

Table S4. Energies, vibrational frequencies, and Cartesian coordinates for all optimized structures. The frequencies and geometries are obtained at M06-2X/6-311+G(d,p) level. The energies are calculated at B2PLYPD3/def2-TZVPP level.

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
2-naphthyl	-385.0159735	173.6744· 191.3683· 367.5500 388.3838· 473.0415· 486.6284 511.6175· 519.4554· 622.9684 623.7067· 753.0440· 759.6488 779.1231· 795.0404· 819.7305 858.1023· 897.4218· 933.4308 979.1946· 995.4084· 1014.8250 1046.8078· 1059.0677· 1141.9555 1159.9397· 1171.4197· 1208.6486 1249.1101· 1281.5483· 1347.1795 1393.6735· 1420.6082· 1466.4921 1481.1590· 1549.8320· 1631.3658 1657.5624· 1694.4691· 3192.9688 3195.6716· 3196.1210· 3200.0961 3214.3611· 3217.5338· 3226.7174	C· 2.33722900· -0.78944500· 0.00000000 C· 1.12403200· -1.42425700· -0.00000100 C· -0.08587900· -0.68191300· 0.00000000 C· -0.01836000· 0.73966400· 0.00000200 C· 1.25258200· 1.36981600· 0.00000000 C· 2.40142100· 0.62427600· 0.00000000 H· -1.38765600· -2.41017700· -0.00000300 H· 3.25361900· -1.36720600· 0.00000000 H· 1.06968500· -2.50765900· -0.00000200 C· -1.35310100· -1.32548200· 0.00000000 C· -1.23335700· 1.48916900· -0.00000100 H· 1.29758600· 2.45347000· -0.00000100 H· 3.36711700· 1.11567800· 0.00000000 C· -2.39364200· 0.79671800· -0.00000100 C· -2.51699000· -0.59492200· 0.00000200 H· -1.19804400· 2.57354300· -0.00000400 H· -3.48591000· -1.07939200· -0.00000200
phenylacet ylene	-308.2473948	141.9778· 159.3160· 367.7094 408.1726· 471.3537· 543.3904 551.2943· 634.6060· 694.8091 706.3839· 732.9992· 778.4730 780.7553· 868.1629· 950.9373 1003.7641· 1018.4455· 1020.8128 1059.5364· 1109.3519· 1179.9667 1200.2874· 1232.3318· 1310.1604 1348.2080· 1485.1804· 1533.4537 1646.0223· 1675.3919· 2246.0525 3204.7124· 3213.9166· 3221.5406 3228.8857· 3233.2590· 3495.9730	C· 0.00000000· 1.20877900· -0.11884100 C· 0.00000000· 1.20485200· -1.50727600 C· 0.00000000· 0.00000000· -2.20412400 C· 0.00000000· -1.20485200· -1.50727600 C· 0.00000000· -1.20877900· -0.11884100 C· 0.00000000· 0.00000000· 0.58611800 H· 0.00000000· 2.14149300· 0.43158300 H· 0.00000000· 2.14439500· -2.04663600 H· 0.00000000· 0.00000000· -3.28751900 H· 0.00000000· -2.14439500· -2.04663600 H· 0.00000000· -2.14149300· 0.43158300 C· 0.00000000· 0.00000000· 3.22201700 H· 0.00000000· 0.00000000· 4.28583300 C· 0.00000000· 0.00000000· 2.02019000
int1-1	-693.3409168	10.4901· 25.8693· 46.5000 93.4505· 139.7642· 178.2513 193.3952· 197.9409· 310.6425 330.2238· 396.1177· 404.1794 408.3079· 476.8368· 481.4134 482.0042· 517.9311· 524.8312 556.7501· 573.1568· 627.7271 637.2027· 649.0871· 687.4937 721.5177· 761.4014· 763.2940 770.5325· 789.6591· 795.3627 822.5958· 849.1706· 860.0363 889.4292· 917.8501· 918.6729 931.9268· 979.7820· 988.7786 993.7558· 999.6188· 1001.2908 1009.7124· 1015.6476· 1048.2484 1049.8623· 1108.6587· 1136.3446 1155.6806· 1163.3763· 1170.6811 1183.4290· 1188.7790· 1207.9956 1226.7470· 1265.4456· 1294.0202 1297.4936· 1321.4020· 1343.2355 1399.8822· 1404.8418· 1430.2309 1470.9563· 1481.4499· 1493.3278 1511.2005· 1563.2879· 1598.9633 1620.3330· 1646.8636· 1673.5728 1705.5469· 1861.9397· 3110.5771 3188.1970· 3191.6563· 3194.0015 3198.4566· 3201.5438· 3206.6132 3208.5759· 3212.3992· 3220.0324 3222.9625· 3224.4900· 3231.0056	C· -1.75387000· 2.32709000· -0.00000200 C· -3.00176000· 1.76674700· -0.00000100 C· -3.16396800· 0.35801300· 0.00000100 C· -2.00222700· -0.46223100· 0.00000000 C· -0.72520100· 0.14619200· -0.00000200 C· -0.58805600· 1.51548900· -0.00000300 H· -5.32484300· 0.37514000· 0.00000200 H· -1.64131700· 3.40606100· -0.00000300 H· -3.88566700· 2.39559100· 0.00000000 C· -4.44288600· -0.25649300· 0.00000200 C· -2.15967400· -1.87459500· 0.00000200 H· 0.15734800· -0.48678500· -0.00000300 C· -3.40647100· -2.43876500· 0.00000300 C· -4.56286500· -1.62033100· 0.00000300 H· -1.27134700· -2.49707400· 0.00000100 H· -3.51520100· -3.51680700· 0.00000400 H· -5.54371100· -2.08053900· 0.00000400 C· 0.73966400· 2.17778300· -0.00000300 C· 1.89097800· 1.56093200· -0.00000200 C· 2.84970200· 0.56104300· -0.00000100 C· 3.36411900· 0.04397500· 1.22010400 C· 3.36410900· 0.04396200· -1.22010500 C· 4.33186800· -0.94190400· 1.20782900 H· 2.98148400· 0.43482600· 2.15498200 C· 4.33185800· -0.94191700· -1.20782700 H· 2.98146700· 0.43480200· -2.15498500 C· 4.82401400· -1.44225900· 0.00000100 H· 4.71095300· -1.32848900· 2.14656900 H· 4.71093500· -1.32851000· -2.14656800 H· 5.58421500· -2.21340000· 0.00000300 H· 0.71967700· 3.26879000· -0.00000200
int1-2	-693.3421137	10.9999· 25.7767· 48.8131 95.7683· 148.0517· 182.4559	C· 0.38673900· 0.61300500· 0.00001100 C· 1.49503100· 1.40914700· 0.00000700

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		187.0769· 188.5804· 311.6836 316.8415· 383.6934· 402.2475 407.6204· 473.4781· 483.8420 483.8882· 522.5895· 525.3502 551.5498· 597.1681· 627.2064 631.8633· 646.7173· 684.9146 735.6947· 758.8500· 765.0542 773.8142· 781.0089· 795.6225 829.4931· 845.0474· 851.8673 889.2129· 902.5633· 913.9465 925.6150· 971.6512· 989.7834 990.1249· 998.5817· 1006.1492 1007.6675· 1016.2975· 1046.8918 1052.0282· 1108.9969· 1135.7976 1155.7733· 1164.5613· 1169.5226 1185.4200· 1194.3711· 1205.0558 1241.5531· 1279.6653· 1288.2106 1297.8306· 1299.2436· 1342.9052 1397.4162· 1405.1704· 1435.4106 1469.4532· 1483.2322· 1491.3918 1512.6494· 1563.1840· 1595.4303 1615.8482· 1649.3587· 1674.7647 1706.2112· 1875.5885· 3101.6465 3186.4672· 3193.3883· 3194.2700 3198.4281· 3202.3262· 3207.3362 3209.8136· 3212.2022· 3220.8666 3223.7745· 3224.4047· 3231.7660	C· 2.80132000· 0.84687500· 0.00000100 C· 2.93489800· -0.56697100· 0.00000000 C· 1.76448700· -1.36869500· 0.00000400 C· 0.51184100· -0.80515000· 0.00000900 H· 3.85980600· 2.72904400· -0.00000300 H· -0.60515100· 1.05196000· 0.00001700 H· 1.39305300· 2.48919100· 0.00001000 C· 3.96870200· 1.64971800· -0.00000300 C· 4.23529800· -1.13393200· -0.00000500 H· 1.87195100· -2.44943400· 0.00000300 C· 5.34719200· -0.33311500· -0.00000900 C· 5.21312100· 1.07501500· -0.00000800 H· 4.33411400· -2.21421800· -0.00000500 H· 6.33589100· -0.77631200· -0.00001300 H· 6.10000100· 1.69729300· -0.00001200 C· -0.68811300· -1.67254700· 0.00001100 C· -1.92202900· -1.24672200· 0.00000900 C· -3.09928600· -0.52864800· 0.00000200 C· -3.72864100· -0.15474700· 1.22152300 C· -3.72863700· -0.15476300· -1.22152500 C· -4.91213800· 0.55605100· 1.20817500 H· -3.26016900· -0.43645100· 2.15649800 C· -4.91213500· 0.55603500· -1.20818900 H· -3.26016200· -0.43647800· -2.15649500 C· -5.51461400· 0.91728800· -0.00001000 H· -5.37628500· 0.83550900· 2.14673900 H· -5.37627900· 0.83548100· -2.14675800 H· -6.44346400· 1.47374100· -0.00001500 H· -0.49150900· -2.74640900· 0.00001700
ii	-693.3281768	25.3943· 40.6392· 49.2681 103.3968· 130.8821· 170.3266 186.0404· 236.4339· 265.0875 318.2310· 381.8892· 406.9933 418.1123· 456.1216· 481.6513 490.2526· 512.4633· 529.8019 541.4041· 602.9461· 628.0406 639.0765· 655.9993· 702.0863 752.7152· 759.4585· 765.3837 773.2221· 792.2269· 836.4857 857.1556· 867.6885· 878.5599 897.7939· 928.8316· 930.5170 964.7969· 986.6534· 989.6893 994.6038· 998.3846· 1001.8432 1008.6362· 1013.5912· 1050.1860 1058.1362· 1129.4773· 1154.0103 1163.9065· 1172.2722· 1182.4897 1195.9812· 1220.0464· 1226.6309 1266.3644· 1291.3025· 1296.2793 1311.6069· 1336.4944· 1340.7041 1395.1018· 1406.9484· 1430.0371 1460.4392· 1479.1248· 1492.7551 1514.8467· 1560.0224· 1605.9076 1645.8944· 1666.0266· 1676.4643 1702.1436· 1727.7373· 3168.5740 3183.1596· 3192.9972· 3194.8548 3196.5491· 3198.1428· 3199.1086 3204.6112· 3210.2892· 3213.7263 3214.6627· 3225.3803· 3226.0595	C· -3.96549500· -1.23545100· -0.62834900 C· -5.33542400· -1.29310300· -0.64694000 C· -6.01864000· -0.25548100· -0.00744800 C· -5.29993600· 0.76599700· 0.61229900 C· -3.91105800· 0.77101600· 0.59939700 C· -3.19052700· -0.24764800· -0.05028300 H· -5.86869400· -2.10256900· -1.13141200 H· -7.10224600· -0.25144200· 0.01197800 H· -5.83030800· 1.56145500· 1.12174300 H· -3.37372200· 1.56002700· 1.11396300 C· -0.90286900· 0.73597400· 0.09021400 H· -1.32479100· 1.71787000· 0.29090500 C· -1.72482700· -0.29816100· -0.12509000 C· 0.56396600· 0.67952400· 0.02818300 C· 1.28150500· 1.87545700· -0.25876500 C· 2.64474100· 1.87809200· -0.35451300 C· 3.38840900· 0.68560400· -0.15798800 C· 2.68622900· -0.51145000· 0.14937600 C· 1.27402800· -0.48146800· 0.24183500 H· 0.72434600· 2.79329800· -0.41329700 H· 3.17740800· 2.79543000· -0.58125100 C· 3.42659600· -1.70452800· 0.36483700 C· 4.79231500· -1.70657900· 0.27129600 H· 5.34688200· -2.62284900· 0.43509400 C· 4.80337800· 0.65274200· -0.24699400 C· 5.48992800· -0.51402800· -0.03926900 H· 6.57089900· -0.52963100· -0.11027900 H· 5.33258600· 1.56979300· -0.48306700 H· 2.88865400· -2.61593200· 0.60289000 H· 0.75495200· -1.39592600· 0.50985200 H· -1.30988000· -1.25858200· -0.41791000
ii2	-693.3297601	22.4722· 40.2734· 53.3422 94.0571· 140.0126· 161.9967 185.3203· 238.0702· 258.7306 321.6347· 377.2893· 405.4717 417.6034· 464.4203· 479.9483 495.5474· 508.3200· 529.8940 543.1051· 603.9740· 628.0836 639.0289· 655.3695· 702.4432 755.5509· 756.9693· 764.3008 771.9286· 792.3142· 838.3241 862.3509· 865.3018· 879.4374 900.9186· 924.1473· 929.5526 962.1389· 986.6571· 990.2810	C· -3.88707300· 0.89902400· 0.30913700 C· -5.24605100· 1.02578900· 0.39338700 C· -6.01215300· -0.10236800· 0.07015300 C· -5.37780500· -1.27915100· -0.31378500 C· -3.98915600· -1.34812400· -0.38118000 C· -3.19044000· -0.23758200· -0.06553100 H· -5.71715900· 1.95359200· 0.69666300 H· -7.09358200· -0.05388100· 0.12111000 H· -5.96851200· -2.15223800· -0.56312800 H· -3.50579800· -2.27243800· -0.68190200 C· -0.90665600· 0.71664200· 0.10630000 H· -1.34542200· 1.68450500· 0.34219300 C· -1.72882500· -0.31115300· -0.13732200

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		991.4755· 998.4973· 1002.7902 1007.5231· 1013.8924· 1049.4147 1053.9911· 1128.7442· 1154.4006 1163.8717· 1172.3555· 1182.6681 1195.7178· 1223.3254· 1229.0036 1257.6673· 1271.1537· 1293.5134 1321.3165· 1341.4557· 1346.2289 1395.2943· 1406.2206· 1429.5572 1464.0674· 1479.5862· 1491.5388 1514.0095· 1560.1103· 1603.4376 1644.8010· 1664.9680· 1675.8243 1702.5239· 1729.2236· 3160.4689 3179.6525· 3188.3849· 3192.8710 3195.1645· 3198.8896· 3200.3887 3201.2590· 3210.1373· 3213.0251 3213.0623· 3225.1396· 3226.1671 1326.5294· 1335.9692· 1342.0294 1359.6464· 1365.4144· 1429.2466 1455.4524· 1490.5232· 1493.5726 1512.9153· 1533.8364· 1547.5090 1598.7697· 1635.2850· 1647.3817 1658.4876· 1672.8378· 1678.1885 3024.7824· 3186.6494· 3188.1964 3189.6192· 3195.8757· 3199.5978 3205.3309· 3206.4111· 3210.3894 3214.8941· 3218.8526· 3224.2139 3226.4309· 3229.2355· 3243.2261	C· 0.55983000· 0.67123400· 0.05271000 C· 1.27143400· 1.88781500· -0.15062800 C· 2.63549300· 1.90611900· -0.23272900 C· 3.38644200· 0.70898400· -0.10525300 C· 2.69040700· -0.51021700· 0.11794700 C· 1.27758300· -0.49598500· 0.19841500 H· 0.70844800· 2.80955800· -0.25052500 H· 3.16316700· 2.83996600· -0.39440200 C· 3.43788600· -1.70964100· 0.26295300 C· 4.80430300· -1.69632600· 0.18249300 H· 5.36419800· -2.61740700· 0.29233700 C· 4.80239600· 0.69153500· -0.18259800 C· 5.49581200· -0.48134000· -0.04370900 H· 6.57748300· -0.48486400· -0.10493800 H· 5.32683000· 1.62560200· -0.35362200 H· 2.90475100· -2.63826300· 0.43670700 H· 0.76465700· -1.43027100· 0.40204000 H· -1.31963700· -1.27538600· -0.42709200
i3	-693.3318065	14.2604· 45.9769· 60.5797 133.8349· 181.2743· 186.5745 241.0672· 259.4226· 313.9525 389.7351· 402.6234· 409.2153 459.8788· 472.7728· 484.9488 513.6876· 522.6640· 540.6892 571.9708· 587.8563· 636.1869 659.6962· 679.3199· 708.9747 762.3068· 767.3547· 777.3920 788.4770· 793.7177· 835.0184 852.1873· 881.1954· 884.7066 900.9153· 923.2333· 930.7029 960.9585· 962.2593· 988.3357 993.4718· 1000.8181· 1005.1850 1015.6856· 1021.8621· 1048.9384 1098.4363· 1138.2169· 1153.3992 1158.8457· 1162.8401· 1175.5865 1179.2662· 1189.1262· 1203.6927 1224.2250· 1231.6192· 1263.9303 1293.1051· 1308.3927· 1329.6393 1378.9057· 1400.2024· 1407.3461 1429.4817· 1456.2444· 1482.8346 1504.3530· 1511.9582· 1564.1651 1606.7841· 1647.1298· 1665.3221 1676.0614· 1709.3931· 3076.8759 3181.6622· 3190.6093· 3194.5602 3198.8174· 3199.0695· 3207.8598 3210.1388· 3212.8952· 3220.5557 3224.9930· 3225.9830· 3251.5582	C· -2.38210900· 0.44225600· 0.41105900 C· -2.80020800· -0.23403500· 1.52962000 C· -3.85447500· -1.14493000· 1.33182600 C· -4.42879300· -1.34846400· 0.06915800 C· -3.99381100· -0.67060300· -1.06757300 C· -2.94292100· 0.23507800· -0.86930800 H· -2.35879800· -0.09145300· 2.50887900 H· -4.23610900· -1.70791200· 2.17524100 H· -5.23770000· -2.06459400· -0.02035800 H· -4.44497500· -0.84905300· -2.03566100 C· -1.37720000· 1.47113200· -0.12468800 H· -1.56245500· 2.48722900· 0.23596900 C· -2.04948800· 1.16138700· -1.47397800 C· 0.09043000· 1.13463800· -0.00979500 C· 1.03027500· 2.14707500· 0.30919800 C· 2.36820700· 1.86601800· 0.39600100 C· 2.84818600· 0.55187300· 0.16967900 C· 1.91298600· -0.47018400· -0.14985200 C· 0.53731900· -0.14554300· -0.23292100 H· 0.67512800· 3.15673200· 0.48696800 H· 3.07876500· 2.64790500· 0.64226200 C· 2.38861800· -1.78966500· -0.37577800 C· 3.72413600· -2.07578200· -0.28873500 H· 4.07636600· -3.08549100· -0.46318800 C· 4.22692200· 0.22393500· 0.25372200 C· 4.65536300· -1.05671000· 0.03014500 H· 5.70966500· -1.29753300· 0.09621800 H· 4.93540900· 1.00812500· 0.49864100 H· 1.67172200· -2.56656400· -0.61892300 H· -0.17346900· -0.93135100· -0.47481800 H· -1.85416600· 1.50910400· -2.47790600
i4	-693.3245788	27.2691· 30.4351· 50.0956 113.5511· 130.1972· 185.7495 194.0897· 235.4173· 292.2293 367.3283· 401.8274· 420.5790 433.6857· 456.5854· 478.4619 487.1314· 515.7454· 528.2530 571.5338· 620.9327· 628.7568 645.5251· 683.4383· 711.1927 737.0206· 752.6264· 766.6900 775.3879· 785.9640· 793.2016 833.9310· 852.2864· 879.5571 886.8488· 923.5432· 939.2461 972.3760· 984.9160· 989.1649 994.5291· 1002.5776· 1012.3619 1014.4844· 1015.4144· 1049.4686	C· -2.13070600· -0.12439600· -1.00714000 C· -2.57771900· -1.38923700· -1.36777100 C· -3.59090400· -2.02213800· -0.64850800 C· -4.17644600· -1.37431300· 0.44193700 C· -3.70002200· -0.12377200· 0.74759000 C· -2.68507100· 0.54721500· 0.09671400 H· -2.13514400· -1.88572500· -2.22283100 H· -3.93148400· -3.00974100· -0.93751600 H· -4.97157200· -1.84016500· 1.01216000 C· -1.02189200· 2.39408900· 0.54497300 H· -0.90889900· 3.44349000· 0.80641300 C· -2.26581100· 1.90155600· 0.51521300 C· 0.23921700· 1.67482300· 0.27388300 C· 1.25928300· 2.32844800· -0.47206600 C· 2.44212100· 1.70060300· -0.75034700

