

1a

B3LYP/CEP121G Etot = -2398.15504599 Hartree/Minimum_Frequency_Value = 37.39 cm-1/Spin_Multiplicity = 7/Point

Group = CS

C	2.78887800	-1.88340000	0.73696300
C	2.78887800	-1.88340000	-0.73696300
C	1.73839000	-2.55227700	-1.42550400
C	0.69818400	-3.31424800	-0.73916400
C	0.69818400	-3.31424800	0.73916400
C	1.73839000	-2.55227700	1.42550400
C	3.26343000	-0.61156700	1.18533200
C	3.54816000	0.19145500	0.00000000
C	3.26343000	-0.61156700	-1.18533200
C	2.71039700	0.00949600	-2.33813200
C	1.15321200	-1.89733900	-2.58852900
C	-0.55320700	-3.06333200	-1.45892000
C	-1.78608400	-2.83071000	-0.73869200
C	-1.78608400	-2.83071000	0.73869200
C	-0.55320700	-3.06333200	1.45892000
C	-0.26278500	-2.19293200	2.59703300
C	1.15321200	-1.89733900	2.58852900
C	1.63586900	-0.64788800	3.03956400
C	2.71039700	0.00949600	2.33813200
C	3.27118500	1.55692200	0.00000000
C	2.69982500	2.19253800	1.18192300
C	2.42308400	1.42309600	2.32368900
C	1.17618000	1.64180900	3.04935500
C	0.69252900	0.35451700	3.50353500
C	-0.68595900	0.07580900	3.50160400
C	-1.18036800	-1.20604200	3.05502000
C	-2.42267000	-0.99710100	2.34206700
C	-2.67424000	-1.78049200	1.17796600
C	-0.26278500	-2.19293200	-2.59703300
C	-3.26023600	1.02575800	-1.18264800
C	-2.70420400	0.41242000	-2.32662000
C	-1.62930800	1.08778500	-3.04486300
C	-1.15870600	2.32245200	-2.60064500
C	-1.73931500	2.95475600	-1.42423800
C	-2.77043000	2.30562400	0.73111200
C	-3.26023600	1.02575800	1.18264800
C	-3.53114000	0.22881500	0.00000000
C	-3.23727700	-1.14340000	0.00000000
C	-2.67424000	-1.78049200	-1.17796600
C	-2.42267000	-0.99710100	-2.34206700
C	-0.68595900	0.07580900	-3.50160400

C	0.69252900	0.35451700	-3.50353500
C	1.17618000	1.64180900	-3.04935500
C	0.27012900	2.60990600	-2.60305800
C	0.56296500	3.40494200	-1.42733600
C	-0.67542400	3.62006900	-0.70363500
C	-0.67542400	3.62006900	0.70363500
C	-1.73931500	2.95475600	1.42423800
C	-2.70420400	0.41242000	2.32662000
C	-1.62930800	1.08778500	3.04486300
C	-1.15870600	2.32245200	2.60064500
C	0.27012900	2.60990600	2.60305800
C	0.56296500	3.40494200	1.42733600
C	1.76296400	3.19306300	0.72823300
C	1.76296400	3.19306300	-0.72823300
C	2.69982500	2.19253800	-1.18192300
C	2.42308400	1.42309600	-2.32368900
C	-1.18036800	-1.20604200	-3.05502000
C	1.63586900	-0.64788800	-3.03956400
C	-2.77043000	2.30562400	-0.73111200
Gd	-0.01848100	-1.13880200	0.00000000

1b

B3LYP/CEP121G Etot = -2398.13735529 Hartree/Minimum_Frequency_Value = 32.59 cm-1/Spin_Multiplicity = 7/Point

Group = C2v

C	-2.33050600	2.60850200	-0.86651900
C	-2.34163900	2.61073900	0.57398900
C	-1.18692700	3.03061100	1.29119500
C	0.00000000	3.45614000	0.55924600
C	0.00000000	3.45658100	-0.83787000
C	-1.18429700	3.02977100	-1.57129800
C	-3.05122600	1.42976300	-1.32621000
C	-3.50577300	0.69799200	-0.15359800
C	-3.05095700	1.43321900	1.02084100
C	-2.62164000	0.72229300	2.15668400
C	-0.74101400	2.30856200	2.44884600
C	1.18692700	3.03061100	1.29119500
C	2.34163900	2.61073900	0.57398900
C	2.33050600	2.60850200	-0.86651900
C	1.18429700	3.02977100	-1.57129800
C	0.73210700	2.30227800	-2.73182400
C	-0.73210700	2.30227800	-2.73182400
C	-1.42497900	1.16812200	-3.17659900
C	-2.60960100	0.72619200	-2.44808800
C	-3.50577300	-0.69799200	-0.15359800

C	-3.05122600	-1.42976300	-1.32621000
C	-2.60960100	-0.72619200	-2.44808800
C	-1.42497900	-1.16812200	-3.17659900
C	-0.70742800	0.00000000	-3.63424300
C	0.70742800	0.00000000	-3.63424300
C	1.42497900	1.16812200	-3.17659900
C	2.60960100	0.72619200	-2.44808800
C	3.05122600	1.42976300	-1.32621000
C	0.74101400	2.30856200	2.44884600
C	3.05095700	-1.43321900	1.02084100
C	2.62164000	-0.72229300	2.15668400
C	1.43537100	-1.16423800	2.90355700
C	0.74101400	-2.30856200	2.44884600
C	1.18692700	-3.03061100	1.29119500
C	2.33050600	-2.60850200	-0.86651900
C	3.05122600	-1.42976300	-1.32621000
C	3.50577300	-0.69799200	-0.15359800
C	3.50577300	0.69799200	-0.15359800
C	3.05095700	1.43321900	1.02084100
C	2.62164000	0.72229300	2.15668400
C	0.72841700	0.00000000	3.39422700
C	-0.72841700	0.00000000	3.39422700
C	-1.43537100	-1.16423800	2.90355700
C	-0.74101400	-2.30856200	2.44884600
C	-1.18692700	-3.03061100	1.29119500
C	0.00000000	-3.45614000	0.55924600
C	0.00000000	-3.45658100	-0.83787000
C	1.18429700	-3.02977100	-1.57129800
C	2.60960100	-0.72619200	-2.44808800
C	1.42497900	-1.16812200	-3.17659900
C	0.73210700	-2.30227800	-2.73182400
C	-0.73210700	-2.30227800	-2.73182400
C	-1.18429700	-3.02977100	-1.57129800
C	-2.33050600	-2.60850200	-0.86651900
C	-2.34163900	-2.61073900	0.57398900
C	-3.05095700	-1.43321900	1.02084100
C	-2.62164000	-0.72229300	2.15668400
C	1.43537100	1.16423800	2.90355700
C	-1.43537100	1.16423800	2.90355700
C	2.34163900	-2.61073900	0.57398900
Gd	0.00000000	0.00000000	0.80187900

2

B3LYP/CEP121G Etot = -2382.15302345 Hartree/Minimum_Frequency_Value = 27.46 cm-1/Spin_Multiplicity = 8/Point

Group = C2v

C	-2.33049700	2.60818800	-0.85912400
C	-2.34166800	2.61035800	0.58141400
C	-1.18663300	3.02911900	1.29857100
C	0.00000000	3.45519700	0.56661000
C	0.00000000	3.45598200	-0.83066700
C	-1.18437100	3.02963700	-1.56410800
C	-3.05154600	1.42966700	-1.31876400
C	-3.50657900	0.69806800	-0.14621400
C	-3.05128600	1.43281600	1.02841100
C	-2.62187800	0.72231100	2.16435000
C	-0.74095100	2.30897400	2.45781600
C	1.18663300	3.02911900	1.29857100
C	2.34166800	2.61035800	0.58141400
C	2.33049700	2.60818800	-0.85912400
C	1.18437100	3.02963700	-1.56410800
C	0.73209000	2.30216200	-2.72472600
C	-0.73209000	2.30216200	-2.72472600
C	-1.42510800	1.16802200	-3.16938900
C	-2.60986500	0.72613100	-2.44086400
C	-3.50657900	-0.69806800	-0.14621400
C	-3.05154600	-1.42966700	-1.31876400
C	-2.60986500	-0.72613100	-2.44086400
C	-1.42510800	-1.16802200	-3.16938900
C	-0.70746300	0.00000000	-3.62710700
C	0.70746300	0.00000000	-3.62710700
C	1.42510800	1.16802200	-3.16938900
C	2.60986500	0.72613100	-2.44086400
C	3.05154600	1.42966700	-1.31876400
C	0.74095100	2.30897400	2.45781600
C	3.05128600	-1.43281600	1.02841100
C	2.62187800	-0.72231100	2.16435000
C	1.43494200	-1.16391000	2.91120000
C	0.74095100	-2.30897400	2.45781600
C	1.18663300	-3.02911900	1.29857100
C	2.33049700	-2.60818800	-0.85912400
C	3.05154600	-1.42966700	-1.31876400
C	3.50657900	-0.69806800	-0.14621400
C	3.50657900	0.69806800	-0.14621400
C	3.05128600	1.43281600	1.02841100
C	2.62187800	0.72231100	2.16435000
C	0.72813500	0.00000000	3.40073400

C	-0.72813500	0.00000000	3.40073400
C	-1.43494200	-1.16391000	2.91120000
C	-0.74095100	-2.30897400	2.45781600
C	-1.18663300	-3.02911900	1.29857100
C	0.00000000	-3.45519700	0.56661000
C	0.00000000	-3.45598200	-0.83066700
C	1.18437100	-3.02963700	-1.56410800
C	2.60986500	-0.72613100	-2.44086400
C	1.42510800	-1.16802200	-3.16938900
C	0.73209000	-2.30216200	-2.72472600
C	-0.73209000	-2.30216200	-2.72472600
C	-1.18437100	-3.02963700	-1.56410800
C	-2.33049700	-2.60818800	-0.85912400
C	-2.34166800	-2.61035800	0.58141400
C	-3.05128600	-1.43281600	1.02841100
C	-2.62187800	-0.72231100	2.16435000
C	1.43494200	1.16391000	2.91120000
C	-1.43494200	1.16391000	2.91120000
C	2.34166800	-2.61035800	0.58141400
Eu	0.00000000	0.00000000	0.77205500

3a

B3LYP/CEP121G Etot = -3295.97673117 Hartree/Minimum_Frequency_Value = 34.19 cm-1/Spin_Multiplicity = 1/Point

Group = CS

Yb	0.66386900	-1.55669600	0.00000000
C	0.86258300	1.03328500	3.59961800
C	-0.40970800	-0.90772600	3.70871500
C	-1.30756300	0.20307100	3.64210500
C	1.06486100	4.53176100	0.69868800
C	-0.17926000	4.38074100	1.41724200
C	1.06486100	4.53176100	-0.69868800
C	-1.38296700	4.31885200	0.72694100
C	-0.51720200	1.40247400	3.59417000
C	0.03503500	3.48984600	2.53209800
C	-0.97447100	2.58261900	2.94864200
C	-2.26319800	2.53559900	2.25111500
C	-3.05373300	1.29008300	2.25518800
C	-2.43767900	3.44312100	1.17670200
C	-3.93994300	1.05590200	1.17510500
C	3.08265500	3.12288600	-0.72806700
C	3.08265500	3.12288600	0.72806700
C	2.06694000	3.77233100	-1.41584500
C	2.06694000	3.77233100	1.41584500
C	1.43430900	3.11323700	2.53301300

