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Supporting Information

Fullerene Anions of Different Sizes and Shapes - A ^{13}C NMR and Density-Functional Study

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$C_{76}(1,D_2)$
Total energy -2895.95336 au

C 2.727319285 0.155806957 2.491846510
C 2.649557758 1.492607102 2.055429476
C 1.704456687 2.316505125 2.733657052
C 1.164735266 3.495687652 2.095713701
C 1.615418178 3.856378395 0.839968698
C 3.363021706 0.695812558 -0.235247614
C 3.049010971 1.802054966 0.682931554
C 2.596943633 3.032667736 0.143077867
C 3.178342313 0.914368010 -1.614859494
C 2.645894044 2.141615636 -2.125770958
C 2.359402961 3.192078181 -1.263661791
C 3.363021706 -0.695812558 0.235247614
C 3.049010971 -1.802054966 -0.682931554
C 3.178342313 -0.914368010 1.614859494
C 2.596943633 -3.032667736 -0.143077867
C -1.154379532 3.978872351 1.450723501
C -0.684881771 4.382066713 0.143668690
C -0.239572906 3.594866943 2.431658928
C 0.684881771 4.382066713 -0.143668690
C 1.154379532 3.978872351 -1.450723501
C -1.615418178 3.856378395 -0.839968698
C -1.164735266 3.495687652 -2.095713701
C 0.239572906 3.594866943 -2.431658928
C -1.743911528 1.816746752 3.212551948
C -2.645894044 2.141615636 2.125770958
C -0.539044790 2.494211064 3.323660286
C -2.359402961 3.192078181 1.263661791
C -2.596943633 3.032667736 -0.143077867
C -3.178342313 0.914368010 1.614859494
C -3.363021706 0.695812558 0.235247614
C -3.049010971 1.802054966 -0.682931554
C -2.649557758 1.492607102 -2.055429476
C -2.727319285 0.155806957 -2.491846510
C -1.704456687 2.316505125 -2.733657052
C -0.680399553 -1.735977549 3.551125151
C -0.647719577 -0.346492196 3.823871751
C -1.799616477 0.391674389 3.430326802
C -2.727319285 -0.155806957 2.491846510
C -2.649557758 -1.492607102 2.055429476
C -1.704456687 -2.316505125 2.733657052
C -1.615418178 -3.856378395 0.839968698

C -1.164735266 -3.495687652 2.095713701
C -3.178342313 -0.914368010 -1.614859494
C -3.363021706 -0.695812558 -0.235247614
C -3.049010971 -1.802054966 0.682931554
C -2.596943633 -3.032667736 0.143077867
C 0.647719577 0.346492196 3.823871751
C 0.680399553 1.735977549 3.551125151
C 0.539044790 -2.494211064 3.323660286
C 1.743911528 -1.816746752 3.212551948
C 1.799616477 -0.391674389 3.430326802
C 0.239572906 -3.594866943 2.431658928
C 2.645894044 -2.141615636 2.125770958
C 2.359402961 -3.192078181 1.263661791
C 1.154379532 -3.978872351 1.450723501
C -1.154379532 -3.978872351 -1.450723501
C -0.684881771 -4.382066713 -0.143668690
C 0.684881771 -4.382066713 0.143668690
C -0.239572906 -3.594866943 -2.431658928
C -1.743911528 -1.816746752 -3.212551948
C -2.645894044 -2.141615636 -2.125770958
C -2.359402961 -3.192078181 -1.263661791
C -0.539044790 -2.494211064 -3.323660286
C -0.680399553 1.735977549 -3.551125151
C -0.647719577 0.346492196 -3.823871751
C -1.799616477 -0.391674389 -3.430326802
C 1.799616477 0.391674389 -3.430326802
C 1.743911528 1.816746752 -3.212551948
C 0.539044790 2.494211064 -3.323660286
C 0.680399553 -1.735977549 -3.551125151
C 0.647719577 -0.346492196 -3.823871751
C 1.615418178 -3.856378395 -0.839968698
C 1.164735266 -3.495687652 -2.095713701
C 1.704456687 -2.316505125 -2.733657052
C 2.649557758 -1.492607102 -2.055429476
C 2.727319285 -0.155806957 -2.491846510

C_{76} (1,D_2) (2-)
Total energy -2896.01058 au

C	2.71571976	0.14156930	2.49430438
C	2.63784043	1.48166079	2.05796418
C	1.69835150	2.30892502	2.74470874
C	1.15635683	3.49152387	2.11261396
C	1.61987004	3.85432740	0.84860586
C	3.35924743	0.69146489	-0.23178662
C	3.03808650	1.79425922	0.68634347
C	2.58282373	3.03356850	0.15461097
C	3.17775302	0.92375120	-1.62491401
C	2.63429853	2.14223317	-2.12602298
C	2.34082492	3.20308428	-1.26623298
C	3.35924743	-0.69146489	0.23178662
C	3.03808650	-1.79425922	-0.68634347
C	3.17775302	-0.92375120	1.62491401
C	2.58282373	-3.03356850	-0.15461097
C	-1.16137409	3.99453480	1.45850995
C	-0.68485914	4.37301456	0.14717454
C	-0.23089637	3.61331270	2.46688541
C	0.68485914	4.37301456	-0.14717454
C	1.16137409	3.99453480	-1.45850995
C	-1.61987004	3.85432740	-0.84860586
C	-1.15635683	3.49152387	-2.11261396
C	0.23089637	3.61331270	-2.46688541
C	-1.73652705	1.82225417	3.22336953
C	-2.63429853	2.14223317	2.12602298
C	-0.53286838	2.51094971	3.34101784
C	-2.34082492	3.20308428	1.26623298
C	-2.58282373	3.03356850	-0.15461097
C	-3.17775302	0.92375120	1.62491401
C	-3.35924743	0.69146489	0.23178662
C	-3.03808650	1.79425922	-0.68634347
C	-2.63784043	1.48166079	-2.05796418
C	-2.71571976	0.14156930	-2.49430438
C	-1.69835150	2.30892502	-2.74470874
C	-0.68515360	-1.73568510	3.58565148
C	-0.64894726	-0.34838381	3.84908774
C	-1.79819010	0.40229052	3.45352901
C	-2.71571976	-0.14156930	2.49430438
C	-2.63784043	-1.48166079	2.05796418
C	-1.69835150	-2.30892502	2.74470874
C	-1.61987004	-3.85432740	0.84860586