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1056.0667·1131.9926·1149.5662 1162.0038·1168.2714·1177.6880 1184.7340·1213.1993·1226.7439 1231.6498·1271.9361·1293.1106 1299.1808·1317.9930·1388.6151 1402.0790·1427.5418·1429.3597 1457.5178·1477.0558·1492.5492 1515.0918·1558.7590·1603.2828 1644.7376·1663.3566·1676.0533 1705.5487·1724.4762·3163.4862 3188.4779·3192.0040·3194.9324 3198.5221·3198.5501·3200.1945 3204.9614·3209.2974·3213.4098 3214.4082·3225.0518·3225.5561	C·2.68988000·0.38217700·-0.28768300 C·1.68766500·-0.26985900·0.48080300 C·0.47331200·0.40597400·0.75111600 H·1.08081600·3.33671200·-0.83035600 H·3.20909900·2.20549100·-1.32792600 C·1.93213600·-1.58637900·0.95443500 C·3.11247900·-2.22112300·0.67487600 H·3.28882500·-3.22619800·1.03910400 C·3.90329200·-0.30034300·-0.55947300 C·4.11043300·-1.57054200·-0.09089200 H·5.04036000·-2.08405000·-0.30409900 H·4.66499100·0.20259500·-1.14572900 H·1.16326700·-2.07991900·1.53913100 H·-0.28411500·-0.09659600·1.34379600 H·-1.34740300·0.36073400·-1.57910500 H·-3.07622400·2.55666300·0.82098600
i5	-693.3813251	65.2628·84.2263·116.8213 168.7525·200.1530·235.5498 260.3761·322.3105·363.7212 406.9371·418.0764·429.1491 450.5532·498.4704·511.2959 524.8277·538.3157·561.0574 569.7869·621.4447·662.9401 692.3505·705.1205·734.9333 753.4104·759.8251·774.3244 804.0507·813.5582·819.9112 834.0800·859.0865·905.0753 909.6340·936.9789·952.0415 960.2932·969.3484·981.9644 993.7402·1011.4324·1019.4332 1073.7489·1080.5490·1109.5289 1117.7720·1146.7473·1156.6184 1179.2001·1181.7454·1193.6807 1216.2655·1230.4936·1236.5808 1243.7646·1246.7139·1293.9634 1304.9959·1324.1404·1327.6134 1338.0116·1369.5223·1398.0222 1443.4640·1464.4473·1490.8920 1522.0734·1533.0830·1543.2988 1585.5762·1637.5366·1647.6476 1663.9948·1669.1951·2921.1860 3187.8543·3189.9989·3190.7456 3194.0957·3195.0252·3208.1953 3210.4025·3211.1736·3214.1730 3223.5575·3225.2395·3236.4068	C·-3.67121400·-0.38566300·-0.04560500 C·-3.63413800·-1.69839200·-0.49452900 C·-2.40682400·-2.32055400·-0.69208800 C·-1.22141100·-1.64851600·-0.39272600 C·-1.24695500·-0.35025400·0.09872800 C·-2.48922100·0.30924500·0.23241400 H·-4.55568400·-2.22490100·-0.71179400 H·-2.36466300·-3.33249700·-1.07688200 H·-0.27634600·-2.14893300·-0.55739200 C·-1.39423700·2.49237500·0.34517500 H·-1.46235100·3.57487600·0.30296800 C·-2.51712600·1.73676700·0.50895700 C·-0.13152600·1.87431000·0.14277300 C·0.95536800·2.54406000·-0.42992200 C·2.13617200·1.90220500·-0.70939300 C·2.35113900·0.52508900·-0.32646500 C·1.33488500·-0.19170100·0.33644600 C·-0.02119800·0.43421500·0.57934200 H·0.83320600·3.58989900·-0.69369400 H·2.94701300·2.43126100·-1.19626200 C·1.62894500·-1.45389200·0.85028300 C·2.87198200·-2.04320400·0.65145800 H·3.07482300·-3.02672500·1.05780600 C·3.59853000·-0.08628100·-0.53518000 C·3.85580000·-1.36167600·-0.06423700 H·4.82439300·-1.81777700·-0.23010300 H·4.37075700·0.46897200·-1.05696700 H·0.87211100·-1.98082100·1.42206600 H·-0.15482900·0.46292800·1.67793400 H·-4.62083400·0.12675600·0.06736000 H·-3.48140800·2.20816800·0.66237300
i6	-693.2831377	20.0768·39.3993·49.2603 105.1575·139.7872·178.7462 227.0456·229.7247·309.7417 333.2033·346.0449·397.7300 432.4832·446.6637·470.0792 517.4882·518.6807·530.0737 548.4140·617.3783·635.0683 640.2657·676.6359·726.7636 753.7576·756.4631·758.4571 770.7600·773.3234·786.2134 825.3621·867.7011·892.5454 901.4489·910.9573·913.1880 957.6192·968.9090·980.8087 996.0042·1005.0357·1008.6296 1016.8938·1021.3078·1050.2565 1057.5746·1111.0418·1136.2834 1147.1433·1157.2412·1164.3488 1174.9842·1181.0548·1206.5046 1239.4841·1270.3343·1295.0660 1297.2957·1311.1161·1367.0229 1380.2497·1398.3540·1422.6604 1454.8033·1479.0920·1485.4038 1493.0045·1495.9698·1550.3735 1605.5433·1628.6800·1654.0764 1678.2226·1766.4902·3152.0075 3186.8749·3192.6412·3195.7781	C·-5.51592600·0.01519500·-0.00001400 C·-4.58934500·-0.99989700·-0.00000700 C·-3.20707900·-0.71512300·0.00000100 C·-2.77413700·0.64059000·0.00000100 C·-3.75463400·1.66901100·-0.00000700 C·-5.09084900·1.36294400·-0.00001400 H·-2.54689600·-2.77731900·0.00000900 H·-6.57467700·-0.21391500·-0.00002000 H·-4.90950100·-2.03647900·-0.00000700 C·-2.21725600·-1.74360500·0.00000900 C·-1.39299400·0.92329300·0.00000800 H·-3.42599000·2.70274500·-0.00000700 H·-5.82865300·2.15648900·-0.00002000 C·-0.42337100·-0.08885100·0.00001500 C·-0.88953500·-1.45240900·0.00001500 H·-1.07245300·1.96048400·0.00000800 H·-0.17237100·-2.26301400·0.00002100 C·0.94494200·0.25579300·0.00002000 C·2.08013600·-0.67908500·0.00002500 C·3.38059700·-0.29007200·-0.67063300 C·3.38060800·-0.29005100·0.67064900 C·4.44277200·0.11342600·-1.45175300 C·4.44279700·0.11347000·1.45173800 C·5.56466100·0.49824200·-0.70044100 H·4.44704200·0.14011400·-2.53432000 C·5.56467300·0.49826300·0.70039500

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		3196.1324·3197.7303·3200.2778 3209.1723·3214.0504·3220.9450 3224.8633·3226.4188·3231.9082	H· 4.44708500· 0.14019000· 2.53430400 H· 6.46315600· 0.81512800· -1.21776500 H· 6.46317700· 0.81516400· 1.21769400 H· 1.20321400· 1.31009000· 0.00001700 H· 1.83050100· -1.73648600· 0.00004400
i8	-693.3280503	13.1531· 42.1596· 53.3068 80.9908· 137.5681· 164.7010 187.4612· 238.4179· 250.2852 317.6844· 373.3489· 409.5214 412.4883· 461.5366· 487.0161 500.5743· 505.2575· 525.5391 538.0041· 609.4793· 631.1755 639.1691· 648.2872· 704.1341 751.2830· 756.6060· 767.8036 774.7571· 792.8416· 833.9657 859.9813· 861.6209· 884.0434 898.0818· 925.7952· 943.5376 982.8646· 995.6029· 999.7733 1003.1321· 1004.2578· 1015.6606 1016.6575· 1018.8466· 1048.2019 1062.2957· 1113.2899· 1147.8232 1164.4249· 1176.2076· 1178.7384 1203.8347· 1209.1370· 1236.4184 1239.5756· 1268.5126· 1312.2575 1343.8340· 1344.5712· 1360.5474 1374.8935· 1391.3810· 1409.0074 1459.4812· 1489.9851· 1508.1227 1538.0520· 1542.9152· 1616.1766 1648.7317· 1668.1227· 1676.1440 1693.0684· 1730.1874· 3157.8826 3183.2870· 3189.2102· 3194.9967 3196.2820· 3203.3908· 3205.5798 3209.3335· 3212.4630· 3217.1691 3220.2714· 3227.0711· 3228.7946	C· 3.89801400· 0.94563800· 0.27359000 C· 5.28461000· 0.91968300· 0.25653300 C· 5.96438300· -0.26851900· -0.00466000 C· 5.24251100· -1.43232400· -0.24277700 C· 3.85304700· -1.40509900· -0.22513200 C· 3.15650800· -0.21665300· 0.02163200 H· 3.38772900· 1.87408100· 0.50112200 H· 5.84049400· 1.82815400· 0.45661900 H· 7.04753200· -0.28559900· -0.01438000 H· 5.76057000· -2.36316800· -0.44084900 H· 3.29268600· -2.31505500· -0.41197700 C· 0.87902600· 0.82563800· -0.02703800 H· 1.29677400· 1.82759400· -0.06768300 C· 1.68911500· -0.23974100· 0.01006600 C· -0.58461300· 0.75417500· -0.03649700 C· -1.36468800· 1.94789400· -0.14474500 C· -2.73250200· 1.90943400· -0.15663400 C· -3.43691300· 0.68010800· -0.06008700 C· -2.68983100· -0.53272900· 0.05031900 C· -1.30084200· -0.40154200· 0.05353400 H· -0.84554600· 2.89812900· -0.21910700 H· -3.30160400· 2.82867700· -0.24012200 C· -3.37744300· -1.77202600· 0.15002900 C· -4.74551900· -1.80223900· -0.13911100 H· -5.26698800· -2.74878000· 0.21533100 C· -4.85286600· 0.60572700· -0.06815000 C· -5.49083600· -0.60247700· 0.02853000 H· -6.57330800· -0.64620000· 0.02114800 H· -5.42230400· 1.52521000· -0.15265400 H· -2.79791100· -2.68370400· 0.23415500 H· 1.23491000· -1.22902800· 0.01264900
i9	-693.332538	24.0007· 41.2831· 54.7813 135.7214· 160.4685· 189.2368 247.7502· 268.2358· 299.4548 341.9291· 412.3735· 413.4587 451.4254· 480.4228· 494.7735 503.9836· 517.0624· 521.0222 589.2232· 617.4979· 628.9293 647.6338· 688.4894· 715.7265 724.1469· 762.1226· 766.6977 778.9217· 800.2332· 829.9986 850.5269· 871.7964· 884.5241 889.6823· 937.9697· 961.2496 981.5338· 997.2603· 1003.8981 1010.8268· 1018.2673· 1021.0099 1022.7056· 1048.7166· 1057.3866 1064.6391· 1111.3240· 1141.6333 1159.5743· 1167.6560· 1174.4409 1176.9044· 1191.6310· 1205.3006 1224.2764· 1225.8077· 1272.2019 1282.3205· 1297.6114· 1344.1480 1367.2210· 1375.2209· 1400.2834 1445.8503· 1462.1565· 1485.8494 1495.6613· 1538.4960· 1564.7725 1626.8807· 1641.6679· 1657.4656 1676.9600· 1681.4052· 3075.5425 3189.6543· 3191.6046· 3192.5710 3195.2170· 3201.5027· 3205.0106 3214.0197· 3214.5403· 3225.6233 3225.9079· 3226.4013· 3254.3722	C· 2.07518500· 0.16313400· 1.02937500 C· 3.11495000· -0.49513100· 1.67172800 C· 4.15820000· -1.04812400· 0.93121300 C· 4.15224700· -0.93763400· -0.45364300 C· 3.10724100· -0.27707900· -1.09577700 C· 2.06133700· 0.27995200· -0.36328900 H· 1.25998200· 0.58963700· 1.60578200 H· 3.11243800· -0.58086900· 2.75203100 H· 4.96865100· -1.56285500· 1.43334500 H· 4.95897900· -1.36565900· -1.03711900 H· 3.10415300· -0.19307400· -2.17774500 C· 0.61068100· 2.42984700· -0.57787900 H· 1.19518500· 3.33803400· -0.56145900 C· 0.93021000· 1.00033300· -1.05483300 C· -0.68684200· 2.04464200· -0.16285100 C· -1.90915900· 2.47037900· 0.43152000 C· -2.85581800· 1.50133700· 0.61775100 C· -2.65672100· 0.12585900· 0.25213800 C· -1.42712400· -0.29919300· -0.34854900 C· -0.48686600· 0.71665300· -0.54614600 H· -2.08740200· 3.49642300· 0.72808400 H· -3.80884600· 1.75991000· 1.06815500 C· -1.24236400· -1.66474600· -0.68488500 C· -2.24112900· -2.57294700· -0.44481600 H· -2.09847100· -3.61629200· -0.70017500 C· -3.65974500· -0.84195500· 0.47819300 C· -3.46081600· -2.15973600· 0.13845100 H· -4.24070500· -2.88930000· 0.32010700 H· -4.59597400· -0.52974000· 0.92912700 H· -0.30022500· -1.97163900· -1.12566300 H· 1.03143300· 0.91188500· -2.14069400
i10	-693.3247542	18.8762· 29.6222· 54.3416 96.4220· 127.9870· 178.5925 199.9029· 230.9330· 287.8965 368.7263· 405.1746· 411.9229 428.2608· 459.2303· 484.2862 502.8425· 506.4136· 527.8935	C· 2.21233900· -0.18753900· 1.11773700 C· 2.58910600· -1.52214700· 1.19873600 C· 3.38407900· -2.08603500· 0.20415800 C· 3.81145400· -1.30300400· -0.86303800 C· 3.44163100· 0.03581200· -0.93827200 C· 2.62407200· 0.60476900· 0.04069500

