Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

for

METALCARBONYL ANALOGUES OF ANNELATED CYCLOOCTATETRAENE AND CYCLODECAPENTAENE DERIVATIVES WITH A PLANAR CORE CYCLE: A QUANTUM CHEMICAL STUDY

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Table of contents: Atomic coordinates of optimized structures 15 – 17, 22, 25, 26 calculated by B3LYP/6-311+G(df,p), PBE0/6-311+G(df,p) and wB97XD/6-311+G(df,p) methods:

15 [B3LYP/6-311+G(df,p)]

D_4

C	-1.627506000	0.666003000	-0.008121000
C	-1.632799000	-0.653078000	0.005412000
C	-0.665988000	-1.627433000	-0.007934000
C	0.653080000	-1.632717000	0.005238000
C	1.627522000	-0.665995000	-0.008110000
C	1.632809000	0.653087000	0.005393000
C	0.665998000	1.627440000	-0.007948000
C	-0.653071000	1.632731000	0.005215000
Cr	2.568567000	-2.588390000	-0.000048000
Cr	-2.588410000	-2.568534000	-0.000060000
Cr	2.588420000	2.568546000	-0.000090000
Cr	-2.568566000	2.588389000	-0.000036000
C	3.890426000	-1.472739000	-0.825971000
C	2.002459000	-3.082348000	-1.780829000
C	1.442111000	-3.901315000	0.825514000
C	3.064378000	-2.023432000	1.780592000
C	2.023490000	3.064419000	1.780550000
C	1.472771000	3.890423000	-0.825986000
C	3.901345000	1.442083000	0.825461000
C	3.082294000	2.002430000	-1.780883000
C	-1.442113000	3.901359000	0.825473000
C	-3.064271000	2.023397000	1.780623000
C	-3.890399000	1.472707000	-0.825947000
C	-2.002536000	3.082404000	-1.780826000
C	-2.023500000	-3.064346000	1.780606000
C	-3.901360000	-1.442055000	0.825433000
C	-1.472758000	-3.890445000	-0.825902000
C	-3.082239000	-2.002465000	-1.780881000
O	4.679962000	-0.837385000	-1.348588000
O	4.685915000	0.800222000	1.347613000
O	0.837421000	4.679964000	-1.348600000
O	-3.338849000	1.707865000	2.839622000
O	-0.800262000	4.685939000	1.347619000
O	-0.837407000	-4.680007000	-1.348483000
O	-3.355936000	-1.686564000	-2.840002000
O	-4.685955000	-0.800179000	1.347529000
O	3.339010000	-1.707928000	2.839586000
O	1.707956000	3.339096000	2.839523000
O	-1.707987000	-3.338988000	2.839593000
O	-1.686668000	3.356205000	-2.839929000
O	3.356010000	1.686519000	-2.839997000
O	-4.679932000	0.837327000	-1.348538000
O	1.686515000	-3.356116000	-2.839919000
O	0.800264000	-4.685878000	1.347694000
C	-3.922175000	3.951106000	0.001837000
C	3.951310000	3.921983000	0.001630000
C	3.922088000	-3.951195000	0.001719000
C	-3.951299000	-3.921973000	0.001678000
O	4.759329000	4.724576000	0.002710000
O	-4.759317000	-4.724568000	0.002767000
O	-4.724925000	4.758970000	0.002962000
O	4.724771000	-4.759126000	0.002767000

15[PBE0/6-311+G(df,p)]

D_4

C	-0.687936000	-1.620152000	0.006820000
C	-1.620152000	-0.687936000	-0.006820000
C	-1.620152000	0.687936000	0.006820000
C	-0.687936000	1.620152000	-0.006820000
C	0.687936000	1.620152000	0.006820000
C	1.620152000	0.687936000	-0.006820000
C	1.620152000	-0.687936000	0.006820000
C	0.687936000	-1.620152000	-0.006820000
Cr	0.000000000	3.597928000	0.000000000
Cr	-3.597928000	0.000000000	0.000000000
Cr	3.597928000	0.000000000	0.000000000
Cr	0.000000000	-3.597928000	0.000000000
C	1.701091000	3.721088000	0.811241000
C	-0.733910000	3.543763000	1.757805000
C	-1.701091000	3.721088000	-0.811241000
C	0.733910000	3.543763000	-1.757805000
C	3.543763000	-0.733910000	-1.757805000
C	3.721088000	-1.701091000	0.811241000
C	3.721088000	1.701091000	-0.811241000
C	3.543763000	0.733910000	1.757805000
C	1.701091000	-3.721088000	-0.811241000
C	-0.733910000	-3.543763000	-1.757805000
C	-1.701091000	-3.721088000	0.811241000
C	0.733910000	-3.543763000	1.757805000
C	-3.543763000	0.733910000	-1.757805000
C	-3.721088000	-1.701091000	-0.811241000
C	-3.721088000	1.701091000	0.811241000
C	-3.543763000	-0.733910000	1.757805000
O	2.709206000	3.807114000	1.333418000
O	3.807114000	2.709206000	-1.333418000
O	3.807114000	-2.709206000	1.333418000
O	-1.145971000	-3.507296000	-2.816311000
O	2.709206000	-3.807114000	-1.333418000
O	-3.807114000	2.709206000	1.333418000
O	-3.507296000	-1.145971000	2.816311000
O	-3.807114000	-2.709206000	-1.333418000
O	1.145971000	3.507296000	-2.816311000
O	3.507296000	-1.145971000	-2.816311000
O	-3.507296000	1.145971000	-2.816311000
O	1.145971000	-3.507296000	2.816311000
O	3.507296000	1.145971000	2.816311000
O	-2.709206000	-3.807114000	1.333418000
O	-1.145971000	3.507296000	2.816311000
O	-2.709206000	3.807114000	-1.333418000
C	0.000000000	-5.490932000	0.000000000
C	5.490932000	0.000000000	0.000000000
C	0.000000000	5.490932000	0.000000000
C	-5.490932000	0.000000000	0.000000000
O	6.627574000	0.000000000	0.000000000
O	-6.627574000	0.000000000	0.000000000
O	0.000000000	-6.627574000	0.000000000
O	0.000000000	6.627574000	0.000000000