C	-1.15635683	-3.49152387	2.11261396
C	-3.17775302	-0.92375120	-1.62491401
C	-3.35924743	-0.69146489	-0.23178662
C	-3.03808650	-1.79425922	0.68634347
C	-2.58282373	-3.03356850	0.15461097
C	0.64894726	0.34838381	3.84908774
C	0.68515360	1.73568510	3.58565148
C	0.53286838	-2.51094971	3.34101784
C	1.73652705	-1.82225417	3.22336953
C	1.79819010	-0.40229052	3.45352901
C	0.23089637	-3.61331270	2.46688541
C	2.63429853	-2.14223317	2.12602298
C	2.34082492	-3.20308428	1.26623298
C	1.16137409	-3.99453480	1.45850995
C	-1.16137409	-3.99453480	-1.45850995
C	-0.68485914	-4.37301456	-0.14717454
C	0.68485914	-4.37301456	0.14717454
C	-0.23089637	-3.61331270	-2.46688541
C	-1.73652705	-1.82225417	-3.22336953
C	-2.63429853	-2.14223317	-2.12602298
C	-2.34082492	-3.20308428	-1.26623298
C	-0.53286838	-2.51094971	-3.34101784
C	-0.68515360	1.73568510	-3.58565148
C	-0.64894726	0.34838381	-3.84908774
C	-1.79819010	-0.40229052	-3.45352901
C	1.79819010	0.40229052	-3.45352901
C	1.73652705	1.82225417	-3.22336953
C	0.53286838	2.51094971	-3.34101784
C	0.68515360	-1.73568510	-3.58565148
C	0.64894726	-0.34838381	-3.84908774
C	1.61987004	-3.85432740	-0.84860586
C	1.15635683	-3.49152387	-2.11261396
C	1.69835150	-2.30892502	-2.74470874
C	2.63784043	-1.48166079	-2.05796418
C	2.71571976	-0.14156930	-2.49430438

C_{76} (1,D_2) (4-)
Total energy -2895.63624 au

C	2.49167379	-0.14545037	2.74291809
C	2.05750929	-1.48256574	2.66709864
C	2.74543931	-2.32415504	1.72198099
C	2.09803486	-3.48516365	1.16043508
C	0.83432304	-3.86097489	1.61770976
C	-0.22860622	-0.69677539	3.38703694
C	0.68918038	-1.79580840	3.06747412
C	0.14921383	-3.04174129	2.60683166
C	-1.62210386	-0.92428732	3.19517306
C	-2.12313042	-2.14315115	2.63948840
C	-1.25685424	-3.20310027	2.35208480
C	0.22860622	0.69677539	3.38703694
C	-0.68918038	1.79580840	3.06747412
C	1.62210386	0.92428732	3.19517306
C	-0.14921383	3.04174129	2.60683166
C	1.44390594	-4.02102013	-1.16511843
C	0.15469544	-4.41912602	-0.70514376
C	2.46960139	-3.62253074	-0.23371973
C	-0.15469544	-4.41912602	0.70514376
C	-1.44390594	-4.02102013	1.16511843
C	-0.83432304	-3.86097489	-1.61770976
C	-2.09803486	-3.48516365	-1.16043508
C	-2.46960139	-3.62253074	0.23371973
C	3.23118115	-1.82454181	-1.75511026
C	2.12313042	-2.14315115	-2.63948840
C	3.32884671	-2.52335159	-0.53319218
C	1.25685424	-3.20310027	-2.35208480
C	-0.14921383	-3.04174129	-2.60683166
C	1.62210386	-0.92428732	-3.19517306
C	0.22860622	-0.69677539	-3.38703694
C	-0.68918038	-1.79580840	-3.06747412
C	-2.05750929	-1.48256574	-2.66709864
C	-2.49167379	-0.14545037	-2.74291809
C	-2.74543931	-2.32415504	-1.72198099
C	3.55234915	1.73594135	-0.68681828
C	3.82405578	0.34801215	-0.64874117
C	3.44779309	-0.41064275	-1.81040627
C	2.49167379	0.14545037	-2.74291809
C	2.05750929	1.48256574	-2.66709864
C	2.74543931	2.32415504	-1.72198099
C	0.83432304	3.86097489	-1.61770976

C	2.09803486	3.48516365	-1.16043508
C	-1.62210386	0.92428732	-3.19517306
C	-0.22860622	0.69677539	-3.38703694
C	0.68918038	1.79580840	-3.06747412
C	0.14921383	3.04174129	-2.60683166
C	3.82405578	-0.34801215	0.64874117
C	3.55234915	-1.73594135	0.68681828
C	3.32884671	2.52335159	0.53319218
C	3.23118115	1.82454181	1.75511026
C	3.44779309	0.41064275	1.81040627
C	2.46960139	3.62253074	0.23371973
C	2.12313042	2.14315115	2.63948840
C	1.25685424	3.20310027	2.35208480
C	1.44390594	4.02102013	1.16511843
C	-1.44390594	4.02102013	-1.16511843
C	-0.15469544	4.41912602	-0.70514376
C	0.15469544	4.41912602	0.70514376
C	-2.46960139	3.62253074	-0.23371973
C	-3.23118115	1.82454181	-1.75511026
C	-2.12313042	2.14315115	-2.63948840
C	-1.25685424	3.20310027	-2.35208480
C	-3.32884671	2.52335159	-0.53319218
C	-3.55234915	-1.73594135	-0.68681828
C	-3.82405578	-0.34801215	-0.64874117
C	-3.44779309	0.41064275	-1.81040627
C	-3.44779309	-0.41064275	1.81040627
C	-3.23118115	-1.82454181	1.75511026
C	-3.32884671	-2.52335159	0.53319218
C	-3.55234915	1.73594135	0.68681828
C	-3.82405578	0.34801215	0.64874117
C	-0.83432304	3.86097489	1.61770976
C	-2.09803486	3.48516365	1.16043508
C	-2.74543931	2.32415504	1.72198099
C	-2.05750929	1.48256574	2.66709864
C	-2.49167379	0.14545037	2.74291809

C_{76} (1,D_2) (6-)
Total energy -2894.87553 au

C	2.78073433	0.14262628	2.50416636
C	2.68292957	1.48537158	2.05466160
C	1.75068726	2.33711020	2.74924348
C	1.18481076	3.48533483	2.09739602
C	1.63335965	3.86203583	0.82046333
C	3.39947848	0.69481123	-0.23209423
C	3.07891651	1.79478945	0.68251480
C	2.62478120	3.05816452	0.13514651
C	3.21173294	0.91539117	-1.64328208
C	2.62994975	2.14188766	-2.14491432
C	2.34443331	3.19902683	-1.27220431
C	3.39947848	-0.69481123	0.23209423
C	3.07891651	-1.79478945	-0.68251480
C	3.21173294	-0.91539117	1.64328208
C	2.62478120	-3.05816452	-0.13514651
C	-1.15445340	4.02217000	1.45785710
C	-0.70637189	4.42348923	0.16291765
C	-0.21430861	3.62030152	2.48201403
C	0.70637189	4.42348923	-0.16291765
C	1.15445340	4.02217000	-1.45785710
C	-1.63335965	3.86203583	-0.82046333
C	-1.18481076	3.48533483	-2.09739602
C	0.21430861	3.62030152	-2.48201403
C	-1.75435132	1.82593134	3.25431900
C	-2.62994975	2.14188766	2.14491432
C	-0.50817103	2.53233678	3.36014046
C	-2.34443331	3.19902683	1.27220431
C	-2.62478120	3.05816452	-0.13514651
C	-3.21173294	0.91539117	1.64328208
C	-3.39947848	0.69481123	0.23209423
C	-3.07891651	1.79478945	-0.68251480
C	-2.68292957	1.48537158	-2.05466160
C	-2.78073433	0.14262628	-2.50416636
C	-1.75068726	2.33711020	-2.74924348
C	-0.69613257	-1.74939083	3.56951939
C	-0.65250060	-0.34777481	3.82382081
C	-1.81542306	0.41742889	3.46246366
C	-2.78073433	-0.14262628	2.50416636
C	-2.68292957	-1.48537158	2.05466160
C	-1.75068726	-2.33711020	2.74924348
C	-1.63335965	-3.86203583	0.82046333