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		566.1039· 619.7911· 630.6168 658.9768· 680.9263· 714.8528 730.8317· 749.1440· 768.7152 773.5127· 789.8416· 794.2797 840.1476· 850.8408· 874.2758 889.1504· 924.8021· 954.6389 984.2145· 992.7429· 997.0590 1006.4985· 1014.2315· 1015.7092 1018.0208· 1022.4540· 1047.7127 1060.0105· 1108.5187· 1145.8791 1164.0069· 1174.6940· 1177.1761 1198.9462· 1203.9385· 1216.0805 1237.0618· 1252.5345· 1271.9629 1317.1157· 1348.7445· 1361.0027 1392.6729· 1413.9355· 1438.4155 1460.0262· 1483.8994· 1508.8546 1535.8844· 1541.1364· 1618.1740 1646.6153· 1671.7649· 1673.0545 1694.0922· 1724.9598· 3166.5141 3186.5329· 3189.1695· 3193.9599 3195.1187· 3200.0095· 3203.5901 3208.1969· 3208.4598· 3215.3638 3216.4454· 3225.7709· 3226.7007	H· 2.26454200· -2.12205400· 2.04092600 H· 3.67616000· -3.12764300· 0.26604200 H· 4.43574100· -1.73337200· -1.63718700 C· 0.98774200· 2.51844500· -0.04576900 H· 0.86921000· 3.59720500· -0.09712700 C· 2.23434700· 2.02971600· -0.05449300 C· -0.27223100· 1.76154500· -0.02362200 C· -1.51565200· 2.45816400· 0.10365200 C· -2.71091500· 1.79153300· 0.11475400 C· -2.76710200· 0.37673900· -0.00497600 C· -1.54485500· -0.34703600· -0.14327000 C· -0.37166000· 0.40953600· -0.15320000 H· -1.49555100· 3.53947700· 0.19647800 H· -3.63978400· 2.34176500· 0.21667300 C· -1.57328700· -1.76201700· -0.26064600 C· -2.76926600· -2.42764900· -0.24069800 H· -2.79122600· -3.50716000· -0.32962800 C· -3.98519600· -0.34883800· 0.00832600 C· -3.98596500· -1.71431300· -0.10584600 H· -4.92319500· -2.25784500· -0.09366400 H· -4.91733800· 0.19657200· 0.11122900 H· -0.63280400· -2.29090000· -0.36527100 H· 1.59538500· 0.25369600· 1.89264200 H· 3.05173800· 2.73900200· -0.15518800 H· 3.77528500· 0.64517800· -1.77129100
i11	-693.3571741	64.3681· 73.1893· 113.8913 176.7891· 206.4477· 233.5006 275.2918· 285.7963· 359.0321 410.2458· 425.1009· 438.8262 477.8493· 486.5587· 493.4347 515.5990· 537.5452· 560.8067 563.3850· 606.6023· 650.3403 667.2278· 697.9841· 730.5774 750.4234· 761.1893· 762.8277 786.0636· 804.7511· 816.0606 848.1467· 855.4029· 874.9810 892.4179· 949.5572· 955.7115 966.9744· 985.0828· 989.3642 996.4563· 1009.0595· 1015.0584 1032.0007· 1056.6076· 1072.6246 1095.5935· 1113.6067· 1161.2486 1166.9643· 1183.4801· 1192.2450 1203.3003· 1222.1496· 1228.3051 1238.8559· 1242.0385· 1288.2164 1305.9900· 1332.2318· 1366.3581 1379.0186· 1404.1742· 1414.0678 1426.4047· 1458.3713· 1474.5355 1505.3149· 1527.9578· 1557.0407 1576.7428· 1629.8128· 1662.9994 1670.9768· 1691.6175· 2831.7570 3189.2703· 3191.9124· 3194.8240 3196.5012· 3198.8515· 3207.9023 3210.6338· 3213.5417· 3219.2306 3223.6164· 3229.8130· 3266.4832	C· -3.71421600· -0.22426100· -0.11066800 C· -3.75644900· -1.58474300· -0.25193500 C· -2.54696200· -2.31093000· -0.30824700 C· -1.34049400· -1.67825000· -0.16251600 C· -1.25444500· -0.27054600· 0.05048900 C· -2.48138700· 0.46380500· 0.01222700 H· -4.70457400· -2.09876400· -0.35321700 H· -2.57054700· -3.37939200· -0.48756900 H· -0.43682200· -2.25716500· -0.27196400 C· -1.27184500· 2.54855100· 0.06449100 H· -1.24569700· 3.63232800· 0.02969800 C· -2.45868800· 1.88187700· 0.05351600 C· -0.04127400· 1.84064500· 0.13513500 C· 1.20239600· 2.57825400· 0.00979700 C· 2.37716200· 1.93868300· -0.25504700 C· 2.46333200· 0.52878700· -0.13588400 C· 1.33520400· -0.13613200· 0.61641200 C· -0.03061800· 0.44788100· 0.22001400 H· 1.14214800· 3.65949800· -0.04448900 H· 3.24892200· 2.49646100· -0.58125400 C· 1.51570100· -1.61509600· 0.77302500 C· 2.60109500· -2.26369000· 0.30348100 H· 2.71139100· -3.32618500· 0.48937300 C· 3.56210500· -0.20790500· -0.58377400 C· 3.63924000· -1.57398200· -0.40840000 H· 4.49201500· -2.12711100· -0.78014400 H· 4.36680900· 0.32231700· -1.08352700 H· 0.78990400· -2.14265600· 1.37914100 H· 1.43568300· 0.26323000· 1.65159200 H· -4.62868600· 0.35936900· -0.11258000 H· -3.39969300· 2.42038600· 0.03223800
i12	-693.2843232	19.3011· 30.2661· 46.6135 124.0283· 149.0850· 166.6839 184.6102· 242.5495· 276.9080 353.8806· 407.3044· 413.7596 425.2364· 474.8584· 481.3121 488.6076· 507.5380· 518.3994 547.9784· 599.2434· 625.9688 654.6334· 656.6498· 685.4468 721.6680· 760.7797· 766.3504 778.4746· 786.6611· 803.6724 839.3781· 844.4712· 862.9166 892.8087· 916.0517· 941.1034 983.9943· 996.0672· 996.6522 997.9288· 1003.6735· 1007.7559 1018.1469· 1048.6838· 1054.0581 1059.0332· 1097.6001· 1140.1659 1150.3757· 1163.1082· 1173.0786	C· 3.45122900· 0.02196200· -1.04454400 C· 4.80453300· -0.24793600· -1.14933600 C· 5.56521800· -0.53434100· -0.01548100 C· 4.94831000· -0.54730300· 1.23727300 C· 3.59799300· -0.27917300· 1.35318600 C· 2.80292500· 0.01483600· 0.21586000 H· 2.88790700· 0.24047100· -1.94268700 H· 5.27598000· -0.23606800· -2.12519600 H· 6.62367800· -0.74455500· -0.10629100 H· 5.52996400· -0.76865200· 2.12451200 H· 3.12428700· -0.29071700· 2.32892800 C· 0.45866200· 0.60371500· -0.67330000 H· 0.85905400· 0.64462900· -1.68282800 C· 1.42093800· 0.28261200· 0.38948400 C· -0.73873900· 1.48346400· -0.37073500 C· -1.66528600· 2.44155000· 0.07016800 C· -2.92389900· 1.92290200· 0.28769400

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1178.8672·1190.8867·1211.7524 1235.6284·1246.9486·1274.8153 1312.9800·1332.9296·1350.6344 1379.5274·1384.9740·1426.4546 1451.0412·1475.2592·1492.9852 1499.9529·1514.5591·1568.8727 1614.7901·1622.2213·1632.3819 1687.6296·1782.7491·3145.5904 3185.2286·3192.8482·3195.3238 3195.3890·3203.3341·3205.4237 3212.9271·3217.3802·3226.1526 3226.6637·3228.1366·3232.3168	C·-3.23533100· 0.53365900· 0.13013000 C·-2.23624800·-0.41325100·-0.27094800 C·-0.99564300· 0.19705600·-0.52628900 H·-1.44323000· 3.48951500· 0.22508300 H·-3.72717300· 2.57863400· 0.60821600 H· 1.01967300· 0.24870800· 1.39754800 C·-2.56122500·-1.78600200·-0.37884300 C·-3.83599500·-2.21118800·-0.10876000 C·-4.83514300·-1.28584600· 0.27542100 C·-4.54301000· 0.04850300· 0.39112300 H·-1.78930700·-2.48451900·-0.67910700 H·-4.08632600·-3.26223300·-0.19105000 H·-5.83832500·-1.63985800· 0.48065600 H·-5.31191000· 0.75333000· 0.68960400
i13	-693.3309042	15.4481· 39.2537· 58.1732 82.4512· 149.2570· 178.6578 192.6966· 224.9638· 248.8876 324.5386· 368.8810· 396.0652 410.0227· 476.1258· 477.4403 498.7914· 501.5995· 531.5270 548.8611· 618.1505· 631.6714 635.6598· 655.2676· 706.1513 750.9458· 762.9427· 763.8778 776.6636· 789.2330· 850.5756 862.5112· 872.9195· 877.6346 892.4032· 906.5754· 919.2932 944.2593· 953.7312· 989.0687 1000.5348·1002.7670·1012.2531 1016.5392·1020.6105·1052.7661 1062.6146·1112.3109·1157.0065 1162.3535·1177.4845·1197.1265 1207.1503·1222.3252·1234.6377 1268.6681·1281.8526·1282.6222 1325.5637·1343.5173·1357.0545 1368.7531·1403.9388·1433.8367 1456.2330·1484.9028·1493.5004 1540.2426·1548.1895·1630.9863 1649.4796·1665.3660·1675.3103 1690.3304·1725.7023·3161.4191 3181.5220·3186.7216·3193.8621 3195.1955·3197.3708·3201.3993 3203.1103·3211.6014·3215.4353 3219.3936·3227.5715·3228.0576	C· 4.20513000·-1.21226700·-0.00001500 C· 5.57487400·-0.97660100·-0.00001800 C· 6.05593200· 0.32726500·-0.00000300 C· 5.15521700· 1.39108100· 0.00001400 C· 3.78896100· 1.15442700· 0.00001600 C· 3.28826500·-0.15493600· 0.00000100 H· 3.83312900·-2.23135300·-0.00002700 H· 6.26522100·-1.81174100·-0.00003100 H· 7.12258000· 0.51651100·-0.00000400 H· 5.52262800· 2.41056700·-0.00002700 H· 3.10767900· 1.99681500· 0.00003100 C· 0.84081700· 0.40725400· 0.00000200 H· 1.03211200· 1.47626300·-0.00000100 C· 1.85459600·-0.46793900· 0.00000200 C·-0.57009500· 0.02309500· 0.00000300 C·-0.99822800·-1.31945100· 0.00001100 C·-2.27005700·-1.75878000· 0.00001200 C·-3.31251300·-0.77802800· 0.00000500 C·-2.95091200· 0.59761100·-0.00000400 C·-1.57926100· 0.96530000·-0.00000400 H· 1.61060100·-1.52862400· 0.00000200 H·-2.52306200·-2.81403400· 0.00001900 C·-3.98119700· 1.57287000·-0.00001100 C·-5.30029400· 1.20096900·-0.00001000 H·-6.07754400· 1.95561700·-0.00001700 C·-4.68209500·-1.13425500· 0.00000600 C·-5.65488000·-0.16730400·-0.00000200 H·-6.70087700·-0.44969600·-0.00000100 H·-4.94904600·-2.18549200· 0.00001300 H·-3.70561000· 2.62199100·-0.00001800 H·-1.32337800· 2.02131700·-0.00001100
i14	-693.3335041	25.9623· 40.9500· 62.0126 124.5986· 171.4646· 213.2824 265.1432· 278.8841· 295.7267 353.7765· 373.0988· 412.5745 436.2912· 467.5075· 478.5614 524.7241· 538.8335· 572.2419 602.2636· 619.9172· 625.4967 630.9532· 703.2649· 715.6796 763.5982· 767.5848· 770.7066 783.2089· 820.1650· 851.9240 856.8855· 871.2454· 879.2468 888.8016· 913.5371· 922.4716 947.3510· 977.3372· 986.1882 1003.4640·1009.4721·1018.2829 1020.6519·1056.2940·1059.8829 1068.0742·1111.4504·1143.7971 1156.7153·1163.4242·1177.0050 1184.1980·1204.8586·1210.9734 1222.7918·1229.2634·1243.4694 1280.7865·1293.4849·1343.4275 1358.7543·1366.8817·1378.5448 1430.5609·1462.1372·1492.8713 1495.1363·1538.0437·1557.9523 1600.5874·1657.7585·1675.5119 1677.3203·1702.8294·3072.2397 3190.5872·3193.1053·3193.7564 3197.3694·3202.7045·3205.9095 3209.5142·3212.7304·3215.1697	C·-3.69373100· 0.02634500·-1.02465200 C·-4.76132700·-0.66268000·-0.45373000 C·-4.66365300·-1.14236700· 0.84634000 C·-3.49379200·-0.93074800· 1.57372400 C·-2.43152800·-0.24357400· 1.00250100 C·-2.52133100· 0.24291700·-0.30457300 H·-3.77232700· 0.39940800·-2.04058400 H·-5.66701100·-0.82384900·-1.02656400 H·-5.49218700·-1.67924300· 1.29266000 H·-3.41074900·-1.30451000· 2.58753500 H·-1.51856700·-0.08315300· 1.56776100 C·-0.80291100· 2.17841300·-0.10588400 H·-1.25450300· 3.09562300· 0.24454000 C·-1.36680700· 1.00012600·-0.91515100 C· 0.47006900· 1.57112600· 0.01251700 C· 0.04010200· 0.41511300·-0.71982900 C· 0.82875200·-0.65440300·-0.94977600 C· 2.17461600·-0.58300400·-0.43910800 C· 2.62398000· 0.57358500· 0.28126900 C· 1.75476600· 1.67604700· 0.51699100 H·-1.58946900· 1.24913000·-1.95727000 H· 0.50404000·-1.54054200·-1.48434800 C· 3.95902200· 0.59105100· 0.76225500 C· 4.80945900·-0.46448400· 0.54966500 H· 5.82476000·-0.42814700· 0.92602600 C· 3.07615600·-1.64985100·-0.63810700 C· 4.36441400·-1.59903900·-0.15848200 H· 5.03871500·-2.43065600·-0.32383900

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		3225.4718·3226.4160·3247.1785	H· 2.73133300·-2.52233900·-1.18292600 H· 4.29791700· 1.46569400· 1.30726700 H· 2.11050900· 2.53514500· 1.07391500
ii5	-693.3258402	25.8052· 31.4974· 63.2940 100.7911· 138.9025· 192.6225 198.3518· 220.8070· 284.7972 381.0708· 389.5520· 404.2935 414.9875· 466.5236· 478.0956 497.9462· 517.5660· 535.2913 569.9907· 626.1068· 630.3794 660.9505· 677.8521· 716.9900 744.5819· 757.4660· 763.4347 771.6199· 792.1167· 796.8605 858.9176· 862.4897· 875.9910 893.2281· 896.8405· 920.4493 947.8785· 958.3609· 992.2864 1007.9468· 1014.0521· 1014.7150 1018.0642· 1023.1606· 1052.0645 1060.6307· 1110.2980· 1153.9545 1160.4886· 1176.2986· 1179.1957 1203.6463· 1205.5539· 1226.6825 1242.1436· 1279.3829· 1283.5910 1321.9889· 1329.5412· 1350.7223 1398.6484· 1418.9625· 1446.3235 1456.5177· 1482.7898· 1490.6815 1536.9914· 1546.7079· 1628.6306 1646.7854· 1664.6358· 1674.2774 1690.5358· 1721.5373· 3164.8907 3178.8659· 3186.9014· 3190.8200 3193.7539· 3195.3572· 3199.2849 3200.1624· 3209.2121· 3213.8337 3216.5453· 3226.1699· 3226.3395	C· 3.93627400· 0.45613700·-0.80288800 C· 4.64184100·-0.74041200·-0.75115900 C· 4.30960300·-1.70567100· 0.19430500 C· 3.27237100·-1.46463200· 1.09075100 C· 2.56180100·-0.27238200· 1.03250600 C· 2.87485600· 0.69741400· 0.07390300 H· 5.45376200·-0.91759800·-1.44657600 H· 4.86285000·-2.63618300· 0.23941500 H· 3.01988400·-2.20430700· 1.84137200 C· 0.81882100· 2.16865800· 0.00155700 H· 0.45969900· 3.19401900· 0.00108200 C· 2.14529600· 1.98065600· 0.00927000 C·-0.24297800· 1.15587600·-0.05840600 C·-0.02305900·-0.20103000·-0.36399200 C·-0.96231800·-1.16215100·-0.46081600 C·-2.32591700·-0.78952800·-0.24778900 C·-2.61924100· 0.56924100· 0.05369000 C·-1.56299800· 1.51427900· 0.13473600 H·-0.71448600·-2.19206200·-0.69686200 C·-3.97088900· 0.94563300· 0.26534900 C·-4.97827500· 0.02050900· 0.18240800 H·-6.00636400· 0.32000400· 0.34656400 C·-3.38654500·-1.72405000·-0.32872000 C·-4.68270000·-1.32922500·-0.11800700 H·-5.48734900·-2.05206100·-0.18170000 H·-3.15518800·-2.75807000·-0.56039400 H·-4.19340700· 1.98219000· 0.49509600 H·-1.80824800· 2.54912600· 0.35816500 H· 4.19819400· 1.20917600·-1.53851200 H· 2.77076100· 2.86851500·-0.03866100 H· 1.76424300·-0.07867900· 1.74082800
ii6	-693.3706509	43.8513· 66.3293· 112.5386 154.7433· 190.5332· 256.8327 267.4848· 301.7501· 341.0192 386.8368· 412.6404· 447.6907 467.2877· 481.7594· 494.1890 511.0964· 527.8514· 559.8058 574.5232· 625.2055· 636.7935 659.0723· 704.3038· 712.9690 755.6114· 763.2319· 765.3908 785.7037· 803.8395· 810.1977 857.4210· 865.2626· 874.0376 911.7126· 915.1802· 919.0696 954.5857· 960.3871· 980.3327 990.4972· 997.7381· 1012.1695 1015.9832· 1050.9525· 1064.8929 1093.4145· 1125.6063· 1157.5135 1168.2388· 1182.1929· 1192.5881 1205.1961· 1220.3502· 1236.0113 1253.5092· 1277.0919· 1291.3163 1305.1661· 1333.3293· 1355.5862 1377.3111· 1406.2701· 1426.0357 1433.5698· 1454.3952· 1491.3879 1509.4196· 1529.4647· 1546.8071 1597.0393· 1642.9878· 1658.8632 1674.2170· 1699.1384· 2850.3186 3186.0861· 3188.5137· 3190.9737 3194.2357· 3198.3719· 3199.8531 3210.0794· 3212.1969· 3212.9347 3224.9827· 3228.5762· 3233.9375	C· 4.00669100· 0.36740800·-0.40588300 C· 4.41778400·-0.95163200·-0.45623100 C· 3.49765800·-1.99911900·-0.12325800 C· 2.25253700·-1.72821000· 0.32006900 C· 1.78676600·-0.32344200· 0.56655800 C· 2.71786900· 0.71914300·-0.00822800 H· 5.41664300·-1.20098300·-0.79001100 H· 3.81258400·-3.02988600·-0.23969600 H· 1.59170200·-2.54306500· 0.58686500 C· 0.94174200· 2.36857200· 0.12596200 H· 0.61183900· 3.40111500· 0.09710200 C· 2.25733900· 2.06318500·-0.03716300 C·-0.07698300· 1.33682800· 0.17536700 C· 0.31841700·-0.04018900· 0.26677700 C·-0.63480900·-1.01601200· 0.18049300 C·-2.01460200·-0.70324200· 0.03259600 C·-2.41123100· 0.65896000·-0.02097700 C·-1.41236000· 1.65675900· 0.04614400 H·-0.36544500·-2.06420100· 0.22891800 C·-3.78914300· 0.97120700·-0.15637800 C·-4.72647000·-0.02477100·-0.23421700 H·-5.77614100· 0.22301400·-0.33743300 C·-3.00587300·-1.71133500·-0.05236200 C·-4.33071900·-1.38210900·-0.18209700 H·-5.08075500·-2.16131200·-0.24596000 H·-2.69882000·-2.75108200·-0.01191800 H·-4.08637300· 2.01361400·-0.19846100 H·-1.70601000· 2.69972800·-0.02689700 H· 4.68165300· 1.15729500·-0.72030400 H· 2.97816100· 2.85098000·-0.23194300 H· 1.85327100·-0.16721300· 1.66669900
ii7	-693.2844519	16.6617· 36.2789· 48.8033 137.4602· 140.4474· 169.4813 205.9030· 264.1958· 275.7059 337.6141· 371.5186· 409.1762 429.7577· 450.7313· 481.1128 490.4757· 498.9949· 541.2574 573.4803· 598.9813· 625.4195 638.7058· 661.5673· 685.7175	C·-3.72472000· 0.00004400·-1.02628400 C·-5.10595500· 0.00004500·-1.11043500 C·-5.89114400·-0.00000300· 0.04271900 C·-5.27047600·-0.00005000· 1.29375900 C·-3.89242900·-0.00005100· 1.38941200 C·-3.07210100·-0.00000500· 0.23186800 H·-3.14323800· 0.00008400·-1.93947000 H·-5.58016800· 0.00008200·-2.08497400