15[wB97XD/6-311+G(df,p)]

D_4

C	-0.688740000	-1.617903000	0.007484000
C	-1.617903000	-0.688740000	-0.007484000
C	-1.617903000	0.688740000	0.007484000
C	-0.688740000	1.617903000	-0.007484000
C	0.688740000	1.617903000	0.007484000
C	1.617903000	0.688740000	-0.007484000
C	1.617903000	-0.688740000	0.007484000
C	0.688740000	-1.617903000	-0.007484000
Cr	0.000000000	3.597079000	0.000000000
Cr	-3.597079000	0.000000000	0.000000000
Cr	3.597079000	0.000000000	0.000000000
Cr	0.000000000	-3.597079000	0.000000000
C	1.720853000	3.730514000	0.803811000
C	-0.722934000	3.516550000	1.775975000
C	-1.720853000	3.730514000	-0.803811000
C	0.722934000	3.516550000	-1.775975000
C	3.516550000	-0.722934000	-1.775975000
C	3.730514000	-1.720853000	0.803811000
C	3.730514000	1.720853000	-0.803811000
C	3.516550000	0.722934000	1.775975000
C	1.720853000	-3.730514000	-0.803811000
C	-0.722934000	-3.516550000	-1.775975000
C	-1.720853000	-3.730514000	0.803811000
C	0.722934000	-3.516550000	1.775975000
C	-3.516550000	0.722934000	-1.775975000
C	-3.730514000	-1.720853000	-0.803811000
C	-3.730514000	1.720853000	0.803811000
C	-3.516550000	-0.722934000	1.775975000
O	2.729749000	3.810767000	1.321777000
O	3.810767000	2.729749000	-1.321777000
O	3.810767000	-2.729749000	1.321777000
O	-1.126132000	-3.444908000	-2.834245000
O	2.729749000	-3.810767000	-1.321777000
O	-3.810767000	2.729749000	1.321777000
O	-3.444908000	-1.126132000	2.834245000
O	-3.810767000	-2.729749000	-1.321777000
O	1.126132000	3.444908000	-2.834245000
O	3.444908000	-1.126132000	-2.834245000
O	-3.444908000	1.126132000	-2.834245000
O	1.126132000	-3.444908000	2.834245000
O	3.444908000	1.126132000	2.834245000
O	-2.729749000	-3.810767000	1.321777000
O	-1.126132000	3.444908000	2.834245000
O	-2.729749000	3.810767000	-1.321777000
C	0.000000000	-5.511069000	0.000000000
C	5.511069000	0.000000000	0.000000000
C	0.000000000	5.511069000	0.000000000
C	-5.511069000	0.000000000	0.000000000
O	6.645641000	0.000000000	0.000000000
O	-6.645641000	0.000000000	0.000000000
O	0.000000000	-6.645641000	0.000000000
O	0.000000000	6.645641000	0.000000000

16 [B3LYP/6-311+G(df,p)]
(the geometry with the help “stable=opt” procedure has been found)

C_s

C	-0.666233000	1.647527000	0.000000000
C	0.646789000	1.655230000	0.000000000
C	1.647567000	0.666179000	0.000000000
C	1.655243000	-0.646844000	0.000000000
C	0.666191000	-1.647623000	0.000000000
C	-0.646832000	-1.655293000	0.000000000
C	-1.647611000	-0.666242000	0.000000000
C	-1.655316000	0.646781000	0.000000000
Fe	2.499769000	-2.470633000	0.000000000
Fe	2.470555000	2.499772000	0.000000000
Fe	-2.470604000	-2.499838000	0.000000000
Fe	-2.499796000	2.470582000	0.000000000
C	2.247034000	-4.280441000	0.000000000
C	2.384509000	-2.356301000	1.832625000
C	4.306602000	-2.197382000	0.000000000
C	2.384509000	-2.356301000	-1.832625000
C	-2.356178000	-2.384641000	-1.832621000
C	-4.280425000	-2.247139000	0.000000000
C	-2.197316000	-4.306657000	0.000000000
C	-2.356178000	-2.384641000	1.832621000
C	-4.306491000	2.196516000	0.000000000
C	-2.384143000	2.356610000	-1.832623000
C	-2.247865000	4.280517000	0.000000000
C	-2.384143000	2.356610000	1.832623000
C	2.356136000	2.384581000	-1.832626000
C	2.197256000	4.306590000	0.000000000
C	4.280376000	2.247065000	0.000000000
C	2.356136000	2.384581000	1.832626000
O	2.042858000	-5.400707000	0.000000000
O	-1.980557000	-5.424559000	0.000000000
O	-5.400686000	-2.042941000	0.000000000
O	-2.297687000	2.272083000	-2.961960000
O	-5.424270000	1.979135000	0.000000000
O	5.400635000	2.042855000	0.000000000
O	2.271225000	2.298433000	2.961957000
O	1.980480000	5.424488000	0.000000000
O	2.298648000	-2.270866000	-2.961939000
O	-2.271254000	-2.298479000	-2.961951000
O	2.271225000	2.298433000	-2.961957000
O	-2.297687000	2.272083000	2.961960000
O	-2.271254000	-2.298479000	2.961951000
O	-2.044286000	5.400893000	0.000000000
O	2.298648000	-2.270866000	2.961939000
O	5.424496000	-1.980588000	0.000000000