C	-1.18481076	-3.48533483	2.09739602
C	-3.21173294	-0.91539117	-1.64328208
C	-3.39947848	-0.69481123	-0.23209423
C	-3.07891651	-1.79478945	0.68251480
C	-2.62478120	-3.05816452	0.13514651
C	0.65250060	0.34777481	3.82382081
C	0.69613257	1.74939083	3.56951939
C	0.50817103	-2.53233678	3.36014046
C	1.75435132	-1.82593134	3.25431900
C	1.81542306	-0.41742889	3.46246366
C	0.21430861	-3.62030152	2.48201403
C	2.62994975	-2.14188766	2.14491432
C	2.34443331	-3.19902683	1.27220431
C	1.15445340	-4.02217000	1.45785710
C	-1.15445340	-4.02217000	-1.45785710
C	-0.70637189	-4.42348923	-0.16291765
C	0.70637189	-4.42348923	0.16291765
C	-0.21430861	-3.62030152	-2.48201403
C	-1.75435132	-1.82593134	-3.25431900
C	-2.62994975	-2.14188766	-2.14491432
C	-2.34443331	-3.19902683	-1.27220431
C	-0.50817103	-2.53233678	-3.36014046
C	-0.69613257	1.74939083	-3.56951939
C	-0.65250060	0.34777481	-3.82382081
C	-1.81542306	-0.41742889	-3.46246366
C	1.81542306	0.41742889	-3.46246366
C	1.75435132	1.82593134	-3.25431900
C	0.50817103	2.53233678	-3.36014046
C	0.69613257	-1.74939083	-3.56951939
C	0.65250060	-0.34777481	-3.82382081
C	1.63335965	-3.86203583	-0.82046333
C	1.18481076	-3.48533483	-2.09739602
C	1.75068726	-2.33711020	-2.74924348
C	2.68292957	-1.48537158	-2.05466160
C	2.78073433	-0.14262628	-2.50416636

$C_{78}(1,D_3)$
Total energy -2972.17052 au

C	-3.20208306	-1.17587829	1.52351867
C	-2.76711830	-1.01914213	2.86492933
C	-2.57192107	0.27625887	3.44554612
C	-3.53091321	0.02010837	0.73508387
C	-3.34561522	1.27454983	1.34964499
C	-2.84214462	1.40473290	2.68287315
C	-2.84214462	-1.40473290	-2.68287315
C	-3.34561522	-1.27454983	-1.34964499
C	-3.53091321	-0.02010837	-0.73508387
C	-2.57192107	-0.27625887	-3.44554612
C	-2.76711830	1.01914213	-2.86492933
C	-3.20208306	1.17587829	-1.52351867
C	-0.51102260	1.32611751	4.30846720
C	-0.76531832	2.47094083	3.44858687
C	-1.40028101	0.24754694	4.30830106
C	-1.92549054	2.52822923	2.70342946
C	-1.89965854	3.10691271	1.38835130
C	-0.67956344	3.57349374	0.81761530
C	-0.66100540	3.67371345	-0.58213525
C	-2.75495463	2.37526607	-0.81761530
C	-2.85102647	2.40930419	0.58213525
C	-1.74083606	3.19860891	-1.38835130
C	0.48575856	-1.33645240	4.30830106
C	1.40396275	-0.22050021	4.30846720
C	-0.89294016	-1.10561731	4.30846720
C	0.91452244	1.08890546	4.30830106
C	1.52520773	2.08921955	3.44554612
C	2.52255668	-0.57268531	3.44858687
C	3.15225601	0.40340911	2.70342946
C	2.63760669	1.75900299	2.68287315
C	0.58270106	3.36102442	1.52351867
C	0.50095617	2.90596581	2.86492933
C	2.77660014	2.26011286	1.34964499
C	1.78287096	3.04780635	0.73508387
C	-1.22676547	-2.93163834	2.70342946
C	0.20453793	-3.16373590	2.68287315
C	-1.75723837	-1.89825552	3.44858687
C	1.04671334	-2.36547842	3.44554612
C	2.26616213	-1.88682368	2.86492933
C	0.56901508	-3.53466269	1.34964499
C	1.74804225	-3.06791472	0.73508387

C	2.61938200	-2.18514613	1.52351867
C	3.43451808	-1.19822766	0.81761530
C	3.51203188	-1.26440926	-0.58213525
C	3.64049460	0.09169620	1.38835130
C	-2.85102647	-2.40930419	-0.58213525
C	-2.75495463	-2.37526607	0.81761530
C	-1.74083606	-3.19860891	1.38835130
C	-0.66100540	-3.67371345	0.58213525
C	-0.67956344	-3.57349374	-0.81761530
C	-1.89965854	-3.10691271	-1.38835130
C	-0.76531832	-2.47094083	-3.44858687
C	-1.92549054	-2.52822923	-2.70342946
C	2.77660014	-2.26011286	-1.34964499
C	1.78287096	-3.04780635	-0.73508387
C	0.58270106	-3.36102442	-1.52351867
C	0.50095617	-2.90596581	-2.86492933
C	3.15225601	-0.40340911	-2.70342946
C	2.63760669	-1.75900299	-2.68287315
C	1.52520773	-2.08921955	-3.44554612
C	2.52255668	0.57268531	-3.44858687
C	3.51203188	1.26440926	0.58213525
C	3.43451808	1.19822766	-0.81761530
C	3.64049460	-0.09169620	-1.38835130
C	0.20453793	3.16373590	-2.68287315
C	0.56901508	3.53466269	-1.34964499
C	1.74804225	3.06791472	-0.73508387
C	1.04671334	2.36547842	-3.44554612
C	2.26616213	1.88682368	-2.86492933
C	2.61938200	2.18514613	-1.52351867
C	-0.89294016	1.10561731	-4.30846720
C	-1.75723837	1.89825552	-3.44858687
C	-1.22676547	2.93163834	-2.70342946
C	0.48575856	1.33645240	-4.30830106
C	0.91452244	-1.08890546	-4.30830106
C	-0.51102260	-1.32611751	-4.30846720
C	-1.40028101	-0.24754694	-4.30830106
C	1.40396275	0.22050021	-4.30846720