C	1.85023100	1.82333200	2.95244900
C	4.03525900	-0.24952300	0.00000000
C	3.54907700	1.83346000	-1.17529500
C	3.98095900	1.11992400	0.00000000
C	2.93792800	1.13784500	2.25102600
C	3.54907700	1.83346000	1.17529500
C	3.64468100	-0.99086900	1.17334600
C	2.98881700	-0.33661200	2.24960100
C	3.64468100	-0.99086900	-1.17334600
C	2.98881700	-0.33661200	-2.24960100
C	2.93792800	1.13784500	-2.25102600
C	1.85023100	1.82333200	-2.95244900
C	1.43430900	3.11323700	-2.53301300
C	0.86258300	1.03328500	-3.59961800
C	3.27425100	-2.31969600	-0.71882200
C	2.31044700	-3.07084300	-1.42425700
C	1.65732900	-2.45250300	-2.54978900
C	1.96330700	-1.10759000	-2.97534100
C	0.93835300	-0.39837400	-3.64191800
C	2.31044700	-3.07084300	1.42425700
C	3.27425100	-2.31969600	0.71882200
C	0.93835300	-0.39837400	3.64191800
C	1.96330700	-1.10759000	2.97534100
C	1.65732900	-2.45250300	2.54978900
C	-0.51720200	1.40247400	-3.59417000
C	-0.97447100	2.58261900	-2.94864200
C	0.03503500	3.48984600	-2.53209800
C	-0.17926000	4.38074100	-1.41724200
C	-1.38296700	4.31885200	-0.72694100
C	-3.05373300	1.29008300	-2.25518800
C	-2.26319800	2.53559900	-2.25111500
C	-2.43767900	3.44312100	-1.17670200
C	-3.93994300	1.05590200	-1.17510500
C	-3.90149100	1.89106100	0.00000000
C	-3.17126200	3.04778300	0.00000000
C	-1.30756300	0.20307100	-3.64210500
C	-2.96730500	-1.19879200	-2.55899000
C	-2.55925100	0.10789800	-2.97690900
C	0.30211100	-2.94223400	-2.57317900
C	-0.75047100	-2.16106000	-3.13151700
C	-0.40970800	-0.90772600	-3.70871500
C	-2.05017200	-2.30679300	-2.58567600
C	-3.37760500	-2.56118200	-0.69902000
C	-3.81905600	-1.38620000	-1.41508400

C	-4.28265800	-0.27344100	-0.72226200
C	-3.37760500	-2.56118200	0.69902000
C	0.08659400	-3.79157200	-1.41970100
C	-1.18974800	-3.76610500	-0.73821100
C	-2.27426400	-3.13685400	-1.41580900
C	0.08659400	-3.79157200	1.41970100
C	1.34243800	-3.89379100	0.71442800
C	1.34243800	-3.89379100	-0.71442800
C	-2.27426400	-3.13685400	1.41580900
C	-1.18974800	-3.76610500	0.73821100
C	-2.05017200	-2.30679300	2.58567600
C	-0.75047100	-2.16106000	3.13151700
C	0.30211100	-2.94223400	2.57317900
C	-4.28265800	-0.27344100	0.72226200
C	-3.81905600	-1.38620000	1.41508400
C	-2.96730500	-1.19879200	2.55899000
C	-2.55925100	0.10789800	2.97690900

3b

B3LYP/CEP121G Etot = -3295.96761340 Hartree/Minimum_Frequency_Value = 28.08 cm-1/Spin_Multiplicity = 1/Point

Group = CS

C	1.29597800	-3.94322900	0.00000000
C	-0.17290400	-4.07362400	0.00000000
C	1.94027800	-3.56592600	1.21790200
C	1.94027800	-3.56592600	-1.21790200
C	-0.88459700	-3.81826100	1.21349100
C	-0.88459700	-3.81826100	-1.21349100
C	1.19668400	-3.36112800	2.42500800
C	1.19668400	-3.36112800	-2.42500800
C	-0.19555600	-3.49461900	2.43519100
C	-0.19555600	-3.49461900	-2.43519100
C	3.01805300	-2.60225200	1.21736300
C	3.01805300	-2.60225200	-1.21736300
C	-2.13463400	-3.09722300	1.21176800
C	-2.13463400	-3.09722300	-1.21176800
C	1.81884200	-2.27878000	3.16588300
C	1.81884200	-2.27878000	-3.16588300
C	-0.99877700	-2.55277200	3.17368100
C	-0.99877700	-2.55277200	-3.17368100
C	3.52400500	-2.07506000	0.00000000
C	-2.77579600	-2.70685200	0.00000000
C	2.92253400	-1.77808600	2.39821400
C	2.92253400	-1.77808600	-2.39821400
C	-2.17419200	-2.25549900	2.40389000

C	-2.17419200	-2.25549900	-2.40389000
C	1.04361900	-1.40276400	3.91437400
C	1.04361900	-1.40276400	-3.91437400
C	-0.39523000	-1.53820700	3.92032500
C	-0.39523000	-1.53820700	-3.92032500
C	3.97476100	-0.72584700	0.00000000
C	-3.51128000	-1.46050900	0.00000000
C	3.21237800	-0.37804700	2.34388100
C	3.21237800	-0.37804700	-2.34388100
C	-2.72979400	-0.94435700	2.35770900
C	-2.72979400	-0.94435700	-2.35770900
C	3.83654400	0.10314800	1.16387700
C	3.83654400	0.10314800	-1.16387700
C	-3.47826800	-0.60031600	1.17127000
C	-3.47826800	-0.60031600	-1.17127000
C	1.36812100	0.00787700	3.93377100
C	1.36812100	0.00787700	-3.93377100
C	-0.96990200	-0.22042600	3.93207500
C	-0.96990200	-0.22042600	-3.93207500
C	2.39730200	0.56223500	3.13256300
C	2.39730200	0.56223500	-3.13256300
C	-2.09153300	0.13363800	3.13297100
C	-2.09153300	0.13363800	-3.13297100
C	0.12340800	0.70913500	4.11470500
C	0.12340800	0.70913500	-4.11470500
C	3.66120700	1.45288400	0.71636100
C	3.66120700	1.45288400	-0.71636100
C	-3.49365500	0.75784600	0.71683300
C	-3.49365500	0.75784600	-0.71683300
C	2.26034800	1.96448100	2.69488100
C	2.26034800	1.96448100	-2.69488100
C	-2.21819300	1.54000900	2.69805300
C	-2.21819300	1.54000900	-2.69805300
C	-0.00059600	2.00944900	3.71181700
C	-0.00059600	2.00944900	-3.71181700
C	2.91933400	2.40765100	1.46251100
C	2.91933400	2.40765100	-1.46251100
C	-2.94503200	1.84927000	1.46748900
C	-2.94503200	1.84927000	-1.46748900
C	1.11328400	2.69245200	3.10554400
C	1.11328400	2.69245200	-3.10554400
C	-1.22839600	2.47087500	3.10607700
C	-1.22839600	2.47087500	-3.10607700
C	2.39494700	3.50211700	0.72474600

C	2.39494700	3.50211700	-0.72474600
C	-2.64355100	3.01807400	0.73048100
C	-2.64355100	3.01807400	-0.73048100
C	0.55760300	3.76412500	2.31557400
C	0.55760300	3.76412500	-2.31557400
C	-0.88970400	3.62349800	2.31486500
C	-0.88970400	3.62349800	-2.31486500
C	1.20589600	4.19011800	1.16354100
C	1.20589600	4.19011800	-1.16354100
C	-1.61546100	3.92578100	-1.16548000
C	-1.61546100	3.92578100	1.16548000
C	0.44482100	4.58950600	0.00000000
C	-0.94687400	4.45986200	0.00000000
Yb	-1.16908600	-0.65625000	0.00000000

3c

B3LYP/CEP121G Etot = -3295.96734124 Hartree/Minimum_Frequency_Value = 17.81 cm-1/Spin_Multiplicity = 1/Point

Group = CS

C	0.00527400	-4.38190500	0.73724900
C	0.00527400	-4.38190500	-0.73724900
C	-1.20949800	-4.06505100	1.41715700
C	1.21916800	-4.06173500	1.41716100
C	-1.20949800	-4.06505100	-1.41715700
C	1.21916800	-4.06173500	-1.41716100
C	-2.42464000	-3.79949100	0.69538600
C	2.43357000	-3.79284300	0.69537900
C	-2.42464000	-3.79949100	-0.69538600
C	2.43357000	-3.79284300	-0.69537900
C	-1.21180400	-3.21736900	2.57949400
C	1.21914900	-3.21403300	2.57948700
C	-1.21180400	-3.21736900	-2.57949400
C	1.21914900	-3.21403300	-2.57948700
C	-3.16848100	-2.78177000	1.41451500
C	3.17462000	-2.77304000	1.41450900
C	-3.16848100	-2.78177000	-1.41451500
C	3.17462000	-2.77304000	-1.41450900
C	0.00301900	-2.73928800	3.13239500
C	0.00301900	-2.73928800	-3.13239500
C	-2.39844500	-2.38391100	2.55686100
C	2.40350000	-2.37733500	2.55685100
C	-2.39844500	-2.38391100	-2.55686100
C	2.40350000	-2.37733500	-2.55685100
C	-3.92484100	-1.84126400	0.72684100
C	3.92845500	-1.83048800	0.72684800

C	-3.92484100	-1.84126400	-0.72684100
C	3.92845500	-1.83048800	-0.72684800
C	0.00122100	-1.43386700	3.70311000
C	0.00122100	-1.43386700	-3.70311000
C	-2.35307200	-1.02549400	2.98007500
C	2.35437600	-1.01902700	2.98010100
C	-2.35307200	-1.02549400	-2.98007500
C	2.35437600	-1.01902700	-2.98010100
C	-1.16556000	-0.60110300	3.64965900
C	1.16574200	-0.59789900	3.64967800
C	-1.16556000	-0.60110300	-3.64965900
C	1.16574200	-0.59789900	-3.64967800
C	-3.94375000	-0.47554400	1.17633800
C	3.94358000	-0.46473700	1.17633600
C	-3.94375000	-0.47554400	-1.17633800
C	3.94358000	-0.46473700	-1.17633600
C	-3.14123800	-0.01972000	2.25886700
C	3.13976900	-0.01111100	2.25885600
C	-3.14123800	-0.01972000	-2.25886700
C	3.13976900	-0.01111100	-2.25885600
C	-4.11727800	0.34237200	0.00000000
C	4.11480800	0.35364200	0.00000000
C	-0.72703600	0.75192000	3.60302600
C	0.72349800	0.75392900	3.60305000
C	-0.72703600	0.75192000	-3.60302600
C	0.72349800	0.75392900	-3.60305000
C	-2.70154500	1.38580000	2.24726600
C	2.69617900	1.39317200	2.24725200
C	-2.70154500	1.38580000	-2.24726600
C	2.69617900	1.39317200	-2.24725200
C	-3.72616700	1.65367100	0.00000000
C	3.72009200	1.66388800	0.00000000
C	-1.46726600	1.76527700	2.94683400
C	1.46100400	1.76935200	2.94696900
C	-1.46726600	1.76527700	-2.94683400
C	1.46100400	1.76935200	-2.94696900
C	-3.11596500	2.22636500	1.17551700
C	3.10837700	2.23499500	1.17550000
C	-3.11596500	2.22636500	-1.17551700
C	3.10837700	2.23499500	-1.17550000
C	-0.73066500	2.92056100	2.53077400
C	0.72139400	2.92280400	2.53098900
C	-0.73066500	2.92056100	-2.53077400
C	0.72139400	2.92280400	-2.53098900

C	-2.32625900	3.34838700	0.72521700
C	2.31593400	3.35519600	0.72532400
C	-2.32625900	3.34838700	-0.72521700
C	2.31593400	3.35519600	-0.72532400
C	-1.17066600	3.74139400	1.42627000
C	1.15928000	3.74515700	1.42661500
C	1.15928000	3.74515700	-1.42661500
C	-1.17066600	3.74139400	-1.42627000
C	-0.00645800	4.24145400	0.71409500
C	-0.00645800	4.24145400	-0.71409500
Yb	0.00246100	1.77351000	0.00000000

4

B3LYP/CEP121G Etot = -3372.20925960 Hartree/Minimum_Frequency_Value = 17.47 cm-1/Spin_Multiplicity = 1/Point

