

Supplementary Materials for

**Interstellar Formation of Glyceric Acid (****HOCH2CH(OH)COOH) –**

**The Simplest Sugar Acid**

Jia Wang *et al.*

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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.

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**Fig. S1**. Infrared spectra of (**A**) CO2−HOCH2CH2OH 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.

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**Fig. S2**. Infrared spectra of (**A**) C18O2−HOCH2CH2OH 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.

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**Fig. S3**. Infrared spectra of (**A**) CO2−HOCD2CD2OH 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.

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**Fig. S4**. Infrared spectra of (**A**) 13CO2−HO13CH213CH2OH 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.

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**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.** (**A**) TPD profiles measured at 11.10 eV with irradiated CO2–HOCH2CH2OH (**16**) ice (*m/z* = 89) and 13CO2–HO13CH213CH2OH 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 CO2–HOCH2CH2OH ice.

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Description automatically generated **Fig. S7.** (**A**) TPD profiles measured at 11.10 eV with irradiated CO2–HOCH2CH2OH (**16**) ice (*m/z* = 76), 13CO2–HO13CH213CH2OH ice (*m/z* = 78) and C18O2–HOCH2CH2OH ice (*m/z* = 80). (**B**) TPD profiles at *m/z* = 76 in irradiated CO2–HOCH2CH2OH ice measured at 11.10 eV and 8.77 eV.

A graph of different colored lines

Description automatically generated with medium confidence **Fig. S8.** (**A**) TPD profiles measured at 11.10 eV with irradiated CO2–HOCH2CH2OH (**16**) ice (*m/z* = 90), 13CO2–HO13CH213CH2OH ice (*m/z* = 93) and C18O2–HOCH2CH2OH ice (*m/z* = 92). (**B**) TPD profiles at *m/z* = 90 in irradiated CO2–HOCH2CH2OH ice measured at 11.10 eV and 8.77 eV.

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**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 (ν1 + ν3) |
| 3595 | combination (2ν2 + ν3) |
| 2348 | C-O asymmetric stretching (ν3) |
| 2278 | C-O asymmetric stretching (ν3 (13CO2)) |
| 662 | O-C-O bending (ν2) |
| **HOCH2CH2OH** | Assignment *(57, 73)* |
| 3396 | OH stretching |
| 2946, 2888 | CH stretching |
| 1462 | CH2 scissoring |
| 1392, 1348 | OH bending and CH2 wagging |
| 1284, 1258, 1202 | CH2 twisting |
| 1090, 1043 | CO stretching and CC stretching |
| 886, 867 | CH2 rocking |
| New absorptions after irradiation (cm−1) | Assignment *(12, 27, 74, 75)* |
| 2140 | ν (CO) |
| 1849 | ν2 (HOĊO) / ν3 (HĊO) |
| 1767 | C=O stretch |
| 1722 | ν2 (H2CO) |
| 1657 | ν2 (H2O) |
| 1500 | ν3 (H2CO) |

**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 (ν1 + ν3) |
| 3512 | combination (2ν2 + ν3) |
| 2313 | C-18O asymmetric stretching (ν3) |
| 2242 | C-18O asymmetric stretching (ν3 (13C18O2)) |
| 661 | O-C-O bending (ν2) |
| **HOCH2CH2OH** | Assignment *(57, 73)* |
| 3393 | OH stretching |
| 2947, 2883 | CH stretching |
| 1461 | CH2 scissoring |
| 1398 | OH bending and CH2 wagging |
| 1282, 1247, 1195 | CH2 twisting |
| 1089, 1042 | CO stretching and CC stretching |
| 884, 865 | CH2 rocking |
| New absorptions after irradiation (cm−1) | Assignment *(12, 76)* |
| 2138 | ν (CO) |
| 2090 | ν (C18O) |
| 1722 | ν2 (H2CO) |
| 1638 | ν2 (H2O) |