16 [PBE0/6-311+G(df,p)]
(the geometry with the help “stable=opt” procedure has been found)

D_{4h}

C	-0.656432000	1.650733000	0.000000000
C	0.656432000	1.650733000	0.000000000
C	1.650733000	0.656432000	0.000000000
C	1.650733000	-0.656432000	0.000000000
C	0.656432000	-1.650733000	0.000000000
C	-0.656432000	-1.650733000	0.000000000
C	-1.650733000	-0.656432000	0.000000000
C	-1.650733000	0.656432000	0.000000000
Fe	2.462826000	-2.462826000	0.000000000
Fe	2.462826000	2.462826000	0.000000000
Fe	-2.462826000	-2.462826000	0.000000000
Fe	-2.462826000	2.462826000	0.000000000
C	2.198872000	-4.245735000	0.000000000
C	2.337042000	-2.337042000	1.806715000
C	4.245735000	-2.198872000	0.000000000
C	2.337042000	-2.337042000	-1.806715000
C	-2.337042000	-2.337042000	-1.806715000
C	-4.245735000	-2.198872000	0.000000000
C	-2.198872000	-4.245735000	0.000000000
C	-2.337042000	-2.337042000	1.806715000
C	-4.245735000	2.198872000	0.000000000
C	-2.337042000	2.337042000	-1.806715000
C	-2.198872000	4.245735000	0.000000000
C	-2.337042000	2.337042000	1.806715000
C	2.337042000	2.337042000	-1.806715000
C	2.198872000	4.245735000	0.000000000
C	4.245735000	2.198872000	0.000000000
C	2.337042000	2.337042000	1.806715000
O	1.983554000	-5.361600000	0.000000000
O	-1.983554000	-5.361600000	0.000000000
O	-5.361600000	-1.983554000	0.000000000
O	-2.236979000	2.236979000	-2.931514000
O	-5.361600000	1.983554000	0.000000000
O	5.361600000	1.983554000	0.000000000
O	2.236979000	2.236979000	2.931514000
O	1.983554000	5.361600000	0.000000000
O	2.236979000	-2.236979000	-2.931514000
O	-2.236979000	-2.236979000	-2.931514000
O	2.236979000	2.236979000	-2.931514000
O	-2.236979000	2.236979000	2.931514000
O	-2.236979000	-2.236979000	2.931514000
O	-1.983554000	5.361600000	0.000000000
O	2.236979000	-2.236979000	2.931514000
O	5.361600000	-1.983554000	0.000000000

16 [wB97XD/6-311+G(df,p)]

D_{4h}

C	-0.655386000	1.650190000	0.000000000
C	0.655386000	1.650190000	0.000000000
C	1.650190000	0.655386000	0.000000000
C	1.650190000	-0.655386000	0.000000000
C	0.655386000	-1.650190000	0.000000000
C	-0.655386000	-1.650190000	0.000000000
C	-1.650190000	-0.655386000	0.000000000
C	-1.650190000	0.655386000	0.000000000
Fe	2.462099000	-2.462099000	0.000000000
Fe	2.462099000	2.462099000	0.000000000
Fe	-2.462099000	-2.462099000	0.000000000
Fe	-2.462099000	2.462099000	0.000000000
C	2.180985000	-4.259342000	0.000000000
C	2.324993000	-2.324993000	1.818933000
C	4.259342000	-2.180985000	0.000000000
C	2.324993000	-2.324993000	-1.818933000
C	-2.324993000	-2.324993000	-1.818933000
C	-4.259342000	-2.180985000	0.000000000
C	-2.180985000	-4.259342000	0.000000000
C	-2.324993000	-2.324993000	1.818933000
C	-4.259342000	2.180985000	0.000000000
C	-2.324993000	2.324993000	-1.818933000
C	-2.180985000	4.259342000	0.000000000
C	-2.324993000	2.324993000	1.818933000
C	2.324993000	2.324993000	-1.818933000
C	2.180985000	4.259342000	0.000000000
C	4.259342000	2.180985000	0.000000000
C	2.324993000	2.324993000	1.818933000
O	1.944099000	-5.368985000	0.000000000
O	-1.944099000	-5.368985000	0.000000000
O	-5.368985000	-1.944099000	0.000000000
O	-2.206703000	2.206703000	-2.938343000
O	-5.368985000	1.944099000	0.000000000
O	5.368985000	1.944099000	0.000000000
O	2.206703000	2.206703000	2.938343000
O	1.944099000	5.368985000	0.000000000
O	2.206703000	-2.206703000	-2.938343000
O	-2.206703000	-2.206703000	-2.938343000
O	2.206703000	2.206703000	-2.938343000
O	-2.206703000	2.206703000	2.938343000
O	-2.206703000	-2.206703000	2.938343000
O	-1.944099000	5.368985000	0.000000000
O	2.206703000	-2.206703000	2.938343000
O	5.368985000	-1.944099000	0.000000000