Group = C1

C	4.27230400	0.32481600	-0.39010000
C	4.18062300	1.44980700	0.51008500
C	4.05839300	-0.86358300	0.39046400
C	3.89893300	0.94284900	1.84366100
C	3.76934600	-0.48100200	1.76469700
C	3.81023200	0.41537400	-1.73385200
C	3.60342400	2.63907000	0.09101200
C	3.48027200	-2.02388800	-0.18349100
C	3.08872600	1.66055800	2.71229200
C	3.08514100	2.75267900	-1.25358300
C	3.21066100	1.68054800	-2.18594000
C	3.36034300	-0.79965000	-2.33903000
C	2.72562200	3.36999600	0.97787800
C	3.18234900	-1.99459900	-1.57508500
C	2.78887400	-1.17012100	2.52628800
C	2.49328000	2.90947000	2.26982800
C	2.65773200	-2.84415400	0.65752400
C	2.12864900	0.97361300	3.53842400
C	2.30594600	-2.40180900	1.97661500
C	1.90508700	3.56190000	-1.19328100
C	2.33312900	-0.79464000	-3.35159600
C	1.63444700	3.88376800	0.20192600
C	1.91155500	-0.42765900	3.43745300
C	2.23187800	1.64945300	-3.21765500
C	2.03915800	-2.72705900	-2.09664000
C	1.18386100	3.01618100	2.82979500
C	1.78991700	0.39581800	-3.80385600
C	1.02205200	1.88249000	3.72834800
C	1.48351700	-1.93888100	-3.17857600

C	1.58665700	-3.65928800	0.14007900
C	1.11068800	2.53554700	-3.21262900
C	0.86109900	3.42622400	-2.12889500
C	1.01474600	-2.92540100	2.28787700
C	1.23040800	-3.55070900	-1.26408100
C	0.31691300	3.94505200	0.70291000
C	0.56902300	-0.95236700	3.74538400
C	0.56407300	-3.73111800	1.17339900
C	0.08386800	3.50989400	2.08585400
C	0.39007300	0.48230200	-4.11070200
C	0.11963900	-2.21155400	3.15330500
C	0.01202000	1.84696400	-3.85095200
C	-0.22006500	1.39244600	4.02052500
C	0.07923600	-1.84544300	-3.38838500
C	-0.44269900	-0.02608800	4.12581300
C	-0.51354000	3.68886700	-1.69280700
C	-0.17552000	-3.60003700	-1.58608400
C	-0.51034000	-0.58683500	-3.84215100
C	-0.78515100	3.93866800	-0.27111700
C	-0.84369400	-3.77417800	0.84488600
C	-0.72490900	-2.74228800	-2.61411800
C	-1.25020000	3.04982600	2.48142500
C	-1.39237000	2.02177900	3.45766700
C	-1.19081400	-3.75011400	-0.55947100
C	-1.26666300	-2.43452700	2.92650700
C	-1.27487600	2.15866200	-3.51106900
C	-1.82623500	-0.23245900	3.80371000
C	-1.55639200	3.16132900	-2.49400800
C	-1.73763200	-3.15269900	1.75947800
C	-2.40789500	1.02178500	3.35719900
C	-1.90092600	-0.25385600	-3.48630900
C	-2.08427700	3.67571300	0.21133400
C	-2.23778600	-1.41811300	3.21982900
C	-2.30824200	3.17136200	1.55991400
C	-2.06649700	-2.41030500	-2.25965500
C	-2.27248600	1.11687400	-3.43087800
C	-2.35405500	-3.02333300	-0.99509300
C	-2.84160000	2.84642300	-1.95665100
C	-2.68518200	-1.18738900	-2.67017700
C	-2.95750700	-2.50028600	1.31444600
C	-3.11649900	3.13288100	-0.62346900
C	-3.26348900	-1.42555500	2.20584700
C	-3.38883700	1.05721700	2.32823200
C	-3.38931600	2.23326500	1.52174300

C	-3.29720600	1.59584000	-2.53853600
C	-3.25944300	-2.40706100	-0.07374700
C	-3.90170200	2.21424400	0.17065800
C	-3.84829300	-0.20883400	1.73602700
C	-3.73145800	-0.70069100	-1.84111700
C	-4.01625500	0.70006100	-1.76072600
C	-3.96811300	-1.26263700	-0.51912300
C	-4.34405700	1.02136000	-0.38088700
C	-4.30648800	-0.19969100	0.38766900
Yb	0.17869800	-1.52683500	-0.05249800

5a

B3LYP/CEP121G Etot = -3372.21267872 Hartree/Minimum_Frequency_Value = 9.03 cm-1/Spin_Multiplicity = 1/Point

Group = CS

C	2.35055400	-3.34069600	0.73346300
C	2.35055400	-3.34069600	-0.73346300
C	1.15975600	-3.61255000	1.45977200
C	1.15975600	-3.61255000	-1.45977200
C	-0.02395700	-3.96590200	0.71706200
C	-0.02395700	-3.96590200	-0.71706200
C	3.28920800	-2.37129700	1.18531900
C	3.28920800	-2.37129700	-1.18531900
C	3.88927500	-1.78298300	0.00000000
C	0.98806100	-2.93450600	2.69815100
C	0.98806100	-2.93450600	-2.69815100
C	-1.34360500	-3.62300400	1.16730400
C	-1.34360500	-3.62300400	-1.16730400
C	3.06014500	-1.59393900	2.35946900
C	3.06014500	-1.59393900	-2.35946900
C	1.93301000	-1.96720500	3.14894500
C	1.93301000	-1.96720500	-3.14894500
C	-2.19000500	-3.42572000	0.00000000
C	-0.34192000	-2.52665900	3.13945600
C	-0.34192000	-2.52665900	-3.13945600
C	-1.49087500	-2.81927900	2.36350400
C	-1.49087500	-2.81927900	-2.36350400
C	4.27069900	-0.46461400	0.00000000
C	1.19109800	-0.97797700	3.90817400
C	1.19109800	-0.97797700	-3.90817400
C	3.48057300	-0.18780000	2.36159500
C	3.48057300	-0.18780000	-2.36159500
C	-0.21336300	-1.28476400	3.85448900
C	-0.21336300	-1.28476400	-3.85448900
C	4.07591500	0.35209100	1.18300900

C	4.07591500	0.35209100	-1.18300900
C	-3.20802900	-2.37994900	0.00000000
C	-2.53965000	-1.84859800	2.37213200
C	-2.53965000	-1.84859800	-2.37213200
C	-3.39756500	-1.64558100	1.22143900
C	-3.39756500	-1.64558100	-1.22143900
C	1.59954800	0.33499500	3.93299500
C	1.59954800	0.33499500	-3.93299500
C	2.76918700	0.74350900	3.16440100
C	2.76918700	0.74350900	-3.16440100
C	-1.18570100	-0.24772900	3.74046000
C	-1.18570100	-0.24772900	-3.74046000
C	3.79424400	1.67127700	0.73178600
C	3.79424400	1.67127700	-0.73178600
C	-2.38323700	-0.58991800	3.04553000
C	-2.38323700	-0.58991800	-3.04553000
C	-3.76845400	-0.25000800	1.21993200
C	-3.76845400	-0.25000800	-1.21993200
C	0.62744000	1.39914300	3.92369200
C	0.62744000	1.39914300	-3.92369200
C	2.54387900	2.08457700	2.73598000
C	2.54387900	2.08457700	-2.73598000
C	2.96651200	2.55644200	1.45836700
C	2.96651200	2.55644200	-1.45836700
C	-0.76145700	1.15130700	3.74539700
C	-0.76145700	1.15130700	-3.74539700
C	-3.15551600	0.39241400	2.34370100
C	-3.15551600	0.39241400	-2.34370100
C	-3.97247200	0.46356900	0.00000000
C	1.27181000	2.51136500	3.28806700
C	1.27181000	2.51136500	-3.28806700
C	2.14721300	3.54096900	0.73271300
C	2.14721300	3.54096900	-0.73271300
C	-1.56156400	2.16713200	3.03914900
C	-1.56156400	2.16713200	-3.03914900
C	-2.77354400	1.76594400	2.31355100
C	-2.77354400	1.76594400	-2.31355100
C	-3.71631500	1.85138700	0.00000000
C	0.53277100	3.46242100	2.64010000
C	0.53277100	3.46242100	-2.64010000
C	1.00902500	4.05754500	1.40000400
C	1.00902500	4.05754500	-1.40000400
C	-0.90500700	3.34688500	2.59521600
C	-0.90500700	3.34688500	-2.59521600

C	-3.19660000	2.51487000	1.17771500
C	-3.19660000	2.51487000	-1.17771500
C	-0.15541200	4.50416700	0.69563300
C	-0.15541200	4.50416700	-0.69563300
C	-1.33476100	4.07123900	1.42454500
C	-1.33476100	4.07123900	-1.42454500
C	-2.45850300	3.65685100	0.72694600
C	-2.45850300	3.65685100	-0.72694600
Yb	-0.91471500	-1.30775600	0.00000000

5b

B3LYP/CEP121G Etot = -3372.21259367 Hartree/Minimum_Frequency_Value = 13.37 cm-1/Spin_Multiplicity = 1/Point

Group = C1

C	-3.68674300	2.03107500	-0.62792300
C	-3.72575500	1.86330800	0.83100200
C	-3.78651800	0.90503800	-1.49137500
C	-3.86432700	0.57155600	1.40936600
C	-4.00971000	-0.38309000	-0.89859800
C	-4.04737700	-0.54672400	0.52838900
C	-2.83517700	3.12642600	-0.93246700
C	-2.89802500	2.85566800	1.42195200
C	-2.35870300	3.65485000	0.33489600
C	-3.05444900	0.96421200	-2.71158400
C	-3.19767600	0.34633800	2.64770300
C	-3.43666500	-1.56255500	-1.46464900
C	-3.50114800	-1.82957700	0.84252000
C	-2.00242100	3.13466200	-2.09172000
C	-2.12829600	2.59522000	2.59521300
C	-2.20478100	2.06848400	-3.01341800
C	-2.37212700	1.34859800	3.23876900
C	-3.12881200	-2.48589200	-0.39370000
C	-2.46292400	-0.23947500	-3.28212000
C	-2.62973000	-0.95896400	2.95749700
C	-2.61401200	-1.48847300	-2.63739000
C	-2.74310300	-2.03209300	2.04311800
C	-1.10359000	4.20000800	0.43101400
C	-1.10573600	1.55186000	-3.80880300
C	-1.31399700	0.65962100	3.95300900
C	-0.66320500	3.72671800	-1.98912700
C	-0.78798700	3.18681200	2.70021400
C	-1.22954200	0.12352400	-3.92651400
C	-1.43347700	-0.75640400	3.73313800
C	-0.23695000	4.24632200	-0.73095400
C	-0.29942500	3.97592600	1.61741000

C	-2.03416800	-3.41930000	-0.47021400
C	-1.52298200	-2.41120500	-2.72373900
C	-1.65715600	-2.97264900	1.98040200
C	-1.25069500	-3.38327600	-1.68272300
C	-1.32734400	-3.70600300	0.76853500
C	0.14245600	2.12372900	-3.73517900
C	-0.06558500	1.22543800	4.07771100
C	0.37463000	3.23830300	-2.82618400
C	0.20746800	2.51599700	3.45861100
C	-0.07944600	-0.71504700	-3.87148800
C	-0.27799300	-1.56591500	3.54845100
C	1.09531800	4.08544900	-0.25954500
C	1.05683200	3.91834700	1.19259200
C	-0.28233900	-2.01657700	-3.31944500
C	-0.44576400	-2.70943700	2.70267400
C	0.18706400	-3.57031200	-1.65927500
C	0.11648900	-3.87611300	0.77340000
C	1.32339400	1.29880000	-3.78785200
C	1.11466500	0.40397000	4.00476900
C	1.72282900	3.13752300	-2.37001600
C	1.57850000	2.51413500	3.06399900
C	2.10123100	3.46693100	-1.03607200
C	2.02461400	3.13443000	1.86069000
C	1.25237000	-0.12082000	-3.77247700
C	1.05277900	-0.97505900	3.66095000
C	0.77441400	-2.73216000	-2.66796500
C	0.64655200	-3.26827400	1.96556300
C	0.89131900	-3.82649500	-0.43806200
C	2.32589000	2.00109900	-3.03915900
C	2.15177400	1.25178100	3.48850900
C	3.16544500	2.70175900	-0.36537200
C	3.12684100	2.53440700	1.09069800
C	2.34584900	-0.85991800	-3.11772200
C	2.18293600	-1.55280100	2.91288900
C	2.08663400	-2.18666000	-2.54421800
C	1.96330900	-2.71291700	2.04071500
C	2.22977400	-3.37690300	-0.35159600
C	3.35068100	1.32005100	-2.44074400
C	3.20937400	0.71786400	2.80514700
C	3.84449300	1.72191200	-1.13188500
C	3.77035800	1.40257100	1.65035900
C	3.41937000	-0.11655900	-2.55693400
C	3.28226100	-0.70879900	2.59598200
C	2.85378300	-2.64284200	-1.43443600

