

C2H5OC2H4-1				
Optimized Cartesian coordinate	C	1.104439000000	0.518394000000	0.031682000000
	O	-0.055708000000	-0.282000000000	-0.029971000000
	H	1.112819000000	1.225870000000	-0.810020000000
	H	1.100359000000	1.108002000000	0.959896000000
	C	2.314365000000	-0.390093000000	-0.020850000000
	H	3.234071000000	0.196069000000	0.025354000000
	H	2.300081000000	-1.085784000000	0.819303000000
	H	2.312731000000	-0.966942000000	-0.946704000000
	C	-1.242503000000	0.475562000000	0.010802000000
	H	-1.275262000000	1.180022000000	-0.836620000000
	H	-1.251591000000	1.095254000000	0.927740000000
	C	-2.409620000000	-0.435837000000	-0.020977000000
	H	-2.287672000000	-1.459828000000	0.301448000000
	H	-3.399959000000	-0.044819000000	-0.204565000000
Frequencies	85.4196 113.6898 131.7166 202.5221 253.8197 394.4895 446.0549 463.4548 823.3305 849.5671 937.716 985.6522 1095.2952 1115.7752 1184.4737 1191.0684 1210.294 1254.0997 1310.9627 1385.8918 1407.3114 1437.7011 1466.5235 1488.3539 1501.3562 1506.3721 1536.8744 2925.7622 2981.2474 3000.1676 3030.1692 3073.3362 3150.5989 3155.0179 3185.8749 3300.8225			
Rotational constants (GHZ)	19.5211390 2.3407506 2.1785877			
ZPE (Hartree/Particle)	0.122071			
C2H5OC2H4-2				
Optimized Cartesian coordinate	C	-2.420848000000	-0.332724000000	0.008935000000
	H	-2.526079000000	-0.847790000000	0.973723000000
	H	-2.413141000000	-1.098992000000	-0.770246000000
	H	-3.297652000000	0.299706000000	-0.134513000000
	C	-1.181511000000	0.482331000000	-0.053152000000
	H	-1.136722000000	1.478310000000	0.383771000000
	O	-0.031255000000	-0.238017000000	-0.014933000000
	C	1.159882000000	0.534733000000	-0.047190000000
	H	1.182546000000	1.117883000000	-0.974641000000
	H	1.155611000000	1.236109000000	0.796720000000
	C	2.339408000000	-0.408720000000	0.036819000000
	H	3.274775000000	0.153270000000	0.012915000000
	H	2.300666000000	-0.984081000000	0.962817000000
	H	2.328456000000	-1.104001000000	-0.803560000000
Frequencies	83.5045 112.3505 180.9905 197.6452 253.2169 432.0638 455.4623 585.1447 821.2482 880.0391 973.6043 1024.2514 1107.3483 1127.9813 1184.4921 1191.4221 1278.8499 1310.6636			

	1377.2057 1401.4762 1422.5786 1461.8894 1472.7796 1488.7557 1497.6064 1506.1632 1530.6132 3011.4227 3028.4304 3069.138 3074.3133 3094.13 3134.8472 3151.8646 3152.4023 3155.9771			
Rotational constants (GHZ)	20.45886 2.26833 2.12738			
ZPE (Hartree/Particle)	0.123549			
C2OC(=O)CH3				
Optimized Cartesian coordinate	C	2.552423000000	-0.400429000000	0.000015000000
	H	2.583868000000	-1.036524000000	-0.885597000000
	H	2.583813000000	-1.036554000000	0.885610000000
	H	3.437259000000	0.238427000000	0.000056000000
	C	1.303967000000	0.452028000000	-0.000023000000
	H	1.243739000000	1.093025000000	0.881999000000
	H	1.243761000000	1.092972000000	-0.882086000000
	O	0.177466000000	-0.439054000000	-0.000004000000
	C	-2.131051000000	-0.881738000000	-0.000001000000
	H	-2.036270000000	-1.518149000000	0.880682000000
	H	-3.094263000000	-0.378771000000	0.000079000000
	H	-2.036363000000	-1.518029000000	-0.880782000000
	C	-1.032574000000	0.144947000000	0.000006000000
	O	-1.187733000000	1.335899000000	0.000012000000
Frequencies	59.8999 80.3881 153.0612 200.95 264.6385 379.934 435.2787 613.6165 651.4554 816.8205 885.4812 972.9331 1022.214 1072.714 1111.395 1153.527 1185.262 1302.430 1312.56 1395.518 1411.292 1442.786 1477.637 1482.565 1491.364 1504.352 1528.970 1858.963 3074.521 3084.166 3089.708 3124.903 3152.233 3158.524 3160.838 3202.250			
Rotational constants (GHZ)	8.5000369 2.1046036 1.7417178			
ZPE (Hartree/Particle)	0.119183			
C2OC2-1O2H-2				
Optimized Cartesian coordinate	C	3.199705000000	-0.786391000000	0.126895000000
	H	2.832621000000	-1.762191000000	-0.193419000000
	H	3.291969000000	-0.788538000000	1.213664000000
	H	4.187845000000	-0.624689000000	-0.307131000000
	C	2.251997000000	0.303800000000	-0.319113000000
	H	2.599369000000	1.291244000000	0.003848000000
	H	2.143503000000	0.313862000000	-1.409449000000
	O	0.978171000000	0.050381000000	0.266166000000
	C	0.016389000000	0.943427000000	-0.035896000000

	H	0.181491000000	1.598175000000	-0.885304000000
	C	-1.336927000000	0.615855000000	0.446977000000
	H	-1.962174000000	1.511288000000	0.496014000000
	H	-1.287771000000	0.143443000000	1.432878000000
	O	-1.929244000000	-0.301497000000	-0.485481000000
	O	-3.247281000000	-0.576789000000	-0.011632000000
	H	-3.187008000000	-1.519500000000	0.183299000000
Frequencies	53.1845 69.2615 92.7715 147.7456 200.5914 212.184 252.886 291.2753 359.7569 439.5933 511.1228 600.3439 821.9572 879.6139 972.5342 985.232 1035.195 1102.581 1130.495 1177.260 1184.406 1262.746 1297.295 1313.038 1364.080 1390.295 1401.697 1430.578 1487.414 1498.250 1506.880 1507.139 1529.738 3040.772 3061.902 3075.755 3081.201 3116.902 3153.844 3158.584 3186.315 3852.676			
Rotational constants (GHZ)	8.5446790 0.9583668 0.9093767			
ZPE (Hartree/Particle)	0.132651			
C2OC2-1O2H-A				
Optimized Cartesian coordinate	C	3.569031000000	-0.404196000000	0.026843000000
	H	3.540679000000	-1.175840000000	-0.746398000000
	H	3.652992000000	-0.913552000000	0.996539000000
	H	4.465590000000	0.199484000000	-0.117312000000
	C	2.357916000000	0.449720000000	-0.048294000000
	H	2.337827000000	1.449072000000	0.381557000000
	O	1.183244000000	-0.236810000000	-0.011614000000
	C	-1.164016000000	-0.368498000000	0.006378000000
	H	-1.135431000000	-0.961010000000	0.926026000000
	H	-1.171256000000	-1.038521000000	-0.857245000000
	O	-2.307199000000	0.464079000000	-0.014832000000
	O	-3.439285000000	-0.395734000000	-0.056192000000
	H	-3.918918000000	-0.116207000000	0.732710000000
	C	0.024147000000	0.571167000000	-0.060450000000
	H	0.002570000000	1.149412000000	-0.989558000000
	H	0.009398000000	1.265716000000	0.787931000000
Frequencies	57.2664 65.7169 112.3668 114.8503 138.4312 166.3527 178.5806 278.5058 345.1224 470.247 540.8939 587.4294 839.2491 928.287 1018.2549 1024.2112 1104.0357 1120.3199 1135.0317 1167.9581 1181.6745 1238.5208 1280.5819 1299.6976 1352.7775 1388.2136 1410.9772 1433.8697 1468.1437 1473.8987 1497.3911 1528.1315 1539.0125 3013.8736 3041.0595 3062.6296 3088.9813 3096.0867 3122.5556 3139.3808 3154.9367 3853.9252			
Rotational	15.9176673 0.8319490 0.8047260			

constants (GHZ)				
ZPE (Hartree/Particle)	0.132269			
C2OC2-1O2H-B				
Optimized	C	3.550138000000	-0.491696000000	0.028065000000
Cartesian coordinate	H	3.413584000000	-1.506670000000	-0.316542000000
	H	4.544906000000	-0.124132000000	0.233984000000
	O	1.200137000000	-0.287198000000	0.041704000000
	C	-1.145351000000	-0.379978000000	0.023748000000
	H	-1.142852000000	-0.962803000000	0.949834000000
	H	-1.149086000000	-1.058942000000	-0.832793000000
	O	-2.275030000000	0.471158000000	-0.026641000000
	O	-3.421631000000	-0.368345000000	-0.078264000000
	H	-3.893556000000	-0.096209000000	0.717836000000
	C	0.062495000000	0.535649000000	-0.031082000000
	H	0.052830000000	1.111668000000	-0.965811000000
	H	0.037712000000	1.243392000000	0.808666000000
	C	2.405151000000	0.445958000000	-0.015250000000
	H	2.453501000000	1.161550000000	0.820711000000
	H	2.420557000000	1.047619000000	-0.943158000000
	Frequencies	59.4236 67.9697 113.5143 116.9448 136.3852 141.3777 184.2053 284.9263 343.4045 408.1804 485.7923 550.0711 841.5316 867.548 976.3059 1017.9084 1098.5364 1105.4294 1127.4712 1169.3448 1175.7928 1216.1841 1236.5564 1258.7183 1299.8058 1352.7845 1402.381 1411.8416 1448.2859 1473.8961 1502.1066 1531.6452 1540.6469 2933.5595 2993.4487 3016.4877 3054.3375 3063.9299 3121.3265 3187.393 3302.3935 3851.7797		
Rotational constants (GHZ)	15.4364512 0.8462392 0.8167916			
ZPE (Hartree/Particle)	0.130930			
C2OC2-1OO				
Optimized	C	2.265846000000	0.500922000000	0.000068000000
Cartesian coordinate	O	1.073615000000	-0.261839000000	-0.000194000000
	H	2.286690000000	1.148394000000	-0.887193000000
	H	2.286440000000	1.148168000000	0.887499000000
	C	3.440583000000	-0.452673000000	0.000118000000
	H	4.379941000000	0.102949000000	0.000336000000
	H	3.410680000000	-1.089201000000	0.885415000000
	H	3.410954000000	-1.088965000000	-0.885357000000
	C	-0.081725000000	0.534115000000	-0.000083000000
	H	-0.118683000000	1.177797000000	-0.889393000000

