902	0.6658
505.4071	21.6154
610.9837	10.2674
621.3036	77.5614
626.0149	28.9363
752.4997	8.3858
1004.3143	49.0245
1037.111	93.3678
1076.0063	71.0006
1168.3854	148.6602
1210.5185	68.6501
1226.3944	40.2841
1263.8796	88.9697
1282.2309	106.2571
1383.6567	96.718
1414.8331	118.6205
1470.3933	60.2644
1517.0531	1.6818
1817.8406	110.2462
2974.1427	77.7769
3019.7859	31.2997
3593.4854	255.9588
3792.1384	93.4113
3796.8047	55.8899
3833.3348	40.7051

19i⁺

C,-0.3316618843,0.3530362996,0.0651206326
C,-0.0285686683,0.4325773823,1.5289500811
C,0.9681915792,-0.3303893973,2.1878607745
O,1.7351909825,-1.1946743046,1.609859278
H,1.5045894783,-1.2411321764,0.6385370538
O,1.1079577545,-0.1318715762,3.4750447103
H,1.8047662762,-0.6887981127,3.8627746348
O,-0.7681460875,1.2921953616,2.1929201711
H,-0.5517631896,1.3344482066,3.1395840194
O,0.489063544,-0.6508662044,-0.5179935078
H,0.3872149972,-0.6870193483,-1.4752451051
H,-1.3958408366,0.123652984,-0.0551791935

H,-0.1470685263,1.33692923,-0.3799259916

E[B3LYP/cc-pVTZ] = -418.70826 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.099763 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.11059 Ha

Frequency and Intensity

32.9108	42.8113
143.8662	8.6069
175.6628	98.287
283.7993	11.9831
337.6554	18.6017
355.2257	6.1479
437.0486	0.692
517.1011	138.0464
530.4636	15.1412
561.8812	121.6484
616.6606	21.1188
664.8191	8.6107
757.6343	4.5001
842.7809	65.7749
993.5925	2.3685
1054.4785	82.5964
1111.955	49.855
1168.4864	149.441
1213.0591	148.6435
1243.8937	3.0353
1312.4607	3.1072
1397.7151	178.4929
1413.4682	162.5915
1467.194	157.8007
1489.1684	20.1949
1577.0022	193.7734
1674.1922	112.3723
3004.4385	8.1386
3039.1521	0.0299
3171.5618	663.337
3691.3287	135.2962
3698.0317	355.638
3812.2251	164.7289

19j

C,-0.2179342238,0.4382322007,0.1096067378

C,-0.0320235827,0.4651160145,1.5951153763

C,0.9775912893,-0.1486458419,2.2161911843

O,1.9361949693,-0.9045873791,1.6171093714

H,1.6150469428,-1.1265952254,0.7235203335

O,1.1462751083,-0.0408579685,3.5627363076
H,1.7316753305,-0.75006335,3.8532382612
O,-0.9902868287,1.2071638502,2.2677584231
H,-0.7506689509,1.2484865661,3.2003932063
O,0.1278223346,-0.8365066727,-0.4731899739
H,-0.5280919434,-1.4826500221,-0.1888262712
H,-1.2526980685,0.7029594823,-0.1168091334
H,0.4275567961,1.1537470924,-0.4033422395

E[B3LYP/cc-pVTZ] = -418.96807 Ha

ZPVE[B3LYP/aug-cc-pVTZ] = 0.099125 Ha

E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.37923 Ha

Frequency and Intensity

88.6741	4.4546
163.0599	19.2782
214.5482	7.4395
239.5324	128.5845
287.0485	10.8225
322.3112	42.7712
341.93	37.7323
374.4241	92.1667
448.7015	29.3356
500.3612	27.4733
611.8056	11.9578
638.5172	20.4824
695.6398	63.9608
762.6248	23.5313
950.1977	56.1447
1003.5217	74.3364
1074.3233	78.7524
1150.9992	177.8792
1194.7131	49.3873
1236.4597	6.6762
1279.1859	161.7739
1354.1769	97.4654
1385.3547	2.5875
1399.0015	114.4103
1431.8314	113.6751
1502.8864	0.9623
1804.1896	112.7445
3031.0584	42.0142
3066.4099	15.5841
3579.0912	229.3119
3788.996	31.0817

	3792.5292	91.5358
	3796.5923	56.8483
	C,-0.415677158,0.3886786251,0.2313752462	
	C,-0.0170450974,0.468092006,1.6719620235	
	C,0.9489726607,-0.3668187329,2.2878645612	
	O,1.6101280513,-1.2974968397,1.6828561198	
	H,1.3378819385,-1.3219161111,0.7216996631	
	O,1.174106465,-0.166989695,3.562716621	
	H,1.8482862956,-0.7705246114,3.9194172853	
	O,-0.6463265338,1.3929908942,2.3614418977	
	H,-0.3787546435,1.4249194848,3.295311831	
	O,0.3783919209,-0.6018952403,-0.4089836672	
	H,0.1054142108,-0.7462180482,-1.321535041	
	H,-1.4831847628,0.1476870763,0.1810424175	
	H,-0.2717341743,1.3752899385,-0.2216673747	
	E[B3LYP/cc-pVTZ] = -418.70826 Ha	
	ZPVE[B3LYP/aug-cc-pVTZ] = 0.099775 Ha	
	E[CCSD(T)-F12b/cc-pVTZ-F12] = -418.11059 Ha	
	Frequency and Intensity	
19j ⁺	35.6162	41.3187
	143.9932	7.7331
	177.0999	100.6115
	283.8253	12.0171
	337.6608	18.5807
	355.1625	6.1519
	437.1037	0.7093
	516.8913	138.1463
	530.4764	15.1497
	561.5491	121.5764
	616.6807	21.1335
	664.8066	8.6069
	757.7323	4.4959
	841.9884	65.698
	993.4965	2.362
	1054.302	82.7538
	1111.8375	49.8645
	1168.4304	149.4913
	1213.1755	148.5849
	1243.7571	3.0272
	1312.4292	3.0549
	1397.7067	177.5054
	1413.4569	164.0637
	1467.2462	157.0655

1489.0824	20.2554
1577.0631	193.5734
1674.347	112.3149
3004.79	8.1608
3039.6368	0.0413
3173.2021	663.2218
3691.6571	135.3196
3698.2928	355.6674
3811.6529	164.6203

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