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		719.6250· 766.5259· 769.3016 777.4525· 789.2901· 843.1619 854.5798· 862.6583· 878.3981 897.8880· 915.6839· 932.1165 936.9280· 948.1332· 991.2965 995.9569· 996.8009· 1008.5570 1013.3227· 1053.7151· 1055.4236 1062.5460· 1094.3140· 1106.7208 1143.8388· 1162.0406· 1167.3088 1172.6485· 1192.1791· 1206.3334 1231.6119· 1242.0346· 1277.7887 1295.8396· 1327.8985· 1350.0910 1357.7361· 1392.7373· 1404.6935 1449.4239· 1481.9687· 1493.2451 1497.4442· 1513.3818· 1586.9871 1614.1859· 1630.5638· 1677.3329 1691.9895· 1762.7630· 3154.1330 3189.9156· 3193.5274· 3196.2329 3196.8929· 3201.9717· 3203.5076 3203.7414· 3213.2031· 3213.3772 3225.1302· 3226.1697· 3231.2096	H· -6.97148400· -0.00000300· -0.03198400 H· -5.87125700· -0.00008700· 2.19569800 H· -3.41590200· -0.00008700· 2.36378400 C· -0.67524000· 0.00002000· -0.70404800 H· -1.07285700· 0.00004700· -1.71517400 C· -1.66333100· -0.00001200· 0.38593000 C· 0.65727100· -0.68226200· -0.51148500 C· 1.74435800· -1.45715100· -0.28149600 C· 2.95671800· -0.71727900· -0.06923800 C· 2.95671900· 0.71728300· -0.06919900 C· 1.74435900· 1.45716700· -0.28141500 C· 0.65727100· 0.68229300· -0.51144800 H· 1.75574600· -2.54102400· -0.25053400 H· -1.25800800· -0.00004800· 1.39231900 H· 1.75574800· 2.54103800· -0.25039600 C· 5.34858300· 0.70592800· 0.36748000 C· 4.18207200· 1.39396200· 0.15485100 C· 4.18207000· -1.39397200· 0.15477600 C· 5.34858200· -0.70595000· 0.36744200 H· 6.27371800· 1.24394100· 0.53633400 H· 4.17916700· 2.47887900· 0.15456000 H· 4.17916400· -2.47888900· 0.15442700 H· 6.27371700· -1.24397300· 0.53626700
TS1-1	-693.263336	388.2858i· 9.1289· 19.0460 24.3351· 55.3056· 82.1569 160.0460· 167.3645· 176.3390 202.7115· 365.5025· 385.5749 390.2077· 408.6418· 474.5867 475.2313· 480.9800· 487.8959 514.0012· 546.0640· 547.5347 620.1607· 621.9904· 633.4553 692.8436· 705.5714· 712.0249 751.4373· 760.3851· 778.4824 779.1036· 781.8243· 804.9515 819.9938· 863.9593· 869.1384 898.6107· 929.0883· 948.4709 974.8838· 992.4633· 1006.3981 1012.5369· 1015.8244· 1022.3483 1043.3521· 1054.9107· 1058.0278 1109.8332· 1144.5578· 1160.0931 1173.4768· 1178.1854· 1199.2894 1211.7561· 1233.0996· 1252.7711 1282.2346· 1309.1861· 1348.6496 1355.4445· 1393.1969· 1420.6247 1467.6995· 1482.1914· 1483.2675 1528.3553· 1549.3755· 1631.0029 1638.6177· 1658.4817· 1666.9404 1695.3587· 2130.7648· 3179.0736 3186.8390· 3195.4638· 3199.7439 3203.3705· 3204.3190· 3212.0556 3213.4270· 3220.8884· 3225.6480 3226.8777· 3232.0689· 3448.8171	C· -1.96372900· 2.40997900· 0.00002000 C· -3.15734400· 1.72845200· 0.00003700 C· -3.18604100· 0.30808100· 0.00001500 C· -1.96137400· -0.41770800· -0.00002500 C· -0.73191000· 0.30281500· -0.00004200 C· -0.78579800· 1.65457800· -0.00002000 H· -5.34089000· 0.14367300· 0.00006300 H· -1.94325200· 3.49448000· 0.00003700 H· -4.09839500· 2.26950100· 0.00006700 C· -4.40936600· -0.41239900· 0.00003200 C· -2.00177100· -1.83630000· -0.00004700 H· 0.21297500· -0.23395400· -0.00007100 C· -3.19876500· -2.50151200· -0.00003000 C· -4.41772400· -1.78159300· 0.00001100 H· -1.06491400· -2.38300000· -0.00007800 H· -3.21779400· -3.58497100· -0.00004600 H· -5.35778800· -2.32013900· 0.00002500 C· 1.32768500· 2.68974600· -0.00003700 C· 2.14626900· 1.79279600· -0.00002300 C· 2.95120300· 0.61718200· -0.00000300 C· 3.34166900· 0.02641600· 1.21108300 C· 3.34172000· 0.02641000· 1.21107000 C· 4.10560800· -1.13181400· 1.20546500 H· 3.03616900· 0.48448300· 2.14379400 C· 4.10565900· -1.13182000· -1.20541300 H· 3.03626000· 0.48447200· -2.14379600 C· 4.48944100· -1.71419600· 0.00003600 H· 4.40219600· -1.58291300· 2.14477500 H· 4.40228700· -1.58292400· -2.14470800 H· 5.08606500· -2.61841400· 0.00005100 H· 0.87448500· 3.65502600· -0.00005100
TS1-2	-693.2634702	374.6653i· 9.7279· 22.7902 25.9858· 51.7587· 80.6443 153.7651· 166.8854· 177.9130 201.0877· 368.8255· 373.1224 389.2108· 408.5886· 474.2145 475.2629· 482.6943· 487.0801 514.5607· 545.3587· 549.3808 620.6012· 621.6466· 633.2299 691.4468· 706.1161· 712.9596 753.7169· 762.3417· 777.8670 779.4763· 782.4440· 800.7777 826.9452· 855.6630· 871.3610 895.0221· 930.0563· 948.8815 981.8766· 994.9490· 1007.8700 1013.6672· 1015.7071· 1022.6335 1045.0536· 1055.5187· 1057.8197 1108.9485· 1144.4152· 1159.6787 1170.5908· 1177.7574· 1199.0836 1210.2388· 1232.6687· 1249.9862	C· 0.35554600· -0.39864600· 0.00001500 C· 1.40110900· -1.28806500· 0.00001100 C· 2.74809900· -0.83176400· 0.00000400 C· 3.01568400· 0.56590000· 0.00000100 C· 1.91780200· 1.47834600· 0.00000600 C· 0.66579700· 0.96489600· 0.00001300 H· 3.63316400· -2.80217200· 0.00000100 H· -0.67644100· -0.73406000· 0.00001900 H· 1.21363000· -2.35721700· 0.00001200 C· 3.84063500· -1.73733800· -0.00000100 C· 4.36304600· 1.00915600· -0.00000600 H· 2.11394500· 2.54682100· 0.00000400 C· 5.39561800· 0.10890500· -0.00001100 C· 5.13211100· -1.28124900· -0.00000800 H· 4.56130800· 2.07564400· -0.00000800 H· 6.42105000· 0.45917800· -0.00001600 H· 5.95751200· -1.98296500· -0.00001200 C· -1.23386000· 2.35756300· 0.00000100 C· -2.20609800· 1.63048000· -0.00000100

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1280.5504·1309.0278·1347.8560 1351.9799·1392.4244·1420.6273 1467.4844·1479.0868·1482.6543 1528.5587·1551.2775·1631.8545 1638.1726·1655.1649·1667.4508 1693.3969·2131.4106·3176.5933 3187.0737·3193.8656·3197.7972 3203.1708·3203.4487·3210.4845 3212.5043·3220.5854·3224.8914 3225.6679·3231.2934·3448.3798	C·-3.23101400· 0.64023400·-0.00000200 C·-3.73426400· 0.14200500·-1.21095900 C·-3.73426400· 0.14200100· 1.21095300 C·-4.71956800·-0.83484400·-1.20536900 H·-3.34215200· 0.52824500·-2.14380100 C·-4.71956700·-0.83484800· 1.20536100 H·-3.34215000· 0.52823800· 2.14379700 C·-5.21486900·-1.32599100·-0.00000500 H·-5.10254200·-1.21510900·-2.14477500 H·-5.10254000·-1.21511700· 2.14476600 H·-5.98430200·-2.08856100·-0.00000600 H·-0.60215000· 3.21663200· 0.00000100
TSint1-1- nt1-2	-693.3335789	39.5890i· 12.6320· 49.0360 84.6351· 115.8729· 154.2058 175.1255· 242.6031· 282.6772 298.6547· 394.2448· 402.7718 422.9992· 463.2278· 474.5747 482.8107· 486.6305· 524.7880 540.0301· 571.7786· 625.8287 629.5718· 660.9981· 678.9355 721.9144· 754.2080· 766.5254 775.7829· 784.8459· 788.4451 808.8695· 840.1148· 845.3832 882.7277· 906.2492· 907.1230 926.3130· 976.1954· 986.6265 988.4800· 994.6941·1001.4308 1003.4592·1015.0637·1045.2521 1049.8754·1109.8546·1127.7519 1154.0993·1161.6020·1169.7239 1180.4310·1189.6961·1204.3687 1229.5112·1268.4901·1289.8649 1298.9897·1311.6180·1343.3933 1380.3347·1401.8631·1426.3211 1468.9156·1475.0477·1490.4540 1510.7761·1556.8590·1591.7124 1613.1236·1645.5320·1673.8006 1707.8378·1909.4878·3081.7258 3194.0203·3195.3333·3195.4341 3198.9167·3201.9047·3207.2244 3213.0910·3214.3870·3220.9393 3224.3878·3225.3520·3231.3380	C·-0.99652200·-1.81274400· 0.30326900 C·-2.20672600·-1.82945300·-0.33495900 C·-3.03712300·-0.67895000·-0.34962100 C·-2.58925500· 0.49600500· 0.31126000 C·-1.32924900· 0.48318900· 0.96385200 C·-0.54369900·-0.64075100· 0.96448900 H·-4.63331500·-1.56499700·-1.50590200 H·-0.36442800·-2.69330700· 0.30710600 H·-2.54616100·-2.72594700·-0.84283500 C·-4.29682500·-0.66483400·-1.00265600 C·-3.41574500· 1.64992300· 0.29731100 H·-0.98755800· 1.38351600· 1.46445300 C·-4.62700700· 1.63436500·-0.34106300 C·-5.07330800· 0.46301400·-0.99921300 H·-3.06985500· 2.54541800· 0.80242600 H·-5.25055600· 2.52043100·-0.34544200 H·-6.03372900· 0.46423600·-1.50064600 C· 0.78532200·-0.65052000· 1.66117000 C· 1.90018000·-0.36007300· 1.06048900 C· 3.03421900·-0.03968100· 0.35492000 C· 3.78608900·-1.04485400·-0.32131100 C· 3.49924100· 1.30632400· 0.28517200 C· 4.92778900·-0.71073800·-1.01995100 H· 3.44299700·-2.07105400·-0.27660000 C· 4.64427500· 1.61321000·-0.42045600 H· 2.93666300· 2.07916100· 0.79402200 C· 5.36918900· 0.61467100·-1.07805800 H· 5.48617600·-1.48725700·-1.52955800 H· 4.98265300· 2.64182000·-0.46432600 H· 6.26634200· 0.86637700·-1.62934000 H· 0.78569900·-0.92701400· 2.71878200
TS1	-693.2484391	2208.2730i· 23.6183· 44.1525 48.1994· 90.2036· 166.0010 169.1505· 188.5634· 240.1827 296.5222· 321.0032· 387.8613 394.9218· 407.3781· 461.4053 472.7554· 487.2718· 510.9020 533.3039· 539.2466· 612.3809 631.5705· 643.5517· 655.6258 708.0130· 755.2899· 760.2355 769.3806· 775.8783· 792.9853 830.2079· 847.6944· 859.4175 888.1772· 888.3648· 925.2497 926.5639· 966.7576· 986.3353 989.0055· 997.0974·1002.4434 1010.4373·1015.3752·1021.0200 1031.9562·1050.4636·1121.7369 1153.3031·1163.3760·1167.3618 1181.8445·1188.2806·1203.4733 1225.7420·1261.9537·1283.8728 1293.3413·1308.0081·1341.9967 1397.0360·1406.0804·1431.7005 1466.1945·1479.5807·1490.3382 1514.5872·1562.6552·1619.9504 1645.4047·1656.6397·1675.1187 1702.1662·1749.5731·1886.0200 3114.4461·3190.9317·3193.0971 3196.5176·3198.4027·3198.6338 3208.1848·3211.7471·3212.1727 3224.5765·3224.6395·3231.7776	C· 3.33663700·-1.08989900·-0.00000800 C· 4.52323500·-1.79693600· 0.00001100 C· 5.68149000·-1.01034300· 0.00002600 C· 5.62584700· 0.38871900· 0.00002000 C· 4.41377300· 1.07609000·-0.00000100 C· 3.26119300· 0.29411400·-0.00001500 H· 1.91616100·-1.00296700·-0.00001900 H· 4.57494300·-2.87786700· 0.00001100 H· 6.65042800·-1.49718000· 0.00004000 H· 6.55461500· 0.94700500· 0.00003400 H· 4.38479500· 2.15898400·-0.00000700 C· 0.82761200· 1.29498600·-0.00002100 H· 1.11204500· 2.34901700·-0.00003100 C· 1.81464000· 0.40660600·-0.00002800 C·-0.61318000· 1.01571200·-0.00001300 C·-1.51635700· 2.11532300· 0.00000200 C·-2.86948700· 1.92092600· 0.00001500 C·-3.41401600· 0.61139200· 0.00001100 C·-2.52185600·-0.49599000·-0.00000800 C·-1.12734800·-0.26282300·-0.00002100 H·-1.11286000· 3.12225000· 0.00000600 H·-3.54555800· 2.76918700· 0.00002600 C·-3.06192400·-1.81072900·-0.00001300 C·-4.41575400·-2.01067900·-0.00000100 H·-4.81637600·-3.01739700·-0.00000400 C·-4.81215000· 0.37235400· 0.00002200 C·-5.30270800·-0.90612200· 0.00001600 H·-6.37225800·-1.07889900· 0.00002400 H·-5.48638700· 1.22219200· 0.00003500 H·-2.37945900·-2.65385700·-0.00002500

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
			H·-0.45798200·-1.11667300·-0.00004800
TS2	-693.3210742	92.0520i· 36.1082· 40.8204 56.3641· 115.2034· 144.7642 184.7262· 234.2360· 267.1003 322.4643· 376.6676· 411.3997 418.6953· 448.6839· 475.0475 483.5246· 517.8711· 530.6276 540.1157· 603.8338· 627.0212 638.5921· 659.8156· 706.1954 748.5768· 765.8919· 767.7936 772.5517· 792.6540· 837.7012 854.8499· 870.3915· 881.0794 893.4994· 927.3906· 931.2162 968.0651· 988.2300· 992.3370 995.6452· 998.9957· 1003.4260 1010.5087· 1015.1961· 1051.1485 1054.9797· 1129.9720· 1154.0102 1164.1850· 1170.8116· 1182.2300 1194.4646· 1223.0760· 1231.1498 1255.1389· 1266.0685· 1292.9153 1310.4451· 1315.6446· 1335.7071 1394.1402· 1406.8317· 1431.0671 1452.2921· 1479.1894· 1491.9860 1514.3658· 1561.0422· 1604.4140 1647.6941· 1667.0399· 1677.5654 1706.7436· 1740.0541· 3162.2764 3167.6515· 3192.9102· 3193.9598 3194.4696· 3196.2590· 3198.2402 3201.9720· 3210.2153· 3212.9086 3213.1820· 3223.9069· 3225.6771	C·-3.98456500· 0.48681800· 1.05757000 C·-5.35395000· 0.58370800· 1.02349300 C·-6.01274800·-0.12008300· 0.01169700 C·-5.27826200·-0.87185400·-0.90164600 C·-3.88998600·-0.93220400·-0.81895800 C·-3.20113500·-0.23503600· 0.18418800 H·-5.90435200· 1.17724700· 1.74405300 H·-7.09346100·-0.07744300·-0.06009700 H·-5.79045900·-1.41373600·-1.68755600 H·-3.32291000·-1.51549400·-1.53685900 C·-0.91838000· 0.61326900·-0.28190200 H·-1.37316400· 1.43800300·-0.82685200 C·-1.71806500·-0.28293300· 0.29613500 C· 0.55418500· 0.60803600·-0.22305200 C· 1.24796100· 1.84246900·-0.36205300 C· 2.61202900· 1.89887200·-0.29140100 C· 3.37759800· 0.72148900·-0.08907000 C· 2.69738800·-0.52058800· 0.03156000 C· 1.28372400·-0.54531900·-0.04589000 H· 0.67323600· 2.74942600·-0.51594800 H· 3.12819800· 2.84761900·-0.39188800 C· 3.45921800·-1.70483000· 0.21740800 C· 4.82539000·-1.65366600· 0.28698200 H· 5.39673400·-2.56286400· 0.43135700 C· 4.79391300· 0.74285200·-0.01423300 C· 5.50164900·-0.41493600· 0.17041400 H· 6.58326500·-0.38869300· 0.22706000 H· 5.30679000· 1.69429700·-0.10631900 H· 2.93751000·-2.65176500· 0.30613100 H· 0.77951100·-1.50430400· 0.01641700 H·-1.29668200·-1.08867700· 0.89304500
TS3	-693.2772441	667.4088i· 34.6699· 45.1966 69.0648· 140.2416· 153.1379 184.1793· 258.0337· 269.1705 324.3217· 388.1377· 401.4669 407.7600· 442.9675· 484.0245 510.0186· 517.0624· 524.5772 542.4657· 582.8253· 602.5661 635.3622· 663.7669· 681.8006 715.7782· 744.5682· 765.1622 774.4769· 776.5401· 792.0321 810.6418· 842.1278· 868.1893 881.3806· 884.6640· 928.2731 932.7760· 962.8709· 984.7761 987.5385· 998.2687· 1000.7922 1006.5073· 1013.7797· 1032.2037 1049.7679· 1127.8223· 1147.4495 1156.3561· 1163.3834· 1168.0786 1182.8200· 1195.1712· 1226.8741 1230.2898· 1258.2975· 1267.5263 1291.3048· 1310.0321· 1349.1460 1388.8508· 1406.0125· 1430.6157 1447.8559· 1465.3719· 1486.6649 1498.3296· 1517.2514· 1563.8562 1605.3681· 1633.1553· 1645.9788 1674.3963· 1703.8030· 3168.9298 3193.7309· 3193.9011· 3194.9967 3197.1009· 3201.3073· 3205.0035 3211.9151· 3214.8550· 3215.3576 3218.0131· 3221.9667· 3226.7552	C·-2.84440500· 0.35557800· 0.49712200 C·-3.79639800· 0.63450500· 1.45638200 C·-5.06511800· 0.08466200· 1.23787500 C·-5.34156700·-0.69547700· 0.10525500 C·-4.37340000·-0.94963600·-0.85655300 C·-3.09889400·-0.40289300·-0.64838700 H·-3.59118300· 1.23092800· 2.33716800 H·-5.85096800· 0.25736900· 1.96511900 H·-6.33755500·-1.10439600·-0.01792900 H·-4.59989800·-1.54887700·-1.73096900 C·-1.11578100· 0.67843600·-0.70919900 H·-1.56120900· 1.66429800·-0.80223400 C·-1.81574500·-0.41104100·-1.28642500 C· 0.32768000· 0.66885400·-0.45143000 C· 1.05491800· 1.89322500·-0.43102000 C· 2.40292000· 1.90657400·-0.21312200 C· 3.11534600· 0.69703500· 0.00737800 C· 2.39789900·-0.53029200· 0.00778200 C· 0.99991900·-0.51075500·-0.21513200 H· 0.51944200· 2.82107900·-0.60132300 H· 2.95023600· 2.84304000·-0.20615100 C· 3.10374000·-1.73973000· 0.24286200 C· 4.45570900·-1.72899700· 0.45889600 H· 4.98576900·-2.65720800· 0.63562100 C· 4.51441600· 0.67642900· 0.23499000 C· 5.16971700·-0.50670100· 0.45414300 H· 6.23936800·-0.51182000· 0.62642600 H· 5.05752900· 1.61538600· 0.23275000 H· 2.55126300·-2.67318300· 0.24658300 H· 0.44925800·-1.44557200·-0.17632200 H·-1.35778800·-1.20970000·-1.85724300
TS4	-693.2662094	759.5513i· 32.6785· 37.7521 82.9029· 101.3495· 176.5495 184.6518· 231.2399· 289.8239 319.6195· 395.4127· 402.3960 410.4618· 456.1131· 481.3801 489.1225· 518.9034· 524.7509 530.8029· 602.0176· 627.3606 648.6957· 656.5910· 668.3238 713.4364· 746.6293· 764.1613 771.5423· 784.2637· 792.6097	C·-2.39878800· 0.57771500· 0.53059000 C·-2.58217400·-0.07502200· 1.73030000 C·-3.18487100·-1.33614400· 1.64604200 C·-3.56933200·-1.88614200· 0.41590100 C·-3.35440300·-1.21365600·-0.78181400 C·-2.74013200· 0.04122900·-0.71232800 H·-2.29120200· 0.34582800· 2.68493500 H·-3.36796200·-1.89738900· 2.55580600 H·-4.03915600·-2.86248000· 0.40336100 H·-3.64371000·-1.65524700·-1.72852500