	H	-0.118642000000	1.177607000000	0.889367000000
	C	-1.258624000000	-0.418544000000	-0.000149000000
	H	-1.269526000000	-1.043747000000	-0.893717000000
	H	-1.269427000000	-1.043982000000	0.893256000000
	O	-2.446061000000	0.397554000000	0.000023000000
	O	-3.526919000000	-0.319708000000	0.000178000000
Frequencies	47.0566 53.213 98.2732 114.6621 142.4121 251.8204 284.5119 348.536 482.5927 564.7454 812.1459 826.6117 911.7683 1035.4067 1080.2513 1112.4369 1141.6278 1184.6322 1188.0034 1213.6314 1234.0042 1298.9898 1300.9323 1313.6528 1350.1284 1398.9146 1427.4704 1473.8708 1488.3858 1504.9921 1509.8272 1526.2714 1542.8908 3010.156 3018.0569 3045.5472 3055.7416 3074.9639 3100.8609 3153.4934 3156.4653 3164.6361			
Rotational constants (GHZ)	15.4674074 0.8461856 0.8188570			
ZPE (Hartree/Particle)	0.134513			
C2OC2-2O2H-1				
Optimized Cartesian coordinate	C	2.982442000000	-0.146660000000	-0.172277000000
	H	3.307458000000	0.821579000000	0.211103000000
	H	2.991235000000	-0.109119000000	-1.262339000000
	H	3.690717000000	-0.909483000000	0.155907000000
	C	1.593392000000	-0.475017000000	0.328140000000
	H	1.248753000000	-1.437754000000	-0.057086000000
	H	1.567522000000	-0.511504000000	1.424695000000
	O	0.717212000000	0.559345000000	-0.118435000000
	C	-0.590805000000	0.411613000000	0.290580000000
	H	-0.666286000000	0.124523000000	1.348060000000
	C	-1.345433000000	1.651228000000	-0.011522000000
	H	-1.075379000000	2.216699000000	-0.892405000000
	H	-2.204939000000	1.931623000000	0.578745000000
	O	-1.103947000000	-0.712697000000	-0.468732000000
	O	-2.328562000000	-1.094694000000	0.136690000000
	H	-2.974282000000	-0.789184000000	-0.512381000000
Frequencies	41.8217 58.2876 98.5406 132.5731 211.1639 252.4516 258.9352 301.4172 367.5503 389.9339 484.8997 559.9741 594.957 822.2896 863.8832 941.1395 1003.6913 1050.4297 1105.6349 1125.7127 1186.5642 1191.4693 1237.0488 1314.2022 1356.6865 1390.2332 1403.4727 1410.4692 1439.3557 1478.1217 1489.5168 1506.7211 1534.7347 3032.8679 3041.0909 3073.9338 3102.497 3151.8184 3156.44 3187.6162 3308.8014 3840.9117			
Rotational constants (GHZ)	5.2298868 1.4675127 1.2215392			

ZPE (Hartree/Particle)	0.130994			
C2OC2-2O2H-A				
Optimized Cartesian coordinate	C	1.330039000000	1.622482000000	-0.013577000000
	H	0.949436000000	2.441228000000	0.597899000000
	H	1.212726000000	1.871475000000	-1.068718000000
	H	2.385554000000	1.465273000000	0.207322000000
	C	0.560985000000	0.360117000000	0.279338000000
	H	0.613953000000	0.072543000000	1.338504000000
	O	-0.758748000000	0.524554000000	-0.123649000000
	C	-1.636222000000	-0.439883000000	0.299664000000
	H	-1.392581000000	-0.913447000000	1.247350000000
	C	-3.034125000000	-0.222708000000	-0.141273000000
	H	-3.467935000000	0.686706000000	0.296668000000
	H	-3.077560000000	-0.115186000000	-1.227878000000
	H	-3.656397000000	-1.069518000000	0.149528000000
	O	1.054924000000	-0.740760000000	-0.489889000000
	O	2.319754000000	-1.078061000000	0.066049000000
	H	2.181309000000	-2.004996000000	0.294330000000
Frequencies	60.5301 94.213 113.1569 181.3894 205.6573 226.3593 236.2758 315.7931 369.2653 418.613 527.7555 549.5779 591.9517 882.1238 912.6275 1002.4896 1021.3143 1045.9765 1133.4852 1142.7373 1172.7773 1221.4004 1259.2509 1367.266 1384.8982 1396.8579 1408.4255 1432.0727 1455.3187 1470.1144 1491.205 1493.0496 1496.2897 3012.5163 3033.1212 3082.5411 3096.5315 3147.1449 3161.9207 3166.3908 3174.8998 3854.2847			
Rotational constants (GHZ)	5.1129177 1.4687606 1.2120336			
ZPE (Hartree/Particle)	0.131700			
C2OC2-2O2H-B				
Optimized Cartesian coordinate	C	1.662149000000	-0.527995000000	0.215535000000
	H	1.374881000000	-1.451040000000	-0.298848000000
	H	1.543424000000	-0.712982000000	1.298271000000
	O	0.788273000000	0.533393000000	-0.159304000000
	C	-0.513336000000	0.377481000000	0.270663000000
	H	-0.558002000000	0.094332000000	1.331858000000
	C	-1.283369000000	1.642776000000	-0.016582000000
	H	-1.204533000000	1.875342000000	-1.079472000000
	H	-2.330764000000	1.511168000000	0.257041000000
	H	-0.869335000000	2.468327000000	0.562981000000
	O	-1.037323000000	-0.736618000000	-0.471033000000

	O	-2.214481000000	-1.160962000000	0.202886000000
	H	-2.883595000000	-1.031134000000	-0.479422000000
	C	3.050396000000	-0.136167000000	-0.113247000000
	H	3.318133000000	0.910665000000	-0.127169000000
	H	3.822998000000	-0.887759000000	-0.183841000000
Frequencies	58.9983 94.5735 138.1646 176.964 209.3653 213.802 250.3184 309.9314 371.7877 418.3546 432.2766 527.1706 597.7188 839.233 891.92 953.6983 1008.7727 1051.2373 1117.6885 1130.4121 1136.2616 1189.8931 1240.6843 1265.1903 1372.5932 1387.3265 1405.1801 1415.2237 1441.1524 1467.2883 1491.4278 1495.2909 1506.8382 2948.8705 3030.4668 3070.3416 3079.5263 3163.9761 3166.7714 3186.8758 3301.2366 3855.5122			
Rotational constants (GHZ)	5.0031067 1.5235239 1.2340731			
ZPE (Hartree/Particle)	0.130790			
C2OC2-2OO				
Optimized Cartesian coordinate	C	-2.951541000000	-0.092082000000	-0.181781000000
	H	-3.251180000000	0.885821000000	0.197351000000
	H	-2.952875000000	-0.057912000000	-1.271808000000
	H	-3.682339000000	-0.833694000000	0.144969000000
	C	-1.575898000000	-0.457446000000	0.328143000000
	H	-1.258468000000	-1.432051000000	-0.053702000000
	H	-1.554847000000	-0.490943000000	1.424520000000
	O	-0.663925000000	0.546995000000	-0.119775000000
	C	0.626909000000	0.367137000000	0.294676000000
	H	0.698634000000	0.071612000000	1.348576000000
	C	1.460623000000	1.574219000000	-0.043174000000
	H	1.106078000000	2.430654000000	0.530385000000
	H	2.504537000000	1.379768000000	0.201924000000
	H	1.364670000000	1.789827000000	-1.107843000000
	O	1.148559000000	-0.794266000000	-0.451659000000
	O	2.223521000000	-1.264485000000	0.096240000000
Frequencies	56.1832 81.0828 136.2216 200.1338 238.1055 254.8405 322.5547 378.4252 431.0528 517.1083 589.4357 823.0929 856.8568 886.5952 980.3979 1084.8796 1110.4733 1131.2248 1186.4849 1196.4342 1257.0136 1304.8059 1318.2432 1370.1184 1382.0568 1406.5396 1420.9098 1460.0223 1489.7196 1490.9289 1494.7949 1506.4874 1533.1158 3036.6117 3061.723 3075.9236 3084.5868 3093.8392 3154.0683 3159.0448 3170.8498 3176.0193			
Rotational constants (GHZ)	4.9470115 1.5197655 1.2395889			
ZPE	0.134205			

(Hartree/Particle)								
C2OC2H3								
Optimized	C	2.435209000000	-0.293790000000	0.026366000000				
Cartesian	H	2.473708000000	-1.373219000000	0.092717000000				
coordinate	H	3.357971000000	0.267123000000	0.004435000000				
	C	1.274539000000	0.346630000000	-0.036333000000				
	H	1.214849000000	1.431636000000	-0.102371000000				
	O	0.083996000000	-0.300565000000	-0.036867000000				
	C	-1.062922000000	0.535541000000	0.050099000000				
	H	-1.055394000000	1.251852000000	-0.780171000000				
	H	-1.033432000000	1.098896000000	0.990073000000				
	C	-2.288133000000	-0.348720000000	-0.011606000000				
	H	-2.282933000000	-1.060209000000	0.814997000000				
	H	-3.193838000000	0.256792000000	0.052955000000				
	H	-2.305061000000	-0.906315000000	-0.948856000000				
	Frequencies	27.706 93.7371 213.8044 255.8222 443.7938 501.9798 712.83 824.0375 870.4931 873.5171 991.3592 997.9948 1110.7644 1180.982 1185.9062 1244.4845 1314.4526 1349.457 1398.1809 1423.6881 1448.8983 1488.9307 1506.3856 1531.8316 1737.909 3030.1578 3069.9379 3076.0344 3154.1655 3157.8873 3158.7515 3197.3174 3295.8783						
Rotational constants (GHZ)	24.1242709 2.3790704 2.2280678							
ZPE (Hartree/Particle)	0.113610							
C2OCC=O								
Optimized	C	2.826668000000	-0.413318000000	0.000008000000				
Cartesian	H	2.806765000000	-1.049976000000	-0.885465000000				
coordinate	H	2.806633000000	-1.050142000000	0.885359000000				
	H	3.757238000000	0.156863000000	0.000130000000				
	C	1.637181000000	0.521790000000	0.000005000000				
	H	1.647840000000	1.169962000000	0.887107000000				
	H	1.647861000000	1.169988000000	-0.887079000000				
	O	0.457234000000	-0.258925000000	-0.000015000000				
	C	-0.710653000000	0.512501000000	-0.000010000000				
	H	-0.775440000000	1.158342000000	-0.887748000000				
	H	-0.775432000000	1.158344000000	0.887727000000				
	C	-1.898166000000	-0.424792000000	-0.000004000000				
	H	-1.638634000000	-1.501008000000	-0.000019000000				
	O	-3.033111000000	-0.039757000000	0.000015000000				
	Frequencies	59.7615 93.4721 121.0379 151.2501 250.6223 372.4086 406.6386 576.3034 745.9566 824.3961 917.083 1061.3599						