$C_{78}(1,D_3)$ (2-)
Total energy -2972.25715 au

C	-2.85600765	1.86354239	-1.52331890
C	-0.18587122	-3.40514637	-1.52331890
C	3.04187887	1.54160398	-1.52331890
C	2.05051989	-2.72487396	1.52331890
C	1.33455013	3.13823929	1.52331890
C	-3.38507001	-0.41336533	1.52331890
C	-2.47310669	1.61335935	-2.88346090
C	-0.16065684	-2.94845289	-2.88346090
C	2.63376353	1.33509354	-2.88346090
C	1.77526980	-2.35957670	2.88346090
C	1.15581847	2.71721710	2.88346090
C	-2.93108827	-0.35764039	2.88346090
C	-2.56725982	0.29500146	-3.45170804
C	1.02815115	-2.37081296	-3.45170804
C	1.53910867	2.07581149	-3.45170804
C	0.46617001	-2.54175813	3.45170804
C	1.96814210	1.67459414	3.45170804
C	-2.43431212	0.86716399	3.45170804
C	-3.44155862	0.77539145	-0.73351324
C	1.04927061	-3.36817292	-0.73351324
C	2.39228801	2.59278147	-0.73351324
C	1.00400073	-3.38194325	0.73351324
C	2.42684841	2.56046177	0.73351324
C	-3.43084914	0.82148149	0.73351324
C	-3.55173900	-0.50322727	-1.34492223
C	2.21167710	-2.82428256	-1.34492223
C	1.34006190	3.32750983	-1.34492223
C	-0.26437628	-3.57745619	1.34492223
C	3.23035608	1.55977152	1.34492223
C	-2.96597980	2.01768467	1.34492223
C	-3.07583168	-0.74478807	-2.68785345
C	2.18292123	-2.29135434	-2.68785345
C	0.89291045	3.03614241	-2.68785345
C	-0.53724850	-3.11878404	2.68785345
C	2.96957046	1.09412117	2.68785345
C	-2.43232195	2.02466287	2.68785345
C	-0.78794592	-1.18655883	-4.31818387
C	1.42156305	-0.08910176	-4.31818387
C	-0.63361713	1.27566060	-4.31818387
C	-1.13115982	-0.86559695	4.31818387
C	1.31520886	-0.54681467	4.31818387

C	-0.18404904	1.41241162	4.31818387
C	-1.28488460	-2.25538232	-3.46464730
C	2.59566069	0.01494846	-3.46464730
C	-1.31077609	2.24043386	-3.46464730
C	-2.16432581	-1.43295905	3.46464730
C	2.32314184	-1.15788161	3.46464730
C	-0.15881603	2.59084066	3.46464730
C	-1.42207859	0.06103169	-4.32002264
C	0.65818430	-1.26207203	-4.32002264
C	0.76389429	1.20104034	-4.32002264
C	0.15607642	-1.41480477	4.32002264
C	1.14721866	0.84256852	4.32002264
C	-1.30329508	0.57223624	4.32002264
C	-2.43874381	-2.04161031	-2.70901655
C	2.98745830	-1.09120894	-2.70901655
C	-0.54871449	3.13281925	-2.70901655
C	-1.87380386	-2.56992279	2.70901655
C	3.16252035	-0.33780035	2.70901655
C	-1.28871650	2.90772314	2.70901655
C	-2.54576767	-2.60271311	-1.39765099
C	3.52689951	-0.90334292	-1.39765099
C	-0.98113183	3.50605603	-1.39765099
C	-2.42648518	-2.71426200	1.39765099
C	3.56386244	-0.74426681	1.39765099
C	-1.13737726	3.45852881	1.39765099
C	-1.46029551	-3.32385761	-0.82185767
C	3.60869288	0.39727580	-0.82185767
C	-2.14839738	2.92658181	-0.82185767
C	-3.21866465	-1.67949106	0.82185767
C	3.06381425	-1.94769982	0.82185767
C	0.15485040	3.62719089	0.82185767
C	-1.47241885	-3.43895789	0.58814247
C	3.71443432	0.44432682	0.58814247
C	-2.24201547	2.99463107	0.58814247
C	-3.33269540	-1.69929103	-0.58814247
C	3.13797690	-2.03655337	-0.58814247
C	0.19471850	3.73584440	-0.58814247

$C_{78}(1,D_3)$ (6-)
Total energy -2971.11172 au

C	-2.85854572	1.86422531	-1.52297596
C	-0.18519362	-3.40768586	-1.52297596
C	3.04373934	1.54346055	-1.52297596
C	2.05137115	-2.72736063	1.52297596
C	1.33627801	3.14021985	1.52297596
C	-3.38764917	-0.41285922	1.52297596
C	-2.47762296	1.61427308	-2.88939860
C	-0.15919002	-2.95282097	-2.88939860
C	2.63681298	1.33854788	-2.88939860
C	1.77648377	-2.36402169	2.88939860
C	1.15906096	2.72049092	2.88939860
C	-2.93554472	-0.35646923	2.88939860
C	-2.56907754	0.29107304	-3.46783513
C	1.03246213	-2.37042294	-3.46783513
C	1.53661542	2.07934990	-3.46783513
C	0.46237206	-2.54383471	3.46783513
C	1.97183945	1.67234330	3.46783513
C	-2.43421151	0.87149141	3.46783513
C	-3.46085162	0.78044484	-0.72894729
C	1.05454075	-3.38740784	-0.72894729
C	2.40631087	2.60696300	-0.72894729
C	1.01033409	-3.40085476	0.72894729
C	2.44005957	2.57540237	0.72894729
C	-3.45039366	0.82545239	0.72894729
C	-3.57707629	-0.51218548	-1.35670843
C	2.23210378	-2.84174619	-1.35670843
C	1.34497250	3.35393168	-1.35670843
C	-0.27161855	-3.60333624	1.35670843
C	3.25639000	1.56643956	1.35670843
C	-2.98477145	2.03689668	1.35670843
C	-3.09427398	-0.75602270	-2.68592283
C	2.20187185	-2.30170852	-2.68592283
C	0.89240213	3.05773122	-2.68592283
C	-0.54722357	-3.13793693	2.68592283
C	2.99114488	1.09505895	2.68592283
C	-2.44392131	2.04287798	2.68592283
C	-0.78851981	-1.20929851	-4.33850420
C	1.44154314	-0.07822893	-4.33850420
C	-0.65302333	1.28752744	-4.33850420
C	-1.15381010	-0.86769155	4.33850420
C	1.32834798	-0.56538308	4.33850420

C	-0.17453788	1.43307464	4.33850420
C	-1.28935563	-2.26451079	-3.49041572
C	2.60580169	0.01564066	-3.49041572
C	-1.31644606	2.24887013	-3.49041572
C	-2.17313456	-1.43803104	3.49041572
C	2.33193869	-1.16297422	3.49041572
C	-0.15880413	2.60100526	3.49041572
C	-1.44363017	0.07220752	-4.34847479
C	0.65928154	-1.28632416	-4.34847479
C	0.78434863	1.21411664	-4.34847479
C	0.16866966	-1.43556001	4.34847479
C	1.15889660	0.86385221	4.34847479
C	-1.32756626	0.57170779	4.34847479
C	-2.45777345	-2.06002878	-2.70922698
C	3.01292398	-1.09847986	-2.70922698
C	-0.55515053	3.15850863	-2.70922698
C	-1.89090734	-2.59014253	2.70922698
C	3.18858290	-0.34250253	2.70922698
C	-1.29767556	2.93264506	2.70922698
C	-2.57770289	-2.63732996	-1.41691032
C	3.57284619	-0.91369121	-1.41691032
C	-0.99514330	3.55102117	-1.41691032
C	-2.45888694	-2.74844256	1.41691032
C	3.60966455	-0.75523728	1.41691032
C	-1.15077761	3.50367984	1.41691032
C	-1.46874016	-3.34108213	-0.81656755
C	3.62783208	0.39857478	-0.81656755
C	-2.15909193	2.94250735	-0.81656755
C	-3.23528534	-1.68906964	0.81656755
C	3.08041988	-1.95730448	0.81656755
C	0.15486546	3.64637411	0.81656755
C	-1.48156621	-3.46327113	0.58827670
C	3.74006388	0.44856159	0.58827670
C	-2.25849767	3.01470954	0.58827670
C	-3.35634187	-1.71004520	-0.58827670
C	3.15911352	-2.05165473	-0.58827670
C	0.19722835	3.76169992	-0.58827670