17 [B3LYP/6-311+G(df,p)]

C_{4h}

C	-1.479964000	0.879824000	0.000000000
C	-1.735728000	-0.405442000	0.000000000
C	-0.879824000	-1.479964000	0.000000000
C	0.405442000	-1.735728000	0.000000000
C	1.479964000	-0.879824000	0.000000000
C	1.735728000	0.405442000	0.000000000
C	0.879824000	1.479964000	0.000000000
C	-0.405442000	1.735728000	0.000000000
Ni	2.777948000	2.075744000	0.000000000
Ni	-2.075744000	2.777948000	0.000000000
Ni	-2.777948000	-2.075744000	0.000000000
Ni	2.075744000	-2.777948000	0.000000000
C	-3.129610000	2.646751000	1.543725000
C	-1.275339000	4.422437000	0.000000000
C	-3.129610000	2.646751000	-1.543725000
C	2.646751000	3.129610000	1.543725000
C	2.646751000	3.129610000	-1.543725000
C	4.422437000	1.275339000	0.000000000
C	3.129610000	-2.646751000	-1.543725000
C	1.275339000	-4.422437000	0.000000000
C	3.129610000	-2.646751000	1.543725000
C	-2.646751000	-3.129610000	-1.543725000
C	-2.646751000	-3.129610000	1.543725000
C	-4.422437000	-1.275339000	0.000000000
O	2.506128000	3.739219000	2.489751000
O	2.506128000	3.739219000	-2.489751000
O	5.396079000	0.691274000	0.000000000
O	-2.506128000	-3.739219000	2.489751000
O	-5.396079000	-0.691274000	0.000000000
O	-2.506128000	-3.739219000	-2.489751000
O	3.739219000	-2.506128000	2.489751000
O	-3.739219000	2.506128000	-2.489751000
O	-3.739219000	2.506128000	2.489751000
O	3.739219000	-2.506128000	-2.489751000
O	0.691274000	-5.396079000	0.000000000
O	-0.691274000	5.396079000	0.000000000

17 [PBE0/6-311+G(df,p)]
(the geometry with the help “stable=opt” procedure has been found)

S_4

C	0.669943000	1.620335000	0.014523000
C	1.620335000	0.669943000	-0.014523000
C	1.620335000	-0.669943000	-0.014523000
C	0.669943000	-1.620335000	0.014523000
C	-0.669943000	-1.620335000	0.014523000
C	-1.620335000	-0.669943000	-0.014523000
C	-1.620335000	0.669943000	-0.014523000
C	-0.669943000	1.620335000	0.014523000
Ni	-3.457797000	0.000000000	-0.031439000
Ni	0.000000000	3.457797000	0.031439000
Ni	3.457797000	0.000000000	-0.031439000
Ni	0.000000000	-3.457797000	0.031439000
C	1.471195000	4.155078000	-0.759264000
C	-1.471195000	4.155078000	-0.759264000
C	0.000000000	3.909910000	1.875791000
C	-3.909910000	0.000000000	-1.875791000
C	-4.155078000	1.471195000	0.759264000
C	-4.155078000	-1.471195000	0.759264000
C	0.000000000	-3.909910000	1.875791000
C	1.471195000	-4.155078000	-0.759264000
C	-1.471195000	-4.155078000	-0.759264000
C	4.155078000	-1.471195000	0.759264000
C	3.909910000	0.000000000	-1.875791000
C	4.155078000	1.471195000	0.759264000
O	-4.081361000	0.000000000	-2.993156000
O	-4.514922000	2.416994000	1.269999000
O	-4.514922000	-2.416994000	1.269999000
O	4.081361000	0.000000000	-2.993156000
O	4.514922000	2.416994000	1.269999000
O	4.514922000	-2.416994000	1.269999000
O	-2.416994000	-4.514922000	-1.269999000
O	0.000000000	4.081361000	2.993156000
O	2.416994000	4.514922000	-1.269999000
O	0.000000000	-4.081361000	2.993156000
O	2.416994000	-4.514922000	-1.269999000
O	-2.416994000	4.514922000	-1.269999000

17 [wB97XD/6-311+G(df,p)]
(the geometry with the help “stable=opt” procedure has been found)

S_4

C	1.644878000	-0.631635000	0.013502000
C	0.631685000	-1.644845000	-0.013473000
C	-0.631635000	-1.644878000	-0.013502000
C	-1.644845000	-0.631685000	0.013473000
C	-1.644878000	0.631635000	0.013502000
C	-0.631685000	1.644845000	-0.013473000
C	0.631635000	1.644878000	-0.013502000
C	1.644845000	0.631685000	0.013473000
Ni	-0.000043000	3.513397000	0.008637000
Ni	3.513397000	0.000043000	-0.008637000
Ni	0.000043000	-3.513397000	0.008637000
Ni	-3.513397000	-0.000043000	-0.008637000
C	4.253838000	-1.489235000	-0.751616000
C	4.253779000	1.489859000	-0.750537000
C	3.961623000	-0.000527000	1.917618000
C	0.000527000	3.961623000	-1.917618000
C	1.489235000	4.253838000	0.751616000
C	-1.489859000	4.253779000	0.750537000
C	-3.961623000	0.000527000	1.917618000
C	-4.253779000	-1.489859000	-0.750537000
C	-4.253838000	1.489235000	-0.751616000
C	-1.489235000	-4.253838000	0.751616000
C	-0.000527000	-3.961623000	-1.917618000
C	1.489859000	-4.253779000	0.750537000
O	0.000811000	4.060254000	-3.041548000
O	2.436770000	4.638661000	1.238052000
O	-2.437765000	4.638661000	1.236195000
O	-0.000811000	-4.060254000	-3.041548000
O	2.437765000	-4.638661000	1.236195000
O	-2.436770000	-4.638661000	1.238052000
O	-4.638661000	2.436770000	-1.238052000
O	4.060254000	-0.000811000	3.041548000
O	4.638661000	-2.436770000	-1.238052000
O	-4.060254000	0.000811000	3.041548000
O	-4.638661000	-2.437765000	-1.236195000
O	4.638661000	2.437765000	-1.236195000