C	2.79285300	-2.91084100	0.90241800
C	4.41917100	0.54982200	-0.54080000
C	4.38318200	0.39161500	0.84071600
C	4.16120200	-0.58387100	-1.41163300
C	4.08636300	-0.90835000	1.41688400
C	3.88065900	-1.82499500	-0.85922300
C	3.84357800	-1.99081100	0.58313800
Yb	-0.57710100	-1.44548600	-0.02200300

6

B3LYP/CEP121G Etot = -3372.21607529 Hartree/Minimum_Frequency_Value = 23.47 cm-1/Spin_Multiplicity = 1/Point

Group = CS

C	1.75675700	-3.75196300	-1.20811100
C	1.75652100	-3.75184200	1.20875300
C	2.47750400	-3.52163100	0.00036400
C	0.36187600	-4.03564800	-1.21305400
C	0.36165400	-4.03550000	1.21346400
C	-0.37472600	-4.15037900	0.00014100
C	2.03109900	-2.96340700	-2.39575300
C	2.03066600	-2.96316900	2.39637100
C	-0.23247500	-3.39549000	-2.38492800
C	-0.23291500	-3.39522100	2.38517900
C	3.54899000	-2.51771700	0.00041800
C	-1.74396600	-3.72364700	-0.00002400
C	0.79881700	-2.69435800	-3.09055700
C	0.79823800	-2.69404600	3.09092000
C	3.03481000	-2.02796400	-2.39898000
C	3.03433200	-2.02769200	2.39966300
C	3.83165900	-1.80933300	-1.20400400
C	3.83142100	-1.80919000	1.20480500
C	-2.33202400	-3.11953200	-1.15810800
C	-2.33222200	-3.11938600	1.15787500
C	-1.55818500	-2.90323200	-2.34789600
C	-1.55860800	-2.90295900	2.34780400
C	0.56307100	-1.42395500	-3.69694800
C	0.56240700	-1.42353000	3.69708400
C	2.85397400	-0.76677900	-3.08901900
C	2.85340900	-0.76642900	3.08954600
C	4.22826300	-0.43949500	-1.20093900
C	4.22803200	-0.43937300	1.20168200
C	-3.31812200	-2.16606900	-0.72551100
C	-3.31827100	-2.16599600	0.72504300
C	-1.83695900	-1.72654600	-3.10460500
C	-1.83750600	-1.72615100	3.10424600

C	1.61396200	-0.39889400	-3.66795700
C	1.61327800	-0.39846900	3.66818700
C	3.67794400	0.18292100	-2.39621400
C	3.67751000	0.18318200	2.39680100
C	4.36656400	0.30717300	0.00034100
C	-0.79137800	-1.00230600	-3.75697300
C	-0.79205100	-1.00183600	3.75674900
C	-3.59477300	-0.97250700	-1.48001100
C	-3.59516100	-0.97231500	1.47934600
C	-2.84823500	-0.78321200	-2.67997500
C	-2.84873200	-0.78286500	2.67938200
C	-1.14679500	0.39674500	-3.75516300
C	-1.14749900	0.39720600	3.75482200
C	4.00120100	1.73605000	0.00023400
C	3.33946000	1.51373400	-2.39806700
C	3.33900100	1.51400000	2.39841600
C	1.25002900	1.02814300	-3.66859500
C	1.24933200	1.02856600	3.66863600
C	-2.41432100	0.53037000	-3.10501500
C	-2.41494600	0.53075300	3.10445300
C	-4.00136300	0.20926700	-0.73091800
C	-4.00158400	0.20931700	0.73006100
C	3.52145800	2.32400200	-1.20156000
C	3.52123700	2.32413700	1.20186900
C	2.16030600	1.94884700	-3.09010200
C	2.15974100	1.94920500	3.09020300
C	-0.16337800	1.41954200	-3.69643500
C	-0.16407300	1.41997900	3.69615300
C	-2.74049000	1.69425900	-2.34945500
C	-2.74090800	1.69449000	2.34857700
C	-3.54444300	1.51036500	-1.16172800
C	-3.54483700	1.51058900	1.16082800
C	2.51517200	3.33464200	-1.20503800
C	2.51493200	3.33477500	1.20505700
C	1.71094800	3.14021500	-2.39978900
C	1.71050700	3.14050700	2.39968500
C	-0.56943300	2.64532400	-3.08857400
C	-0.57003100	2.64578300	3.08819700
C	-3.28918400	2.31386300	-0.00045300
C	1.92737200	3.81959700	-0.00008200
C	-1.81256900	2.76184200	-2.38277400
C	-1.81300900	2.76209400	2.38200500
C	0.38020000	3.47778100	-2.39717400
C	0.37974700	3.47805200	2.39679000

C	-2.29471100	3.35549100	-0.00044200
C	-1.59731500	3.61066900	-1.21312400
C	-1.59750700	3.61078400	1.21232400
C	0.50393400	4.18220600	-0.00022700
C	-0.23785300	4.03666000	-1.20951000
C	-0.23805400	4.03679800	1.20893200
Yb	-1.61886200	-0.04970500	0.00020400

7a

B3LYP/CEP121G Etot = -3448.43349680 Hartree/Minimum_Frequency_Value = 11.06 cm-1/Spin_Multiplicity = 1/Point

Group = C1

Yb	1.65180900	0.19065900	-0.00770100
C	-3.97380900	-1.41353700	1.04615400
C	-4.01265100	-1.87333400	-0.31229000
C	-3.92918600	-0.95404000	-1.40076000
C	-4.18978300	0.39333600	-1.08463100
C	-4.35435400	0.82752300	0.27296200
C	-4.05749600	-0.04399700	1.36330200
C	-3.31083700	0.45161200	2.51456300
C	-2.38885900	-0.45616900	3.21230700
C	-2.26900900	-1.86309100	2.81250200
C	-3.16366500	-2.33138200	1.82038300
C	-2.83932700	-3.43844100	0.96766100
C	-3.34136500	-3.14052700	-0.36181800
C	-2.60046400	-3.47124900	-1.47935100
C	-2.48161400	-2.54254400	-2.58474700
C	-3.07123400	-1.24824200	-2.54357400
C	-2.39489600	-0.13979000	-3.23285900
C	-2.63080200	1.25278900	-2.83427700
C	-3.62338500	1.48394400	-1.85167700
C	-3.59088700	2.63533800	-0.99658100
C	-4.01785600	2.22120900	0.32777800
C	-3.39335700	2.72345000	1.45256800
C	-3.05988300	1.85148900	2.56027800
C	-1.85741800	2.36949300	3.13928300
C	-1.00284000	1.52087200	3.80968900
C	-1.29160200	0.11454200	3.89328700
C	-0.02786500	-0.56668300	4.02961600
C	0.14979900	-1.89099500	3.57314500
C	-1.00303100	-2.58709200	3.00038400
C	-0.73074500	-3.70243500	2.15575800
C	-1.63375600	-4.10027000	1.12043900
C	-0.85510400	-4.46615200	-0.05675100
C	-1.32285100	-4.15366100	-1.32003700

C	-0.41404200	-3.64427700	-2.31016400
C	-1.18243200	-2.74655900	-3.15055200
C	-0.55733400	-1.71237800	-3.81372100
C	-1.18369100	-0.42091900	-3.90181500
C	-0.12649300	0.55199300	-4.02565900
C	-0.28629800	1.87859200	-3.56894300
C	-1.58133800	2.26776100	-3.00995500
C	-1.60110400	3.41406200	-2.16308300
C	-2.58473100	3.57484100	-1.13758600
C	-1.93327400	4.12072300	0.04689400
C	-2.32209400	3.70044900	1.30551300
C	-1.32599600	3.43047700	2.30564200
C	0.06347300	3.51803500	2.02878300
C	0.95777700	2.65300000	2.81108900
C	0.41230800	1.71024900	3.72250900
C	1.01879100	0.41443100	3.92540900
C	2.26840900	0.09033600	3.33796900
C	2.49922600	-1.26875100	2.99589900
C	1.47463200	-2.25302800	3.16709400
C	1.67658000	-3.24397600	2.14945200
C	0.60686300	-3.96064400	1.65984900
C	0.53713400	-4.29191100	0.25531100
C	1.45285200	-3.72736700	-0.67875100
C	0.95078700	-3.38502800	-2.01817800
C	1.61171800	-2.32505000	-2.79202200
C	0.85986600	-1.54589300	-3.71074900
C	1.12917300	-0.13993100	-3.90860500
C	2.25373600	0.48222400	-3.30904000
C	2.13759700	1.85557100	-2.96656900
C	0.90369700	2.55672900	-3.15020900
C	0.84486500	3.56641600	-2.13220800
C	-0.37408000	3.99475800	-1.65423700
C	-0.53813000	4.29690700	-0.25062200
C	0.47900400	3.97560600	0.69375600
C	1.78417900	3.56946400	0.16077400
C	2.65708700	2.78912200	0.98126400
C	2.24462500	2.34047100	2.27447800
C	2.90841400	1.09740900	2.54528000
C	3.75255100	0.76860600	1.42275900
C	3.90351900	-0.61344400	1.01690100
C	3.29316200	-1.61286400	1.82893100
C	2.73014800	-2.82277300	1.27020400
C	2.61231700	-3.01259400	-0.13308000
C	3.27695300	-2.04095100	-0.94616100

C	2.77651000	-1.70487400	-2.24266200
C	3.11656000	-0.33641100	-2.50931800
C	3.84544500	0.18846600	-1.38039400
C	3.63946200	1.56419000	-0.97334900
C	2.81001400	2.38384700	-1.79225000
C	1.96070100	3.41740900	-1.24136800
C	3.60387700	1.83351100	0.44470800
C	3.95605300	-0.88235600	-0.40208100

7b

B3LYP/CEP121G Etot = -3448.40659329 Hartree/Minimum_Frequency_Value = 21.56 cm-1/Spin_Multiplicity = 1/Point

Group = C1

Yb	1.73467200	-0.39560200	0.05092800
C	-0.04129500	-3.91195600	-1.11291600
C	-0.43782300	-4.14734100	0.24983700
C	0.37903200	-3.71633600	1.33706200
C	1.72381000	-3.41709100	1.01488400
C	2.18186200	-3.38068400	-0.34697500
C	1.24771800	-3.43761200	-1.43290300
C	1.39836200	-2.53885600	-2.56873100
C	0.19624400	-2.04711900	-3.25384200
C	-1.13998600	-2.50306400	-2.85208000
C	-1.20795500	-3.52657200	-1.87279100
C	-2.34500500	-3.67819100	-1.01167100
C	-1.86639400	-4.03818500	0.30902000
C	-2.45343500	-3.49538100	1.43927600
C	-1.64618200	-3.04176300	2.54711200
C	-0.22187700	-3.06916000	2.49514700
C	0.52927800	-2.01944700	3.19489300
C	1.89467600	-1.67325300	2.78767700
C	2.51842600	-2.49429400	1.79251800
C	3.57915600	-2.00578400	0.94474600
C	3.34420000	-2.53496500	-0.39536500
C	3.54720900	-1.73512700	-1.52487700
C	2.59952700	-1.75482000	-2.61799800
C	2.58981300	-0.43638800	-3.18011500
C	1.46384500	0.02642000	-3.82091700
C	0.27866600	-0.80173100	-3.91862200
C	-0.83870500	0.08284100	-4.04480400
C	-2.12399200	-0.28640700	-3.57902400
C	-2.30233000	-1.62691000	-3.02510800
C	-3.42863600	-1.82868400	-2.16924100
C	-3.42879800	-2.82531300	-1.14699400
C	-4.06741600	-2.27049600	0.04067900