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		837.4196· 855.7611· 877.4651 879.7839· 911.2947· 924.5265 949.3912· 960.3764· 966.6579 980.4953· 986.2602· 999.0737 1007.6902· 1013.0529· 1031.3892 1051.0024· 1098.8915· 1128.3946 1153.3552· 1162.8261· 1166.6726 1182.0529· 1195.4424· 1222.3081 1231.9843· 1262.1066· 1269.4611 1292.2320· 1309.2446· 1381.4235 1386.3693· 1402.9312· 1430.9979 1432.1539· 1455.7221· 1485.9877 1491.4176· 1511.2795· 1560.5410 1607.5411· 1635.1082· 1646.4704 1674.0976· 1703.3670· 3113.7416 3189.7581· 3193.0743· 3195.5174 3196.4247· 3198.1643· 3206.3369 3207.2760· 3209.5654· 3211.9791 3218.4855· 3223.4909· 3224.4562	C· -1.37536300· 1.84891200· -0.88373800 H· -1.38901800· 2.93552100· -0.99337500 C· -2.33542500· 1.10022300· -1.60114500 C· -0.04868600· 1.34611600· -0.44280300 C· 0.69016800· 2.11468300· 0.50072700 C· 1.92298700· 1.71053700· 0.92695000 C· 2.50796500· 0.51386000· 0.43300300 C· 1.78603800· -0.24906900· -0.52377800 C· 0.51069700· 0.19727800· -0.95033100 H· 0.25009900· 3.02681000· 0.89028700 H· 2.47364600· 2.30148800· 1.65120200 C· 2.37036300· -1.43937100· -1.03096300 C· 3.60526200· -1.85043800· -0.60386000 H· 4.03977400· -2.76217500· -0.99635100 C· 3.78429200· 0.06516300· 0.85486300 C· 4.32190600· -1.09027600· 0.35073100 H· 5.29793400· -1.42604100· 0.67996700 H· 4.32895900· 0.65367200· 1.58566000 H· 1.81793600· -2.02009900· -1.76184700 H· -0.02868300· -0.38484800· -1.69032800 H· -2.91164500· 1.49136900· -2.43088600
TSS	-693.3216275	355.7155i· 43.1451· 63.5630 75.5741· 130.6092· 169.1551 196.4507· 255.6539· 257.7900 370.3083· 403.1207· 405.6406 429.4635· 449.7894· 485.7933 490.2398· 520.3209· 527.9296 573.6255· 586.1582· 617.1535 645.8453· 689.5836· 708.8730 736.7633· 744.1140· 772.6056 781.8521· 789.3041· 799.3013 831.1682· 854.0867· 871.2161 882.4267· 890.1573· 930.3378 964.5455· 983.5173· 986.3604 991.9376· 1001.9668· 1004.2009 1009.0767· 1014.7288· 1052.9628 1053.2902· 1130.7499· 1147.1587 1162.5676· 1170.4689· 1177.7162 1179.1519· 1204.0740· 1230.7253 1234.5635· 1268.4908· 1272.2320 1289.5043· 1323.0732· 1366.5515 1390.8423· 1416.1093· 1433.6175 1456.0058· 1473.3976· 1489.0447 1508.3972· 1551.3533· 1601.7505 1623.7921· 1648.9400· 1659.1664 1685.9390· 1696.2045· 3172.9103 3184.6702· 3187.7397· 3188.5314 3192.4221· 3193.8911· 3195.1857 3197.4614· 3204.7898· 3211.5138 3212.3103· 3222.4139· 3224.1518	C· -3.80689600· -0.18128900· -0.13569500 C· -3.93802300· -1.50089300· -0.55641900 C· -2.81999900· -2.32302800· -0.67486600 C· -1.55180600· -1.82279800· -0.35777200 C· -1.47319700· -0.51645900· 0.05206800 C· -2.54693800· 0.35147500· 0.18185800 H· -4.92012300· -1.89061800· -0.79561400 H· -2.93089400· -3.34945600· -1.00594800 H· -0.66573900· -2.44511100· -0.43460100 C· -1.25028100· 2.45372600· 0.57365600 H· -1.28240300· 3.53039300· 0.71542700 C· -2.40446500· 1.76557300· 0.55702600 C· 0.05149300· 1.83353100· 0.30431800 C· 0.93743200· 2.39610300· -0.64683500 C· 2.08217300· 1.74221300· -1.01914900 C· 2.42360800· 0.48480300· -0.44637400 C· 1.57209300· -0.07368500· 0.54103400 C· 0.36920000· 0.61198900· 0.89053100 H· 0.68167100· 3.34792700· -1.09979700 H· 2.74568700· 2.17553400· -1.75945400 C· 1.92269000· -1.30536700· 1.14160700 C· 3.06829400· -1.96390500· 0.76926000 H· 3.32852000· -2.90809300· 1.23255200 C· 3.59973900· -0.21540300· -0.81038600 C· 3.91421700· -1.41296500· -0.21905200 H· 4.81598500· -1.94030700· -0.50659800 H· 4.24929700· 0.21230500· -1.56663400 H· 1.26529100· -1.72297200· 1.89749500 H· -0.16557800· 0.29426300· 1.77911200 H· -4.68524200· 0.45193900· -0.05445000 H· -3.33248700· 2.30248400· 0.72965000
TS6	-693.3338727	1014.1221i· 81.0751· 87.4060 127.3434· 171.7939· 209.4070 253.1943· 273.2082· 321.1158 376.5615· 417.9934· 431.0386 436.4700· 458.2911· 473.0851 510.9017· 522.8674· 537.2221 546.5877· 561.0597· 586.3322 602.5881· 632.1284· 688.4497 695.6033· 707.7885· 758.7361 763.3182· 772.8675· 777.5313 823.7743· 825.0241· 840.7560 862.0063· 870.0725· 898.8612 906.7014· 968.5944· 986.6053 987.5261· 1001.2999· 1001.7981 1015.3760· 1021.6519· 1033.2966 1066.3215· 1082.9243· 1131.3463 1155.5589· 1158.6017· 1176.1567 1183.6542· 1192.5760· 1223.2781 1240.3973· 1242.7997· 1256.8944 1283.4788· 1326.5872· 1353.6663 1369.9139· 1393.1715· 1417.6037	C· -3.72252400· -0.21743600· 0.12812700 C· -3.80534500· -1.54510300· -0.22000100 C· -2.63387200· -2.24489700· -0.54709100 C· -1.40111700· -1.63359000· -0.45116100 C· -1.28145000· -0.29387700· -0.02780800 C· -2.47553300· 0.43776700· 0.19506100 H· -4.76841900· -2.03745600· -0.27892400 H· -2.69576300· -3.27010200· -0.89208800 H· -0.52156300· -2.18255600· -0.75475400 C· -1.24531200· 2.52330900· 0.20044800 H· -1.21809600· 3.60727100· 0.22076000 C· -2.41224100· 1.85607900· 0.38673200 C· -0.02137800· 1.81963100· -0.00011000 C· 1.18064600· 2.53516600· -0.26894200 C· 2.36070000· 1.88802500· -0.44273900 C· 2.45390800· 0.47448600· -0.23339600 C· 1.29608400· -0.26808700· 0.10443000 C· -0.00207400· 0.40564300· 0.13459300 H· 1.12267300· 3.61389100· -0.36533200 H· 3.26271400· 2.43484000· -0.69381000 C· 1.47319800· -1.60129800· 0.53588200

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1451.6143·1462.6388·1464.0723 1493.7268·1541.1923·1549.4553 1577.9586·1627.7632·1661.2076 1671.6988·1679.1059·1692.4260 3195.5494·3197.1418·3198.1895 3198.7430·3209.2267·3210.1618 3213.7222·3215.2629·3223.7589 3225.4210·3234.2127·3250.7522	C· 2.71057400·-2.20438500· 0.50888400 H· 2.81808300·-3.22424900· 0.85835100 C· 3.70890600·-0.17133400·-0.28342400 C· 3.83749000·-1.49530200· 0.05943000 H· 4.80662000·-1.97819100· 0.02653500 H· 4.57865300· 0.40986400·-0.57031500 H· 0.63153900·-2.14091000· 0.94896600 H·-0.18604300· 0.42861500· 1.91665500 H·-4.62076300· 0.35688200· 0.32782000 H·-3.33359600· 2.39332300· 0.58264500
TS7	-693.2733302	701.2558i· 26.7049· 38.5342 51.5217· 102.4666· 131.2312 179.0522· 210.2579· 244.5293 312.5956· 328.2052· 354.9059 406.7731· 456.7947· 473.6026 479.7832· 496.9240· 523.9400 528.6952· 569.6726· 617.3737 637.4767· 650.8244· 715.7041 750.3025· 756.1558· 761.5572 767.1473· 789.3803· 797.9687 833.3364· 849.0841· 876.9995 896.5591· 900.1057· 914.6197 932.0178· 965.2800· 983.3990 986.2177· 989.8406·1000.3078 1012.4500·1014.1170·1024.3041 1050.8681·1113.9257·1150.8559 1162.5130·1166.7365·1175.3115 1184.2346·1194.1575·1209.0751 1230.2726·1267.3747·1283.9988 1295.5836·1311.7929·1350.1634 1383.0606·1403.4045·1428.0961 1443.3464·1478.8938·1482.3920 1502.6712·1513.5217·1557.2368 1618.4243·1632.5794·1664.0599 1690.7881·1728.4788·3181.8448 3191.8704·3192.8798·3194.2143 3195.1053·3198.6974·3208.3756 3208.7968·3210.4799·3213.4131 3220.8217·3224.3187·3225.7487	C·-3.20719200·-0.72678800· 0.52010000 C·-4.28715200·-0.95667900· 1.35562500 C·-5.50953200·-0.50387600· 0.83850300 C·-5.60293800· 0.16369400·-0.38936700 C·-4.47581500· 0.42405000·-1.17610800 C·-3.29730500·-0.06952800·-0.64519900 H·-4.22798500·-1.44959000· 2.31784700 H·-6.41611000·-0.67057200· 1.41077800 H·-6.57698700· 0.49708300·-0.72777300 H·-4.54329900· 0.97051200·-2.10884000 C·-0.97501200· 0.82253400·-0.19423300 H·-1.43579100· 1.75854700· 0.10713700 C·-1.82432600·-0.19895200·-0.62181800 C· 0.45782900· 0.73015900·-0.07465700 C· 1.19044400· 1.91525600· 0.25345700 C· 2.54791600· 1.90201000· 0.37279700 C· 3.28601600· 0.70108200· 0.18176400 C· 2.57531200·-0.49014600·-0.13304900 C· 1.16790700·-0.44856600·-0.25282900 H· 0.64005700· 2.83794700· 0.40232800 H· 3.08581800· 2.81127100· 0.61896800 C· 3.30661000·-1.69487500·-0.31466200 C· 4.67068700·-1.71082900·-0.19406600 H· 5.21758400·-2.63538100·-0.33551100 C· 4.69547700· 0.65373800· 0.30034200 C· 5.37484100·-0.52342000· 0.11641700 H· 6.45389900·-0.54931000· 0.20930800 H· 5.23000600· 1.56663900· 0.54051600 H· 2.76352600·-2.60338900·-0.55205200 H· 0.64853100·-1.37469100·-0.47304200 H·-1.40183900·-1.09225700·-1.06776600
TS8	-693.2739975	685.3662i· 31.2800· 38.0187 50.0029· 108.1803· 141.2705 180.5807· 208.7927· 229.2185 317.9093· 326.8323· 355.4788 401.0723· 431.7963· 477.6175 493.6602· 508.8821· 527.4260 528.7625· 572.1114· 620.5566 638.8969· 648.4454· 716.5752 750.4884· 761.7698· 767.1602 771.6936· 790.5551· 795.9856 832.9655· 845.5752· 880.9310 896.1261· 904.0188· 912.5308 922.4529· 964.0466· 970.5336 985.1923· 986.1784· 999.3361 1012.0965·1014.4831·1024.0781 1051.4909·1114.0105·1150.8766 1164.1893·1171.2436·1180.8181 1187.1438·1197.8518·1209.2348 1247.2394·1271.9963·1287.3812 1297.6699·1306.8285·1348.1748 1378.3217·1404.0975·1430.3987 1443.9045·1479.4479·1484.7714 1501.6928·1516.3137·1559.1886 1618.6144·1629.9964·1662.5473 1689.9973·1728.9126·3182.7873 3188.7471·3191.9236·3194.4476 3196.2819·3198.5770·3202.6440 3209.5372·3212.8349·3221.3713 3224.9603·3225.2726·3227.9374	C· 5.51281700· 0.04122700· 0.22434200 C· 4.57969000· 1.03284100· 0.05313000 C· 3.20375000· 0.72029400·-0.04184700 C· 2.79281900·-0.63768500· 0.04366200 C· 3.78029600·-1.64229900· 0.22137100 C· 5.10699000·-1.31075600· 0.30918800 H· 2.51814900· 2.76006800·-0.26821300 H· 6.56474000· 0.29028800· 0.29552800 H· 4.88546600· 2.07162600·-0.01182000 C· 2.20665900· 1.72221500·-0.21543200 C· 1.41671900·-0.94693900·-0.05063500 H· 3.46527300·-2.67824000· 0.28628800 H· 5.85238900·-2.08537500· 0.44430200 C· 0.45318500· 0.03514900·-0.23217900 C· 0.88671500· 1.39855300·-0.30747200 H· 1.11098900·-1.98669000· 0.01597600 H· 0.15432400· 2.18752300·-0.42336100 C·-0.93077200·-0.34382400·-0.33522400 C·-1.99893700· 0.51971900·-0.59070900 C·-3.40863300· 0.07387600·-0.62311700 C·-3.40650600· 0.55828800· 0.62729600 C·-4.47709600·-0.58212700·-1.20795900 C·-4.47190000· 0.42302900· 1.50168000 C·-5.59691500·-0.68995600·-0.37645000 H·-4.46897800·-0.98839600·-2.21196800 C·-5.59212400·-0.20403600· 0.93736000 H·-4.47566000· 0.77147100· 2.52684200 H·-6.49227400·-1.17360100·-0.74913800 H·-6.48676800·-0.32303600· 1.53953500 H·-1.16760000·-1.38972700·-0.16401400 H·-1.80058200· 1.53866400·-0.90198700
TS9	-693.2480403	2199.1123i· 27.0888· 42.7434	C· 2.29517300·-1.02818100· 0.40802900