22 [B3LYP/6-311+G(df,p)]

D_{4h}

C	0.645115000	1.659147000	0.000000000
C	1.659147000	0.645115000	0.000000000
C	1.659147000	-0.645115000	0.000000000
C	0.645115000	-1.659147000	0.000000000
C	-0.645115000	-1.659147000	0.000000000
C	-1.659147000	-0.645115000	0.000000000
C	-1.659147000	0.645115000	0.000000000
C	-0.645115000	1.659147000	0.000000000
Ni	0.000000000	-3.439168000	0.000000000
Ni	3.439168000	0.000000000	0.000000000
Ni	-3.439168000	0.000000000	0.000000000
Ni	0.000000000	3.439168000	0.000000000
C	-1.472564000	-4.495185000	0.000000000
C	1.472564000	-4.495185000	0.000000000
C	-4.495185000	1.472564000	0.000000000
C	-4.495185000	-1.472564000	0.000000000
C	-1.472564000	4.495185000	0.000000000
C	1.472564000	4.495185000	0.000000000
C	4.495185000	1.472564000	0.000000000
C	4.495185000	-1.472564000	0.000000000
O	-2.414822000	-5.128962000	0.000000000
O	-5.128962000	-2.414822000	0.000000000
O	-5.128962000	2.414822000	0.000000000
O	-2.414822000	5.128962000	0.000000000
O	5.128962000	-2.414822000	0.000000000
O	5.128962000	2.414822000	0.000000000
O	2.414822000	5.128962000	0.000000000
O	2.414822000	-5.128962000	0.000000000

22 [PBE0/6-311+G(df,p)]

D_{4h}

C	0.646227000	1.657913000	0.000000000
C	1.657913000	0.646227000	0.000000000
C	1.657913000	-0.646227000	0.000000000
C	0.646227000	-1.657913000	0.000000000
C	-0.646227000	-1.657913000	0.000000000
C	-1.657913000	-0.646227000	0.000000000
C	-1.657913000	0.646227000	0.000000000
C	-0.646227000	1.657913000	0.000000000
Ni	0.000000000	-3.413552000	0.000000000
Ni	3.413552000	0.000000000	0.000000000
Ni	-3.413552000	0.000000000	0.000000000
Ni	0.000000000	3.413552000	0.000000000
C	-1.464714000	-4.447246000	0.000000000
C	1.464714000	-4.447246000	0.000000000
C	-4.447246000	1.464714000	0.000000000
C	-4.447246000	-1.464714000	0.000000000
C	-1.464714000	4.447246000	0.000000000
C	1.464714000	4.447246000	0.000000000
C	4.447246000	1.464714000	0.000000000
C	4.447246000	-1.464714000	0.000000000
O	-2.414422000	-5.065541000	0.000000000
O	-5.065541000	-2.414422000	0.000000000
O	-5.065541000	2.414422000	0.000000000
O	-2.414422000	5.065541000	0.000000000
O	5.065541000	-2.414422000	0.000000000
O	5.065541000	2.414422000	0.000000000
O	2.414422000	5.065541000	0.000000000
O	2.414422000	-5.065541000	0.000000000

22[wB97XD/6-311+G(df,p)]

D_{4h}

C	0.642218000	1.658814000	0.000000000
C	1.658814000	0.642218000	0.000000000
C	1.658814000	-0.642218000	0.000000000
C	0.642218000	-1.658814000	0.000000000
C	-0.642218000	-1.658814000	0.000000000
C	-1.658814000	-0.642218000	0.000000000
C	-1.658814000	0.642218000	0.000000000
C	-0.642218000	1.658814000	0.000000000
Ni	0.000000000	-3.421834000	0.000000000
Ni	3.421834000	0.000000000	0.000000000
Ni	-3.421834000	0.000000000	0.000000000
Ni	0.000000000	3.421834000	0.000000000
C	-1.481686000	-4.454909000	0.000000000
C	1.481686000	-4.454909000	0.000000000
C	-4.454909000	1.481686000	0.000000000
C	-4.454909000	-1.481686000	0.000000000
C	-1.481686000	4.454909000	0.000000000
C	1.481686000	4.454909000	0.000000000
C	4.454909000	1.481686000	0.000000000
C	4.454909000	-1.481686000	0.000000000
O	-2.435616000	-5.063256000	0.000000000
O	-5.063256000	-2.435616000	0.000000000
O	-5.063256000	2.435616000	0.000000000
O	-2.435616000	5.063256000	0.000000000
O	5.063256000	-2.435616000	0.000000000
O	5.063256000	2.435616000	0.000000000
O	2.435616000	5.063256000	0.000000000
O	2.435616000	-5.063256000	0.000000000

25 [B3LYP/6-311+G(df,p)]