	1081.2319 1116.0139 1175.8143 1189.1177 1217.2431 1255.784 1313.9601 1352.0168 1398.296 1413.3184 1448.4229 1488.1124 1491.0479 1505.3125 1535.7164 1879.6397 2978.6455 3005.5984 3012.1209 3041.8237 3046.6263 3075.0452 3153.6862 3156.5768			
Rotational constants (GHZ)	19.1063437 1.3618881 1.3024287			
ZPE (Hartree/Particle)	0.118263			
C2OCY(COC)				
Optimized Cartesian coordinate	C	-2.632824000000	0.080857000000	-0.282699000000
	H	-2.848767000000	1.098026000000	0.046288000000
	H	-2.555324000000	0.078650000000	-1.370620000000
	H	-3.460355000000	-0.566823000000	0.011939000000
	C	-1.339808000000	-0.404902000000	0.334815000000
	H	-1.108550000000	-1.428557000000	0.012510000000
	H	-1.408150000000	-0.404658000000	1.430857000000
	O	-0.299494000000	0.467817000000	-0.080551000000
	C	0.917015000000	0.128759000000	0.467506000000
	C	1.834999000000	-0.745286000000	-0.276169000000
	O	2.007032000000	0.672680000000	-0.186717000000
	H	0.945196000000	0.173997000000	1.556999000000
	H	1.514922000000	-1.096344000000	-1.251632000000
	H	2.584432000000	-1.334839000000	0.241088000000
Frequencies	78.6353 80.6926 203.7109 251.1124 379.6328 493.8822 515.0668 824.0634 839.4166 925.6468 961.5403 1010.6134 1096.6701 1111.4968 1155.2365 1166.0995 1185.9301 1193.617 1221.0547 1311.575 1327.2618 1394.7735 1420.2037 1456.4607 1488.3204 1505.7597 1530.4098 1540.2373 3016.1396 3050.8043 3075.8785 3113.4159 3131.7106 3153.9867 3158.416 3231.9969			
Rotational constants (GHZ)	12.3917185 1.8362876 1.7608777			
ZPE (Hartree/Particle)	0.119835			
CCY(COCCO)				
Optimized Cartesian coordinate	C	-1.397403000000	0.769330000000	0.102396000000
	C	-1.388563000000	-0.769833000000	-0.027710000000
	C	0.684137000000	-0.026707000000	-0.379434000000
	H	-1.967846000000	1.243324000000	-0.700815000000
	H	-1.780880000000	1.107902000000	1.065656000000
	H	-1.717494000000	-1.085183000000	-1.024681000000
	H	-1.984392000000	-1.278321000000	0.728006000000
	H	0.657994000000	-0.100232000000	-1.479805000000

	C	2.090330000000	0.008430000000	0.150580000000
	H	2.621516000000	-0.896109000000	-0.146703000000
	H	2.612355000000	0.878376000000	-0.248342000000
	H	2.058780000000	0.072429000000	1.238464000000
	O	-0.024944000000	1.128675000000	0.019146000000
	O	-0.028936000000	-1.107364000000	0.167507000000
Frequencies	42.6909 197.4342 223.3367 332.8934 522.1315 709.5881 721.8884 862.1306 883.2982 904.875 965.8988 1089.7745 1116.1744 1126.9769 1154.2229 1177.2849 1201.1795 1243.5888 1266.5434 1353.4657 1382.3495 1396.2927 1401.4566 1461.5145 1490.6095 1492.0372 1523.931 1540.3439 2977.9155 3045.5233 3072.0233 3082.7028 3122.8639 3154.504 3167.4344 3171.1124			
Rotational constants (GHZ)	7.1082221 3.4417012 2.5441112			
ZPE (Hartree/Particle)	0.122060			
CCY(COCO)C				
Optimized Cartesian coordinate	C	-1.976999000000	0.681438000000	0.000020000000
	H	-2.608090000000	0.613670000000	-0.888284000000
	H	-2.608098000000	0.613608000000	0.888314000000
	H	-1.450430000000	1.636226000000	0.000055000000
	C	-0.982361000000	-0.443205000000	-0.000016000000
	H	-1.467400000000	-1.427877000000	-0.000045000000
	C	0.982361000000	-0.443206000000	-0.000010000000
	H	1.467403000000	-1.427876000000	-0.000037000000
	O	-0.000002000000	-0.358099000000	-1.030889000000
	O	0.000003000000	-0.358157000000	1.030872000000
	C	1.976997000000	0.681438000000	0.000016000000
	H	2.608106000000	0.613609000000	0.888303000000
	H	2.608080000000	0.613672000000	-0.888295000000
	H	1.450427000000	1.636226000000	0.000057000000
Frequencies	88.4539 210.1749 221.4745 348.8906 352.4774 460.4203 508.5072 780.9141 880.2296 895.4813 945.3077 955.396 1074.6515 1124.1667 1127.7264 1168.1314 1170.7198 1209.7603 1288.3569 1365.1804 1386.3973 1399.2835 1422.2501 1464.4348 1479.9617 1483.1199 1492.2435 1501.0863 3034.2559 3042.0761 3072.1236 3072.661 3153.45 3153.6076 3165.4213 3167.4482			
Rotational constants (GHZ)	7.4243061 2.7486974 2.6578679			
ZPE (Hartree/Particle)	0.119983			
CH3CHO				

Optimized Cartesian coordinate	C	1.164755000000	-0.147189000000	0.000006000000
	H	1.698074000000	0.222612000000	-0.879937000000
	H	1.148964000000	-1.235591000000	0.001182000000
	H	1.699330000000	0.224402000000	0.878429000000
	C	-0.234797000000	0.398753000000	0.000064000000
	H	-0.317577000000	1.504619000000	0.000027000000
	O	-1.226067000000	-0.278179000000	-0.000016000000
Frequencies	150.2409 513.8767 777.1461 900.8443 1137.4843 1144.404 1381.2442 1430.4519 1467.283 1476.3944 1872.8273 2945.0324 3063.6222 3129.9179 3181.6598			
Rotational constants (GHZ)	57.1335322 10.2259735 9.1636106			
ZPE (Hartree/Particle)	0.055980			
HOC2OC2-1O				
Optimized Cartesian coordinate	C	0.020716000000	0.067059000000	0.013647000000
	H	0.030618000000	0.123220000000	1.107641000000
	H	1.053032000000	0.125109000000	-0.348283000000
	C	-0.765658000000	1.237524000000	-0.537258000000
	H	-0.778472000000	1.191520000000	-1.633957000000
	H	-1.802271000000	1.188453000000	-0.179391000000
	O	-0.139671000000	2.419992000000	-0.094293000000
	C	-0.782332000000	3.585688000000	-0.547971000000
	H	-1.820830000000	3.624844000000	-0.192853000000
	H	-0.794769000000	3.624987000000	-1.645433000000
	C	-0.005220000000	4.771449000000	0.000879000000
	H	1.050051000000	4.727827000000	-0.319057000000
	H	0.043401000000	4.729855000000	1.102539000000
	O	-0.629012000000	-1.104999000000	-0.444018000000
	H	-0.156139000000	-1.874003000000	-0.121010000000
	O	-0.512260000000	5.986198000000	-0.359956000000
Frequencies	56.5234 68.9429 110.1786 129.2522 154.2226 209.3981 277.3289 337.6305 389.882 472.2443 550.6028 841.1699 907.8274 1040.9527 1059.1657 1090.3186 1120.5283 1130.8083 1163.9405 1209.645 1220.7626 1247.5217 1254.3481 1290.6129 1313.0858 1329.1342 1374.9913 1399.2868 1449.4505 1488.721 1520.5336 1533.7198 1540.8081 2969.7429 2989.4516 3016.6126 3024.4326 3042.6675 3059.0146 3062.091 3092.0446 3923.8749			
Rotational constants (GHZ)	16.41192 0.81488 0.79168			
ZPE (Hartree/Particle)	0.133190			

HOC2OC2-2O	
Optimized Cartesian coordinate	C -2.026269000000 -0.514334000000 -0.232803000000 H -2.023089000000 -1.485138000000 0.274996000000 H -1.957918000000 -0.684790000000 -1.312586000000 C -0.825928000000 0.289253000000 0.218665000000
R1-P15	H -0.802530000000 1.251171000000 -0.301752000000
Optimized Cartesian coordinate	H -0.840892000000 -0.457563000000 0.299486000000 H -3.071486000000 -0.847905000000 0.125470000000 H -3.925061000000 -0.345982000000 -0.499243000000 H -3.286871000000 -0.472683000000 -0.083414000000 C -1.322778000000 0.347653000000 -0.228614000000 H -1.650887000000 0.254558000000 -1.007138000000 C -0.659206000000 -0.833402000000 -0.023168000000 H 2.707859000000 -0.494677000000 -0.997295000000 H 0.644848000000 -0.400883000000 -0.421472000000 H 2.407434000000 -0.066446000000 -0.568535000000 C 2.372822000000 -0.036482000000 -0.316967000000
Frequencies	50.74963 2953.40650000 38.8030 383.44580000 3.4215 0.02145000 311.8328 336.1451 405.2928 525.0447 605.7252 839.6414 889.2557 918.4565 1014.8343 1047.473 1073.9243 1122.9061 1164.0224 1167.3265 1192.01 1218.0415 1247.2068 1256.6679 1313.941 1326.0989 1388.1993 1398.9459 1481.9551 1483.8305 1496.5416 1528.338 1538.4975 2896.0098 3028.5199 3042.8915 3080.2733 3091.1453 3106.0422 3178.5805 3189.4561 3925.4917
Rotational constants (GHZ)	7.6971477 1.1279679 1.0283207
ZPE (Hartree/Particle)	0.133711