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		52.5061· 104.3142· 137.5850 183.3985· 199.5987· 260.5232 290.5580· 372.6320· 396.1449 404.9389· 417.8856· 456.8607 484.3548· 498.0918· 515.9548 531.8545· 551.3617· 607.7858 633.9950· 650.6111· 691.1248 709.0177· 744.9765· 766.3612 771.9940· 779.5472· 792.4891 795.0576· 826.9367· 854.0883 886.3913· 894.0118· 924.1244 942.0397· 970.8770· 984.4241 987.4053· 997.5535· 1000.5656 1013.7607· 1016.2539· 1031.2337 1035.3973· 1050.7018· 1122.2643 1151.6568· 1158.8594· 1164.8816 1181.3597· 1185.2333· 1195.3030 1225.5160· 1261.3176· 1276.7847 1293.1068· 1307.5606· 1354.1304 1393.0315· 1406.2885· 1428.9749 1464.8788· 1478.3424· 1489.1572 1512.1185· 1558.4679· 1618.1307 1645.1533· 1656.6321· 1673.4631 1702.3962· 1738.3073· 1892.9260 3178.1248· 3192.9090· 3194.2773 3195.0095· 3197.5717· 3197.9419 3211.6550· 3212.2120· 3213.1547 3225.0028· 3225.6432· 3232.3723	C· 3.36774300· -1.89082500· 0.62835500 C· 4.69170900· -1.49668300· 0.40414300 C· 5.01332200· -0.21021100· -0.04450500 C· 3.93273700· 0.62423800· -0.25515100 C· 2.61313500· 0.25103700· -0.04583600 H· 3.17603100· -2.89624900· 0.98428300 H· 5.48993600· -2.20759400· 0.58701400 H· 6.03999500· 0.09079100· -0.20726900 H· 3.36267000· 1.87989900· -0.58693300 C· 0.86196700· 2.19527200· -0.46378600 H· 0.87899600· 3.25926000· -0.68187900 C· 2.01069300· 1.53354400· -0.38103000 C· -0.45691600· 1.57281600· -0.23662800 C· -1.48805400· 2.33074300· 0.38639500 C· -2.70954800· 1.77414500· 0.64396300 C· -2.98683600· 0.42790600· -0.28718200 C· -1.97254600· -0.32844100· -0.35994000 C· -0.71701200· 0.27568100· -0.61414300 H· -1.28561400· 3.35848700· 0.66742900 H· -3.48648000· 2.35675800· 1.12744600 C· -2.24931500· -1.66943000· -0.73598600 C· -3.47004400· -2.23121600· -0.47215300 H· -3.67096600· -3.25585500· -0.76145700 C· -4.24116800· -0.18046700· 0.54562500 C· -4.47791900· -1.47871700· 0.17746200 H· -5.43940400· -1.93507200· 0.38004500 H· -5.01122800· 0.40130400· 1.04095500 H· -1.47499900· -2.24078300· -1.23724700 H· 0.04201700· -0.29382700· -1.14093600 H· 1.27631600· -1.34437900· 0.59656500
TS10	-693.2859919	1924.0878i· 26.9433· 46.8222 54.9817· 108.7734· 160.9343 175.0428· 203.7864· 254.9704 306.6881· 322.6698· 408.8992 412.4564· 423.6285· 471.0389 490.0838· 501.2749· 518.7603 529.3937· 535.0216· 629.4021 633.1080· 651.1330· 661.4936 706.4093· 745.2298· 751.0705 764.8524· 776.4569· 799.4342 832.5632· 867.7696· 875.4601 885.1840· 896.0133· 934.6763 946.5691· 980.9728· 994.1373 1003.9600· 1005.7932· 1013.2310 1015.8636· 1021.2850· 1045.8590 1056.5634· 1059.3946· 1108.1184 1142.2167· 1162.9500· 1169.9334 1176.8645· 1179.3499· 1199.6587 1231.0070· 1232.4074· 1266.1849 1305.6163· 1327.2503· 1347.2654 1377.4498· 1380.9714· 1403.1678 1470.6580· 1481.0345· 1495.3130 1524.5414· 1559.1612· 1622.9480 1638.7018· 1652.8571· 1665.1772 1690.1549· 1706.3307· 1749.2980 3191.5951· 3193.9663· 3195.4636 3200.2035· 3204.7323· 3205.1794 3211.6163· 3213.2599· 3216.4122 3220.0096· 3226.7170· 3228.7156	C· -3.27197700· -1.19527700· -0.60139400 C· -4.60406000· -1.58048900· -0.53843100 C· -5.53833600· -0.76720500· 0.09718600 C· -5.13198000· 0.43262000· 0.67582600 C· -3.80058200· 0.82030000· 0.61904400 C· -2.85433600· 0.01697000· -0.03617200 H· -2.54123800· -1.82537500· -1.09560000 H· -4.91503800· -2.51766000· -0.98445800 H· -6.57707600· -1.07049900· 0.14895400 H· -5.85404100· 1.06271200· 1.18168100 H· -3.47708100· 1.74265400· -1.08755300 C· -0.81660100· 1.58588800· -0.22470700 H· -1.28419900· 2.55818400· -0.34745600 C· -1.47005600· 0.42963200· -0.12052500 C· 0.64818800· 1.38554900· -0.17916400 C· 1.69444000· 2.33002700· -0.24006800 C· 2.99566900· 1.89054500· -0.16460000 C· 3.30993900· 0.51502800· -0.02387300 C· 2.25261800· -0.45127400· 0.04207200 C· 0.95513000· 0.05496900· -0.05029400 H· 1.47423100· 3.38719100· -0.34135900 H· 3.81302100· 2.60204700· -0.21034900 C· 2.57574400· -1.82901900· 0.18742000 C· 3.88051500· -2.22885600· 0.26316800 H· 4.12008700· -3.27962200· 0.37490100 C· 4.65172600· 0.05434600· 0.05579400 C· 4.93095700· -1.27749800· 0.19551100 H· 5.95918100· -1.61341200· -0.25571700 H· 5.45425000· 0.78271700· 0.00418100 H· 1.76648700· -2.54816800· 0.23783600 H· -0.38056900· -0.39831400· -0.05236000
TS11	-693.2793143	572.7934i· 40.4674· 51.0993 59.9211· 113.4768· 169.2197 208.3338· 224.7671· 273.2473 318.8027· 358.0006· 411.8777 416.2956· 458.1583· 477.8239 500.8106· 514.5205· 528.8285 545.6545· 580.3754· 622.7458 631.1707· 655.5009· 707.6487 717.7344· 740.1001· 743.5417 771.9690· 778.4616· 792.7937 814.6458· 835.0680· 870.3172 887.9991· 897.8779· 933.4383	C· 3.14517800· 0.50258600· 0.92496000 C· 4.39264200· 0.02278900· 1.30170700 C· 5.08549200· -0.85108000· 0.46816700 C· 4.52437800· -1.24496900· -0.74417300 C· 3.28091700· -0.75882100· -1.12352200 C· 2.58031700· 0.13198300· -0.30132000 H· 2.58791800· 1.15410200· 1.58912400 H· 4.82021800· 0.31805000· 2.25253900 H· 6.05515300· -1.23160100· 0.76644000 H· 5.05826400· -1.92990600· -1.39212000 H· 2.84359800· -1.06083800· -2.06943600 C· 0.74362700· 1.89240900· -0.27379600

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		952.2589·984.7671·997.0512 1005.6733·1011.7735·1014.3927 1017.6408·1022.5157·1051.9536 1059.1819·1107.9986·1130.3663 1159.7872·1165.6002·1171.5548 1178.3395·1200.7687·1218.4409 1228.6298·1247.5308·1268.7592 1317.8582·1331.3846·1348.3697 1366.7387·1377.5056·1417.4526 1458.8868·1474.2012·1476.3201 1508.1885·1540.4057·1558.7340 1615.5221·1642.4507·1651.1976 1671.7179·1683.4920·3176.8224 3192.8140·3195.5088·3195.6543 3200.4787·3205.3366·3208.3690 3210.5858·3216.2901·3216.5737 3218.3111·3226.8902·3227.8761	H·1.32863300·2.71135900·0.12811000 C·1.27307200·0.65333500·-0.71620000 C·-0.66001000·1.66878900·-0.15911600 C·-1.84835300·2.45564100·-0.10714700 C·-3.04025400·1.80039200·0.00362200 C·-3.12570600·0.36956900·0.06146800 C·-1.93877700·-0.42751600·0.02202200 C·-0.72945100·0.29131600·-0.07343600 H·-1.80789600·3.53741500·-0.15979300 H·-3.96808300·2.36114200·0.04488700 C·-2.03967300·-1.83745700·0.09103800 C·-3.26852600·-2.44048900·0.18876400 H·-3.34082400·-3.52030300·0.24078300 C·-4.37244200·-0.28955000·0.16247700 C·-4.44467700·-1.66037200·0.22384100 H·-5.40884700·-2.14868600·0.29982500 H·-5.27780200·0.30818900·0.18651300 H·-1.12772900·-2.42261300·0.06624600 H·0.89087200·0.25236200·-1.64924700
TS12	-693.2681938	694.0249i·29.4892·38.0047 62.5798·122.3866·168.0104 194.4010·237.5306·266.2413 310.8306·407.2760·409.7444 414.8972·457.0730·479.8387 497.9469·514.9354·520.3195 539.0685·606.3130·629.1872 639.3731·661.6673·704.7962 708.0257·737.2018·761.7382 772.9176·777.7996·784.4127 828.4296·848.8012·862.3035 889.4581·910.6129·926.1164 951.2324·985.0046·997.5029 999.7893·1014.0088·1014.7054 1014.9845·1018.2796·1053.4452 1060.5991·1103.3008·1116.3419 1129.6553·1165.2535·1171.0036 1176.5602·1205.8264·1228.0898 1230.0573·1258.3350·1269.3438 1317.8538·1323.0496·1351.8843 1371.5572·1404.7628·1418.5893 1437.2682·1473.0711·1480.4664 1501.1694·1534.0027·1559.3814 1617.2174·1643.0500·1650.4735 1669.2483·1684.6985·3112.3301 3189.2788·3191.1397·3196.2725 3200.7311·3204.7671·3206.5628 3209.4735·3215.0751·3216.6726 3217.0805·3225.8250·3227.1336	C·2.04039400·0.40414500·1.03567000 C·2.58895300·-0.62314300·1.78854300 C·3.24289300·-1.68650900·1.16831500 C·3.35050100·-1.70419800·-0.21702100 C·2.80340000·-0.67346900·-0.97362600 C·2.12886300·0.38681800·-0.36199400 H·1.53796500·1.22850300·1.52860800 H·2.51192100·-0.59179700·2.86913700 H·3.67019300·-2.48593000·1.76127700 H·3.86430200·-2.51947300·-0.71291300 H·2.89284900·-0.69132100·-2.05511600 C·0.83759900·2.59141600·-0.78318300 H·1.00795000·3.60837900·-1.11699300 C·1.58571300·1.47457500·-1.22037700 C·-0.37237500·2.05120600·-0.24180200 C·-1.37218300·2.42233400·0.70241300 C·-2.34279300·1.50569100·0.99192400 C·-2.37506200·0.20593600·0.38659000 C·-1.39546000·-0.16302900·-0.58707500 C·-0.43931500·0.82855700·-0.87815600 H·-1.35296300·3.38955200·1.19106000 H·-3.11733200·1.74321600·1.71341300 C·-1.43031600·-1.45044500·-1.17135600 C·-2.40438600·-2.34608400·-0.80762400 H·-2.42759600·-3.33374900·-1.25226600 C·-3.36665400·-0.74271600·0.72758700 C·-3.38132800·-1.98782400·0.14665800 H·-4.14607600·-2.70384700·0.42301900 H·-4.11564800·-0.47331400·1.46499800 H·-0.67138600·-1.70859100·-1.90063500 H·2.15515400·1.57880900·-2.14651000
TS13	-693.31676	422.7641i·46.2624·53.6722 95.0101·162.8875·175.7941 189.8786·225.8586·280.3239 375.0021·392.9336·412.5751 429.8342·457.7424·494.5920 497.6936·503.1246·524.4640 564.5715·586.7740·615.7318 659.0365·670.6393·713.4821 734.9121·745.1058·751.8620 769.1624·780.0978·791.8133 840.3708·843.7339·877.1782 884.3879·892.8443·964.0286 973.3862·981.4318·990.4761 993.6858·1001.0111·1009.3604 1015.0676·1035.1060·1050.8136 1054.0080·1099.5816·1143.5411 1164.3165·1172.4750·1175.5456 1189.1010·1191.3321·1211.6685 1233.8450·1237.7966·1270.4551 1319.9511·1331.6757·1352.5915 1386.1825·1406.1332·1430.6556 1453.0986·1465.8989·1500.9824 1529.5740·1541.3186·1605.2205	C·1.77757600·-0.29511600·0.93848900 C·1.92358100·-1.69851600·0.88291600 C·2.74600700·-2.27982000·-0.06511400 C·3.50272500·-1.47845300·-0.92561300 C·3.43162000·-0.09211600·-0.82729100 C·2.57923300·0.51483700·0.09097800 H·1.39579700·-2.31597600·1.60036500 H·2.83482600·-3.35873500·-0.11646200 H·4.15924100·-1.93605700·-1.65549100 C·1.19849600·2.54432000·0.21476900 H·1.13032400·3.62778200·0.21845600 C·2.40911100·1.96828500·0.13420900 C·-0.07514100·1.81768500·0.14399700 C·-1.28066700·2.54274600·-0.10609900 C·-2.47896800·1.89939800·-0.23740700 C·-2.56398200·0.48446100·-0.14746900 C·-1.37290700·-0.26822100·0.09516600 C·-0.17743300·0.45549800·0.23608500 H·-1.22945100·3.62398100·-0.18781400 H·-3.38679800·2.46443900·-0.41805700 C·-1.45894500·-1.68521100·0.16262500 C·-2.66386700·-2.31851300·0.01418700 H·-2.71612300·-3.39968400·0.06278300

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1616.2600·1637.9704·1654.3662 1680.9733·1703.6930·3178.4865 3179.4260·3187.7587·3194.3670 3195.0540·3198.4797·3202.7239 3208.2303·3209.9509·3214.8859 3221.8742·3226.0191·3243.7764	C·-3.79325200·-0.20632800·-0.29374300 C·-3.84504000·-1.57267000·-0.21170300 H·-4.79067200·-2.08887900·-0.32663800 H·-4.69425100· 0.36966500·-0.47722300 H·-0.55083000·-2.25319500· 0.31472600 H· 1.37497500· 0.15055300· 1.84208200 H· 3.29213100· 2.59185500· 0.03140200 H· 4.03195200· 0.53065200·-1.48202100
TS14	-693.327006	1186.2338i· 76.7818· 84.2321 122.8335· 176.6785· 209.7710 248.3178· 281.2140· 308.2941 372.4819· 411.6992· 431.4761 438.6354· 484.1553· 505.1975 512.9156· 525.9270· 546.6698 558.5516· 577.9457· 610.2636 615.1771· 643.8412· 684.6881 696.4379· 706.6699· 761.9163 763.2266· 773.0475· 776.4875 819.4160· 824.9777· 845.6404 862.0419· 864.6862· 898.0768 914.4294· 967.4655· 985.2793 988.0845·1000.2776·1003.1030 1014.2789·1017.0325·1039.2521 1054.4700·1077.9589·1132.2621 1149.1609·1160.4596·1175.3173 1183.0708·1195.1959·1218.6472 1237.4352·1242.2964·1257.1002 1278.0324·1322.5347·1364.4996 1378.8660·1401.9630·1418.9123 1451.4083·1454.2757·1464.4517 1488.3116·1543.2756·1546.1399 1569.9451·1623.0009·1661.9046 1674.2181·1679.3691·1696.6726 3195.2304·3196.6150·3197.7350 3198.2779·3208.0440·3208.8290 3213.3018·3215.1250·3225.0807 3226.2584·3243.0581·3259.9369	C·-3.73926200·-0.20290400· 0.11163700 C·-3.82322400·-1.54539400·-0.15493100 C·-2.64777900·-2.26313400·-0.44570400 C·-1.41969000·-1.65007700·-0.38775900 C·-1.28725200·-0.28167700·-0.03032300 C·-2.49046300· 0.45953700· 0.14204900 H·-4.78592500·-2.04103300·-0.18508800 H·-2.71124600·-3.30397300·-0.74015200 H·-0.54683700·-2.21213800·-0.68412900 C·-1.25853500· 2.53494500· 0.15066700 H·-1.22016700· 3.61848600· 0.17157800 C·-2.43930400· 1.87953100·-0.27004000 C·-0.03112700· 1.81592900· 0.02720000 C· 1.19187800· 2.54233800·-0.14942600 C· 2.36795000· 1.90013600·-0.36894100 C· 2.45481000· 0.48815800·-0.21799600 C· 1.28719800·-0.23193100· 0.22582600 C·-0.02439200· 0.41488600· 0.05418400 H· 1.14026700· 3.62492800·-0.18556100 H· 3.26870100· 2.45474900·-0.60757800 C· 1.45814300·-1.63000400· 0.51763300 C· 2.67999500·-2.23406200· 0.41561000 H· 2.78421900·-3.27623500· 0.69342700 C· 3.69218100·-0.17783700·-0.32250800 C· 3.81198700·-1.51319600·-0.02716100 H· 4.77096000·-2.00934400·-0.11085200 H· 4.56007400· 0.39701100·-0.62777100 H· 0.62695800·-2.18187300· 0.93150900 H· 1.41887300· 0.29139600· 1.80141000 H·-4.63685000· 0.38354300· 0.27617400 H·-3.36770000· 2.42302500· 0.40644000
TS15	-693.2753795	633.8252i· 28.6496· 33.6840 42.7108· 110.4627· 156.2137 164.6896· 181.8053· 268.4001 283.5247· 350.4386· 399.5201 410.1994· 420.7656· 485.4740 491.0952· 503.4732· 512.9393 513.9502· 576.3792· 606.0236 628.9534· 657.6408· 694.2837 709.0728· 761.2132· 764.3094 770.4995· 779.5553· 821.7675 835.6526· 852.1086· 860.1673 874.3582· 889.7258· 933.0013 946.6020· 968.6797· 985.2349 996.6489·1001.3884·1010.0050 1015.9574·1016.1611·1048.3139 1059.1970·1112.5143·1124.1919 1161.7345·1170.3200·1177.4833 1193.7002·1198.8466·1226.2003 1243.2762·1254.0810·1288.2733 1305.6866·1322.3570·1344.3703 1357.6360·1378.0679·1419.5918 1446.5567·1482.0942·1497.2083 1514.8897·1529.5103·1572.4939 1626.4564·1635.6072·1653.8094 1683.4072·1740.4363·3181.1143 3192.0767·3195.6841·3196.9069 3198.9142·3205.2229·3205.8127 3213.5656·3217.2024·3223.6420 3225.0695·3226.9958·3230.0484	C· 3.41313200·-0.33729500·-1.00855300 C· 4.71293700·-0.81343000·-1.06135300 C· 5.52690000·-0.77894100· 0.07043000 C· 5.02204700·-0.26636000· 1.26294500 C· 3.72124400· 0.20876000· 1.32084900 C· 2.88795400· 0.19225400· 0.18637400 H· 2.79424900·-0.38955700·-1.89590400 H· 5.09613600·-1.22028200·-1.98977600 H· 6.54244100·-1.15270100· 0.02299900 H· 5.64477700·-0.23989600· 2.14931100 H· 3.33097200· 0.60642500· 2.25158300 C· 0.63391100· 0.85090700·-0.75003400 H· 0.97295600· 0.72004700·-1.77089700 C· 1.54458100· 0.70747000· 0.29824700 C·-0.74966800· 1.33614200·-0.55055700 C·-1.65598900· 2.35542100·-0.19954100 C·-2.92216100· 1.90654300· 0.09160500 C·-3.26644700· 0.51721800· 0.08786600 C·-2.29633500·-0.48777800·-0.23391000 C·-1.03842400· 0.04599400·-0.59516400 H·-1.39381800· 3.40501600·-0.15337700 H·-3.70034300· 2.61416400· 0.35770500 H· 1.20296800· 0.97548000· 1.29385000 C·-4.89978400·-1.24080400· 0.45859200 C·-3.92893500·-2.22316800· 0.15378100 C·-2.65378600·-1.85525400·-0.18957300 C·-4.57761800· 0.09125400· 0.42411800 H·-5.90498800·-1.54750400· 0.72206800 H·-4.20095600·-3.27141500· 0.18884500 H·-1.90114200·-2.59540100·-0.43360200 H·-5.32461900· 0.84202100· 0.66046600
TS16	-693.2753571	627.6371i· 25.1608· 33.3072 65.2744· 130.4460· 139.7509 183.6002· 205.5135· 274.7337	C·-1.73420700·-0.58457900·-0.35687600 C·-2.34390100·-1.77295900·-0.73277900 C·-3.68138000·-2.01689500·-0.43176700