$C_{78}(2,C_{2v})$
Total energy -2972.25680 au

C	4.27828472	0.72171060	1.15859503
C	3.44919499	1.15971989	2.26569079
C	4.23340222	1.41920434	-0.05747707
C	2.71637031	2.33149389	2.16449855
C	1.40418529	2.40369456	2.74538615
C	4.13512410	-0.70606768	-1.30510194
C	4.23340222	-1.41920434	-0.05747707
C	4.13512410	0.70606768	-1.30510194
C	4.27828472	-0.72171060	1.15859503
C	3.44919499	-1.15971989	2.26569079
C	3.41032926	-2.61530599	-0.17443226
C	2.71869374	-3.10246269	0.93323385
C	2.71637031	-2.33149389	2.16449855
C	2.83779051	0.00000000	2.87773412
C	1.47526697	0.00000000	3.31002986
C	0.73506435	1.26274996	3.26903620
C	1.16315254	-1.41850826	-3.41725652
C	2.35918229	-0.73835835	-3.04288151
C	3.23284723	-1.42643653	-2.16147344
C	1.46530150	-3.14115019	-1.63516376
C	0.71308439	-2.60470889	-2.71383721
C	2.78707570	-2.62890815	-1.46186152
C	2.35918229	0.73835835	-3.04288151
C	3.23284723	1.42643653	-2.16147344
C	0.00000000	-0.70591110	-3.83788466
C	0.00000000	0.70591110	-3.83788466
C	1.16315254	1.41850826	-3.41725652
C	-1.16315254	-1.41850826	-3.41725652
C	-2.35918229	-0.73835835	-3.04288151
C	-3.23284723	-1.42643653	-2.16147344
C	-1.46530150	-3.14115019	-1.63516376
C	-0.71308439	-2.60470889	-2.71383721
C	-2.78707570	-2.62890815	-1.46186152
C	-0.73673116	-3.68784182	-0.48510569
C	1.41183235	-3.67893660	0.76715796
C	0.73673116	-3.68784182	-0.48510569
C	-1.41183235	-3.67893660	0.76715796
C	0.71308439	2.60470889	-2.71383721
C	1.46530150	3.14115019	-1.63516376
C	2.78707570	2.62890815	-1.46186152
C	3.41032926	2.61530599	-0.17443226

C	2.71869374	3.10246269	0.93323385
C	-0.73673116	3.68784182	-0.48510569
C	0.73673116	3.68784182	-0.48510569
C	1.41183235	3.67893660	0.76715796
C	-1.41183235	3.67893660	0.76715796
C	-0.68153308	3.38754262	1.97605273
C	0.68153308	3.38754262	1.97605273
C	-0.71308439	2.60470889	-2.71383721
C	-2.78707570	2.62890815	-1.46186152
C	-1.46530150	3.14115019	-1.63516376
C	-2.35918229	0.73835835	-3.04288151
C	-1.16315254	1.41850826	-3.41725652
C	-3.23284723	1.42643653	-2.16147344
C	-4.23340222	1.41920434	-0.05747707
C	-3.41032926	2.61530599	-0.17443226
C	-2.71869374	3.10246269	0.93323385
C	-4.27828472	0.72171060	1.15859503
C	-4.23340222	-1.41920434	-0.05747707
C	-4.13512410	-0.70606768	-1.30510194
C	-4.13512410	0.70606768	-1.30510194
C	-4.27828472	-0.72171060	1.15859503
C	-2.71637031	-2.33149389	2.16449855
C	-2.71869374	-3.10246269	0.93323385
C	-3.41032926	-2.61530599	-0.17443226
C	-3.44919499	-1.15971989	2.26569079
C	0.68153308	-3.38754262	1.97605273
C	-1.40418529	-2.40369456	2.74538615
C	-0.68153308	-3.38754262	1.97605273
C	-2.71637031	2.33149389	2.16449855
C	-1.40418529	2.40369456	2.74538615
C	-0.73506435	1.26274996	3.26903620
C	-3.44919499	1.15971989	2.26569079
C	-2.83779051	0.00000000	2.87773412
C	-1.47526697	0.00000000	3.31002986
C	-0.73506435	-1.26274996	3.26903620
C	0.73506435	-1.26274996	3.26903620
C	1.40418529	-2.40369456	2.74538615

$C_{78}(2,C_{2v})$ (4-)
Total energy -2971.87660 au

C	0.72896128	4.26194989	-1.17848922
C	1.16794359	3.45247480	-2.28218217
C	1.42396412	4.22581903	0.05199632
C	2.35362691	2.70133705	-2.19011762
C	2.44817250	1.42362524	-2.78465257
C	-0.70843596	4.12775912	1.29533512
C	-1.42396412	4.22581903	0.05199632
C	0.70843596	4.12775912	1.29533512
C	-0.72896128	4.26194989	-1.17848922
C	-1.16794359	3.45247480	-2.28218217
C	-2.61517959	3.39724892	0.17211342
C	-3.11186974	2.70197349	-0.93263187
C	-2.35362691	2.70133705	-2.19011762
C	0.00000000	2.82635499	-2.86947028
C	0.00000000	1.45545192	-3.30511158
C	1.27116164	0.72194524	-3.29578237
C	-1.42229944	1.16028419	3.44014991
C	-0.74029718	2.35739181	3.05178175
C	-1.42793400	3.22619259	2.16549681
C	-3.15293438	1.45914226	1.64905106
C	-2.61847816	0.71179604	2.74012310
C	-2.63229806	2.77852612	1.46710434
C	0.74029718	2.35739181	3.05178175
C	1.42793400	3.22619259	2.16549681
C	-0.71339914	0.00000000	3.87002726
C	0.71339914	0.00000000	3.87002726
C	1.42229944	1.16028419	3.44014991
C	-1.42229944	-1.16028419	3.44014991
C	-0.74029718	-2.35739181	3.05178175
C	-1.42793400	-3.22619259	2.16549681
C	-3.15293438	-1.45914226	1.64905106
C	-2.61847816	-0.71179604	2.74012310
C	-2.63229806	-2.77852612	1.46710434
C	-3.71547027	-0.73000603	0.50894040
C	-3.70421588	1.40930332	-0.76125902
C	-3.71547027	0.73000603	0.50894040
C	-3.70421588	-1.40930332	-0.76125902
C	2.61847816	0.71179604	2.74012310
C	3.15293438	1.45914226	1.64905106
C	2.63229806	2.77852612	1.46710434
C	2.61517959	3.39724892	0.17211342