C	-3.59154600	-2.59330500	1.30015200
C	-3.48191300	-1.56985700	2.29740700
C	-2.34029800	-1.93176200	3.12825900
C	-1.64412200	-0.95793800	3.80137400
C	-0.20295100	-1.02416100	3.88668400
C	0.26464300	0.31846200	4.03315400
C	1.54171200	0.70935500	3.56648300
C	2.41016500	-0.31373800	2.98423100
C	3.49449400	0.13586400	2.13889500
C	4.06195300	-0.69544200	1.10756200
C	4.28839600	0.14207100	-0.07397600
C	4.02831500	-0.36290500	-1.35618500
C	3.35888400	0.46061900	-2.32990800
C	2.87271300	1.76703200	-2.02466700
C	1.72880400	2.27460700	-2.80648700
C	1.07604900	1.39655900	-3.72494200
C	-0.35070000	1.43683300	-3.91735900
C	-1.13689300	2.44756500	-3.30873000
C	-2.47588400	2.10523300	-2.95978300
C	-2.97318200	0.77891000	-3.15290200
C	-3.95770800	0.55823100	-2.12704300
C	-4.19182100	-0.70936600	-1.65845200
C	-4.46262000	-0.92278100	-0.24798000
C	-4.30843400	0.12783500	0.69584300
C	-3.78961100	-0.21285100	2.02991600
C	-3.08758600	0.81139000	2.82376200
C	-2.05709000	0.40853100	3.73206300
C	-0.87810400	1.20180100	3.92871300
C	-0.75966600	2.49268700	3.34738400
C	0.55095100	2.93468400	3.00468500
C	1.68572400	2.07477900	3.16679000
C	2.62295600	2.42915500	2.13958800
C	3.52147400	1.49587400	1.65378300
C	3.86087700	1.48687700	0.24636300
C	3.13379700	2.30520200	-0.68134400
C	2.24328100	3.34156400	-0.13440900
C	1.19966500	3.84481500	-0.95048500
C	0.95198300	3.32679300	-2.26622300
C	-0.46140900	3.42335800	-2.51756900
C	-1.08618500	3.99151600	-1.35712700
C	-2.38924600	3.56613100	-0.94523900
C	-3.10382700	2.67077500	-1.78400200
C	-3.98995900	1.68513600	-1.23483600
C	-4.11574300	1.48577500	0.17039900

C	-3.49137500	2.45503800	0.99781200
C	-2.99594200	2.12445200	2.30858700
C	-1.85930000	2.96442500	2.57507800
C	-1.64217300	3.79375100	1.42380500
C	-0.32153400	4.14601600	1.01394200
C	0.76837500	3.76446000	1.84290300
C	2.04410700	3.41670900	1.27753100
C	-0.06295200	4.25242600	-0.39157600
C	-2.65938700	3.48983900	0.45604000

La@C₆₀_hexagon

B3LYP/CEP121G Etot = -2317.64623148 Hartree/Minimum_Frequency_Value = 44.69 cm-1/Spin_Multiplicity = 2/Point

Group = C1

C	-3.30255900	-0.75466900	0.79632400
C	-2.53426200	-1.46140300	1.81372900
C	-1.84206500	-0.77769000	2.85291500
C	-1.84632700	0.69853300	2.87112800
C	-2.54251100	1.40310400	1.84793000
C	-3.30699700	0.71716500	0.81430700
C	-3.10435000	-1.46122900	-0.46613400
C	-2.24505600	-2.61847000	-0.21551900
C	-1.90742500	-2.62658400	1.19504000
C	-0.63694100	-3.06672300	1.62812800
C	-0.55296200	-1.22781200	3.28130200
C	-0.55969000	1.14490400	3.30963600
C	0.04011600	2.30517500	2.74482300
C	-0.65379700	3.02205800	1.70064600
C	-1.92192000	2.58609800	1.25730600
C	-2.25981600	2.61073200	-0.15322200
C	-3.11243500	1.45498100	-0.43150200
C	-2.92949000	0.75144200	-1.68244100
C	-2.92563000	-0.72697500	-1.70048700
C	-1.28542000	-3.05377000	-1.17285500
C	-1.11830500	-2.32283300	-2.41586900
C	-1.91419000	-1.15584500	-2.63767300
C	-1.29953900	0.03487300	-3.20805400
C	-1.92032200	1.20824900	-2.60920700
C	-1.13091100	2.37347400	-2.35944500
C	-1.30227400	3.07427700	-1.09975400
C	-0.00462800	3.51612600	-0.64074500
C	0.31845400	3.49873100	0.72969800
C	0.25592300	-0.04238400	3.55061700
C	3.36849000	1.43088700	0.47654500
C	3.19754100	0.71657600	1.67514500

C	3.20162400	-0.73958600	1.65753600
C	3.37660100	-1.42381200	0.44229000
C	3.55088000	-0.68552300	-0.79333000
C	2.84481000	1.45363000	-1.80849300
C	2.22711500	2.62137400	-1.19375600
C	2.56080600	2.60759200	0.22410700
C	1.62027000	3.04040600	1.16631000
C	1.44332700	2.29858400	2.41056400
C	2.22551700	1.15572200	2.64857700
C	2.23190600	-1.20738400	2.62017600
C	1.45638700	-2.34842300	2.35482100
C	1.63730800	-3.05899600	1.09316700
C	2.57554000	-2.59888200	0.16165100
C	2.24165600	-2.57996400	-1.25619400
C	2.85257300	-1.39431500	-1.84245400
C	2.16713000	-0.69142700	-2.84387700
C	2.16330800	0.77105400	-2.82649600
C	0.97726400	3.06918100	-1.62052500
C	0.26943200	2.36392100	-2.68343900
C	0.86838800	1.22509200	-3.27089300
C	0.06685200	0.04257400	-3.53216300
C	0.87488500	-1.14165100	-3.29912200
C	0.28184600	-2.29717100	-2.73881400
C	0.99394700	-3.02391900	-1.69330200
C	0.01484900	-3.49954800	-0.72456600
C	0.33786600	-3.51395200	0.64575800
C	1.61185500	-0.03460000	3.22623700
C	0.05287800	-2.37100600	2.68890600
C	3.54699200	0.72366500	-0.77633400
La	-0.97836900	-0.00143500	-0.01985800

Ce@C₆₀_66_bond

B3LYP/CEP121G Etot = -2324.96286900 Hartree/Minimum_Frequency_Value = 39.42 cm-1/Spin_Multiplicity = 3/Point

Group = C2v

C	-2.33011500	2.60836400	-0.84303700
C	-2.34104300	2.61050200	0.59746900
C	-1.18622100	3.03037800	1.31495800
C	0.00000000	3.45735900	0.58280500
C	0.00000000	3.45768800	-0.81520800
C	-1.18426700	3.03102200	-1.54861500
C	-3.05176400	1.42974400	-1.30256500
C	-3.50720100	0.69820300	-0.13014200
C	-3.05113200	1.43256600	1.04476900
C	-2.62297800	0.72257000	2.18174800

C	-0.74056400	2.31063000	2.47515800
C	1.18622100	3.03037800	1.31495800
C	2.34104300	2.61050200	0.59746900
C	2.33011500	2.60836400	-0.84303700
C	1.18426700	3.03102200	-1.54861500
C	0.73216000	2.30316300	-2.70924800
C	-0.73216000	2.30316300	-2.70924800
C	-1.42524400	1.16836100	-3.15312000
C	-2.61020800	0.72619900	-2.42494900
C	-3.50720100	-0.69820300	-0.13014200
C	-3.05176400	-1.42974400	-1.30256500
C	-2.61020800	-0.72619900	-2.42494900
C	-1.42524400	-1.16836100	-3.15312000
C	-0.70746400	0.00000000	-3.60980000
C	0.70746400	0.00000000	-3.60980000
C	1.42524400	1.16836100	-3.15312000
C	2.61020800	0.72619900	-2.42494900
C	3.05176400	1.42974400	-1.30256500
C	0.74056400	2.31063000	2.47515800
C	3.05113200	-1.43256600	1.04476900
C	2.62297800	-0.72257000	2.18174800
C	1.43453300	-1.16397000	2.92690100
C	0.74056400	-2.31063000	2.47515800
C	1.18622100	-3.03037800	1.31495800
C	2.33011500	-2.60836400	-0.84303700
C	3.05176400	-1.42974400	-1.30256500
C	3.50720100	-0.69820300	-0.13014200
C	3.50720100	0.69820300	-0.13014200
C	3.05113200	1.43256600	1.04476900
C	2.62297800	0.72257000	2.18174800
C	0.72778600	0.00000000	3.41478700
C	-0.72778600	0.00000000	3.41478700
C	-1.43453300	-1.16397000	2.92690100
C	-0.74056400	-2.31063000	2.47515800
C	-1.18622100	-3.03037800	1.31495800
C	0.00000000	-3.45735900	0.58280500
C	0.00000000	-3.45768800	-0.81520800
C	1.18426700	-3.03102200	-1.54861500
C	2.61020800	-0.72619900	-2.42494900
C	1.42524400	-1.16836100	-3.15312000
C	0.73216000	-2.30316300	-2.70924800
C	-0.73216000	-2.30316300	-2.70924800
C	-1.18426700	-3.03102200	-1.54861500
C	-2.33011500	-2.60836400	-0.84303700

C	-2.34104300	-2.61050200	0.59746900
C	-3.05113200	-1.43256600	1.04476900
C	-2.62297800	-0.72257000	2.18174800
C	1.43453300	1.16397000	2.92690100
C	-1.43453300	1.16397000	2.92690100
C	2.34104300	-2.61050200	0.59746900
Ce	0.00000000	0.00000000	0.73836400

Pr@C₆₀_66_bond

B3LYP/CEP121G Etot = -2333.48504811 Hartree/Minimum_Frequency_Value = 23.26 cm-1/Spin_Multiplicity = 4/Point

Group = C2v

C	-2.33089000	2.60827600	-0.83809900
C	-2.34170600	2.61063600	0.60224000
C	-1.18662800	3.03027900	1.31908200
C	0.00000000	3.45658100	0.58702200
C	0.00000000	3.45636400	-0.81049800
C	-1.18453800	3.03003000	-1.54396900
C	-3.05173400	1.42970600	-1.29754800
C	-3.50729300	0.69817400	-0.12478700
C	-3.05233300	1.43284500	1.05010100
C	-2.62462600	0.72279700	2.18669100
C	-0.74066100	2.30914000	2.47783800
C	1.18662800	3.03027900	1.31908200
C	2.34170600	2.61063600	0.60224000
C	2.33089000	2.60827600	-0.83809900
C	1.18453800	3.03003000	-1.54396900
C	0.73235700	2.30231900	-2.70415300
C	-0.73235700	2.30231900	-2.70415300
C	-1.42524600	1.16780600	-3.14908900
C	-2.61023000	0.72599400	-2.41990200
C	-3.50729300	-0.69817400	-0.12478700
C	-3.05173400	-1.42970600	-1.29754800
C	-2.61023000	-0.72599400	-2.41990200
C	-1.42524600	-1.16780600	-3.14908900
C	-0.70806600	0.00000000	-3.60743600
C	0.70806600	0.00000000	-3.60743600
C	1.42524600	1.16780600	-3.14908900
C	2.61023000	0.72599400	-2.41990200
C	3.05173400	1.42970600	-1.29754800
C	0.74066100	2.30914000	2.47783800
C	3.05233300	-1.43284500	1.05010100
C	2.62462600	-0.72279700	2.18669100
C	1.43485800	-1.16399600	2.92905200
C	0.74066100	-2.30914000	2.47783800