	H	2.568737000000	1.015960000000	0.245845000000
	H	2.164694000000	-0.300368000000	1.355930000000
Frequencies		-762.7616 42.8187 91.1764 103.0856 152.8222 196.1625 319.7484 498.7125 681.4317 703.749 833.3524 884.9177 913.0798 1024.1191 1044.8501 1098.6973 1121.5013 1220.7302 1325.7705 1392.7669 1401.2927 1455.8945 1476.3621 1481.9382 1482.5315 1492.218 1507.7514 3019.7222 3041.3622 3042.4613 3105.409 3111.587 3146.2504 3146.9219 3154.96 3243.7328		
Rotational constants (GHZ)		13.1670211 2.2148354	2.1171776	
ZPE (Hartree/Particle)		0.118373		
R1-P17				
Optimized Cartesian coordinate	C	-2.368058000000	-0.237253000000	-0.160318000000
	H	-2.834290000000	-0.748361000000	1.813465000000
	H	-2.410343000000	-1.302623000000	-0.344292000000
	H	-3.283202000000	0.335885000000	-0.180318000000
	C	-1.193091000000	0.395828000000	-0.074736000000
	H	-1.124605000000	1.473257000000	0.060970000000
	O	-0.018984000000	-0.265935000000	-0.116521000000
	C	1.142541000000	0.527383000000	0.108462000000
	H	1.181604000000	1.330633000000	-0.636339000000
	H	1.083033000000	0.981387000000	1.103953000000
	C	2.349657000000	-0.375814000000	-0.004599000000
	H	3.263921000000	0.196173000000	0.162445000000
	H	2.295339000000	-1.173993000000	0.736551000000
	H	2.394116000000	-0.825736000000	-0.997123000000
Frequencies		-456.1625 46.2031 86.328 205.9479 234.4303 252.8075 320.2523 443.3987 502.5691 754.8052 823.7154 872.3629 900.4434 978.9147 1001.7777 1111.0491 1176.2737 1184.9627 1252.5397 1315.1931 1397.4923 1423.6493 1448.6425 1487.8827 1506.0728 1530.299 1694.4524 3035.2782 3076.4999 3076.7 3155.1035 3159.3809 3164.6133 3197.1306 3298.384		
Rotational constants (GHZ)		19.8366486 2.2547956	2.1500527	
ZPE (Hartree/Particle)		0.114946		
R1-R2				
Optimized Cartesian coordinate	C	2.071483000000	-0.264319000000	-0.189030000000
	H	2.660679000000	0.658793000000	-0.200457000000
	H	1.931011000000	-0.584674000000	-1.222945000000
	H	2.639667000000	-1.025841000000	0.347970000000

	C	0.746003000000	-0.033144000000	0.468322000000
	H	0.775331000000	0.129273000000	1.553178000000
	O	-0.035615000000	0.901737000000	-0.201510000000
	C	-1.407314000000	0.537788000000	-0.007334000000
	H	-1.742853000000	0.879082000000	0.979875000000
	H	-1.982664000000	1.056889000000	-0.774313000000
	C	-1.463319000000	-0.971557000000	-0.092240000000
	H	-2.103326000000	-1.502917000000	0.605263000000
	H	-1.448266000000	-1.395122000000	-1.094027000000
	H	-0.125780000000	-1.041995000000	0.339226000000
Frequencies	-1761.3469	133.7881	190.4316	223.5615
	562.9695	680.1071	845.3822	886.5014
	1033.1594	1065.7079	1123.962	1174.1015
	1278.6815	1352.0875	1384.2706	1435.1919
	1479.5971	1494.3932	1520.7499	1722.1269
	3049.5773	3117.9881	3124.7203	3133.0302
Rotational constants (GHZ)	10.3533248	3.3482992	2.8480579	
ZPE (Hartree/Particle)	0.119251			
R2-P16				
Optimized Cartesian coordinate	C	2.149829000000	-0.637766000000	0.169217000000
	H	2.049928000000	-1.535521000000	-0.429326000000
	H	2.524930000000	-0.752430000000	1.178547000000
	C	1.739116000000	0.568838000000	-0.293306000000
	H	1.933407000000	1.471605000000	0.269189000000
	H	1.461949000000	0.697533000000	-1.332555000000
	O	-0.184546000000	0.632023000000	0.337130000000
	C	-0.938330000000	-0.410783000000	-0.198457000000
	H	-0.714700000000	-1.367872000000	0.288773000000
	H	-0.760091000000	-0.519858000000	-1.277953000000
	C	-2.404717000000	-0.047981000000	0.040582000000
	H	-2.648854000000	0.892516000000	-0.454427000000
	H	-3.048937000000	-0.835591000000	-0.356163000000
	H	-2.596649000000	0.059586000000	1.108665000000
Frequencies	-580.3789	70.4712	87.8906	165.7023
	403.0431	429.227	823.0691	829.6619
	998.4576	1020.9176	1047.2397	1162.3705
	1284.7856	1314.7454	1363.5923	1394.0849
	1504.2414	1534.7577	1592.7811	2998.8201
	3147.6925	3158.8245	3168.4676	3180.6534
Rotational constants (GHZ)	13.7080944	2.2608140	2.1093217	

ZPE (Hartree/Particle)	0.120739			
R2-P17				
Optimized Cartesian coordinate	C	1.085245000000	0.520775000000	-0.002337000000
	O	-0.051683000000	-0.332659000000	-0.035026000000
	H	1.076413000000	1.171313000000	-0.885565000000
	H	1.027825000000	1.154838000000	0.890678000000
	C	2.321641000000	-0.349337000000	0.019504000000
	H	3.217779000000	0.272704000000	0.051115000000
	H	2.313797000000	-0.994744000000	0.898609000000
	H	2.361699000000	-0.976725000000	-0.871853000000
	C	-1.242175000000	0.293962000000	-0.178063000000
	H	-1.210959000000	1.256605000000	-0.685666000000
	H	-1.192573000000	1.330970000000	1.403395000000
	C	-2.403151000000	-0.355912000000	0.029041000000
	H	-2.410993000000	-1.350739000000	0.453475000000
	H	-3.338880000000	0.140123000000	-0.182844000000
Frequencies	-834.4094 70.6149 129.6786 216.9213 254.123 425.2768 461.3625 500.95 512.6779 686.4335 823.8841 848.5007 875.6876 995.0713 1038.2784 1110.0318 1173.4121 1184.7388 1244.8363 1309.0292 1324.7243 1394.2034 1419.7997 1446.8066 1488.4496 1505.6457 1527.8202 1647.0327 3028.1899 3067.8584 3075.6271 3150.6728 3154.0516 3157.9125 3195.5461 3300.521			
Rotational constants (GHZ)	20.02259 2.33334 2.20380			
ZPE (Hartree/Particle)	0.115609			
W1-P1				
Optimized Cartesian coordinate	C	2.843031000000	0.175242000000	0.035072000000
	H	3.033426000000	0.829960000000	-0.816240000000
	H	2.948182000000	0.756172000000	0.952229000000
	H	3.592048000000	-0.618334000000	0.038927000000
	C	1.459854000000	-0.427278000000	-0.053322000000
	H	1.240756000000	-1.076693000000	0.795472000000
	H	1.327631000000	-1.008138000000	-0.972073000000
	O	0.519338000000	0.657646000000	-0.070967000000
	C	-0.790149000000	0.319693000000	-0.087926000000
	H	-1.074924000000	-0.503887000000	-1.075071000000
	C	-1.706199000000	1.509435000000	-0.073313000000
	H	-1.420299000000	2.212310000000	-0.853926000000
	H	-2.732873000000	1.178570000000	-0.220366000000
	H	-1.625231000000	2.001404000000	0.899662000000

	O	-1.159338000000	-0.713990000000	0.752985000000
	O	-1.375992000000	-1.597895000000	-0.390978000000
Frequencies	-1667.5694 49.4981 115.2718 133.0811 201.1881 207.4205 254.9322 363.2969 382.0944 458.6438 568.5373 689.8549 819.212 871.0313 922.0062 937.5283 1011.1149 1070.7377 1103.9616 1123.6802 1140.071 1184.6431 1283.4708 1302.9221 1319.3193 1403.9635 1410.6262 1443.8583 1480.3159 1486.6813 1490.4288 1506.7057 1530.7152 1966.4701 3064.1546 3074.2092 3075.49 3126.9961 3154.6927 3157.3841 3158.8631 3188.6996			
Rotational constants (GHZ)	4.26055 1.76223 1.36600			
ZPE (Hartree/Particle)	0.128110			
W1-P3				
Optimized Cartesian coordinate	C	-0.431774000000	0.800659000000	0.465465000000
	O	0.700191000000	0.608920000000	-0.191059000000
	H	-0.407074000000	0.627229000000	1.538433000000
	C	-1.508866000000	1.422348000000	-0.162576000000
	H	-2.141808000000	0.292598000000	-0.460497000000
	H	-2.200868000000	1.948921000000	0.485018000000
	H	-1.301513000000	1.881150000000	-1.123979000000
	C	1.651054000000	-0.265032000000	0.437032000000
	H	1.205864000000	-1.260044000000	0.499828000000
	H	1.846070000000	0.103374000000	1.449881000000
	C	2.905548000000	-0.261390000000	-0.404391000000
	H	3.320462000000	0.745031000000	-0.471830000000
	H	3.652776000000	-0.918818000000	0.042783000000
	H	2.686455000000	-0.618296000000	-1.411158000000
	O	-1.234882000000	-1.235218000000	0.287407000000
	O	-2.259826000000	-0.996284000000	-0.416554000000
Frequencies	-1065.4775 46.419 116.3058 140.7223 190.6896 241.6882 266.4648 407.2196 454.739 476.9833 545.0923 650.152 688.2885 823.3095 881.6009 978.5496 996.2274 1023.6374 1111.8624 1151.2783 1185.0919 1274.525 1313.0457 1323.4508 1338.4946 1389.9205 1403.9332 1429.9676 1450.0965 1489.9589 1506.848 1526.5906 1618.8098 1646.3724 3057.2839 3078.2887 3122.2319 3152.6918 3157.2685 3163.017 3175.0302 3246.986			
Rotational constants (GHZ)	4.54981 1.45943 1.21413			
ZPE (Hartree/Particle)	0.128127			
W1-W2				

Optimized Cartesian coordinate	C	-0.555956000000	0.255287000000	0.345700000000	
	O	0.701005000000	0.486970000000	-0.143965000000	
	H	-0.552883000000	0.096693000000	1.433569000000	
	C	-1.527538000000	1.346764000000	-0.061270000000	
	H	-2.498602000000	0.405130000000	-0.092411000000	
	H	-1.756660000000	2.124424000000	0.659772000000	
	H	-1.411116000000	1.676925000000	-1.091128000000	
	C	1.694657000000	-0.415764000000	0.348371000000	
	H	1.429881000000	-1.434851000000	0.051306000000	
	H	1.707860000000	-0.366350000000	1.444191000000	
	C	3.026152000000	-0.000974000000	-0.234742000000	
	H	3.269476000000	1.020687000000	0.060209000000	
	H	3.815258000000	-0.665688000000	0.120774000000	
	H	2.992837000000	-0.050322000000	-1.323642000000	
	O	-1.093753000000	-0.922031000000	-0.282184000000	
	O	-2.459745000000	-0.804755000000	-0.030226000000	
Frequencies	-2172.4964	54.6741	99.5361	149.4567	224.7588
	256.5424	358.5194	426.1372	438.4619	561.0662
	609.5632	687.4134	822.3262	896.0987	917.9904
	997.0358	1033.1789	1056.8058	1100.3874	1116.9262
	1137.253	1175.9628	1185.8516	1248.313	1316.0477
	1344.6823	1385.7068	1410.0015	1442.2136	1477.5717
	1489.1116	1505.5882	1530.9036	1758.6754	3028.6783
	3038.1178	3075.6927	3091.9291	3136.9426	3153.9028
	3158.7601	3240.5665			
Rotational constants (GHZ)	6.64151	1.38979	1.22030		
ZPE (Hartree/Particle)	0.127895				
W1-W3					
Optimized Cartesian coordinate	C	1.005522000000	-0.192473000000	0.324379000000	
	O	-0.217377000000	-0.854133000000	0.058298000000	
	H	1.047793000000	0.089968000000	1.383667000000	
	C	2.143296000000	-1.066775000000	-0.124525000000	
	H	3.091155000000	-0.562091000000	0.058834000000	
	H	2.119390000000	-2.005656000000	0.427720000000	
	H	2.040460000000	-1.273993000000	-1.189732000000	
	C	-1.324747000000	-0.114320000000	0.428008000000	
	H	-0.905324000000	1.114764000000	0.150711000000	
	H	-1.429387000000	-0.030612000000	1.516974000000	
	C	-2.551392000000	-0.514587000000	-0.333991000000	
	H	-2.805274000000	-1.558031000000	-0.121635000000	
	H	-3.397058000000	0.111433000000	-0.048173000000	