C_s

C	2.045239000	0.713409000	0.000000000
C	1.237625000	1.776226000	0.000000000
C	-0.047100000	2.164341000	0.000000000
C	-1.308105000	1.726516000	0.000000000
C	-2.074606000	0.624692000	0.000000000
C	-2.046288000	-0.709899000	0.000000000
C	-1.234453000	-1.778681000	0.000000000
C	0.043321000	-2.164693000	0.000000000
C	1.311094000	-1.724087000	0.000000000
C	2.073612000	-0.628425000	0.000000000
Fe	-1.315373000	3.781064000	0.000000000
Fe	-4.003222000	-0.083430000	0.000000000
Fe	3.188699000	2.420604000	0.000000000
Fe	3.287363000	-2.286399000	0.000000000
Fe	-1.157329000	-3.831921000	0.000000000
C	-0.336192000	5.315363000	0.000000000
C	-3.034347000	4.379701000	0.000000000
C	-1.268638000	3.645101000	1.833043000
C	-1.268638000	3.645101000	-1.833043000
C	3.073819000	2.333960000	-1.833007000
C	3.224972000	4.240271000	0.000000000
C	3.073819000	2.333960000	1.833007000
C	4.951168000	1.965687000	0.000000000
C	5.029700000	-1.759883000	0.000000000
C	-1.115247000	-3.694687000	-1.833115000
C	-0.117864000	-5.326161000	0.000000000
C	-2.851075000	-4.498648000	0.000000000
C	3.169866000	-2.203777000	1.833028000
C	-3.859251000	-0.080751000	-1.833018000
C	-5.102829000	-1.533888000	0.000000000
C	-3.859251000	-0.080751000	1.833018000
C	-5.160724000	1.321409000	0.000000000
C	3.169866000	-2.203777000	-1.833028000
C	3.395828000	-4.103164000	0.000000000
C	-1.115247000	-3.694687000	1.833115000
O	6.060477000	1.704860000	0.000000000
O	2.977025000	2.261157000	-2.963007000
O	3.273287000	5.378815000	0.000000000
O	6.127456000	-1.454007000	0.000000000
O	-5.811329000	-2.426438000	0.000000000
O	-3.738191000	-0.078458000	-2.963026000
O	-5.904191000	2.185028000	0.000000000
O	-3.738191000	-0.078458000	2.963026000
O	-3.902062000	-4.939118000	0.000000000
O	0.255692000	6.289147000	0.000000000
O	-4.101992000	4.778146000	0.000000000
O	3.488381000	-5.238953000	0.000000000
O	3.071290000	-2.134380000	-2.963086000
O	0.511634000	-6.276082000	0.000000000
O	-1.079891000	-3.579412000	-2.963176000
O	2.977025000	2.261157000	2.963007000
O	3.071290000	-2.134380000	2.963086000
O	-1.229162000	3.530610000	2.963045000
O	-1.229162000	3.530610000	-2.963045000
O	-1.079891000	-3.579412000	2.963176000

25 [PBE0/6-311+G(df,p)]

C_s

C	-0.696287000	2.052319000	0.000000000
C	-1.770099000	1.250775000	0.000000000
C	-2.167037000	-0.027884000	0.000000000
C	-1.736141000	-1.296680000	0.000000000
C	-0.642893000	-2.069500000	0.000000000
C	0.696978000	-2.052172000	0.000000000
C	1.769766000	-1.251153000	0.000000000
C	2.167153000	0.028560000	0.000000000
C	1.736810000	1.296323000	0.000000000
C	0.642436000	2.069516000	0.000000000
Fe	-3.755140000	-1.275107000	0.000000000
Fe	0.051851000	-3.965469000	0.000000000
Fe	-2.372675000	3.177830000	0.000000000
Fe	2.288590000	3.238696000	0.000000000
Fe	3.787550000	-1.175914000	0.000000000
C	-5.264124000	-0.301220000	0.000000000
C	-4.354083000	-2.968133000	0.000000000
C	-3.603157000	-1.222556000	1.808041000
C	-3.603157000	-1.222556000	-1.808041000
C	-2.276228000	3.049235000	-1.808028000
C	-4.167892000	3.226165000	0.000000000
C	-2.276228000	3.049235000	1.808028000
C	-1.911690000	4.913658000	0.000000000
C	1.778455000	4.960630000	0.000000000
C	3.633645000	-1.128844000	-1.808014000
C	5.268180000	-0.159607000	0.000000000
C	4.434961000	-2.851157000	0.000000000
C	2.196320000	3.107135000	1.807971000
C	0.049029000	-3.804761000	-1.808023000
C	1.475914000	-5.059618000	0.000000000
C	0.049029000	-3.804761000	1.808023000
C	-1.340857000	-5.099419000	0.000000000
C	2.196320000	3.107135000	-1.807971000
C	4.081899000	3.337893000	0.000000000
C	3.633645000	-1.128844000	1.808014000
O	-1.638849000	6.017703000	0.000000000
O	-2.190704000	2.935141000	-2.933373000
O	-5.304074000	3.275750000	0.000000000
O	1.473751000	6.056309000	0.000000000
O	2.365887000	-5.767636000	0.000000000
O	0.046567000	-3.662039000	-2.933354000
O	-2.210077000	-5.832774000	0.000000000
O	0.046567000	-3.662039000	2.933354000
O	4.863151000	-3.904728000	0.000000000
O	-6.229932000	0.299267000	0.000000000
O	-4.751277000	-4.033781000	0.000000000
O	5.216171000	3.420344000	0.000000000
O	2.114322000	2.990459000	-2.933315000
O	6.216373000	0.468323000	0.000000000
O	3.496883000	-1.086915000	-2.933304000
O	-2.190704000	2.935141000	2.933373000
O	2.114322000	2.990459000	2.933315000
O	-3.468167000	-1.175987000	2.933363000
O	-3.468167000	-1.175987000	-2.933363000
O	3.496883000	-1.086915000	2.933304000