C	1.18662800	-3.03027900	1.31908200
C	2.33089000	-2.60827600	-0.83809900
C	3.05173400	-1.42970600	-1.29754800
C	3.50729300	-0.69817400	-0.12478700
C	3.50729300	0.69817400	-0.12478700
C	3.05233300	1.43284500	1.05010100
C	2.62462600	0.72279700	2.18669100
C	0.72664100	0.00000000	3.41272300
C	-0.72664100	0.00000000	3.41272300
C	-1.43485800	-1.16399600	2.92905200
C	-0.74066100	-2.30914000	2.47783800
C	-1.18662800	-3.03027900	1.31908200
C	0.00000000	-3.45658100	0.58702200
C	0.00000000	-3.45636400	-0.81049800
C	1.18453800	-3.03003000	-1.54396900
C	2.61023000	-0.72599400	-2.41990200
C	1.42524600	-1.16780600	-3.14908900
C	0.73235700	-2.30231900	-2.70415300
C	-0.73235700	-2.30231900	-2.70415300
C	-1.18453800	-3.03003000	-1.54396900
C	-2.33089000	-2.60827600	-0.83809900
C	-2.34170600	-2.61063600	0.60224000
C	-3.05233300	-1.43284500	1.05010100
C	-2.62462600	-0.72279700	2.18669100
C	1.43485800	1.16399600	2.92905200
C	-1.43485800	1.16399600	2.92905200
C	2.34170600	-2.61063600	0.60224000
Pr	0.00000000	0.00000000	0.70032700

Nd@C₆₀_66_bond

B3LYP/CEP121G Etot = -2343.41179919 Hartree/Minimum_Frequency_Value = 31.86 cm⁻¹/Spin_Multiplicity = 5/Point

Group = C2v

C	-3.09857600	1.19051600	0.95996200
C	-3.46466400	0.34354600	-0.16033500
C	-3.30928300	-1.09656000	-0.03904500
C	-2.79746000	-1.65420600	1.18832500
C	-2.46410300	-0.82972500	2.29095200
C	-2.61560600	0.63807400	2.16636000
C	-2.46866200	2.41392900	0.44432600
C	-2.41410700	2.29849200	-0.99471200
C	-3.01516200	1.00669500	-1.36133400
C	-2.44682700	0.27875400	-2.43519500
C	-2.70482900	-1.83583500	-1.13059400
C	-1.91404000	-2.78412900	0.86413900

C	-0.76764000	-3.03104100	1.63591800
C	-0.43952700	-2.18871400	2.76805200
C	-1.29067200	-1.08946500	3.07174800
C	-0.70172500	0.19987000	3.42325000
C	-1.53685500	1.26358800	2.88347900
C	-0.93222800	2.45347300	2.38999700
C	-1.40801600	3.01889500	1.15019400
C	-1.30238300	2.78942800	-1.70565000
C	-0.20902700	3.42510200	-0.97643800
C	-0.26054800	3.53580800	0.41394700
C	0.92745800	3.26999400	1.21182100
C	0.50358400	2.59681800	2.43063000
C	1.30711300	1.56981700	2.96258900
C	0.68714300	0.34759200	3.46276000
C	1.55613600	-0.77857800	3.15636200
C	0.98849500	-2.02484600	2.80652400
C	-1.86100100	-2.90032400	-0.57614800
C	2.71344900	-2.39069700	-0.44852800
C	1.67139400	-3.00557100	-1.14674400
C	1.18386700	-2.43211500	-2.39106500
C	1.77688100	-1.25196000	-2.88383300
C	2.85547800	-0.61993400	-2.16086100
C	3.66623200	-0.31964600	0.15671900
C	3.24401000	-0.98937300	1.36394500
C	2.65908400	-2.27585300	0.99758200
C	1.56389100	-2.77960700	1.70224100
C	0.47474700	-3.41573400	0.97594800
C	0.52625000	-3.52560000	-0.41482300
C	-0.24843800	-2.59711000	-2.43303900
C	-1.06407200	-1.56392500	-2.96463300
C	-0.44745200	-0.34092400	-3.46357600
C	0.94049600	-0.19073900	-3.42511300
C	1.53006600	1.09684000	-3.07358000
C	2.70389900	0.83133500	-2.28218300
C	3.03366300	1.65438900	-1.19392600
C	3.51922000	1.08295400	0.03982400
C	2.68703400	-0.26315600	2.42705800
C	2.53543200	1.18889700	2.30710600
C	2.94532300	1.83569900	1.13417000
C	2.11478900	2.89789900	0.57828200
C	2.16818900	2.78268600	-0.86922200
C	1.03073900	3.04343000	-1.63535200
C	0.69137700	2.18814600	-2.76479000
C	-0.74083300	2.04497800	-2.80981100

C	-1.31732900	0.78824900	-3.15484600
C	-0.66184400	-3.26120900	-1.21641100
C	-2.28924700	-1.18821600	-2.31168000
C	3.32722300	-1.17087800	-0.96365200
Nd	-0.73405100	-0.02802200	0.00229100

Pm@C₆₀_66_bond

B3LYP/CEP121G Etot = -2354.72442011 Hartree/Minimum_Frequency_Value = 17.09 cm-1/Spin_Multiplicity = 6/Point

Group = C2v

C	-2.33057400	2.60812800	-0.85100000
C	-2.34176400	2.61030900	0.58938400
C	-1.18674900	3.02975600	1.30656500
C	0.00000000	3.45544900	0.57455000
C	0.00000000	3.45608100	-0.82278500
C	-1.18440000	3.02972900	-1.55625100
C	-3.05166400	1.42959900	-1.31069100
C	-3.50721000	0.69811900	-0.13798400
C	-3.05208500	1.43296500	1.03654800
C	-2.62285700	0.72241000	2.17247800
C	-0.74091800	2.30864600	2.46494800
C	1.18674900	3.02975600	1.30656500
C	2.34176400	2.61030900	0.58938400
C	2.33057400	2.60812800	-0.85100000
C	1.18440000	3.02972900	-1.55625100
C	0.73220600	2.30225900	-2.71678900
C	-0.73220600	2.30225900	-2.71678900
C	-1.42518800	1.16800700	-3.16153300
C	-2.61009900	0.72615000	-2.43286100
C	-3.50721000	-0.69811900	-0.13798400
C	-3.05166400	-1.42959900	-1.31069100
C	-2.61009900	-0.72615000	-2.43286100
C	-1.42518800	-1.16800700	-3.16153300
C	-0.70768000	0.00000000	-3.61936500
C	0.70768000	0.00000000	-3.61936500
C	1.42518800	1.16800700	-3.16153300
C	2.61009900	0.72615000	-2.43286100
C	3.05166400	1.42959900	-1.31069100
C	0.74091800	2.30864600	2.46494800
C	3.05208500	-1.43296500	1.03654800
C	2.62285700	-0.72241000	2.17247800
C	1.43538500	-1.16400900	2.91783200
C	0.74091800	-2.30864600	2.46494800
C	1.18674900	-3.02975600	1.30656500
C	2.33057400	-2.60812800	-0.85100000

C	3.05166400	-1.42959900	-1.31069100
C	3.50721000	-0.69811900	-0.13798400
C	3.50721000	0.69811900	-0.13798400
C	3.05208500	1.43296500	1.03654800
C	2.62285700	0.72241000	2.17247800
C	0.72770500	0.00000000	3.40492100
C	-0.72770500	0.00000000	3.40492100
C	-1.43538500	-1.16400900	2.91783200
C	-0.74091800	-2.30864600	2.46494800
C	-1.18674900	-3.02975600	1.30656500
C	0.00000000	-3.45544900	0.57455000
C	0.00000000	-3.45608100	-0.82278500
C	1.18440000	-3.02972900	-1.55625100
C	2.61009900	-0.72615000	-2.43286100
C	1.42518800	-1.16800700	-3.16153300
C	0.73220600	-2.30225900	-2.71678900
C	-0.73220600	-2.30225900	-2.71678900
C	-1.18440000	-3.02972900	-1.55625100
C	-2.33057400	-2.60812800	-0.85100000
C	-2.34176400	-2.61030900	0.58938400
C	-3.05208500	-1.43296500	1.03654800
C	-2.62285700	-0.72241000	2.17247800
C	1.43538500	1.16400900	2.91783200
C	-1.43538500	1.16400900	2.91783200
C	2.34176400	-2.61030900	0.58938400
Pm	0.00000000	0.00000000	0.75174800

Sm@C₆₀_hexagon

B3LYP/CEP121G Etot = -2367.61102076 Hartree/Minimum_Frequency_Value = 35.69 cm-1/Spin_Multiplicity = 7/Point

Group = C2v

C	-2.33062100	2.60842200	-0.85627200
C	-2.34154600	2.61036300	0.58432400
C	-1.18656400	3.02971100	1.30162800
C	0.00000000	3.45572000	0.56947900
C	0.00000000	3.45634800	-0.82779000
C	-1.18437400	3.02987200	-1.56127900
C	-3.05156300	1.42975200	-1.31589300
C	-3.50652700	0.69805100	-0.14330400
C	-3.05126400	1.43280200	1.03134500
C	-2.62219300	0.72230500	2.16745900
C	-0.74092500	2.30956500	2.46081700
C	1.18656400	3.02971100	1.30162800
C	2.34154600	2.61036300	0.58432400
C	2.33062100	2.60842200	-0.85627200

C	1.18437400	3.02987200	-1.56127900
C	0.73219500	2.30250000	-2.72196200
C	-0.73219500	2.30250000	-2.72196200
C	-1.42513500	1.16812400	-3.16645500
C	-2.61007700	0.72618500	-2.43801700
C	-3.50652700	-0.69805100	-0.14330400
C	-3.05156300	-1.42975200	-1.31589300
C	-2.61007700	-0.72618500	-2.43801700
C	-1.42513500	-1.16812400	-3.16645500
C	-0.70755500	0.00000000	-3.62385900
C	0.70755500	0.00000000	-3.62385900
C	1.42513500	1.16812400	-3.16645500
C	2.61007700	0.72618500	-2.43801700
C	3.05156300	1.42975200	-1.31589300
C	0.74092500	2.30956500	2.46081700
C	3.05126400	-1.43280200	1.03134500
C	2.62219300	-0.72230500	2.16745900
C	1.43471900	-1.16388900	2.91328200
C	0.74092500	-2.30956500	2.46081700
C	1.18656400	-3.02971100	1.30162800
C	2.33062100	-2.60842200	-0.85627200
C	3.05156300	-1.42975200	-1.31589300
C	3.50652700	-0.69805100	-0.14330400
C	3.50652700	0.69805100	-0.14330400
C	3.05126400	1.43280200	1.03134500
C	2.62219300	0.72230500	2.16745900
C	0.72783800	0.00000000	3.40236400
C	-0.72783800	0.00000000	3.40236400
C	-1.43471900	-1.16388900	2.91328200
C	-0.74092500	-2.30956500	2.46081700
C	-1.18656400	-3.02971100	1.30162800
C	0.00000000	-3.45572000	0.56947900
C	0.00000000	-3.45634800	-0.82779000
C	1.18437400	-3.02987200	-1.56127900
C	2.61007700	-0.72618500	-2.43801700
C	1.42513500	-1.16812400	-3.16645500
C	0.73219500	-2.30250000	-2.72196200
C	-0.73219500	-2.30250000	-2.72196200
C	-1.18437400	-3.02987200	-1.56127900
C	-2.33062100	-2.60842200	-0.85627200
C	-2.34154600	-2.61036300	0.58432400
C	-3.05126400	-1.43280200	1.03134500
C	-2.62219300	-0.72230500	2.16745900
C	1.43471900	1.16388900	2.91328200

C	-1.43471900	1.16388900	2.91328200
C	2.34154600	-2.61036300	0.58432400
Sm	0.00000000	0.00000000	0.76808900