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		280.1237· 372.0746· 404.1268 413.0641· 478.4611· 483.1861 490.0239· 494.0927· 514.1571 514.9315· 590.3270· 624.3013 636.9293· 668.7105· 696.6594 727.4948· 735.6541· 763.2628 766.1913· 775.5968· 805.4715 832.4342· 845.7973· 857.0797 861.3641· 889.3534· 940.2783 956.0785· 959.6765· 983.7665 996.2808· 1003.0298· 1009.4928 1018.0547· 1018.0965· 1048.2129 1059.9976· 1116.4300· 1123.5707 1131.2661· 1163.1777· 1171.2684 1177.8796· 1206.8172· 1225.6287 1239.6423· 1248.9737· 1288.7468 1307.3243· 1339.2042· 1357.4373 1376.7350· 1404.0525· 1421.5503 1448.3539· 1479.1239· 1497.0092 1509.2463· 1529.2875· 1568.1963 1625.4551· 1633.7526· 1653.2915 1683.2214· 1735.7689· 3176.6263 3192.2696· 3193.2680· 3196.2342 3197.5842· 3203.3665· 3205.8508 3213.6643· 3218.6697· 3225.9886 3227.4593· 3227.7120· 3258.8269	C· -4.41132600· -1.05805800· 0.26774400 C· -3.80682300· 0.12645500· 0.65335100 C· -2.45931500· 0.40262500· 0.34219400 H· -0.69007500· -0.43858600· -0.59445600 H· -1.76465700· -2.51967500· -1.26316700 H· -4.14812000· -2.94718700· -0.73228100 H· -5.45082700· -1.23825000· 0.51488600 H· -4.37797300· 0.86761500· 1.20237900 C· -0.68613400· 2.26697600· 0.50610200 H· -0.52181000· 3.24269200· 0.94882200 C· -1.91741500· 1.66513200· 0.79217700 C· 0.32964500· 1.79603800· -0.45968800 C· 0.70132200· 1.47698500· -1.78119100 C· 1.75471300· 0.59993300· -1.87300400 C· 2.37156100· 0.01482600· -0.71984600 C· 1.92808500· 0.33951000· 0.60399200 C· 0.90636300· 1.31729000· 0.63118400 H· 0.19748500· 1.86469400· -2.65758500 H· 2.13047600· 0.30236600· -2.84641800 H· -2.54997100· 2.21465400· 1.48268000 C· 2.52101600· -0.29149800· 1.72189300 C· 3.52607800· -1.20674200· 1.54364200 C· 3.98620800· -1.52033800· 0.24371700 C· 3.42648000· -0.92402700· -0.85668600 H· 2.16339900· -0.03346300· 2.71143600 H· 3.97761500· -1.69146900· 2.40105100 H· 4.78726500· -2.23936500· 0.12023400 H· 3.78137100· -1.16807400· -1.85265700
TS17	-693.2689886	778.7774i· 20.4825· 34.3927 40.0348· 101.0722· 113.0180 167.9301· 187.8115· 211.0761 240.0038· 304.2565· 359.4019 398.9750· 408.7268· 445.1833 478.5114· 483.2406· 491.4283 522.0042· 527.2606· 557.2415 587.0129· 598.8218· 632.3314 641.8597· 664.5587· 672.9746 703.0633· 768.0050· 773.4618 780.0999· 791.4088· 805.1966 843.3238· 868.8950· 885.4059 912.4064· 927.7389· 949.3472 978.0594· 990.0325· 1003.2773 1006.0452· 1016.1999· 1016.7010 1022.1583· 1050.9988· 1058.3082 1109.7045· 1143.1986· 1163.8457 1169.3258· 1178.6146· 1184.0233 1201.4011· 1223.2459· 1264.6975 1291.8159· 1309.7694· 1331.3166 1348.0202· 1382.7034· 1406.1545 1428.9229· 1478.1663· 1483.3179 1509.3553· 1536.0096· 1559.3769 1639.7723· 1643.6860· 1668.6970 1675.1425· 1705.3879· 2264.7394 3196.1879· 3199.8087· 3201.3984 3204.0124· 3209.7970· 3211.7071 3214.3926· 3220.7876· 3225.5700 3226.3900· 3226.6816· 3231.9293	C· -1.34706300· 1.81521000· -0.32318300 C· -2.70801600· 1.86463900· -0.22187600 C· -3.47176200· 0.68135700· -0.03784700 C· -2.79403600· -0.56473000· 0.04451800 C· -1.38176100· -0.59102600· -0.05684000 C· -0.66342300· 0.56966100· -0.23574300 H· -5.39856200· 1.65725300· -0.00061700 H· -0.76778400· 2.71811700· -0.47215200 H· -3.22557300· 2.81557900· -0.28594500 C· -4.88570500· 0.70363800· 0.06365600 C· -3.55228400· -1.75094000· 0.22675800 H· -0.86174600· -1.54009500· 0.00899100 C· -4.91714400· -1.69855800· 0.32204200 C· -5.59195700· -0.45696100· 0.23948300 H· -3.03014500· -2.69953700· 0.28952100 H· -5.48773800· -2.60894600· 0.46120100 H· -6.67230700· -0.42967400· 0.31620200 C· 0.77420300· 0.51136700· -0.31540200 C· 1.94515800· 0.23430400· -0.12867300 C· 3.34527100· 0.00271900· -0.01572500 C· 4.16495800· 0.93064700· 0.64320400 C· 3.91919100· -1.15361300· -0.56413700 C· 5.52960000· 0.70309700· 0.74744100 H· 3.71819100· 1.82207700· 1.06581500 C· 5.28452800· -1.37305600· -0.45330500 H· 3.28384500· -1.86687200· -1.07459400 C· 6.09287200· -0.44746100· 0.20167000 H· 6.15645800· 1.42525200· 1.25657500 H· 5.72052500· -2.26808100· -0.88050600 H· 7.15874000· -0.62191600· 0.28574700 H· 0.95031400· 1.71507400· -1.78649600
TS18	-693.2693793	740.7017i· 16.9151· 32.8960 39.5985· 98.8763· 112.5618 166.6092· 180.9054· 207.4243 230.7670· 304.6767· 362.6713 401.5949· 408.4460· 433.5380 481.7039· 488.2771· 504.7972 522.2428· 526.0671· 551.3569 583.4047· 610.0926· 627.7753 636.8970· 663.8010· 680.0341 703.4431· 767.6972· 772.7824 780.1855· 792.7931· 800.9068 842.5193· 868.2549· 884.5405 913.9403· 927.1629· 949.7191 976.9959· 989.6157· 1002.5549	C· -4.04223800· -1.09298300· 0.67276700 C· -5.42742300· -1.12183300· 0.74796900 C· -6.18433800· -0.12956800· 0.13065400 C· -5.55002800· 0.89561500· -0.56620700 C· -4.16549700· 0.93288800· -0.64706300 C· -3.39727500· -0.06258800· -0.02640000 H· -3.44535200· -1.86000400· 1.15054600 H· -5.91874700· -1.92124000· 1.28947200 H· -7.26563500· -0.15537800· 0.19182800 H· -6.13674400· 1.66773600· -1.04917000 H· -3.66399000· 1.72533400· -1.18882500 C· -0.76816900· -0.09171800· -0.24958700 H· -0.69602500· -1.42682700· -1.64122300 C· -1.97526600· -0.02844700· -0.10450600

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1005.4655·1016.3827·1016.7708 1022.0966·1050.3889·1058.5329 1109.5013·1141.3445·1163.0334 1168.3147·1179.0728·1182.7127 1201.5316·1223.9012·1264.0775 1291.6484·1309.4591·1320.9805 1347.9214·1383.8860·1407.8283 1428.8268·1476.2673·1483.0808 1509.8606·1536.7288·1554.6012 1640.2788·1644.2963·1668.6243 1675.7693·1706.3573·2266.8082 3196.4330·3200.1487·3201.3764 3204.4229·3209.1585·3212.4484 3214.4236·3221.0084·3225.5589 3226.2544·3227.4499·3232.4445	C· 0.64632600· 0.15468700·-0.12941300 C· 1.07010900· 1.47211500· 0.21374500 C· 2.39709700· 1.75532700· 0.36615300 C· 3.38369100· 0.74902100· 0.19001400 C· 2.96617300·-0.56527600·-0.15203000 C· 1.58481300·-0.83482600·-0.30976000 H· 0.31816300· 2.23909900· 0.35166300 H· 2.71445500· 2.75933000· 0.62625800 C· 3.94801700·-1.57513500·-0.32982400 C· 5.27820200·-1.29027300·-0.17397500 H· 6.02034200·-2.06746200·-0.31158000 C· 4.76785300· 1.01393100· 0.34382100 C· 5.69319700· 0.01937800· 0.16683500 H· 6.74888000· 0.23140700· 0.28680900 H· 5.08111400· 2.01908200· 0.60477000 H· 3.62432600·-2.57649300·-0.59220200 H· 1.26774800·-1.83648000·-0.57749900
TS19	-693.2904772	1889.5424i· 26.0047· 38.3202 60.7840· 107.9322· 167.8647 196.6759· 216.7035· 231.8169 318.2470· 338.7596· 379.7200 395.6360· 408.9317· 475.7009 479.6626· 503.1425· 524.0040 552.4269· 563.7402· 620.1264 629.8713· 668.9404· 670.6336 706.7211· 763.3712· 767.3437 770.9243· 777.5164· 787.1281 858.7483· 867.6655· 871.0130 898.1997· 899.2418· 904.5675 918.0068· 947.2024· 964.6502 988.2848·1004.4279·1014.0139 1015.6296·1021.2492·1055.9206 1059.7966·1069.7874·1108.7568 1151.1111·1160.7598·1168.5478 1177.9007·1199.6682·1208.6328 1217.5205·1246.3335·1263.7005 1278.6264·1310.7713·1348.4612 1353.2474·1391.0775·1443.2644 1459.5768·1481.5059·1492.8765 1525.6260·1563.8923·1638.8985 1656.7617·1665.3767·1670.5259 1682.5774·1696.2754·1759.9395 3189.5190·3190.4269·3193.8549 3195.9801·3198.3834·3199.4787 3203.8599·3211.7136·3213.0077 3219.3534·3224.0039·3228.6702	C· 3.75697600· 1.15170300·-0.48541900 C· 5.14023200· 1.25944300·-0.44080600 C· 5.90670300· 0.21826400· 0.07526800 C· 5.28174300·-0.93112000· 0.55286000 C· 3.89893400·-1.04253900· 0.51266200 C· 3.11857700·-0.00607800·-0.02231700 H· 3.15605500· 1.96026100·-0.88584000 H· 5.62229000· 2.15787300·-0.80731300 H· 6.98589000· 0.30514600· 0.11369900 H· 5.87427000·-1.73882800· 0.96610100 H· 3.40847300·-1.92687300· 0.90299400 C· 0.81070000·-1.12603900·-0.26530000 H· 1.08230800·-2.15487300·-0.48154500 C· 1.67694300·-0.12693400·-0.08740500 C·-0.58263000·-0.66474600·-0.16154100 C·-0.60526100· 0.73264900· 0.09506300 C·-1.73104500· 1.45541600· 0.25338800 C·-2.98759500· 0.76403900· 0.14525400 C·-2.99677300·-0.63562000·-0.11314000 C·-1.76377300·-1.34206700·-0.26316200 H· 0.78430800· 0.88887200· 0.08842800 H·-1.72793600· 2.52197400· 0.45216700 C·-4.24303500·-1.29910600·-0.21540400 C·-5.42345900·-0.61314400·-0.07105000 H·-6.36874300·-1.13621500·-0.15259300 C·-4.21754300· 1.44518100· 0.28848700 C·-5.41141500· 0.77388200· 0.18353100 H·-6.34703200· 1.30839500· 0.29635800 H·-4.20248600· 2.51203500· 0.48442600 H·-4.24941700·-2.36600800·-0.41170600 H·-1.78764900·-2.41086900·-0.45279900
TS20	-693.275857	718.3449i· 36.9166· 47.9835 64.8995· 113.9117· 185.2989 220.7936· 232.7769· 254.2406 317.1452· 356.2378· 377.5632 416.1220· 425.6226· 472.8305 482.9778· 527.7685· 542.9520 550.4589· 580.4044· 619.7912 630.3961· 654.2658· 693.9627 709.0729· 745.3046· 765.7927 766.4379· 776.2704· 790.2421 820.9239· 860.6688· 870.6098 879.5934· 897.9008· 905.4659 914.1436· 953.1229· 968.1558 988.1721·1006.6410·1011.2170 1017.4661·1023.6073·1051.3528 1059.5169·1109.1754·1143.8439 1158.4438·1162.1405·1178.9488 1191.8645·1202.1340·1212.1718 1235.8847·1243.1521·1261.6186 1277.5145·1331.7298·1349.5933 1363.0351·1395.5330·1419.9021 1443.5187·1465.5653·1490.6829 1510.0031·1540.5182·1554.4420 1615.8282·1644.2571·1651.0078 1672.5377·1683.5142·3160.0412	C· 3.81690300· 0.77462800·-0.99623100 C· 5.11899800· 0.96513300·-0.55464100 C· 5.55705900· 0.34054400· 0.61029500 C· 4.68420900·-0.46701100· 1.33485000 C· 3.38000100·-0.65174900· 0.89622000 C· 2.93400800·-0.04697200·-0.28530300 H· 3.47449300· 1.25736900·-1.90550900 H· 5.79371500· 1.59923600·-1.11728800 H· 6.57242800· 0.49032000· 0.95749000 H· 5.01816700·-0.94109900· 2.25012500 H· 2.68931600·-1.25141300· 1.47864000 C· 0.79726900·-1.40981500·-0.48047900 H· 1.20310200·-2.35106300·-0.13068900 C· 1.56492100·-0.25617500·-0.77005300 C·-0.55959800·-0.95460700·-0.38523800 C·-0.37862600· 0.43749900·-0.19006700 C·-1.38236900· 1.31137900· 0.05187700 C·-2.70962600· 0.76737500· 0.10918800 C·-2.92253900·-0.63302500·-0.09215900 C·-1.82624200·-1.49929300·-0.34292400 H· 1.30207500· 0.31368200·-1.65677700 H·-1.23440900· 2.37535300· 0.20171600 C·-4.25174600·-1.13197800·-0.03055300 C·-5.31146600·-0.30006800· 0.21471200 H·-6.31775500·-0.69928700· 0.25710100

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		3192.7878·3196.0002·3196.1877 3197.4934·3199.2054·3201.2581 3209.7962·3211.2778·3218.0599 3219.6522·3224.0226·3228.1468	C·-3.82779400·1.59891800·0.36318700 C·-5.09753100·1.08317300·0.41418800 H·-5.94111900·1.73482400·0.60825100 H·-3.65975700·2.65956500·0.51683100 H·-4.41174800·-2.19403000·-0.18339500 H·-2.00349800·-2.56119700·-0.47771800
TS21	-693.2648062	815.5866i·32.1469·43.9781 66.1500·115.4681·179.6429 202.4613·245.5039·270.1610 295.6881·378.4885·399.4902 410.0829·443.8199·460.2470 474.0558·521.0684·532.7351 541.8284·619.9982·626.5672 628.5859·641.1444·703.0451 710.0866·758.1691·762.1540 765.2659·776.2642·777.9641 846.3906·860.6309·864.0830 887.5492·904.2722·912.3323 921.5278·942.9594·966.3571 988.0941·1001.3502·1010.3611 1015.9662·1016.8923·1052.1816 1059.3769·1100.7102·1114.3099 1146.1838·1158.5349·1175.5744 1180.0571·1204.0964·1213.0790 1224.5808·1236.8381·1276.7841 1315.8820·1323.2499·1349.4270 1376.3182·1393.3013·1405.9738 1435.0537·1450.1003·1491.6778 1498.9874·1532.4455·1554.8804 1621.9528·1645.1088·1650.0066 1669.1527·1684.9855·3119.3288 3191.7342·3193.6001·3196.5916 3198.2203·3202.2206·3203.0475 3210.8652·3212.5636·3213.9935 3218.2731·3224.9803·3228.1442	C·-3.47307000·-0.20185200·-0.94202200 C·-4.12085700·-1.33047300·-0.45504400 C·-3.85642100·-1.78689400·0.83196000 C·-2.94511300·-1.09764900·1.62878900 C·-2.29608600·0.02882800·1.14395300 C·-2.54086200·0.48332800·-0.15709700 H·-3.68183200·0.15092100·-1.94677300 H·-4.83594900·-1.85152300·-1.08081700 H·-4.36293500·-2.66416500·1.21568700 H·-2.74506800·-1.43582500·2.63878800 H·-1.59552200·0.56518100·1.77344200 C·-0.87874000·2.46024100·-0.08440400 H·-0.85676200·3.54308900·-0.08221500 C·-1.89137800·1.69997300·-0.71195100 C·0.27059700·1.59721700·0.01737300 C·-0.02132700·0.64165600·-0.98749000 C·0.79562000·-0.37197700·-1.34952900 C·2.04811600·-0.45751200·-0.65408200 C·2.37760100·0.49762900·0.35865500 C·1.46903100·1.53884100·0.69172600 H·-2.53394900·2.21411600·-1.42918000 H·0.55378300·-1.10028100·-2.11561200 C·3.62860800·0.37951600·1.02078800 C·4.50659100·-0.62342400·0.70552900 H·5.45579700·-0.69773600·1.22241600 C·2.98007500·-1.48036100·-0.95723100 C·4.17835800·-1.56537500·-0.29590700 H·4.87794800·-2.35601900·-0.53958800 H·2.72524600·-2.20117000·-1.72667000 H·3.87701500·1.10502600·1.78812900 H·1.73777100·2.25811300·1.45829500
TS22	-693.3186861	388.8031i·39.4379·68.0046 88.7356·154.5308·182.2739 201.3837·224.7946·282.9854 357.2000·383.6597·399.8302 405.3152·462.3327·478.6792 496.8493·507.8555·526.4238 568.1339·617.7290·627.1664 658.1670·666.6781·701.1808 741.6747·758.7849·765.1685 774.4053·783.8202·791.9871 845.4108·862.1295·870.8390 890.3200·896.4751·916.1331 916.7535·967.3604·979.7121 990.9307·1004.0250·1009.4009 1013.1890·1031.6885·1052.0101 1054.7567·1100.2886·1149.9882 1158.9905·1170.5704·1173.9036 1192.7036·1198.4363·1223.7485 1233.2674·1266.8208·1282.2607 1319.1066·1331.3212·1336.0981 1396.1642·1416.3549·1440.5094 1447.2833·1466.4791·1488.7563 1529.2358·1546.6639·1618.5956 1629.0810·1640.4059·1661.3601 1684.2590·1696.4303·3173.4283 3175.9045·3177.9382·3183.9523 3193.8862·3196.0119·3197.7837 3198.1763·3203.5448·3212.0023 3214.9842·3224.5893·3225.6081	C·3.74122400·0.36939200·-0.88646600 C·4.16201800·-0.95206000·-1.01375300 C·3.66874400·-1.93007900·-0.14761300 C·2.77413500·-1.58656000·0.85280500 C·2.30645700·-0.26402000·0.95902100 C·2.80973000·0.72932700·0.08304500 H·4.87662500·-1.21927300·-1.78266400 H·4.01162200·-2.95401100·-0.23912900 H·2.43148300·-2.33202700·1.56095900 C·0.92698600·2.32394900·0.22512600 H·0.57777800·3.35194200·0.22333600 C·2.24499900·2.08468600·0.13040400 C·-0.11597000·1.29142300·0.20324600 C·0.18711500·-0.08538700·0.28336400 C·-0.71246000·-1.08858000·0.21295000 C·-2.09050500·-0.75285100·0.03215500 C·-2.45273800·0.62082200·-0.04884700 C·-1.44631300·1.61864500·0.03877000 H·-0.41817800·-2.13186800·0.28868000 C·-3.82039500·0.95796700·-0.21959900 C·-4.77901400·-0.01739100·-0.30613600 H·-5.81987100·0.25314300·-0.43696400 C·-3.10220500·-1.73925700·-0.06027700 C·-4.41569800·-1.38148900·-0.22576200 H·-5.18165800·-2.14467500·-0.29615100 H·-2.81893100·-2.78449500·0.00181500 H·-4.09461800·2.00572700·-0.28178900 H·-1.73984900·2.66261300·-0.03417200 H·4.11943600·1.12735900·-1.56421800 H·2.92616600·2.92255300·0.01374000 H·1.81333100·0.05179300·1.87196400
TS23	-693.3340848	1106.2522i·58.6705·65.7304 132.8615·163.7106·183.8321 268.6230·275.3675·306.5773 352.5216·390.3493·411.2465 449.0595·468.6121·477.3774	C·4.07035600·0.39414300·-0.13702100 C·4.52017300·-0.90975300·-0.12134300 C·3.59312700·-1.96432800·-0.04745100 C·2.24838500·-1.70623400·0.05231500 C·1.76077200·-0.36987900·0.14656100