	H	-2.378952000000	-0.416673000000	-1.406405000000
	O	1.013807000000	0.980483000000	-0.452324000000
	O	0.076210000000	1.856127000000	0.077128000000
Frequencies	-1811.4446	125.3995	174.5026	198.6705
	289.2685	319.8224	419.9137	472.1545
	572.0992	633.964	860.1912	883.7873
	975.5129	1072.1446	1109.1909	1138.0755
	1172.3917	1196.327	1227.6566	1288.3685
	1382.4864	1396.5672	1421.3485	1450.0485
	1488.1743	1492.3089	1495.6973	1668.4403
	3057.2269	3058.1974	3090.3892	3131.6393
	3176.4318	3179.0448		3163.7888
Rotational constants (GHZ)	4.02912	2.04035	1.48377	
ZPE (Hartree/Particle)	0.128546			
W1-W4				
Optimized Cartesian coordinate	C	0.913339000000	-0.098642000000	0.292361000000
	O	0.090467000000	-1.135578000000	-0.156126000000
	H	0.801173000000	0.030078000000	1.376550000000
	C	2.327208000000	-0.406724000000	-0.132956000000
	H	2.999231000000	0.380089000000	0.207491000000
	H	2.632766000000	-1.361550000000	0.292938000000
	H	2.368790000000	-0.473268000000	-1.220629000000
	C	-1.250986000000	-1.116799000000	0.309994000000
	H	-1.266173000000	-0.953670000000	1.395697000000
	H	-1.645993000000	-2.118402000000	0.116171000000
	C	-2.079696000000	-0.072365000000	-0.387029000000
	H	-3.080975000000	0.080911000000	0.010015000000
	H	-1.419118000000	1.060992000000	-0.076463000000
	H	-2.010460000000	-0.076550000000	-1.473282000000
	O	0.578235000000	1.143546000000	-0.312616000000
	O	-0.523507000000	1.691851000000	0.328404000000
Frequencies	-1890.8815	127.8098	185.7275	208.1003
	329.7517	365.5187	436.0364	538.6855
	593.4314	676.5526	833.2562	865.1895
	948.6596	1067.2699	1075.3769	1086.933
	1158.1661	1175.1796	1194.6174	1236.3886
	1376.0017	1387.5803	1414.6395	1435.5252
	1486.6878	1490.659	1497.1096	1498.9003
	3051.8824	3087.2634	3088.6306	3117.284
	3179.3886	3213.6741		3172.3856
Rotational	3.92545	2.36744	1.62447	

constants (GHZ)					
ZPE (Hartree/Particle)	0.128192				
W2-P2					
Optimized Cartesian coordinate	C	0.72053100	-0.54471300	0.40873700	
	O	-0.56235400	-0.73952000	-0.04476800	
	H	0.75405300	-0.26006300	1.46659400	
	C	1.64948900	-1.58706500	-0.04367300	
	H	2.56390800	-1.77734800	0.49573300	
	H	1.44196000	-2.08483500	-0.97890600	
	C	-1.43411300	0.37546400	0.15939900	
	H	-1.12355500	1.19727600	-0.48901200	
	H	-1.34411600	0.71491300	1.19884200	
	C	-2.84200300	-0.08345500	-0.14884600	
	H	-3.13336700	-0.90150500	0.51177300	
	H	-3.54371700	0.74189500	-0.01548400	
	H	-2.90800100	-0.43121900	-1.18085100	
	O	1.52413400	0.28160000	-0.36138300	
	O	1.12563500	1.90826300	0.00805100	
	H	2.03008700	2.23676000	-0.07759300	
Frequencies	-1002.2514	71.8138	94.1736	144.7823	164.2985
	208.3538	253.4349	260.7122	357.5525	397.2024
	481.4514	547.4976	631.9216	784.9858	820.6369
	865.9245	967.9332	994.3051	1058.1861	1096.7937
	1155.4489	1178.0415	1187.26	1220.6592	1314.1391
	1327.6484	1387.0228	1409.4103	1443.025	1487.5418
	1490.0077	1505.929	1534.491	3040.3925	3066.4867
	3072.6974	3114.1776	3150.8851	3154.4664	3206.4155
	3336.3053	3863.5331			
Rotational constants (GHZ)	3.84737	1.79290	1.29468		
ZPE (Hartree/Particle)	0.129509				
W2-P3					
Optimized Cartesian coordinate	C	0.78010600	-0.88638500	0.32951200	
	O	-0.40929300	-0.74157500	-0.26285500	
	H	0.77712500	-1.02280700	1.40809100	
	C	1.85083500	-1.30097300	-0.43230000	
	H	2.78952500	-1.53791200	0.04459300	
	H	1.77989700	-1.29436700	-1.51163400	
	C	-1.43154700	-0.15860400	0.55182100	
	H	-1.06150700	0.78640400	0.95484100	

	H	-1.64887000	-0.84130600	1.38163200
	C	-2.64483400	0.05288300	-0.32340900
	H	-2.98421100	-0.89326300	-0.74750300
	H	-3.45756600	0.48536800	0.26260500
	H	-2.39833700	0.73562600	-1.13733500
	O	1.34948300	0.96635900	0.59786400
	O	0.73840800	1.70517000	-0.38486500
	H	1.44779800	1.90110500	-1.01019100
Frequencies	-673.9401	26.4007	119.2433	152.5418
	229.7972	242.526	284.5628	366.5861
	488.0836	508.3469	576.722	765.9615
	872.0706	942.1511	997.479	1082.3868
	1163.1226	1186.2632	1255.902	1280.6618
	1392.2466	1400.9736	1420.3064	1448.2709
	1505.7316	1521.0489	1559.8347	3046.6098
	3119.581	3153.3091	3159.6829	3167.2027
	3308.9068	3816.4029		3193.1886
Rotational constants (GHZ)	3.62173	1.87453	1.42861	
ZPE (Hartree/Particle)	0.130281			
W2-W3				
Optimized Cartesian coordinate	C	-0.65426900	0.50761300	0.47141000
	O	0.35423300	-0.48761400	0.55979500
	H	-1.12439700	0.56134100	1.45443200
	C	-0.00638600	1.76349100	-0.04731700
	H	0.48564800	2.37171600	0.70606100
	H	-0.55539200	2.31756300	-0.80115500
	C	1.29550000	-0.28121300	-0.46330600
	H	1.01111200	1.00864400	-0.63801800
	H	1.01228100	-0.75438000	-1.40664300
	C	2.70124900	-0.51365400	-0.00385400
	H	2.83358300	-1.55220600	0.31707100
	H	3.40665700	-0.31321800	-0.81196300
	H	2.93623800	0.13102100	0.84524400
	O	-1.61617000	0.13285400	-0.48597200
	O	-2.28910600	-1.01112800	0.00932400
	H	-1.61395200	-1.70080000	-0.07180600
Frequencies	-1743.1733	84.3415	137.9697	155.2913
	270.3645	335.4995	386.1446	404.5395
	600.1934	631.2468	779.3953	871.5766
	906.0072	933.4971	1046.0828	1053.6394
	1114.6741	1147.6125	1169.0841	1181.3806
				1344.9846

	1361.4961	1387.8805	1393.2541	1426.8462	1435.1814
	1451.6638	1478.7639	1493.4299	1733.82	3050.0256
	3094.6939	3118.9429	3123.9873	3147.4814	3151.1321
	3242.2256	3790.8602			
Rotational constants (GHZ)	4.83325	1.70723	1.41093		
ZPE (Hartree/Particle)	0.127814				
W3-P4					
Optimized Cartesian coordinate	C	0.82593800	1.91506900	-0.22923800	
	H	0.51636900	2.58456100	0.57321700	
	H	0.03792700	1.89400000	-0.98489600	
	H	1.74090900	2.30578100	-0.68781800	
	C	1.01929100	0.55566300	0.33431000	
	H	1.62990100	0.37674700	1.21109000	
	O	-0.71424000	0.18434600	1.11945700	
	C	-1.43416400	-0.57363200	0.42508500	
	H	-1.36323100	-1.65816800	0.56635900	
	C	-2.30640400	-0.05771000	-0.67898500	
	H	-2.50565700	1.00545400	-0.53217900	
	H	-1.81461400	-0.19025200	-1.65087300	
	H	-3.25227100	-0.60371900	-0.71939800	
	O	1.13128800	-0.38498000	-0.64109400	
	O	1.37035900	-1.64511900	-0.01717200	
	H	2.08345600	-1.98472600	-0.57205800	
Frequencies	-662.2219	46.4223	93.8758	117.1812	128.1697
	164.7042	180.1941	215.0228	240.6652	298.2136
	442.9622	508.4621	528.553	712.1794	826.8456
	906.0879	910.2635	1023.7224	1036.7103	1044.9288
	1121.9457	1155.5615	1205.9321	1333.3558	1373.0772
	1390.2175	1419.8601	1436.1073	1459.9634	1473.338
	1475.3518	1491.8002	1517.8959	3029.423	3044.7147
	3065.9506	3098.8728	3119.7941	3145.4795	3161.3756
	3209.3198	3850.7864			
Rotational constants (GHZ)	3.06136	2.06971	1.56791		
ZPE (Hartree/Particle)	0.127589				
W3-P5					
Optimized Cartesian coordinate	C	0.60405000	0.54211400	-0.43819000	
	O	-0.73219600	1.00873400	-0.35912400	
	H	0.95744500	0.55513800	-1.47646400	