Tb@C₆₀_66_bond

B3LYP/CEP121G Etot = -2415.92215204 Hartree/Minimum_Frequency_Value = 41.00 cm-1/Spin_Multiplicity = 6/Point

Group = C1

C	-2.91578800	0.69540000	-1.67774000
C	-2.82065400	-0.78065100	-1.81196900
C	-2.97814900	-1.59418000	-0.65697000
C	-3.25415700	-1.01528600	0.63427800
C	-3.35618800	0.43167300	0.76803300
C	-3.16878900	1.26570600	-0.40583200
C	-1.94852000	1.28683800	-2.56551600
C	-1.24107800	0.20133400	-3.22679900
C	-1.79409400	-1.07041400	-2.77126400
C	-0.92657800	-2.19003800	-2.61226200
C	-2.06640800	-2.73658800	-0.47853200
C	-2.47617300	-1.75830500	1.61059100
C	-1.84645800	-1.11760800	2.69449700
C	-1.94469300	0.35014600	2.82857300
C	-2.67252800	1.08404300	1.86359500
C	-2.11394100	2.35629800	1.38988600
C	-2.41854100	2.47103200	-0.01653800
C	-1.47707500	3.04480300	-0.89761400
C	-1.23683700	2.46637800	-2.19655500
C	0.12438200	0.31385300	-3.51015900
C	0.84994100	1.52285200	-3.13582100
C	0.17325900	2.57062100	-2.48208200
C	0.81771100	3.23892800	-1.35974400
C	-0.20831900	3.53707200	-0.37227100
C	0.07885700	3.43099900	0.98932900
C	-0.88728700	2.82563400	1.89935500
C	-0.16397500	2.07347900	2.89658600
C	-0.69990500	0.83545000	3.34673700
C	-1.76611100	-2.84415200	0.93127800
C	2.24922800	-1.28133600	2.56802400
C	1.55454600	-2.44771600	2.19458100
C	1.80622000	-3.04028800	0.89068000
C	2.72664800	-2.45503400	0.01767600
C	3.44649900	-1.24873000	0.40864300
C	3.10997800	0.77383000	1.79583100
C	2.09476400	1.07181200	2.77543300
C	1.54479900	-0.19850800	3.23769200

C	0.18195300	-0.31319300	3.51673400
C	-0.53942100	-1.52164900	3.13510900
C	0.14597300	-2.57594500	2.48240700
C	0.54050400	-3.53512500	0.37186100
C	0.25262200	-3.42875200	-0.99033600
C	1.21475300	-2.82466400	-1.89946400
C	2.42643300	-2.34529400	-1.39870600
C	2.97008400	-1.07549000	-1.87267000
C	3.60743000	-0.41053100	-0.76144400
C	3.51750400	0.99444800	-0.63385900
C	3.26596800	1.58424800	0.66126400
C	1.24413800	2.18102800	2.60584700
C	1.40388300	3.02322900	1.42831200
C	2.38620700	2.73169600	0.48042500
C	2.08717000	2.84057800	-0.93803900
C	2.78532900	1.75698100	-1.62042500
C	2.16332000	1.11490300	-2.69953000
C	2.25675100	-0.34047100	-2.83079500
C	1.00510900	-0.83123300	-3.35053400
C	0.47569400	-2.06132700	-2.89596800
C	-0.48526900	-3.23511500	1.36103600
C	-1.07463600	-3.01766900	-1.43165500
C	3.20335100	-0.68011200	1.66389700
Tb	-0.85194800	-0.00922000	0.00488400

Dy@C₆₀_66_bond

B3LYP/CEP121G Etot = -2435.52265070 Hartree/Minimum_Frequency_Value = 22.62 cm⁻¹/Spin_Multiplicity = 5/Point

Group = C2v

C	-2.32997100	2.60797900	-0.88166000
C	-2.34164600	2.60949600	0.55904300
C	-1.18611900	3.02631700	1.27641600
C	0.00000000	3.45273000	0.54456300
C	0.00000000	3.45596600	-0.85243100
C	-1.18422100	3.02950200	-1.58592800
C	-3.05140300	1.42958000	-1.34154600
C	-3.50590000	0.69792400	-0.16889000
C	-3.05018900	1.43249400	1.00538300
C	-2.61866700	0.72164400	2.14099800
C	-0.74118400	2.30747700	2.43626800
C	1.18611900	3.02631700	1.27641600
C	2.34164600	2.60949600	0.55904300
C	2.32997100	2.60797900	-0.88166000
C	1.18422100	3.02950200	-1.58592800
C	0.73185400	2.30223100	-2.74693000

C	-0.73185400	2.30223100	-2.74693000
C	-1.42503800	1.16847100	-3.19153800
C	-2.60925900	0.72629900	-2.46320500
C	-3.50590000	-0.69792400	-0.16889000
C	-3.05140300	-1.42958000	-1.34154600
C	-2.60925900	-0.72629900	-2.46320500
C	-1.42503800	-1.16847100	-3.19153800
C	-0.70695200	0.00000000	-3.64858000
C	0.70695200	0.00000000	-3.64858000
C	1.42503800	1.16847100	-3.19153800
C	2.60925900	0.72629900	-2.46320500
C	3.05140300	1.42958000	-1.34154600
C	0.74118400	2.30747700	2.43626800
C	3.05018900	-1.43249400	1.00538300
C	2.61866700	-0.72164400	2.14099800
C	1.43545900	-1.16344900	2.89319000
C	0.74118400	-2.30747700	2.43626800
C	1.18611900	-3.02631700	1.27641600
C	2.32997100	-2.60797900	-0.88166000
C	3.05140300	-1.42958000	-1.34154600
C	3.50590000	-0.69792400	-0.16889000
C	3.50590000	0.69792400	-0.16889000
C	3.05018900	1.43249400	1.00538300
C	2.61866700	0.72164400	2.14099800
C	0.72994400	0.00000000	3.39030300
C	-0.72994400	0.00000000	3.39030300
C	-1.43545900	-1.16344900	2.89319000
C	-0.74118400	-2.30747700	2.43626800
C	-1.18611900	-3.02631700	1.27641600
C	0.00000000	-3.45273000	0.54456300
C	0.00000000	-3.45596600	-0.85243100
C	1.18422100	-3.02950200	-1.58592800
C	2.60925900	-0.72629900	-2.46320500
C	1.42503800	-1.16847100	-3.19153800
C	0.73185400	-2.30223100	-2.74693000
C	-0.73185400	-2.30223100	-2.74693000
C	-1.18422100	-3.02950200	-1.58592800
C	-2.32997100	-2.60797900	-0.88166000
C	-2.34164600	-2.60949600	0.55904300
C	-3.05018900	-1.43249400	1.00538300
C	-2.61866700	-0.72164400	2.14099800
C	1.43545900	1.16344900	2.89319000
C	-1.43545900	1.16344900	2.89319000
C	2.34164600	-2.60949600	0.55904300

Dy 0.00000000 0.00000000 0.85508000

Ho@C₆₀_66_bond

B3LYP/CEP121G Etot = -2457.00961703 Hartree/Minimum_Frequency_Value = 34.25 cm⁻¹/Spin_Multiplicity = 4/Point

Group = C2v

C	-2.32991200	2.60826000	-0.88921700
C	-2.34123700	2.60948800	0.55152000
C	-1.18594100	3.02620100	1.26887600
C	0.00000000	3.45283100	0.53711800
C	0.00000000	3.45641700	-0.85990900
C	-1.18419900	3.02985200	-1.59343500
C	-3.05113700	1.42973100	-1.34887600
C	-3.50484200	0.69787400	-0.17611100
C	-3.04887800	1.43232100	0.99791000
C	-2.61733000	0.72158400	2.13380900
C	-0.74113700	2.30693100	2.42847500
C	1.18594100	3.02620100	1.26887600
C	2.34123700	2.60948800	0.55152000
C	2.32991200	2.60826000	-0.88921700
C	1.18419900	3.02985200	-1.59343500
C	0.73190000	2.30250800	-2.75434000
C	-0.73190000	2.30250800	-2.75434000
C	-1.42498400	1.16859500	-3.19868400
C	-2.60906000	0.72636100	-2.47043600
C	-3.50484200	-0.69787400	-0.17611100
C	-3.05113700	-1.42973100	-1.34887600
C	-2.60906000	-0.72636100	-2.47043600
C	-1.42498400	-1.16859500	-3.19868400
C	-0.70683700	0.00000000	-3.65536500
C	0.70683700	0.00000000	-3.65536500
C	1.42498400	1.16859500	-3.19868400
C	2.60906000	0.72636100	-2.47043600
C	3.05113700	1.42973100	-1.34887600
C	0.74113700	2.30693100	2.42847500
C	3.04887800	-1.43232100	0.99791000
C	2.61733000	-0.72158400	2.13380900
C	1.43489400	-1.16331900	2.88699100
C	0.74113700	-2.30693100	2.42847500
C	1.18594100	-3.02620100	1.26887600
C	2.32991200	-2.60826000	-0.88921700
C	3.05113700	-1.42973100	-1.34887600
C	3.50484200	-0.69787400	-0.17611100
C	3.50484200	0.69787400	-0.17611100
C	3.04887800	1.43232100	0.99791000

C	2.61733000	0.72158400	2.13380900
C	0.73042700	0.00000000	3.38778700
C	-0.73042700	0.00000000	3.38778700
C	-1.43489400	-1.16331900	2.88699100
C	-0.74113700	-2.30693100	2.42847500
C	-1.18594100	-3.02620100	1.26887600
C	0.00000000	-3.45283100	0.53711800
C	0.00000000	-3.45641700	-0.85990900
C	1.18419900	-3.02985200	-1.59343500
C	2.60906000	-0.72636100	-2.47043600
C	1.42498400	-1.16859500	-3.19868400
C	0.73190000	-2.30250800	-2.75434000
C	-0.73190000	-2.30250800	-2.75434000
C	-1.18419900	-3.02985200	-1.59343500
C	-2.32991200	-2.60826000	-0.88921700
C	-2.34123700	-2.60948800	0.55152000
C	-3.04887800	-1.43232100	0.99791000
C	-2.61733000	-0.72158400	2.13380900
C	1.43489400	1.16331900	2.88699100
C	-1.43489400	1.16331900	2.88699100
C	2.34123700	-2.60948800	0.55152000
Ho	0.00000000	0.00000000	0.88072900

Er@C₆₀_66_bond

B3LYP/CEP121G Etot = -2480.46009324 Hartree/Minimum_Frequency_Value = 34.22 cm-1/Spin_Multiplicity = 3/Point

Group = C2v

C	-3.38134400	-0.72067200	-0.17219000
C	-2.92750100	-1.47898700	0.97918200
C	-2.51515800	-0.83678500	2.16897600
C	-2.51636800	0.64488500	2.23776100
C	-2.92854000	1.39053700	1.10536600
C	-3.37948900	0.73904300	-0.10473700
C	-2.83504100	-1.37290300	-1.34308000
C	-2.10014600	-2.57557900	-0.92489000
C	-2.15884900	-2.64268800	0.51564200
C	-1.05088000	-3.10825400	1.25012700
C	-1.38233400	-1.31627100	2.91183800
C	-1.38250400	1.05272200	3.01557600
C	-0.64680700	2.22417000	2.68026000
C	-1.04622000	2.98360000	1.51714800
C	-2.15392700	2.58838600	0.74532300
C	-2.09620500	2.65375400	-0.69555000
C	-2.82901900	1.49321700	-1.21693800
C	-2.32657000	0.84970200	-2.36851700