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		490.8953· 507.2675· 543.0948 547.3933· 565.6923· 586.5818 592.9476· 632.3429· 658.4242 704.8596· 734.7918· 756.7380 762.4490· 766.4325· 775.0614 807.7075· 820.5966· 827.7910 868.0977· 886.4780· 897.7575 914.7388· 916.2265· 919.2028 978.8784· 993.3164· 1000.5119 1004.2824· 1011.8883· 1012.3570 1043.9298· 1065.5708· 1128.3805 1153.0408· 1164.1523· 1177.9608 1188.3047· 1199.5053· 1224.6001 1238.2231· 1267.9838· 1290.7247 1303.5880· 1320.4168· 1350.6666 1371.1676· 1394.9427· 1439.9775 1444.8130· 1467.1378· 1484.4217 1490.6541· 1528.4635· 1549.3597 1597.5630· 1636.6946· 1661.2194 1672.1070· 1690.9528· 1705.6073 3191.0565· 3195.1316· 3196.8241 3198.5649· 3200.9299· 3209.7599 3213.3322· 3214.9868· 3217.3632 3226.7811· 3227.4978· 3245.3283	C· 2.70274900· 0.69112800· -0.04854700 H· 5.57966600· -1.12289900· -0.19182400 H· 3.94137700· -2.98978500· -0.07923300 H· 1.55705100· -2.53564300· 0.11303500 C· 0.92830800· 2.35046900· 0.03062300 H· 0.59642200· 3.38292300· 0.04131500 C· 2.24195600· 2.05297300· -0.04708200 C· -0.08170000· 1.31746200· 0.04854200 C· 0.31606100· -0.05879800· 0.06393400 C· -0.66156300· -1.03283200· 0.03750800 C· -2.03206600· -0.70978200· -0.00050700 C· -2.42566900· 0.65945100· -0.00477800 C· -1.42668300· 1.64578400· 0.01886300 H· -0.39795000· -2.08324100· 0.04820800 C· -3.81320700· 0.97921800· -0.03843300 C· -4.75506500· -0.0091900· -0.06550700 H· -5.80843400· 0.24304100· -0.09058000 C· -3.04038700· -1.71434800· -0.03055400 C· -4.36324500· -1.37503000· -0.06157300 H· -5.12260300· -2.14747600· -0.08340800 H· -2.73766400· -2.75601200· -0.02710900 H· -4.10630000· 2.02352500· -0.04203200 H· -1.71657600· 2.69211100· 0.00719100 H· 4.77424900· 1.21460100· -0.22703800 H· 2.98361100· 2.84226000· -0.10425700 H· 1.76334200· -0.20654900· 1.86243200
TS24	-693.2741867	700.5358i· 32.2913· 36.2521 44.9162· 115.5473· 153.9421 167.1417· 204.4286· 265.2661 288.0998· 342.2665· 366.4373 408.7941· 420.3184· 473.4115 482.0101· 499.3133· 503.7876 530.7261· 599.4487· 628.1921 632.1644· 644.9165· 687.6811 696.8513· 758.5612· 763.9525 774.0546· 779.6405· 818.7788 856.7088· 862.0716· 871.3568 897.8652· 909.0175· 915.6127 922.6603· 935.1051· 982.3523 989.6264· 999.6831· 1009.7734 1011.8077· 1014.6969· 1052.1315 1059.4290· 1111.4998· 1137.0469 1157.0386· 1163.8933· 1176.5099 1197.2479· 1206.3055· 1212.8163 1227.7231· 1245.3485· 1274.5589 1298.9451· 1325.5717· 1343.0544 1355.9487· 1389.1457· 1400.0831 1442.5528· 1473.0035· 1490.3700 1512.0535· 1528.9561· 1576.9071 1633.9048· 1638.6951· 1653.0742 1690.5328· 1730.0365· 3184.0194 3194.9649· 3196.1637· 3196.9901 3198.7384· 3202.8573· 3205.1410 3208.0207· 3213.6740· 3213.8175 3222.6089· 3226.1568· 3229.7440	C· -3.70795400· 0.57344200· -0.83925200 C· -5.07088100· 0.82102400· -0.81989600 C· -5.87903100· 0.25882200· 0.16757500 C· -5.30557600· -0.55204700· 1.14396200 C· -3.94204200· -0.80050200· 1.12965800 C· -3.11224500· -0.25170600· 0.13405800 H· -3.09666900· 1.03722500· -1.60388300 H· -5.50875600· 1.46244500· -1.57563400 H· -6.94394700· 0.45649500· 0.17809200 H· -5.92414600· -0.98878800· 1.91902200 H· -3.49856300· -1.43191600· 1.89210200 C· -0.77381300· -0.17478300· -0.81584900 H· -1.11986400· 0.21893600· -1.76488700 C· -1.70077400· -0.55120000· 0.15726700 C· 0.67571900· -0.42708900· -0.69257000 C· 1.76906200· -1.23532200· -0.70567800 C· 2.97885700· -0.60967400· -0.27068800 C· 2.97671200· 0.75110000· 0.17984200 C· 1.76583900· 1.52033600· 0.20047000 C· 0.67309200· 0.87279400· -0.28476800 H· 1.76617500· -2.27736900· -1.00538400 H· -1.32285500· -1.08086900· 1.02652100 H· 1.77792700· 2.53783400· 0.57482200 C· 5.36462900· 0.60123600· 0.60966200 C· 4.20059000· 1.32344400· 0.61441400 C· 4.20370700· -1.32606100· -0.25978700 C· 5.36642900· -0.74097900· 0.16693000 H· 6.28805700· 1.05714900· 0.94645100 H· 4.19595200· 2.35365800· 0.95416600 H· 4.20171800· -2.35614700· -0.60019100 H· 6.29104700· -1.30565900· 0.16670400
TS25	-693.2737619	692.3990i· 28.4041· 39.1528 58.6309· 130.9179· 142.3564 195.7325· 218.3832· 274.2355 293.4184· 342.5392· 374.3988 411.9711· 455.6847· 469.0789 485.1429· 492.0656· 516.1640 530.8696· 615.7968· 628.8932 637.1757· 649.5641· 696.4617 729.3375· 741.9770· 768.3936 774.0336· 779.3060· 804.5239 823.3153· 859.1908· 873.7803 895.1075· 912.4095· 922.8242 929.1384· 939.2805· 963.7634 991.6583· 1003.0270· 1009.5899 1013.5362· 1017.0324· 1052.6669 1060.9956· 1111.7084· 1124.1215	C· 1.88680500· -0.71757900· 0.00390900 C· 2.44941600· -1.98057400· -0.10998400 C· 3.83066700· -2.14350800· -0.17964400 C· 4.65528300· -1.02084700· -0.14499900 C· 4.09987400· 0.24304900· -0.03846000 C· 2.70501200· 0.42957400· 0.04958900 H· 0.81070100· -0.62677800· 0.04312900 H· 1.80049200· -2.84763200· -0.14831500 H· 4.26000300· -3.13434100· -0.26613800 H· 5.73130300· -1.13344500· -0.20475400 H· 4.74578100· 1.11443300· -0.01673100 C· 0.91544800· 2.25632700· 0.35961000 H· 0.80626500· 3.33095600· 0.45943200 C· 2.21826200· 1.78567100· 0.15646600 C· -0.30455500· 1.46389800· 0.61057400 C· -1.12011400· 0.70723800· 1.39272900

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
		1155.4812·1157.4836·1177.6234 1184.6440·1206.2540·1211.3378 1224.0242·1247.3473·1274.6800 1307.0688·1339.1030·1358.6804 1388.7007·1392.1172·1401.7697 1445.7111·1473.5347·1491.7241 1507.9158·1529.7774·1576.7866 1630.9341·1636.4590·1654.9606 1690.5394·1728.6205·1777.1956 3191.8974·3193.8057·3195.1013 3197.4051·3202.5544·3204.7305 3207.4590·3213.0061·3214.4565 3225.5559·3227.5083·3256.9909	C·-2.21358700· 0.10011900· 0.70101200 C·-2.36955600· 0.27277400·-0.71391600 C·-1.44471900· 1.07035700·-1.46701000 C·-0.46700100· 1.65986700·-0.72800000 H·-0.97217500· 0.52987400· 2.45205500 H· 2.96847300· 2.55698600· 0.01350900 H·-1.56588300· 1.16930000·-2.53997500 C·-4.19431100·-1.30859000· 0.73823500 C·-3.15436100·-0.70563500· 1.39434800 C·-3.46023400·-0.36724000·-1.35887300 C·-4.34907500·-1.13706200·-0.65644500 H·-4.90159400·-1.91961700· 1.28611100 H·-3.03235800·-0.83514300· 2.46451400 H·-3.57647600·-0.23366700·-2.42911800 H·-5.17405400·-1.61795300·-1.16843700
benzo[c]phenanthrene (P1)	-692.8457242	81.0801· 86.3203· 128.6288 172.9507· 211.3474· 256.6514 282.0640· 322.6482· 379.9846 418.6852· 440.0365· 440.5912 478.6406· 515.3313· 523.5902 527.2633· 554.6249· 590.7288 592.2520· 628.0407· 684.7796 691.8731· 706.4883· 760.3735 762.9775· 770.5599· 777.3398 804.6723· 825.9216· 838.2335 857.7508· 866.3989· 894.1585 906.7421· 967.5972· 988.7327 988.9033·1002.8133·1003.6483 1016.0196·1021.6210·1038.6268 1064.2983·1084.8210·1136.1479 1155.0968·1159.8965·1178.0320 1184.5978·1197.4000·1219.2723 1239.9311·1244.5315·1262.7241 1281.3897·1332.0431·1364.2467 1378.7977·1408.5448·1429.1204 1452.8297·1464.7532·1466.2267 1494.9364·1548.5227·1551.2217 1580.8547·1636.5402·1676.6162 1678.4102·1683.2291·1703.8674 3195.1272·3196.4203·3197.3465 3197.9904·3208.1368·3208.8336 3213.8052·3215.3179·3224.0294 3224.7455·3241.1331·3257.2574	C· 3.82816400·-1.51515900·-0.11474300 C· 2.67463900·-2.22803700·-0.48821700 C· 1.43949000·-1.62417500·-0.46159000 C· 1.28189500·-0.27492100·-0.05488800 C· 2.46682600· 0.46735900· 0.19804600 C· 3.72108700·-0.18392200· 0.20025100 C· 0.00000000· 0.40424500· 0.00000000 C·-1.28189500·-0.27492100· 0.05488800 C·-1.43949000·-1.62417500· 0.46159000 C·-2.46682600· 0.46735900·-0.19804600 C·-2.39563700· 1.88485900·-0.36355100 C·-1.21708700· 2.53230400·-0.20033800 C· 0.00000000· 1.80834900· 0.00000000 C· 1.21708700· 2.53230400· 0.20033800 C· 2.39563700· 1.88485900· 0.36355100 H· 3.31103900· 2.43233800· 0.55918400 H· 1.16803000· 3.61476800· 0.24548400 H· 4.79559600·-2.00250800·-0.12000800 H· 4.60564300· 0.40147100· 0.42734500 H·-3.31103900· 2.43233800·-0.55918400 H·-1.16803000· 3.61476800·-0.24548400 C·-2.67463900·-2.22803700· 0.48821700 C·-3.72108700·-0.18392200·-0.20025100 H·-4.60564300· 0.40147100·-0.42734500 C·-3.82816400·-1.51515900· 0.11474300 H·-4.79559600·-2.00250800·-0.12000800 H· 2.76003700·-3.25563200·-0.82108600 H· 0.58287300·-2.17807400·-0.81696500 H·-0.58287300·-2.17807400· 0.81696600 H·-2.76003700·-3.25563200· 0.82108600
2-(phenylacetylene)naphthalene (P2)	-692.7762435	24.9562· 38.5225· 38.5557 102.4592· 133.4052· 180.7868 198.9573· 226.3520· 318.3446 345.3176· 395.7141· 408.8026 439.4521· 481.0099· 483.9908 507.8708· 524.8743· 536.1866 570.9081· 592.7334· 629.3361 639.4680· 658.5246· 670.5562 707.3007· 769.4512· 774.3686 782.8604· 791.6474· 802.0944 846.6826· 872.5661· 886.8124 913.4424· 928.6157· 950.8908 978.8499· 991.8284·1005.6151 1007.3776·1017.3948·1017.7660 1022.6062·1051.8193·1059.4064 1109.6342·1143.7126·1164.1212 1170.8162·1179.5667·1182.7334 1203.0094·1224.8012·1265.1151 1292.2816·1309.7753·1334.4557 1348.8815·1383.8897·1408.2276 1429.8596·1478.4035·1484.4471 1511.3827·1541.2268·1559.0695 1642.6011·1643.7419·1670.8920 1678.2339·1705.9905·2353.8933 3194.5933·3198.0567·3199.4096 3202.0961·3208.3667·3209.6826 3212.7933·3218.9554·3224.2745 3224.7151·3224.9368·3230.2189	C·-3.98067600·-1.30050700· 0.00001200 C·-5.36194100·-1.43687900· 0.00000200 C·-6.17792100·-0.30895800·-0.00001300 C·-5.60567600· 0.96011600·-0.00002100 C·-4.22520700· 1.10472800·-0.00001300 C·-3.39842500·-0.02627600· 0.00000900 H·-3.33944000·-2.17332300· 0.00002500 H·-5.80330800·-2.42631400· 0.00000800 H·-7.25571100·-0.41856000·-0.00002000 H·-6.23725300· 1.84040400·-0.00003600 H·-3.77306000· 2.08890300·-0.00001900 C·-0.77439600· 0.23123700· 0.00001700 C·-1.97598300· 0.11697100· 0.00001700 C· 0.64643800· 0.38183800·-0.00001400 C· 1.21631200· 1.68872200· 0.00001100 C· 2.57176300· 1.85270000· 0.00000500 C· 3.44403000· 0.73165400· 0.00000000 C· 2.88203400·-0.57373900· 0.00000000 C· 1.47419700·-0.72015300· 0.00000700 H· 0.55304100· 2.54472300· 0.00001100 H· 3.00144200· 2.84858200· 0.00000200 C· 3.75074900·-1.69703800·-0.00000800 C· 5.10944500·-1.52866500·-0.00001200 H· 5.76411700·-2.39189900·-0.00001900 C· 4.85450900· 0.87399400·-0.00000500 C· 5.66834200·-0.22801900·-0.00001100 H· 6.74517500·-0.10879200·-0.00001400 H· 5.27808900· 1.87257500·-0.00000400

Species	Energy (Hartree)	Frequencies (cm ⁻¹)	Cartesian coordinates
			H· 3.31746100·-2.69137200·-0.00001000 H· 1.04388000·-1.71529200· 0.00000500
tetracene (P3)	-692.8501307	64.7958· 66.1125· 143.7880 166.2825· 183.9475· 268.6782 289.3820· 309.1314· 359.9266 398.4800· 429.5638· 453.4661 476.3064· 496.8453· 520.3398 538.6056· 551.4697· 578.2104 585.9407· 632.1789· 660.8970 695.3146· 740.6037· 758.0533 764.8959· 765.4600· 775.9772 779.0420· 815.4598· 827.0040 863.8581· 888.0802· 889.7833 907.7518· 916.9646· 918.8724 981.9311· 993.8405· 1003.7764 1004.0747· 1012.0748· 1013.3236 1041.7884· 1074.5151· 1129.2830 1154.7132· 1164.6146· 1180.6650 1188.0319· 1198.4020· 1226.2388 1242.1025· 1270.3703· 1294.4155 1305.7016· 1328.2017· 1353.8507 1376.2257· 1391.5147· 1443.7243 1446.3748· 1473.3592· 1490.1480 1502.4441· 1527.6261· 1553.8820 1619.3373· 1638.9818· 1663.9781 1684.0659· 1704.3857· 1707.2611 3190.2802· 3194.8007· 3196.5952 3196.7011· 3200.6328· 3208.0034 3213.6782· 3214.7652· 3215.3302 3225.1406· 3226.8137· 3239.3186	C·-4.08585500· 0.38938400·-0.00001000 C·-4.53795400·-0.91231400·-0.00000600 C·-3.61166400·-1.96301700·-0.00000100 C·-2.25707500·-1.69787500· 0.00000100 C·-1.77002900·-0.37793900·-0.00000400 C·-2.70890700· 0.67799800·-0.00000800 H·-5.60058300·-1.12273200·-0.00000800 H·-3.95771300·-2.98967500· 0.00000200 H·-1.56738400·-2.53156600· 0.00000500 C·-0.94198500· 2.35058500·-0.00001100 H·-0.60965700· 3.38297100·-0.00001300 C·-2.25443100· 2.04888500·-0.00001300 C· 0.06359900· 1.31513100·-0.00000500 C·-0.33909600·-0.06144900·-0.00000200 C· 0.64840800·-1.03458900· 0.00000500 C· 2.01528000·-0.71106000· 0.00000700 C· 2.40905800· 0.65961500· 0.00000300 C· 1.41078200· 1.64351400·-0.00000300 H· 0.38651900·-2.08558900· 0.00000800 C· 3.79825400· 0.97961200· 0.00000500 C· 4.74003100·-0.00777800· 0.00001100 H· 5.79369100· 0.24445200· 0.00001300 C· 3.02692900·-1.71580100· 0.00001300 C· 4.34855300·-1.37555700· 0.00001500 H· 5.10915500·-2.14711300· 0.00002000 H· 2.72472700·-2.75764500· 0.00001600 H· 4.09081700· 2.02409700· 0.00000200 H· 1.69983900· 2.69020400·-0.00000600 H·-4.78992400· 1.21465200·-0.00001400 H·-3.00288700· 2.83387000·-0.00001600