	C	1.48063600	1.34008900	0.48674600
	H	2.51798800	1.02530800	0.39669400
	H	1.39219900	2.39543900	0.22135500
	H	1.14191500	1.19576100	1.51329200
	C	-1.43693300	-0.16211200	-0.46083100
	H	-1.52251200	-0.58354700	-1.45996700
	C	-2.49282400	-0.38870800	0.54816500
	H	-3.30606800	0.33738100	0.41899200
	H	-2.90976800	-1.39119300	0.44967300
	H	-2.08158900	-0.25734600	1.55050700
	O	0.39514600	-0.82483000	-0.04514800
	O	1.97186000	-1.31271000	0.11453200
	H	1.80232900	-2.23479900	-0.11149900
Frequencies	-1059.5733	73.1419	104.1319	141.2773
	191.4595	247.8172	297.3455	364.9306
	451.8094	499.5252	653.295	767.9051
	913.6812	963.986	1033.3526	1097.4881
	1150.6479	1164.683	1193.0984	1221.0977
	1380.2982	1392.6721	1424.9271	1448.6275
	1478.5465	1484.9596	1493.631	3030.8225
	3081.1871	3114.51	3147.8504	3160.7021
	3188.5521	3882.1485		3167.0977
Rotational constants (GHZ)	4.18321	1.89267	1.48003	
ZPE (Hartree/Particle)	0.129519			
W4-P1				
Optimized Cartesian coordinate	C	1.72522700	-0.67026300	0.95123300
	H	2.20592500	-0.09267900	1.73640400
	H	1.75972800	-1.74377300	1.10763200
	C	1.87883400	-0.15457900	-0.46023200
	H	2.80979200	0.38200300	-0.63936400
	H	1.77669800	-0.95679600	-1.19401400
	O	0.81826900	0.81119800	-0.67035600
	C	-0.27789600	0.42007000	0.03914400
	H	0.37396900	-0.24783900	0.98656600
	C	-1.15894700	1.54270200	0.48770900
	H	-1.49289700	2.10964900	-0.38678900
	H	-2.02868300	1.15103200	1.01332100
	H	-0.59802700	2.20542300	1.14644600
	O	-0.93196500	-0.58114500	-0.71346100
	O	-1.91830000	-1.17670400	0.11848300
	H	-1.55384500	-2.06139400	0.24535200

Frequencies	-1770.8309 80.9933 135.3143 157.8718 176.7411 197.5134 293.2085 315.4675 408.3154 528.5261 540.0437 601.6574 692.2927 845.5678 882.9154 920.0767 963.1291 1031.0411 1036.0939 1058.7189 1119.6458 1169.3178 1187.6514 1269.658 1289.2095 1386.061 1396.8542 1403.8435 1433.1184 1462.2484 1481.359 1485.3562 1522.9497 1721.4602 3062.9618 3089.4095 3137.3331 3145.7493 3147.836 3178.692 3227.5642 3844.3288				
Rotational constants (GHZ)	3.75768 2.03124 1.68108				
ZPE (Hartree/Particle)	0.127641				
W4-P6					
Optimized Cartesian coordinate	C 1.90285400 -0.17737800 0.33028000 H 2.83951200 -0.66298000 0.04508300 H 1.92745000 0.03475900 1.40632300 O 0.87560300 -1.10994100 0.03187200 C -0.37510100 -0.56236800 0.32794400 H -0.51763100 -0.49513300 1.41501900 C -1.42473200 -1.41144800 -0.34362400 H -2.42090400 -1.05395000 -0.09498900 H -1.27807400 -1.36662000 -1.42346500 H -1.30753800 -2.44261200 -0.00760800 C 1.62046700 1.05497700 -0.45275000 H 1.76527800 2.03104200 -0.01131000 H 1.63139600 0.98693900 -1.53210900 O -0.37702400 0.80068300 -0.16524700 O -1.90697400 1.23148300 0.21923600 H -1.71325400 2.16805800 0.34507200				
Frequencies	-1061.5813 73.8988 127.5056 166.25 219.0082 274.4881 291.4405 337.605 428.6524 485.6193 542.8688 599.6761 630.0194 814.3254 856.3066 877.5066 928.1153 1045.1357 1083.1473 1121.1118 1142.3733 1155.417 1182.9322 1196.3885 1295.8779 1358.1845 1388.2847 1395.936 1438.6638 1470.6038 1486.6328 1494.9529 1503.0923 3034.9195 3039.1202 3086.691 3101.8257 3164.3475 3180.8929 3196.3572 3290.7815 3879.5229				
Rotational constants (GHZ)	3.86172 2.28942 1.58358				
ZPE (Hartree/Particle)	0.130736				

W4-P7	
Optimized Cartesian coordinate	C 0.96146400 -0.06292500 0.29691600 O 0.10730500 -0.96089900 -0.37052100 H 0.79387300 -0.16445700 1.37984700 C 2.39014300 -0.38593600 -0.08719600 H 3.07625200 0.31992500 0.38039700 H 2.63136500 -1.39767600 0.23895600 H 2.48985500 -0.32426900 -1.17113000 C -1.17382300 -1.16250500 0.21862900 H -1.07536600 -1.19754500 1.31035700 H -1.49551800 -2.15197700 -0.12022900 C -2.18259500 -0.12470500 -0.16526000 H -2.39139600 0.00342300 -1.22078000 H -2.98459100 0.10035500 0.52592800 O 0.74856100 1.26814300 -0.07237700 O -0.85219400 1.35254400 0.15305200 H -1.04498500 1.95033800 -0.58311300
Frequencies	-1262.7852 122.8544 164.7565 217.2362 271.5288 327.3804 337.9577 417.8003 458.7185 484.5398 562.2645 576.4642 607.2747 811.6042 856.7236 872.2546 927.0431 1013.8604 1087.0497 1117.7277 1127.1886 1149.7411 1184.1989 1215.2993 1317.0272 1369.0568 1388.1837 1411.5589 1439.124 1460.3149 1486.2617 1490.9539 1495.3061 3008.9512 3041.72 3083.047 3089.9676 3164.3727 3168.3573 3170.9197 3272.806 3847.0931
Rotational constants (GHZ)	4.50716 2.20892 1.59468
ZPE (Hartree/Particle)	0.131260
W4-P8	
Optimized Cartesian coordinate	C 2.33923100 0.39292800 0.25176400 H 2.23089000 0.78529100 1.25552800 H 2.81880900 1.03727800 -0.47227300 O 0.50058700 1.15753800 -0.37309200 C -0.51032400 0.47974400 0.20502400 H -0.31671200 0.21017600 1.25374600 C -1.77842400 1.32438500 0.09228200 H -1.94731200 1.57902700 -0.95440000 H -2.62312100 0.75184900 0.47782500 H -1.66757600 2.23751000 0.67608900 O -0.66709100 -0.76325700 -0.51378300

	O	-1.51502000	-1.59090400	0.27543400	
	H	-2.24274300	-1.75836800	-0.33447500	
	C	2.14158900	-0.92150900	-0.00776900	
	H	2.31758200	-1.33040200	-0.99444500	
	H	1.72993100	-1.59266000	0.73613000	
Frequencies	-411.5843	75.0956	81.9846	113.6965	178.9347
	215.5156	220.0669	255.4994	308.9686	390.2771
	424.5883	502.8729	549.2592	825.5148	873.6673
	936.6673	958.397	1003.0954	1011.0536	1036.1254
	1082.3439	1116.6693	1210.4608	1237.5113	1326.0517
	1332.84	1367.2067	1382.1199	1403.0273	1472.0089
	1487.8542	1490.5073	1602.4287	3012.3785	3078.4168
	3164.5141	3173.1581	3174.8199	3183.1058	3261.4628
	3284.9378	3857.6636			
Rotational constants (GHZ)	3.61589	1.90192	1.35049		
ZPE (Hartree/Particle)	0.129087				
W5-P9					
Optimized Cartesian coordinate	C	-1.50713700	-0.45031500	-0.20953200	
	O	-1.08625900	0.87260100	0.09841500	
	H	-1.29088900	-0.66335200	-1.26458800	
	H	-0.94859200	-1.17657800	0.39358600	
	C	-2.98985800	-0.54216800	0.07647000	
	H	-3.35364900	-1.54869800	-0.13777400	
	H	-3.18692400	-0.31653800	1.12554800	
	H	-3.54131000	0.16893700	-0.54008100	
	C	0.23563000	1.16023300	-0.28837000	
	H	0.37531400	2.22994400	-0.12601000	
	H	0.40015800	0.92670700	-1.34840900	
	C	1.23657500	0.38806400	0.53428300	
	H	2.47208400	0.66379800	0.14570800	
	H	1.21365800	0.49611600	1.62020200	
	O	1.49730800	-0.90775400	0.11411300	
	O	2.84006200	-0.47924900	-0.28069000	
Frequencies	-1828.6875	63.4941	94.7135	117.068	146.2179
	237.2228	274.761	338.5232	426.4703	535.3302
	644.3078	828.131	866.8941	888.6846	927.6652
	940.4109	1059.8689	1097.2026	1098.3387	1152.8955
	1173.0284	1183.4447	1192.9903	1296.0997	1333.2739
	1367.9125	1404.3415	1421.4999	1454.9913	1483.2288
	1488.891	1506.2124	1533.5541	2015.8039	3029.5309

	3040.8313	3060.3877	3068.6198	3126.7767	3137.3845
	3138.8832	3149.2131			
Rotational constants (GHZ)	6.47588	1.27511	1.13473		
ZPE (Hartree/Particle)	0.128364				
W5-W6					
Optimized Cartesian coordinate	C	-1.92245700	0.29339600	0.44826300	
	O	-0.76569600	-0.32447500	-0.10946300	
	H	-2.13557100	-0.16368100	1.42241800	
	H	-1.71009100	1.35648900	0.60621400	
	C	-3.07081900	0.10017900	-0.51563400	
	H	-3.97330600	0.57013300	-0.12150900	
	H	-2.83416700	0.55155900	-1.47958300	
	H	-3.26717000	-0.96197000	-0.66673900	
	C	0.33662000	-0.29575600	0.68321000	
	H	0.13574500	-0.50466700	1.73929100	
	H	0.99847300	0.84259700	0.61618500	
	C	1.53419600	-0.98166100	0.03571100	
	H	2.22366600	-1.31854200	0.81587900	
	H	1.25709100	-1.79843900	-0.63126600	
	O	2.13094300	0.03075300	-0.75476800	
	O	2.13976500	1.13491800	0.08795800	
Frequencies	-2172.9116	59.1664	81.585	148.6147	201.2291
	259.4742	321.15	416.1125	446.405	595.3861
	761.5406	820.5113	887.4555	932.7271	969.1398
	1007.2259	1064.5724	1071.4602	1103.3699	1166.1716
	1184.0993	1242.7312	1258.8222	1286.7686	1316.431
	1350.9218	1389.6176	1416.1127	1458.1194	1485.0773
	1489.6044	1504.6858	1526.4095	1739.2871	3034.4137
	3065.7475	3077.1194	3078.2729	3081.7866	3154.7949
	3156.0969	3161.5205			
Rotational constants (GHZ)	6.69643	1.19823	1.15649		
ZPE (Hartree/Particle)	0.129336				
W5-W7					
Optimized Cartesian coordinate	C	1.18946500	-0.04440500	0.37078900	
	O	0.64843800	1.04678200	-0.27674100	
	H	1.05290500	0.00236700	1.45990500	
	H	0.43154200	-1.03981300	0.07419800	