25 [wB97XD/6-311+G(df,p)]

C_s

C	0.706586000	-2.044381000	0.000000000
C	1.771425000	-1.240316000	0.000000000
C	2.161739000	0.040197000	0.000000000
C	1.726881000	1.301679000	0.000000000
C	0.629892000	2.068885000	0.000000000
C	-0.704177000	2.044822000	0.000000000
C	-1.772732000	1.238376000	0.000000000
C	-2.161678000	-0.038080000	0.000000000
C	-1.725179000	-1.303575000	0.000000000
C	-0.631851000	-2.068415000	0.000000000
Fe	3.745458000	1.292566000	0.000000000
Fe	-0.072010000	3.962432000	0.000000000
Fe	2.387069000	-3.163335000	0.000000000
Fe	-2.270996000	-3.247511000	0.000000000
Fe	-3.789452000	1.155807000	0.000000000
C	5.270008000	0.312503000	0.000000000
C	4.339298000	3.004843000	0.000000000
C	3.580835000	1.235419000	1.821674000
C	3.580835000	1.235419000	-1.821674000
C	2.281861000	-3.024568000	-1.821714000
C	4.199097000	-3.198841000	0.000000000
C	2.281861000	-3.024568000	1.821714000
C	1.926182000	-4.916156000	0.000000000
C	-1.745585000	-4.982065000	0.000000000
C	-3.622651000	1.105263000	-1.821676000
C	-5.276330000	0.119460000	0.000000000
C	-4.446490000	2.844921000	0.000000000
C	-2.171340000	-3.104613000	1.821673000
C	-0.068431000	3.788188000	-1.821693000
C	-1.517397000	5.055883000	0.000000000
C	-0.068431000	3.788188000	1.821693000
C	1.330880000	5.110000000	0.000000000
C	-2.171340000	-3.104613000	-1.821673000
C	-4.080488000	-3.349928000	0.000000000
C	-3.622651000	1.105263000	1.821676000
O	1.653444000	-6.018439000	0.000000000
O	2.182294000	-2.893256000	-2.942141000
O	5.333943000	-3.237915000	0.000000000
O	-1.432080000	-6.073461000	0.000000000
O	-2.412778000	5.754232000	0.000000000
O	-0.065111000	3.623292000	-2.942103000
O	2.199014000	5.841951000	0.000000000
O	-0.065111000	3.623292000	2.942103000
O	-4.873838000	3.896960000	0.000000000
O	6.234497000	-0.286816000	0.000000000
O	4.726773000	4.072218000	0.000000000
O	-5.213101000	-3.431120000	0.000000000
O	-2.076978000	-2.969330000	-2.942086000
O	-6.217373000	-0.516034000	0.000000000
O	-3.464811000	1.057416000	-2.942083000
O	2.182294000	-2.893256000	2.942141000
O	-2.076978000	-2.969330000	2.942086000
O	3.425009000	1.181461000	2.942088000
O	3.425009000	1.181461000	-2.942088000
O	-3.464811000	1.057416000	2.942083000

26 [B3LYP/6-311+G(df,p)]

C_1

C	1.830604000	-1.083480000	0.012036000
C	2.134041000	0.182374000	0.012462000
C	1.595481000	1.405990000	-0.003652000
C	0.485417000	2.086261000	-0.010940000
C	-0.844327000	1.951154000	-0.003922000
C	-1.833342000	1.104561000	0.008160000
C	-2.114567000	-0.201787000	0.016413000
C	-1.617807000	-1.405186000	0.005213000
C	-0.462596000	-2.077656000	-0.012554000
C	0.835061000	-1.975053000	-0.008135000
Ni	2.059147000	3.395863000	-0.048258000
Ni	3.866788000	-0.907993000	0.070680000
Ni	0.332442000	-3.959355000	-0.072856000
Ni	-2.594929000	3.005450000	0.000128000
Ni	-3.661949000	-1.537314000	0.052086000
C	3.294691000	3.305600000	-1.433328000
C	1.101899000	4.924054000	-0.309820000
C	4.269017000	-1.696381000	-1.594147000
C	4.154361000	-2.082529000	1.483041000
C	5.022281000	0.478768000	0.316553000
C	2.016765000	-4.636027000	-0.227934000
C	-0.388627000	-4.610271000	1.536754000
C	-0.617116000	-4.564561000	-1.558886000
C	-3.797765000	-3.353424000	0.031812000
C	-4.566376000	-0.902704000	-1.456829000
C	-4.457638000	-0.958535000	1.647421000
C	-4.353283000	2.570124000	0.194126000
C	-2.171539000	4.149266000	1.405805000
C	-2.410781000	3.849793000	-1.674027000
C	2.900956000	3.534823000	1.634245000
O	5.728902000	1.353458000	0.481078000
O	4.487089000	-2.159202000	-2.606565000
O	4.305546000	-2.782428000	2.363988000
O	3.389108000	3.601464000	2.655910000
O	0.492227000	5.867068000	-0.484518000
O	-1.902898000	4.821128000	2.280477000
O	-5.445980000	2.284128000	0.319521000
O	-2.288972000	4.333467000	-2.692886000
O	-4.910310000	-0.609255000	2.627602000
O	-5.087439000	-0.511623000	-2.386138000
O	-3.869206000	-4.487626000	0.023127000
O	-0.821906000	-4.977927000	2.518642000
O	-1.184150000	-4.904054000	-2.481829000
O	3.071937000	-5.044404000	-0.334557000
O	4.027198000	3.231149000	-2.297482000