**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 (ν1 + ν3) |
| 3595 | combination (2ν2 + ν3) |
| 2346 | C-O asymmetric stretching (ν3) |
| 2278 | C-O asymmetric stretching (ν3 (13CO2)) |
| 662 | O-C-O bending (ν2) |
| **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 CD2 scissoring |
| 979, 964 | CD2 wagging |
| 951, 898 | CD2 twisting |
| 740, 768 | CD2 rocking |
| New absorptions after irradiation (cm−1) | Assignment *(12, 30, 74, 75)* |
| 2141 | ν (CO) |
| 1844 | ν2 (HOĊO) / ν4 (HĊO) |
| 1703 | ν2 (D2CO) |

**Table S4.** Absorption peaks observed in 13CO2−HO13CH213CH2OH ice before and after electron irradiation (30 nA, 60 minutes) at 5 K.

|  |  |
| --- | --- |
| Pristine ice, absorptions before irradiation (cm−1) |  |
| 13**CO2** | Assignment *(27)* |
| 3621 | combination (ν1 + ν3) |
| 3506 | combination (2ν2 + ν3) |
| 2347 | C-O asymmetric stretching (ν3 (CO2)) |
| 2282 | 13C-O asymmetric stretching (ν3) |
| 650 | O-13C-O bending (ν2) |
| **HO**13**CH2**13**CH2OH** | Assignment *(57, 73)* |
| 3379 | OH stretching |
| 2938, 2872 | 13CH stretching |
| 1456 | 13CH2 scissoring |
| 1399 | OH bending and 13CH2 wagging |
| 1253, 1194 | 13CH2 twisting |
| 1064, 1022 | 13CO stretching and 13C13C stretching |
| 875, 849 | 13CH2 rocking |
| New absorptions after irradiation (cm−1) | Assignment *(12, 27, 29-31, 74, 75)* |
| 2092 | ν (13CO) |
| 1811 | ν2 (HO13ĊO) / ν3 (H13ĊO) |
| 1709 | 13C=O stretch |
| 1681 | ν2 (H213CO) |
| 1658 | ν2 (H2O) |
| 1500 | ν3 (H213CO) |