C	3.11186974	2.70197349	-0.93263187
C	3.71547027	-0.73000603	0.50894040
C	3.71547027	0.73000603	0.50894040
C	3.70421588	1.40930332	-0.76125902
C	3.70421588	-1.40930332	-0.76125902
C	3.39162741	-0.68205677	-1.96470008
C	3.39162741	0.68205677	-1.96470008
C	2.61847816	-0.71179604	2.74012310
C	2.63229806	-2.77852612	1.46710434
C	3.15293438	-1.45914226	1.64905106
C	0.74029718	-2.35739181	3.05178175
C	1.42229944	-1.16028419	3.44014991
C	1.42793400	-3.22619259	2.16549681
C	1.42396412	-4.22581903	0.05199632
C	2.61517959	-3.39724892	0.17211342
C	3.11186974	-2.70197349	-0.93263187
C	0.72896128	-4.26194989	-1.17848922
C	-1.42396412	-4.22581903	0.05199632
C	-0.70843596	-4.12775912	1.29533512
C	0.70843596	-4.12775912	1.29533512
C	-0.72896128	-4.26194989	-1.17848922
C	-2.35362691	-2.70133705	-2.19011762
C	-3.11186974	-2.70197349	-0.93263187
C	-2.61517959	-3.39724892	0.17211342
C	-1.16794359	-3.45247480	-2.28218217
C	-3.39162741	0.68205677	-1.96470008
C	-2.44817250	-1.42362524	-2.78465257
C	-3.39162741	-0.68205677	-1.96470008
C	2.35362691	-2.70133705	-2.19011762
C	2.44817250	-1.42362524	-2.78465257
C	1.27116164	-0.72194524	-3.29578237
C	1.16794359	-3.45247480	-2.28218217
C	0.00000000	-2.82635499	-2.86947028
C	0.00000000	-1.45545192	-3.30511158
C	-1.27116164	-0.72194524	-3.29578237
C	-1.27116164	0.72194524	-3.29578237
C	-2.44817250	1.42362524	-2.78465257

$C_{78}(2,C_{2v})$ (6-)
Total energy -2971.10453 au

C	4.29059623	0.72146737	1.19622571
C	3.45414659	1.16248957	2.28328785
C	4.25476347	1.44682829	-0.05204563
C	2.69755363	2.34786537	2.18767598
C	1.42300440	2.45049238	2.79656769
C	4.12373273	-0.70983172	-1.29295706
C	4.25476347	-1.44682829	-0.05204563
C	4.12373273	0.70983172	-1.29295706
C	4.29059623	-0.72146737	1.19622571
C	3.45414659	-1.16248957	2.28328785
C	3.43030518	-2.61754301	-0.17154146
C	2.70329865	-3.12214968	0.93343957
C	2.69755363	-2.34786537	2.18767598
C	2.83070857	0.00000000	2.89584217
C	1.46037997	0.00000000	3.33220955
C	0.71936419	1.27028633	3.32619116
C	1.16564229	-1.41919616	-3.46573384
C	2.36165011	-0.73522266	-3.07836431
C	3.23348334	-1.42847177	-2.17545792
C	1.45976347	-3.13978720	-1.64777428
C	0.71273459	-2.60796782	-2.74751234
C	2.78309093	-2.62142688	-1.00000000
C	2.36165011	0.73522266	-3.07836431
C	3.23348334	1.42847177	-2.17545792
C	0.00000000	-0.71297060	-3.90855711
C	0.00000000	0.71297060	-3.90855711
C	1.16564229	1.41919616	-3.46573384
C	-1.16564229	-1.41919616	-3.46573384
C	-2.36165011	-0.73522266	-3.07836431
C	-3.23348334	-1.42847177	-2.17545792
C	-1.45976347	-3.13978720	-1.64777428
C	-0.71273459	-2.60796782	-2.74751234
C	-2.78309093	-2.62142688	-1.47033623
C	-0.72429893	-3.72311601	-0.51587020
C	1.42768762	-3.72869287	0.76839381
C	0.72429893	-3.72311601	-0.51587020
C	-1.42768762	-3.72869287	0.76839381
C	0.71273459	2.60796782	-2.74751234
C	1.45976347	3.13978720	-1.64777428
C	2.78309093	2.62142688	-1.47033623
C	3.43030518	2.61754301	-0.17154146

C	2.70329865	3.12214968	0.93343957
C	-0.72429893	3.72311601	-0.51587020
C	0.72429893	3.72311601	-0.51587020
C	1.42768762	3.72869287	0.76839381
C	-1.42768762	3.72869287	0.76839381
C	-0.68286042	3.38509974	1.96606421
C	0.68286042	3.38509974	1.96606421
C	-0.71273459	2.60796782	-2.74751234
C	-2.78309093	2.62142688	-1.47033623
C	-1.45976347	3.13978720	-1.64777428
C	-2.36165011	0.73522266	-3.07836431
C	-1.16564229	1.41919616	-3.46573384
C	-3.23348334	1.42847177	-2.17545792
C	-4.25476347	1.44682829	-0.05204563
C	-3.43030518	2.61754301	-0.17154146
C	-2.70329865	3.12214968	0.93343957
C	-4.29059623	0.72146737	1.19622571
C	-4.25476347	-1.44682829	-0.05204563
C	-4.12373273	-0.70983172	-1.29295706
C	-4.12373273	0.70983172	-1.29295706
C	-4.29059623	-0.72146737	1.19622571
C	-2.69755363	-2.34786537	2.18767598
C	-2.70329865	-3.12214968	0.93343957
C	-3.43030518	-2.61754301	-0.17154146
C	-3.45414659	-1.16248957	2.28328785
C	0.68286042	-3.38509974	1.96606421
C	-1.42300440	-2.45049238	2.79656769
C	-0.68286042	-3.38509974	1.96606421
C	-2.69755363	2.34786537	2.18767598
C	-1.42300440	2.45049238	2.79656769
C	-0.71936419	1.27028633	3.32619116
C	-3.45414659	1.16248957	2.28328785
C	-2.83070857	0.00000000	2.89584217
C	-1.46037997	0.00000000	3.33220955
C	-0.71936419	-1.27028633	3.32619116
C	0.71936419	-1.27028633	3.32619116
C	1.42300440	-2.45049238	2.79656769