26 [PBE0/6-311+G(df,p)]

C_1

C	-0.590278000	-2.044754000	0.006984000
C	0.716343000	-2.020260000	-0.002238000
C	1.763591000	-1.193165000	-0.011286000
C	2.144634000	0.056883000	-0.003796000
C	1.682156000	1.308505000	0.010772000
C	0.610692000	2.056764000	0.008159000
C	-0.722633000	2.003533000	-0.006481000
C	-1.765043000	1.215223000	-0.008119000
C	-2.127521000	-0.068998000	0.002064000
C	-1.700362000	-1.304219000	0.008497000
Ni	3.762599000	-1.129059000	-0.039159000
Ni	0.088419000	-3.925906000	0.011149000
Ni	-3.706143000	-1.296795000	0.024096000
Ni	2.237112000	3.230319000	0.050330000
Ni	-2.379829000	3.124293000	-0.045518000
C	4.005301000	-2.119818000	-1.583005000
C	4.986257000	0.188611000	-0.057443000
C	-0.879080000	-4.512073000	-1.445213000
C	-0.681813000	-4.463181000	1.612155000
C	1.717158000	-4.682531000	-0.084750000
C	-3.915895000	-3.075112000	0.196461000
C	-4.572584000	-0.508900000	1.442802000
C	-4.450172000	-0.790389000	-1.604780000
C	-4.134475000	2.769352000	-0.223723000
C	-1.894818000	4.174027000	-1.475792000
C	-2.135863000	4.007766000	1.573476000
C	1.358442000	4.794834000	0.178156000
C	3.339119000	3.111212000	1.523435000
C	3.202449000	3.244583000	-1.534754000
C	4.050882000	-2.144020000	1.480216000
O	2.758201000	-5.128716000	-0.146453000
O	-1.478584000	-4.828010000	-2.353031000
O	-1.155996000	-4.748340000	2.599908000
O	4.184358000	-2.756994000	2.423234000
O	5.733682000	1.041721000	-0.072421000
O	3.991893000	3.004448000	2.443010000
O	0.775169000	5.763615000	0.266907000
O	3.771021000	3.213061000	-2.513539000
O	-1.957008000	4.515483000	2.569390000
O	-1.571580000	4.786248000	-2.372643000
O	-5.232471000	2.511367000	-0.344400000
O	-5.065788000	-0.008441000	2.331558000
O	-4.864252000	-0.464595000	-2.606704000
O	-4.015640000	-4.199197000	0.311218000
O	4.114573000	-2.714536000	-2.540524000

26 [wB97XD/6-311+G(df,p)]

C_1

C	-1.705405000	1.253178000	0.017625000
C	-2.128115000	0.031111000	-0.004389000
C	-1.714918000	-1.247312000	-0.028808000
C	-0.685020000	-2.027794000	-0.006824000
C	0.658284000	-2.032740000	0.039928000
C	1.717356000	-1.291935000	0.024861000
C	2.140720000	-0.017055000	-0.028071000
C	1.761002000	1.218995000	-0.032568000
C	0.679286000	2.016318000	0.003260000
C	-0.613683000	2.036745000	0.022611000
Ni	-2.357338000	-3.137501000	-0.124646000
Ni	-3.702818000	1.268226000	0.018830000
Ni	0.064378000	3.916965000	0.094182000
Ni	2.263370000	-3.217273000	0.190252000
Ni	3.756399000	1.154172000	-0.177131000
C	-3.212886000	-3.021296000	-1.800597000
C	-1.537222000	-4.750836000	-0.050326000
C	-3.881352000	2.707006000	-1.112257000
C	-4.016654000	1.809685000	1.824826000
C	-4.945682000	0.022539000	-0.422812000
C	-1.474816000	4.644367000	0.727728000
C	1.450697000	4.511206000	1.133877000
C	0.319835000	4.477483000	-1.720674000
C	3.948981000	2.859753000	-0.768110000
C	4.685792000	0.061577000	-1.322080000
C	4.463950000	1.012186000	1.593772000
C	4.013461000	-2.887474000	0.524072000
C	1.630138000	-4.252359000	1.588207000
C	2.095927000	-4.138881000	-1.455860000
C	-3.598234000	-3.014426000	1.255000000
O	-5.682185000	-0.790812000	-0.705362000
O	-3.922286000	3.582540000	-1.829039000
O	-4.139645000	2.118815000	2.904225000
O	-4.326609000	-2.874787000	2.109678000
O	-0.982191000	-5.738161000	-0.016722000
O	1.212926000	-4.832632000	2.465615000
O	5.092331000	-2.629236000	0.755352000
O	1.942592000	-4.650204000	-2.452197000
O	4.828074000	0.897109000	2.656872000
O	5.200045000	-0.632053000	-2.054458000
O	4.006297000	3.922255000	-1.157755000
O	2.315844000	4.812077000	1.799761000
O	0.478718000	4.746645000	-2.805940000
O	-2.454242000	5.037514000	1.140178000
O	-3.692215000	-2.900161000	-2.817207000