**Table S5.** Error analysis of adiabatic ionization energies (IEs) and relative energies (*Δ*E) of distinct C3H6O4 isomers **1**, **18**,and **19**; IEs and *Δ*E 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 | *Δ*E  (kJ mol-1) | Computed IE (eV) | Corrected IE ranges (eV) |
| Glyceric acid  (2,3-Dihydroxypropanoic acid) | **1a** | | A molecule model of a chemical compound  Description automatically generated | 19.8 | 9.83 | 9.75 – 9.83 |
| **1b** | | A molecule model of a chemical compound  Description automatically generated with medium confidence | 31.0 | 9.97 | 9.89 – 9.97 |
| **1c** | | A molecule model of a chemical compound  Description automatically generated | 26.3 | 9.91 | 9.83 – 9.91 |
| **1d** | | A molecule model of a chemical compound  Description automatically generated with medium confidence | 16.2 | 9.88 | 9.80 – 9.88 |
| **1e** | |  | 24.4 | 9.79 | 9.71 – 9.79 |
| **1f** | | A molecule model of a chemical compound  Description automatically generated with medium confidence | 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** | | A molecule model of a chemical compound  Description automatically generated with medium confidence | 13.9 | 10.17 | 10.09 – 10.17 |
| 2-Hydroxyethyl hydrogen carbonate | | **18a** | A molecule model of a chemical compound  Description automatically generated | 21.9 | 9.87 | 9.79 – 9.87 |
| **18b** | A molecule model of a chemical compound  Description automatically generated with medium confidence | 7.9 | 11.07 | 10.99 – 11.07 |
| **18c** | A molecule model of a molecule  Description automatically generated with medium confidence | 1.3 | 10.17 | 10.09 – 10.17 |
| **18d** | A molecule model of a molecule  Description automatically generated | 6.2 | 10.09 | 10.01 – 10.09 |
| **18e** | A molecule model of a chemical compound  Description automatically generated with medium confidence | 0.0 | 10.08 | 10.00 – 10.08 |
| **18f** | A molecule model of a chemical compound  Description automatically generated with medium confidence | 7.9 | 11.09 | 11.01 – 11.09 |
| Propene-1,1,2,3-tetrol | | **19a** | A molecule model of a molecule  Description automatically generated | 122.8 | 7.43 | 7.35 – 7.43 |
| **19b** | A molecule model of a molecule  Description automatically generated | 118.7 | 7.44 | 7.36 – 7.44 |
| **19c** | A molecule model of a molecule  Description automatically generated | 118.7 | 7.32 | 7.24 – 7.32 |
| **19d** | A molecule model of a molecule  Description automatically generated | 114.4 | 7.39 | 7.31 – 7.39 |
| **19e** | A molecule model of a chemical compound  Description automatically generated with medium confidence | 111.8 | 7.42 | 7.34 – 7.42 |
| **19f** | A molecule model of a chemical compound  Description automatically generated with medium confidence | 114.4 | 7.39 | 7.31 – 7.39 |
| **19g** | A molecule model of a chemical compound  Description automatically generated | 126.2 | 7.53 | 7.45 – 7.53 |
| **19h** | A molecule model of a molecule  Description automatically generated | 139.6 | 7.40 | 7.32 – 7.40 |
| **19i** | A molecule model of a molecule  Description automatically generated | 118.7 | 7.32 | 7.24 – 7.32 |
| **19j** | A molecule model of a molecule  Description automatically generated | 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) |
| CO2−HOCH2CH2OH | 2.1 ± 0.7 : 1 | 750 ± 80 | - | - | - | - | 11.10 |
| CO2−HOCH2CH2OH | 3.1 ± 1.2 : 1 | 750 ± 80 | 31 ± 4 | 3600 ± 10 | 1.8 ± 0.3 | 3.1 ± 0.5 | 11.10 |
| C18O2−HOCH2CH2OH | 1.5 ± 0.6 : 1 | 750 ± 80 | 29 ± 1 | 3600 ± 10 | 1.8 ± 0.3 | 2.9 ± 0.5 | 11.10 |
| CO2−HOCD2CD2OH | 2.3 ± 0.5 : 1 | 770 ± 80 | 28 ± 2 | 3600 ± 10 | 1.6 ± 0.3 | 3.0 ± 0.5 | 11.10 |
| 13CO2−HO13CH213CH2OH | 1.4 ± 0.3 : 1 | 770 ± 80 | 32 ± 6 | 3600 ± 10 | 1.9 ± 0.3 | 3.3 ± 0.5 | 11.10 |
| CO2−HOCH2CH2OH | 1.9 ± 0.5 : 1 | 750 ± 80 | 31 ± 2 | 3600 ± 10 | 1.8 ± 0.3 | 3.1 ± 0.5 | 8.77 |
| CO2−HOCH2CH2OH | 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 | ω1 laser wavelength (nm) | ω1 Dye | ω2 laser wavelength (nm) |
| 11.10  (2ω1 + ω2) | Xenon | 249.628 | Coumarin 503 | 1064 |
| 8.77  (2ω1 − ω2) | 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**).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C3H6O4 isomers | Differences in IEs (eV) | | Differences in relative energies (kJ mol−1) | |
| PBE0a | ωB97XDb | PBE0a | ωB97XDb |
| **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//ωB97XD/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) |
| **1a** | 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  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 |
| **1a+** | 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  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 |
| **1d** | 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  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 |
| **1d+** | 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  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 |
| **1e** | 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  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 |
| **1g** | 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  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 |
| **1g+** | 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  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 |
| **1h** | 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  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 |
| **1h+** | 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  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 |
| **1i** | 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 |
| **18b** | 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  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 |
| **18b+** | 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  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 |
| **18c** | 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  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 |
| **18c+** | 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  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 |
| **18d** | 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  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  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 |
| **18f+** | 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  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 |
| **19a** | 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  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 |
| **19a+** | 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  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 |
| **19d** | 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  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 |
| **19d+** | 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  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 |
| **19e** | 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  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 |
| **19g+** | 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  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 |
| **19h** | 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  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 |
| **19j+** | 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  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 |