$C_{84}(22, D_2)$
Total energy -3200.87981 au

C	1.28402588	0.55406342	3.83156785
C	0.12543008	1.38348651	3.88925586
C	4.21912862	0.68298750	0.02563042
C	2.33897388	1.28502248	3.13865250
C	3.28760376	0.60700921	2.33791005
C	3.80676075	1.35442202	1.23881543
C	3.80936112	1.46697337	-1.12103373
C	3.24545651	0.85929176	-2.26999307
C	2.20188088	1.59204990	-2.99016633
C	1.19046880	0.84943118	-3.75220053
C	0.47051452	3.36507734	-2.61334354
C	3.31117112	2.70015689	-0.59155387
C	2.34532898	3.39692763	-1.28047494
C	1.83167677	2.87197974	-2.50915468
C	1.84039424	2.57201882	2.79268468
C	2.21264781	3.22886072	1.58548944
C	3.26634821	2.62178028	0.86185220
C	0.48089452	2.64324131	3.28488277
C	1.28082488	4.08344978	-0.56100468
C	1.19146119	3.99643597	0.85464503
C	0.12374774	4.07460232	-1.39170093
C	-1.28402588	-0.55406342	3.83156785
C	1.28402588	-0.55406342	-3.83156785
C	-1.28402588	0.55406342	-3.83156785
C	-0.12543008	-1.38348651	3.88925586
C	0.12543008	-1.38348651	-3.88925586
C	-0.12543008	1.38348651	-3.88925586
C	-4.21912862	-0.68298750	0.02563042
C	4.21912862	-0.68298750	-0.02563042
C	-4.21912862	0.68298750	-0.02563042
C	-2.33897388	-1.28502248	3.13865250
C	2.33897388	-1.28502248	-3.13865250
C	-2.33897388	1.28502248	-3.13865250
C	-3.28760376	-0.60700921	2.33791005
C	3.28760376	-0.60700921	-2.33791005
C	-3.28760376	0.60700921	-2.33791005
C	-3.80676075	-1.35442202	1.23881543
C	3.80676075	-1.35442202	-1.23881543
C	-3.80676075	1.35442202	-1.23881543
C	-3.80936112	-1.46697337	-1.12103373
C	3.80936112	-1.46697337	1.12103373

C	-3.80936112	1.46697337	1.12103373
C	-3.24545651	-0.85929176	-2.26999307
C	3.24545651	-0.85929176	2.26999307
C	-3.24545651	0.85929176	2.26999307
C	-2.20188088	-1.59204990	-2.99016633
C	2.20188088	-1.59204990	2.99016633
C	-2.20188088	1.59204990	2.99016633
C	-1.19046880	-0.84943118	-3.75220053
C	1.19046880	-0.84943118	3.75220053
C	-1.19046880	0.84943118	3.75220053
C	-0.47051452	-3.36507734	-2.61334354
C	0.47051452	-3.36507734	2.61334354
C	-0.47051452	3.36507734	2.61334354
C	-3.31117112	-2.70015689	-0.59155387
C	3.31117112	-2.70015689	0.59155387
C	-3.31117112	2.70015689	0.59155387
C	-2.34532898	-3.39692763	-1.28047494
C	2.34532898	-3.39692763	1.28047494
C	-2.34532898	3.39692763	1.28047494
C	-1.83167677	-2.87197974	-2.50915468
C	1.83167677	-2.87197974	2.50915468
C	-1.83167677	2.87197974	2.50915468
C	-1.84039424	-2.57201882	2.79268468
C	1.84039424	-2.57201882	-2.79268468
C	-1.84039424	2.57201882	-2.79268468
C	-2.21264781	-3.22886072	1.58548944
C	2.21264781	-3.22886072	-1.58548944
C	-2.21264781	3.22886072	-1.58548944
C	-3.26634821	-2.62178028	0.86185220
C	3.26634821	-2.62178028	-0.86185220
C	-3.26634821	2.62178028	-0.86185220
C	-0.48089452	-2.64324131	3.28488277
C	0.48089452	-2.64324131	-3.28488277
C	-0.48089452	2.64324131	-3.28488277
C	-1.28082488	-4.08344978	-0.56100468
C	1.28082488	-4.08344978	0.56100468
C	-1.28082488	4.08344978	0.56100468
C	-1.19146119	-3.99643597	0.85464503
C	1.19146119	-3.99643597	-0.85464503
C	-1.19146119	3.99643597	-0.85464503
C	-0.12374774	-4.07460232	-1.39170093
C	0.12374774	-4.07460232	1.39170093
C	-0.12374774	4.07460232	1.39170093

$C_{84}(22, D_2)$ (2-)
Total energy -3200.96839 au

C	1.29662924	0.54713710	3.83929137
C	0.12568090	1.39883308	3.90232569
C	4.22691413	0.68427017	0.03180896
C	2.33858004	1.26595507	3.15189823
C	3.29562468	0.59241671	2.34076686
C	3.81852396	1.34569184	1.25158550
C	3.82130170	1.47914544	-1.10985116
C	3.24805309	0.86864664	-2.26056539
C	2.19627171	1.60012123	-2.97551700
C	1.18884430	0.85472223	-3.74705325
C	0.47194327	3.38298956	-2.60876895
C	3.31912990	2.70454619	-0.57396303
C	2.34837475	3.41262099	-1.26060982
C	1.82621910	2.88259409	-2.49348903
C	1.83186889	2.55867171	2.80117111
C	2.20704503	3.21656125	1.59323057
C	3.27328985	2.61920104	0.87413818
C	0.47978244	2.64009451	3.30099588
C	1.29371775	4.09344001	-0.55220985
C	1.19051498	3.99343518	0.86012874
C	0.12590012	4.08543860	-1.40680910
C	-1.29662924	-0.54713710	3.83929137
C	1.29662924	-0.54713710	-3.83929137
C	-1.29662924	0.54713710	-3.83929137
C	-0.12568090	-1.39883308	3.90232569
C	0.12568090	-1.39883308	-3.90232569
C	-0.12568090	1.39883308	-3.90232569
C	-4.22691413	-0.68427017	0.03180896
C	4.22691413	-0.68427017	-0.03180896
C	-4.22691413	0.68427017	-0.03180896
C	-2.33858004	-1.26595507	3.15189823
C	2.33858004	-1.26595507	-3.15189823
C	-2.33858004	1.26595507	-3.15189823
C	-3.29562468	-0.59241671	2.34076686
C	3.29562468	-0.59241671	-2.34076686
C	-3.29562468	0.59241671	-2.34076686
C	-3.81852396	-1.34569184	1.25158550
C	3.81852396	-1.34569184	-1.25158550
C	-3.81852396	1.34569184	-1.25158550
C	-3.82130170	-1.47914544	-1.10985116
C	3.82130170	-1.47914544	1.10985116

C	-3.82130170	1.47914544	1.10985116
C	-3.24805309	-0.86864664	-2.26056539
C	3.24805309	-0.86864664	2.26056539
C	-3.24805309	0.86864664	2.26056539
C	-2.19627171	-1.60012123	-2.97551700
C	2.19627171	-1.60012123	2.97551700
C	-2.19627171	1.60012123	2.97551700
C	-1.18884430	-0.85472223	-3.74705325
C	1.18884430	-0.85472223	3.74705325
C	-1.18884430	0.85472223	3.74705325
C	-0.47194327	-3.38298956	-2.60876895
C	0.47194327	-3.38298956	2.60876895
C	-0.47194327	3.38298956	2.60876895
C	-3.31912990	-2.70454619	-0.57396303
C	3.31912990	-2.70454619	0.57396303
C	-3.31912990	2.70454619	0.57396303
C	-2.34837475	-3.41262099	-1.26060982
C	2.34837475	-3.41262099	1.26060982
C	-2.34837475	3.41262099	1.26060982
C	-1.82621910	-2.88259409	-2.49348903
C	1.82621910	-2.88259409	2.49348903
C	-1.82621910	2.88259409	2.49348903
C	-1.83186889	-2.55867171	2.80117111
C	1.83186889	-2.55867171	-2.80117111
C	-1.83186889	2.55867171	-2.80117111
C	-2.20704503	-3.21656125	1.59323057
C	2.20704503	-3.21656125	-1.59323057
C	-2.20704503	3.21656125	-1.59323057
C	-3.27328985	-2.61920104	0.87413818
C	3.27328985	-2.61920104	-0.87413818
C	-3.27328985	2.61920104	-0.87413818
C	-0.47978244	-2.64009451	3.30099588
C	0.47978244	-2.64009451	-3.30099588
C	-0.47978244	2.64009451	-3.30099588
C	-1.29371775	-4.09344001	-0.55220985
C	1.29371775	-4.09344001	0.55220985
C	-1.29371775	4.09344001	0.55220985
C	-1.19051498	-3.99343518	0.86012874
C	1.19051498	-3.99343518	-0.86012874
C	-1.19051498	3.99343518	-0.86012874
C	-0.12590012	-4.08543860	-1.40680910
C	0.12590012	-4.08543860	1.40680910
C	-0.12590012	4.08543860	1.40680910