	C	2.58210600	-0.32807300	-0.10860300
	H	2.97625300	-1.22173600	0.37592700
	H	2.58641500	-0.47667700	-1.18927100
	H	3.23849500	0.51608000	0.12373200
	C	-0.66227300	1.39778400	0.15010800
	H	-0.87046000	2.37216000	-0.29492600
	H	-0.67778300	1.49557500	1.24333100
	C	-1.72363800	0.40469200	-0.28522600
	H	-2.70858900	0.78277200	-0.00002000
	H	-1.68980600	0.23356500	-1.36421200
	O	-1.59666900	-0.84610700	0.38483200
	O	-0.63338500	-1.60620900	-0.25697400
Frequencies	-1930.094	108.0024	175.3823	221.6318
	293.8661	353.3741	406.8683	494.8829
	615.0194	843.5598	870.4618	918.1526
	1007.7141	1098.4099	1117.4913	1122.648
	1170.1387	1216.1656	1299.6216	1303.6447
	1374.8599	1400.2879	1419.0406	1428.802
	1480.2429	1488.5992	1497.0071	1562.4235
	3041.3473	3058.6789	3077.1701	3130.657
	3137.9409	3162.5486		3132.8713
Rotational constants (GHZ)	4.11361	2.05198	1.48948	
ZPE (Hartree/Particle)	0.129277			
W5-W8				
Optimized Cartesian coordinate	C	-1.81316200	0.21939700	-0.08293500
	O	-0.85456300	1.15173400	0.37433000
	H	-2.73253000	0.45139800	0.46791900
	H	-2.02296200	0.38297500	-1.14804300
	C	-1.43529700	-1.21339800	0.17257200
	H	-2.07230900	-1.95700200	-0.30363900
	H	-0.19395600	-1.41652300	-0.36067000
	H	-1.17178000	-1.43965300	1.20557500
	C	0.28099500	1.29248400	-0.45531200
	H	0.45988500	2.36117400	-0.61085900
	H	0.10348000	0.83510600	-1.43344500
	C	1.53625100	0.70327700	0.16676000
	H	2.37207000	0.83152200	-0.53092100
	H	1.76729300	1.19731300	1.11225600
	O	1.41391900	-0.66510400	0.52737300
	O	0.95040400	-1.39373800	-0.55228700
Frequencies	-1861.8757	123.9414	175.5026	235.5877
				255.5589

	383.9376	423.9773	477.3638	584.7296	610.2401
	653.4272	809.3745	855.1673	871.8268	908.7959
	1010.4746	1049.1732	1059.3704	1132.0531	1142.0971
	1159.2072	1203.7136	1213.2062	1296.4726	1319.2106
	1333.524	1388.0675	1410.8772	1431.5076	1444.5353
	1476.3544	1491.6977	1505.9211	1518.4377	3025.4981
	3046.5174	3063.2366	3067.275	3101.22	3108.7517
	3134.2078	3197.2622			
Rotational constants (GHZ)	3.58528	2.51121	1.69417		
ZPE (Hartree/Particle)	0.129171				
W6-P2					
Optimized Cartesian coordinate	C	-3.21553200	0.54050300	0.37015300	
	H	-2.90870500	1.29870100	1.09107700	
	H	-3.57651600	-0.33363400	0.91320900	
	H	-4.03318400	0.94087500	-0.23115300	
	C	-2.05665600	0.16818700	-0.52363400	
	H	-2.33544300	-0.60809900	-1.24363900	
	H	-1.66672000	1.03289200	-1.06742700	
	O	-1.00055400	-0.33650100	0.30861800	
	C	0.04522700	-0.83830400	-0.31610300	
	H	-0.05308600	-1.12177800	-1.35817900	
	C	1.34296700	-0.84920200	0.36591700	
	H	2.00388100	-1.67770800	0.09861500	
	H	1.26428600	-0.72323400	1.44842400	
	O	1.64352000	0.32599000	-0.30839000	
	O	3.25584600	0.72871600	0.19056200	
	H	3.41895000	1.31923200	-0.55525100	
Frequencies	-868.0275	48.308	71.2597	88.1082	117.5388
	199.6396	227.1197	258.1378	275.737	391.6986
	453.4931	503.1802	677.4867	820.0225	884.7979
	967.8827	985.0993	1094.5228	1104.9178	1154.1524
	1176.8704	1184.9931	1217.2842	1309.6852	1320.2966
	1329.3499	1397.0394	1429.6965	1490.0326	1497.3953
	1505.2556	1521.1148	1549.6932	3056.1425	3062.7307
	3078.1885	3105.9508	3126.5661	3156.9549	3163.0097
	3206.5119	3871.9643			
Rotational constants (GHZ)	7.91670	0.99330	0.95046		
ZPE (Hartree/Particle)	0.130037				

W6-P3					
Optimized Cartesian coordinate	C	2.88014600	-0.77928900	0.17187600	
	H	2.42905900	-1.75639400	-0.00566700	
	H	3.01783100	-0.65099600	1.24595400	
	H	3.85775600	-0.75323300	-0.31212100	
	C	1.99970600	0.31838300	-0.37985500	
	H	2.44047100	1.30511100	-0.20293400	
	H	1.84167600	0.19745800	-1.45733700	
	O	0.73919600	0.24845700	0.28706300	
	C	-0.18647600	1.13422300	-0.12143000	
	H	0.05721000	1.71919000	-1.00417800	
	C	-1.41860300	1.15828000	0.46123000	
	H	-2.11130500	1.93364500	0.16670200	
	H	-1.56424900	0.68053900	1.42063700	
	O	-2.36044400	-0.29055200	-0.45876100	
	O	-1.93023600	-1.44688000	0.14359700	
	H	-1.20520900	-1.75311200	-0.41717500	
Frequencies	-589.8878	47.1218	61.9873	89.2175	113.1068
	196.5354	255.0157	300.3287	331.7897	388.8648
	445.9761	505.6154	772.9737	823.1445	870.7636
	916.4816	981.6363	1012.3127	1049.3403	1112.2629
	1166.0312	1184.7697	1253.4269	1312.6858	1316.7544
	1396.3122	1409.9268	1424.6814	1448.9867	1489.0063
	1506.0559	1529.829	1604.7477	3041.7974	3077.1258
	3084.8715	3155.9303	3160.0154	3177.9866	3194.8866
	3295.3416	3804.3494			
Rotational constants (GHZ)	4.64979	1.28280	1.07789		
ZPE (Hartree/Particle)	0.130562				
W6-P9					
Optimized Cartesian coordinate	C	-1.16965900	-0.83191100	-0.32474700	
	C	-0.34400700	-0.32699100	0.75132400	
	O	-2.44419100	-0.62052600	-0.26745300	
	O	-1.87583900	1.54567000	-0.11677700	
	H	-0.66819500	-0.89448200	-1.30495400	
	H	-0.81228800	-1.85806300	0.21751900	
	H	-0.82952300	-0.19270700	1.71505700	
	H	-2.81283000	1.63012300	0.10597000	
	O	0.92895000	-0.13471300	0.77101100	
	C	1.66325000	-0.14722300	-0.48148500	
	H	1.13022600	0.49679500	-1.18330900	
	H	1.66414800	-1.17356800	-0.85632000	

	C	3.05691900	0.34820400	-0.18448300
	H	3.64390300	0.35125900	-1.10398200
	H	3.02398200	1.36360700	0.21087700
	H	3.55020500	-0.29887900	0.54123800
Frequencies	-782.0203	44.0876	97.6135	143.9987
	205.6342	223.0987	267.0093	280.5973
	397.7727	432.005	484.9913	659.3273
	864.338	967.7526	1040.6156	1081.2928
	1184.5877	1200.6892	1264.7469	1311.1307
	1347.6858	1395.5443	1417.8541	1444.664
	1504.0298	1516.0011	1581.2204	2175.4592
	3080.3902	3082.3738	3136.7015	3162.1654
	3208.5773	3863.2139		3169.3197
Rotational constants (GHZ)	5.20264	1.23895	1.1377	
ZPE (Hartree/Particle)	0.126571			
W7-P6				
Optimized Cartesian coordinate	C	-0.19905400	1.66731800	0.12738900
	C	1.03325100	0.88590200	-0.30895100
	H	1.10269400	0.85064600	-1.40057200
	H	1.93196000	1.35633300	0.09778700
	H	-0.28672400	2.61466000	-0.40330900
	O	-1.33292400	0.87894000	-0.19985600
	C	-1.24751300	-0.30726800	0.43639100
	H	-1.13986700	-0.26561500	1.51727300
	C	-1.88952800	-1.45916100	-0.23317700
	H	-1.53334300	-1.53700300	-1.26247800
	H	-1.65306300	-2.38048900	0.29929700
	H	-2.98063400	-1.34764600	-0.25931900
	H	-0.17603300	1.84910100	1.20814600
	O	0.91063500	-0.42423600	0.20787000
	O	2.45922900	-0.95074200	-0.00479700
	H	2.25655100	-1.89242100	0.04752900
Frequencies	-942.4203	88.9936	118.387	134.0201
	212.664	275.7169	317.9232	356.8954
	477.9167	600.9101	733.6201	895.1458
	950.3625	1029.145	1070.2854	1100.0855
	1151.0756	1182.0121	1239.2576	1262.7449
	1372.1205	1390.7188	1404.7057	1450.9554
	1484.8543	1511.2717	1515.7941	3034.0458
	3060.764	3110.2752	3115.864	3152.4507
	3166.3204	3877.7899		3152.9676

Rotational constants (GHZ)	3.65399	1.99942	1.38661		
ZPE (Hartree/Particle)	0.130911				
W7-P8					
Optimized Cartesian coordinate	C	3.30818000	0.63050800	-0.37136800	
	H	3.16767600	1.51595300	0.26377000	
	H	2.95977400	0.87639600	-1.37543600	
	H	4.37741700	0.41334600	-0.39240000	
	C	2.53182400	-0.52096900	0.17911400	
	H	2.97449200	-1.11513700	0.98775700	
	O	1.34098900	-0.73720300	-0.15527300	
	C	-1.17771000	-0.25101600	-0.11615500	
	H	-1.29912400	-1.31408000	0.11126200	
	H	-1.04299800	-0.12739800	-1.19381200	
	O	-2.33302800	0.47110400	0.30249600	
	O	-3.42891000	-0.02640100	-0.46624600	
	H	-4.00041800	-0.38077500	0.22511600	
	C	-0.01837200	0.32157900	0.62481400	
	H	0.28742000	1.32578400	0.35439000	
	H	0.07982100	0.06529700	1.67309700	
Frequencies	-775.4441	13.0581	44.2857	85.6063	101.6259
	122.6073	135.6449	198.2899	289.0591	332.2637
	488.3616	505.1887	693.5966	707.4127	840.1015
	912.3563	950.5084	995.348	1037.5515	1087.1258
	1119.2993	1125.1265	1185.8439	1273.9267	1317.4738
	1376.5711	1394.1057	1402.6368	1455.312	1475.7801
	1487.3458	1506.2304	1527.6477	3022.4126	3053.8358
	3064.588	3109.0437	3117.173	3153.5989	3159.2791
	3255.5689	3852.7961			
Rotational constants (GHZ)	10.09533	0.82289	0.80843		
ZPE (Hartree/Particle)	0.127522				
W7-P9					
Optimized Cartesian coordinate	C	1.29948300	-0.41094400	-0.27437600	
	O	1.15637400	0.96784300	-0.39135400	
	H	0.96536400	-0.95720300	-1.16312900	
	C	2.62294000	-0.80903700	0.29811600	
	H	2.67606400	-1.89245800	0.41671100	
	H	3.44116900	-0.49635000	-0.35991100	
	H	2.77625400	-0.33576300	1.26981200	