C	-2.32961500	-0.63036800	-2.43659200
C	-0.93782500	-2.97690600	-1.60885500
C	-0.44474700	-2.21983500	-2.73614400
C	-1.14442100	-1.04502800	-3.12841400
C	-0.39439800	0.15651200	-3.47443400
C	-1.13944600	1.32444300	-3.02368400
C	-0.44056000	2.45807200	-2.52876400
C	-0.93282200	3.11491100	-1.34135000
C	0.21192900	3.53340600	-0.54234000
C	0.15655100	3.46914900	0.85055300
C	-0.66775800	-0.15252000	3.41798800
C	3.15735800	1.36373700	1.34988000
C	2.66712400	0.62224100	2.43418200
C	2.66595200	-0.84005600	2.36800600
C	3.15392600	-1.48309200	1.22355000
C	3.65756300	-0.71505400	0.10596200
C	3.24758000	1.46747500	-0.98334100
C	2.50497600	2.63339700	-0.51869100
C	2.44686600	2.56740600	0.93152700
C	1.29812000	2.97997300	1.60805800
C	0.79142300	2.20916400	2.73529900
C	1.47956900	1.04409900	3.13412500
C	1.47639300	-1.32233700	3.02813900
C	0.78985700	-2.44618700	2.52862100
C	1.29521800	-3.11595500	1.33895700
C	2.44364300	-2.64491900	0.70086900
C	2.50076000	-2.57929400	-0.74938800
C	3.24764100	-1.37965900	-1.10996000
C	2.84881300	-0.63543000	-2.22945100
C	2.84953400	0.82662100	-2.16295900
C	1.41308400	3.11004500	-1.24599200
C	1.00048700	2.44259500	-2.47154700
C	1.71800700	1.31492900	-2.91546100
C	1.00124900	0.15243900	-3.42278400
C	1.71677300	-1.05113600	-3.02026600
C	0.99423900	-2.21206500	-2.67731500
C	1.40673100	-2.98610900	-1.51458600
C	0.20613800	-3.46921400	-0.85011500
C	0.15114200	-3.53304900	0.54281300
C	0.72819600	-0.15551000	3.47678700
C	-0.65064800	-2.45420600	2.47264200
C	3.65791500	0.69688600	0.17019600
Er	-0.89520100	-0.00065700	-0.00238400

Tm@C₆₀_66_bondB3LYP/CEP121G Etot = -2505.99559876 Hartree/Minimum_Frequency_Value = 31.11 cm⁻¹/Spin_Multiplicity = 2/Point

Group = C2v

C	-2.32982600	2.60823700	-0.89885900
C	-2.34165900	2.60964200	0.54198800
C	-1.18571400	3.02467100	1.25918900
C	0.00000000	3.45211500	0.52771000
C	0.00000000	3.45605700	-0.86914900
C	-1.18422200	3.02968300	-1.60272800
C	-3.05100900	1.42964400	-1.35859800
C	-3.50430000	0.69774800	-0.18580300
C	-3.04825400	1.43230100	0.98824700
C	-2.61607600	0.72138700	2.12383800
C	-0.74122300	2.30640000	2.41928800
C	1.18571400	3.02467100	1.25918900
C	2.34165900	2.60964200	0.54198800
C	2.32982600	2.60823700	-0.89885900
C	1.18422200	3.02968300	-1.60272800
C	0.73180300	2.30242700	-2.76379200
C	-0.73180300	2.30242700	-2.76379200
C	-1.42492600	1.16869000	-3.20799900
C	-2.60900800	0.72643600	-2.48013700
C	-3.50430000	-0.69774800	-0.18580300
C	-3.05100900	-1.42964400	-1.35859800
C	-2.60900800	-0.72643600	-2.48013700
C	-1.42492600	-1.16869000	-3.20799900
C	-0.70660200	0.00000000	-3.66450200
C	0.70660200	0.00000000	-3.66450200
C	1.42492600	1.16869000	-3.20799900
C	2.60900800	0.72643600	-2.48013700
C	3.05100900	1.42964400	-1.35859800
C	0.74122300	2.30640000	2.41928800
C	3.04825400	-1.43230100	0.98824700
C	2.61607600	-0.72138700	2.12383800
C	1.43455400	-1.16281900	2.87884600
C	0.74122300	-2.30640000	2.41928800
C	1.18571400	-3.02467100	1.25918900
C	2.32982600	-2.60823700	-0.89885900
C	3.05100900	-1.42964400	-1.35859800
C	3.50430000	-0.69774800	-0.18580300
C	3.50430000	0.69774800	-0.18580300
C	3.04825400	1.43230100	0.98824700
C	2.61607600	0.72138700	2.12383800
C	0.73109900	0.00000000	3.38243000

C	-0.73109900	0.00000000	3.38243000
C	-1.43455400	-1.16281900	2.87884600
C	-0.74122300	-2.30640000	2.41928800
C	-1.18571400	-3.02467100	1.25918900
C	0.00000000	-3.45211500	0.52771000
C	0.00000000	-3.45605700	-0.86914900
C	1.18422200	-3.02968300	-1.60272800
C	2.60900800	-0.72643600	-2.48013700
C	1.42492600	-1.16869000	-3.20799900
C	0.73180300	-2.30242700	-2.76379200
C	-0.73180300	-2.30242700	-2.76379200
C	-1.18422200	-3.02968300	-1.60272800
C	-2.32982600	-2.60823700	-0.89885900
C	-2.34165900	-2.60964200	0.54198800
C	-3.04825400	-1.43230100	0.98824700
C	-2.61607600	-0.72138700	2.12383800
C	1.43455400	1.16281900	2.87884600
C	-1.43455400	1.16281900	2.87884600
C	2.34165900	-2.60964200	0.54198800
Tm	0.00000000	0.00000000	0.90374800

Yb@C₆₀_66_bond

B3LYP/CEP121G Etot = -2533.71386488 Hartree/Minimum_Frequency_Value = 35.48 cm-1/Spin_Multiplicity = 1/Point

Group = C2v

C	-2.32967700	2.60835800	-0.90496400
C	-2.34152800	2.60989400	0.53597700
C	-1.18600700	3.02564400	1.25328800
C	0.00000000	3.45268000	0.52182500
C	0.00000000	3.45654100	-0.87496600
C	-1.18412700	3.02969000	-1.60851700
C	-3.05073200	1.42960100	-1.36464500
C	-3.50383600	0.69771800	-0.19176100
C	-3.04798200	1.43271000	0.98197400
C	-2.61500000	0.72109600	2.11704500
C	-0.74116400	2.30617900	2.41233200
C	1.18600700	3.02564400	1.25328800
C	2.34152800	2.60989400	0.53597700
C	2.32967700	2.60835800	-0.90496400
C	1.18412700	3.02969000	-1.60851700
C	0.73167700	2.30240000	-2.76968500
C	-0.73167700	2.30240000	-2.76968500
C	-1.42491800	1.16880800	-3.21382800
C	-2.60875600	0.72651300	-2.48613700
C	-3.50383600	-0.69771800	-0.19176100

C	-3.05073200	-1.42960100	-1.36464500
C	-2.60875600	-0.72651300	-2.48613700
C	-1.42491800	-1.16880800	-3.21382800
C	-0.70635800	0.00000000	-3.67024400
C	0.70635800	0.00000000	-3.67024400
C	1.42491800	1.16880800	-3.21382800
C	2.60875600	0.72651300	-2.48613700
C	3.05073200	1.42960100	-1.36464500
C	0.74116400	2.30617900	2.41233200
C	3.04798200	-1.43271000	0.98197400
C	2.61500000	-0.72109600	2.11704500
C	1.43431600	-1.16294400	2.87330300
C	0.74116400	-2.30617900	2.41233200
C	1.18600700	-3.02564400	1.25328800
C	2.32967700	-2.60835800	-0.90496400
C	3.05073200	-1.42960100	-1.36464500
C	3.50383600	-0.69771800	-0.19176100
C	3.50383600	0.69771800	-0.19176100
C	3.04798200	1.43271000	0.98197400
C	2.61500000	0.72109600	2.11704500
C	0.73146300	0.00000000	3.37787200
C	-0.73146300	0.00000000	3.37787200
C	-1.43431600	-1.16294400	2.87330300
C	-0.74116400	-2.30617900	2.41233200
C	-1.18600700	-3.02564400	1.25328800
C	0.00000000	-3.45268000	0.52182500
C	0.00000000	-3.45654100	-0.87496600
C	1.18412700	-3.02969000	-1.60851700
C	2.60875600	-0.72651300	-2.48613700
C	1.42491800	-1.16880800	-3.21382800
C	0.73167700	-2.30240000	-2.76968500
C	-0.73167700	-2.30240000	-2.76968500
C	-1.18412700	-3.02969000	-1.60851700
C	-2.32967700	-2.60835800	-0.90496400
C	-2.34152800	-2.60989400	0.53597700
C	-3.04798200	-1.43271000	0.98197400
C	-2.61500000	-0.72109600	2.11704500
C	1.43431600	1.16294400	2.87330300
C	-1.43431600	1.16294400	2.87330300
C	2.34152800	-2.60989400	0.53597700
Yb	0.00000000	0.00000000	0.92172800

Lu@C₆₀_hexagon

B3LYP/CEP121G Etot = -2563.48484415 Hartree/Minimum_Frequency_Value = 31.92 cm⁻¹/Spin_Multiplicity = 2/Point

Group = CS

C	2.43181900	1.44381000	2.32325500
C	2.71005700	0.02784100	2.33792800
C	3.25797900	-0.59759900	1.18514200
C	3.54830200	0.20326700	0.00000000
C	3.28136400	1.57046900	0.00000000
C	2.71365400	2.21033500	1.18159700
C	1.18645100	1.67132100	3.04870200
C	0.69339500	0.38750400	3.50084300
C	1.63073400	-0.62088300	3.03613600
C	1.13728800	-1.86319600	2.57900500
C	2.77621200	-1.86591900	0.73705500
C	3.25797900	-0.59759900	-1.18514200
C	2.71005700	0.02784100	-2.33792800
C	2.43181900	1.44381000	-2.32325500
C	2.71365400	2.21033500	-1.18159700
C	1.78418000	3.21807300	-0.72807400
C	1.78418000	3.21807300	0.72807400
C	0.58587800	3.43833500	1.42742500
C	0.28713700	2.64606000	2.60289000
C	-0.68603200	0.11803000	3.49930300
C	-1.62282000	1.13695100	3.04427300
C	-1.14361800	2.36837100	2.60057500
C	-1.72010800	3.00420800	1.42405400
C	-0.65104400	3.66158200	0.70315800
C	-0.65104400	3.66158200	-0.70315800
C	0.58587800	3.43833500	-1.42742500
C	0.28713700	2.64606000	-2.60289000
C	1.18645100	1.67132100	-3.04870200
C	2.77621200	-1.86591900	-0.73705500
C	-1.18994100	-1.16009700	-3.05287000
C	-0.27894300	-2.15037100	-2.58898300
C	-0.57400200	-3.03114400	-1.45997800
C	-1.80447900	-2.78344900	-0.73916900
C	-2.68350800	-1.72345800	-1.17708400
C	-2.70215800	0.46923900	-2.32595200
C	-1.62282000	1.13695100	-3.04427300
C	-0.68603200	0.11803000	-3.49930300
C	0.69339500	0.38750400	-3.50084300
C	1.63073400	-0.62088300	-3.03613600
C	1.13728800	-1.86319600	-2.57900500
C	0.67927500	-3.30281100	-0.74220200
C	0.67927500	-3.30281100	0.74220200
C	-0.57400200	-3.03114400	1.45997800

C	-1.80447900	-2.78344900	0.73916900
C	-2.68350800	-1.72345800	1.17708400
C	-3.24348500	-1.08369100	0.00000000
C	-3.52970600	0.29033400	0.00000000
C	-3.25363800	1.08546000	-1.18227900
C	-1.14361800	2.36837100	-2.60057500
C	-1.72010800	3.00420800	-1.42405400
C	-2.75521600	2.36255200	-0.73097100
C	-2.75521600	2.36255200	0.73097100
C	-3.25363800	1.08546000	1.18227900
C	-2.70215800	0.46923900	2.32595200
C	-2.42957700	-0.94261400	2.34095900
C	-1.18994100	-1.16009700	3.05287000
C	-0.27894300	-2.15037100	2.58898300
C	1.71942200	-2.52915000	-1.42128800
C	1.71942200	-2.52915000	1.42128800
C	-2.42957700	-0.94261400	-2.34095900
Lu	-0.02140300	-1.21169100	0.00000000