|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Neutral | | | | Ionization potential (eV) | Cationic | | | |
| Structure | Abs. energy (hartree) | XYZ coordinates (Angstroms) | Frequencies | Structure | Abs. energy (hartree) | XYZ coordinates (Angstroms) | Frequencies |
|  | -210.046669 | |  |  |  |  |  | | --- | --- | --- | --- | --- | | C | 0 | -2.135053 | -0.421918 | 0.000020 | | C | 0 | -0.667295 | -0.092347 | 0.000003 | | O | 0 | -0.228109 | 1.034820 | -0.000083 | | H | 0 | -2.373535 | -1.031479 | 0.878503 | | H | 0 | -2.373525 | -1.031618 | -0.878370 | | H | 0 | -2.735248 | 0.487804 | -0.000055 | | H | 0 | 0.032434 | -0.951283 | 0.000074 | | H | 0 | 1.940701 | 0.452686 | -0.000023 | | N | 0 | 2.549562 | -0.363783 | 0.000045 | | H | 0 | 3.150596 | -0.286236 | 0.814765 | | H | 0 | 3.150606 | -0.286364 | -0.814680 | | |  |  | | --- | --- | | A | 72.3084 | | A | 94.8064 | | A | 139.4851 | | A | 140.5437 | | A | 164.8536 | | A | 198.1965 | | A | 364.1886 | | A | 514.4461 | | A | 798.1636 | | A | 888.3063 | | A | 1096.9646 | | A | 1129.3874 | | A | 1152.5691 | | A | 1375.4958 | | A | 1433.1532 | | A | 1460.6920 | | A | 1470.6580 | | A | 1672.8154 | | A | 1702.2841 | | A | 1795.9631 | | A | 2930.0403 | | A | 3021.4110 | | A | 3076.0578 | | A | 3134.7308 | | A | 3447.1223 | | A | 3559.9915 | | A | 3583.5427 | | 7.96 |  | -209.754250 | |  |  |  |  |  | | --- | --- | --- | --- | --- | | C | 0 | -2.439005 | 0.004112 | 0.000000 | | C | 0 | -0.998018 | -0.365718 | 0.000000 | | O | 0 | -0.027163 | 0.333327 | 0.000000 | | H | 0 | -2.911918 | -0.446497 | 0.877023 | | H | 0 | -2.911916 | -0.446495 | -0.877026 | | H | 0 | -2.570459 | 1.089678 | 0.000001 | | H | 0 | 2.925934 | -1.051497 | -0.000047 | | H | 0 | 1.603923 | 0.028892 | 0.000000 | | N | 0 | 2.659316 | -0.063893 | 0.000000 | | H | 0 | 3.044327 | 0.388053 | 0.833403 | | H | 0 | 3.044332 | 0.388134 | -0.833357 | | |  |  | | --- | --- | | A | -11.0214 | | A | 69.2864 | | A | 82.7233 | | A | 116.9469 | | A | 241.2182 | | A | 339.8902 | | A | 342.6523 | | A | 500.9942 | | A | 894.4594 | | A | 953.0959 | | A | 1076.0112 | | A | 1363.4217 | | A | 1433.3092 | | A | 1444.0426 | | A | 1446.6574 | | A | 1529.2211 | | A | 1535.0929 | | A | 1737.1760 | | A | 1738.7460 | | A | 1858.7940 | | A | 2856.3070 | | A | 3024.8370 | | A | 3106.4928 | | A | 3118.5241 | | A | 3424.9528 | | A | 3509.3335 | | A | 3511.9758 | |