	C	-0.22874200	1.29118500	-0.30765800	
	H	-0.73509900	1.07869000	-1.25593100	
	H	-0.29816100	2.35482400	-0.08054700	
	C	-0.79678500	0.38168700	0.77091000	
	H	0.21317700	-0.53920300	0.56644400	
	H	-0.76104000	0.73613900	1.79901200	
	O	-2.04599500	-0.16314000	0.57305400	
	O	-1.95949300	-1.01805100	-0.58260400	
	H	-2.86620900	-0.95923600	-0.90717900	
Frequencies	-1737.2855	72.1866	133.1358	151.9212	178.6475
	196.6271	234.4132	348.187	418.223	512.3133
	565.5362	644.1112	792.1212	881.4567	899.7189
	943.6683	999.96	1066.3665	1106.1822	1128.2354
	1144.4824	1155.1062	1174.0362	1267.7904	1323.2536
	1368.4875	1380.8233	1402.9236	1434.6358	1443.9893
	1478.6426	1494.6537	1508.5705	1726.4555	3045.3682
	3059.0692	3066.0125	3115.3897	3139.6952	3150.7296
	3168.831	3863.3256			
Rotational constants (GHZ)	4.62219	1.52720	1.34743		
ZPE (Hartree/Particle)	0.127999				
W7-P11					
Optimized Cartesian coordinate	C	1.35456200	-0.07256000	0.42222500	
	O	0.60920400	-1.02637300	-0.14754400	
	H	1.30129200	0.01340500	1.50384200	
	C	2.57115600	0.30330200	-0.33450200	
	H	2.29755300	0.59379300	-1.35085400	
	H	3.08241800	1.13429400	0.15111000	
	H	3.27054000	-0.54051800	-0.40399500	
	C	-0.72153300	-1.21726100	0.34382000	
	H	-0.76903200	-0.96864400	1.40895200	
	H	-0.92682600	-2.27974000	0.20609200	
	C	-1.75513800	-0.39658200	-0.43323800	
	H	-2.74219500	-0.84359900	-0.27225200	
	H	-1.50665500	-0.45368600	-1.50107800	
	O	-1.87474500	0.92565100	-0.00669300	
	O	-0.27886400	1.28905400	0.11544300	
	H	-0.34614700	2.13664400	0.57870600	
Frequencies	-1027.1388	106.9968	159.7233	161.3522	193.5588
	210.1856	320.4568	348.6257	396.6796	407.8961
	495.1546	540.9802	735.4215	830.9211	927.8784
	963.8579	1023.6672	1073.4765	1086.2749	1095.1529

	1150.127	1177.8743	1233.0045	1285.6828	1324.8942
	1378.3855	1398.8041	1406.8046	1446.9306	1469.7277
	1473.2193	1483.8433	1500.8955	3019.6384	3030.8961
	3067.4509	3093.7229	3106.3224	3139.0773	3155.3015
	3170.9392	3836.4478			
Rotational constants (GHZ)	4.68234	1.91552	1.49399		
ZPE (Hartree/Particle)	0.130831				
W8-P9					
Optimized Cartesian coordinate	C	-2.04952500	-0.18577500	-0.24418200	
	O	-0.93257900	-1.01303700	-0.53181700	
	H	-2.72348000	-0.29697000	-1.09741900	
	H	-2.56453800	-0.56867800	0.64793800	
	C	-1.64343800	1.25424100	-0.03622300	
	H	-2.28527500	1.85329600	0.60504300	
	H	-1.29200200	1.77111100	-0.92656400	
	C	-0.01943100	-1.05970100	0.54590400	
	H	0.73975800	-1.79875600	0.28141900	
	H	-0.52700100	-1.39568300	1.46195700	
	C	0.60311900	0.29057500	0.80686400	
	H	-0.46981500	1.05632500	0.63634300	
	H	1.01847500	0.44164800	1.80582400	
	O	1.41168000	0.78578500	-0.20574400	
	O	2.55803100	-0.08416700	-0.33666500	
	H	2.46246700	-0.36698400	-1.25489900	
Frequencies	-1600.6763	42.5053	131.434	152.7243	244.1316
	271.1169	366.7317	434.918	474.8365	594.8587
	600.2074	682.2897	851.3277	873.8924	889.1015
	903.0011	945.9765	1027.4723	1093.3049	1101.7645
	1148.022	1163.926	1173.3916	1279.6426	1334.0989
	1341.0401	1369.5505	1376.5507	1406.1977	1421.7851
	1450.8342	1485.9995	1498.7301	1519.0503	3014.522
	3017.3195	3093.8245	3106.5052	3116.0719	3123.2402
	3214.6451	3845.0413			
Rotational constants (GHZ)	4.89724	1.70609	1.48409		
ZPE (Hartree/Particle)	0.127991				
W8-P12					
Optimized Cartesian	C	0.62145800	-0.82405600	0.66768700	
	C	-0.49865600	-1.37891300	-0.19004000	

coordinate	C	-1.59580200	0.68698400	-0.46975400	
	C	-0.71601800	1.49474000	0.42278500	
	H	0.29487400	-0.71687300	1.70641300	
	H	1.48952700	-1.48255900	0.63778500	
	H	-0.17535200	-1.37730900	-1.23993600	
	H	-0.72283000	-2.40362000	0.11142000	
	H	-1.21745800	0.73313000	-1.50021100	
	H	-2.61794700	1.08322400	-0.46795800	
	H	-0.35255000	2.44709000	0.06117700	
	H	-0.84977800	1.39949100	1.49415700	
	O	1.03818600	0.46116200	0.19051200	
	O	-1.70663700	-0.65787500	-0.04947900	
	O	2.47604300	0.12433500	-0.50416400	
	H	2.82488800	1.02391700	-0.48186100	
Frequencies	-1009.4125	50.7327	151.0114	187.9751	214.4485
	323.222	344.1583	411.6243	451.8182	458.8572
	560.8646	627.7671	803.4312	855.2068	882.4122
	923.2446	1013.0016	1054.9978	1080.6014	1109.1841
	1137.4744	1161.9374	1192.9153	1269.1259	1304.5957
	1339.1555	1375.1897	1400.3088	1424.2143	1460.6878
	1477.3963	1483.7354	1493.8698	3021.0704	3031.4704
	3064.9224	3073.265	3127.8825	3145.0889	3164.6128
	3271.8551	3871.9045			
Rotational constants (GHZ)	4.20078	2.00866	1.57112		
ZPE (Hartree/Particle)	0.131672				
W8-P13					
Optimized Cartesian coordinate	C	-0.82433200	-1.32649600	-0.18744100	
	O	0.51083500	-1.11117500	-0.60385300	
	H	-1.36488100	-1.56192400	-1.10578800	
	H	-0.87865800	-2.20209800	0.47745500	
	C	-1.52252500	-0.16375600	0.52105000	
	H	-1.10988800	0.00839900	1.52292200	
	H	-2.57577200	-0.44148200	0.64809400	
	C	1.42548300	-0.67529700	0.38648100	
	H	2.26670700	-1.38116200	0.39491700	
	H	0.97516800	-0.69833900	1.38453700	
	C	1.90985900	0.70451800	0.07500000	
	H	2.29377800	0.87310100	-0.92486000	
	H	2.33827000	1.30153400	0.86993900	
	O	0.02420800	1.46450100	-0.08167800	
	O	-1.53405500	1.03719000	-0.19392400	

	H	0.11646700	1.74402100	-1.00211000	
Frequencies	-1091.5783	98.7115	160.1931	226.2775	294.2167
	335.0839	380.9432	392.1863	457.179	487.8397
	555.7869	584.7381	796.7215	831.7199	869.6883
	907.5713	985.7308	1061.6922	1093.0269	1117.0606
	1156.8305	1198.3884	1216.0135	1298.1517	1309.086
	1317.6114	1383.8973	1412.1665	1425.699	1459.2003
	1467.9793	1492.4266	1507.9073	3002.6232	3023.1817
	3035.8546	3075.6613	3081.6084	3124.4265	3157.5204
	3266.1774	3868.1259			
Rotational constants (GHZ)	3.61568	2.58970	1.72427		
ZPE (Hartree/Particle)	0.131944				
W8-P14					
Optimized Cartesian coordinate	C	-0.82433200	-1.32649600	-0.18744100	
	O	0.51083500	-1.11117500	-0.60385300	
	H	-1.36488100	-1.56192400	-1.10578800	
	H	-0.87865800	-2.20209800	0.47745500	
	C	-1.52252500	-0.16375600	0.52105000	
	H	-1.10988800	0.00839900	1.52292200	
	H	-2.57577200	-0.44148200	0.64809400	
	C	1.42548300	-0.67529700	0.38648100	
	H	2.26670700	-1.38116200	0.39491700	
	H	0.97516800	-0.69833900	1.38453700	
	C	1.90985900	0.70451800	0.07500000	
	H	2.29377800	0.87310100	-0.92486000	
	H	2.33827000	1.30153400	0.86993900	
	O	0.02420800	1.46450100	-0.08167800	
	O	-1.53405500	1.03719000	-0.19392400	
	H	0.11646700	1.74402100	-1.00211000	
Frequencies	-513.898	48.3836	64.2293	95.33	112.762
	134.3515	185.4034	210.2115	276.6065	386.9582
	412.9177	508.3006	826.1415	844.3073	935.8481
	989.4226	1013.7097	1018.7726	1055.0822	1115.7929
	1143.3666	1162.3572	1234.5392	1238.0178	1284.8658
	1321.3242	1335.6902	1397.6527	1413.3581	1468.8956
	1528.5338	1537.9076	1598.7295	3014.451	3062.3451
	3066.2855	3125.4541	3168.2941	3182.4525	3257.4063
	3282.9455	3851.0366			
Rotational constants (GHZ)	10.16690	0.84699	0.81220		
ZPE	0.129652				

(Hartree/Particle)	
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