C_{84}(22, D_2) (4-)
Total energy -3200.65739 au

C	1.30096856	0.55373845	3.84513978
C	0.11880217	1.40419985	3.89533833
C	4.22070313	0.69318347	0.02893519
C	2.32860953	1.26986621	3.16188664
C	3.28041969	0.59321804	2.33871364
C	3.80369413	1.34965789	1.24855323
C	3.82975996	1.48417752	-1.10181929
C	3.23870293	0.87247404	-2.26185661
C	2.20557156	1.60391722	-2.98310933
C	1.19591719	0.86010264	-3.73940361
C	0.49842416	3.40889070	-2.62418438
C	3.30839235	2.71190633	-0.56085497
C	2.34797729	3.42670727	-1.25752240
C	1.83557651	2.91492973	-2.50617160
C	1.82064580	2.58403480	2.81639632
C	2.19649462	3.23082291	1.60506544
C	3.27375307	2.64257146	0.88336231
C	0.46975726	2.65298481	3.30239630
C	1.29562942	4.11682874	-0.54856894
C	1.18210767	4.01210831	0.87004664
C	0.13525274	4.10823988	-1.40996873
C	-1.30096856	-0.55373845	3.84513978
C	1.30096856	-0.55373845	-3.84513978
C	-1.30096856	0.55373845	-3.84513978
C	-0.11880217	-1.40419985	3.89533833
C	0.11880217	-1.40419985	-3.89533833
C	-0.11880217	1.40419985	-3.89533833
C	-4.22070313	-0.69318347	0.02893519
C	4.22070313	-0.69318347	-0.02893519
C	-4.22070313	0.69318347	-0.02893519
C	-2.32860953	-1.26986621	3.16188664
C	2.32860953	-1.26986621	-3.16188664
C	-2.32860953	1.26986621	-3.16188664
C	-3.28041969	-0.59321804	2.33871364
C	3.28041969	-0.59321804	-2.33871364
C	-3.28041969	0.59321804	-2.33871364
C	-3.80369413	-1.34965789	1.24855323
C	3.80369413	-1.34965789	-1.24855323
C	-3.80369413	1.34965789	-1.24855323
C	-3.82975996	-1.48417752	-1.10181929
C	3.82975996	-1.48417752	1.10181929

C	-3.82975996	1.48417752	1.10181929
C	-3.23870293	-0.87247404	-2.26185661
C	3.23870293	-0.87247404	2.26185661
C	-3.23870293	0.87247404	2.26185661
C	-2.20557156	-1.60391722	-2.98310933
C	2.20557156	-1.60391722	2.98310933
C	-2.20557156	1.60391722	2.98310933
C	-1.19591719	-0.86010264	-3.73940361
C	1.19591719	-0.86010264	3.73940361
C	-1.19591719	0.86010264	3.73940361
C	-0.49842416	-3.40889070	-2.62418438
C	0.49842416	-3.40889070	2.62418438
C	-0.49842416	3.40889070	2.62418438
C	-3.30839235	-2.71190633	-0.56085497
C	3.30839235	-2.71190633	0.56085497
C	-3.30839235	2.71190633	0.56085497
C	-2.34797729	-3.42670727	-1.25752240
C	2.34797729	-3.42670727	1.25752240
C	-2.34797729	3.42670727	1.25752240
C	-1.83557651	-2.91492973	-2.50617160
C	1.83557651	-2.91492973	2.50617160
C	-1.83557651	2.91492973	2.50617160
C	-1.82064580	-2.58403480	2.81639632
C	1.82064580	-2.58403480	-2.81639632
C	-1.82064580	2.58403480	-2.81639632
C	-2.19649462	-3.23082291	1.60506544
C	2.19649462	-3.23082291	-1.60506544
C	-2.19649462	3.23082291	-1.60506544
C	-3.27375307	-2.64257146	0.88336231
C	3.27375307	-2.64257146	-0.88336231
C	-3.27375307	2.64257146	-0.88336231
C	-0.46975726	-2.65298481	3.30239630
C	0.46975726	-2.65298481	-3.30239630
C	-0.46975726	2.65298481	-3.30239630
C	-1.29562942	-4.11682874	-0.54856894
C	1.29562942	-4.11682874	0.54856894
C	-1.29562942	4.11682874	0.54856894
C	-1.18210767	-4.01210831	0.87004664
C	1.18210767	-4.01210831	-0.87004664
C	-1.18210767	4.01210831	-0.87004664
C	-0.13525274	-4.10823988	-1.40996873
C	0.13525274	-4.10823988	1.40996873
C	-0.13525274	4.10823988	1.40996873

C_{84}(22, D_2) (6-)
Total energy -3199.91102 eV

C	1.30722277	0.54714631	3.84125904
C	0.13095320	1.40718761	3.89500281
C	4.23373836	0.69897611	0.04142016
C	2.35117211	1.26113943	3.17229334
C	3.29337569	0.58493688	2.34573871
C	3.85292706	1.35054271	1.25748219
C	3.83158756	1.49795227	-1.09553079
C	3.24046491	0.87942798	-2.26158438
C	2.19674215	1.61365461	-2.97669332
C	1.19173560	0.87023124	-3.73998736
C	0.47951448	3.42222503	-2.62134166
C	3.32569989	2.72824686	-0.55967959
C	2.34094503	3.45008172	-1.25504281
C	1.82388177	2.92890684	-2.49978333
C	1.83954092	2.59039854	2.82955490
C	2.20648417	3.23010500	1.60210282
C	3.28418316	2.64326812	0.87752423
C	0.49391600	2.66083351	3.30905778
C	1.31096507	4.15384792	-0.55592820
C	1.18804717	4.01927066	0.86963362
C	0.12234687	4.13072827	-1.42073803
C	-1.30722277	-0.54714631	3.84125904
C	1.30722277	-0.54714631	-3.84125904
C	-1.30722277	0.54714631	-3.84125904
C	-0.13095320	-1.40718761	3.89500281
C	0.13095320	-1.40718761	-3.89500281
C	-0.13095320	1.40718761	-3.89500281
C	-4.23373836	-0.69897611	0.04142016
C	4.23373836	-0.69897611	-0.04142016
C	-4.23373836	0.69897611	-0.04142016
C	-2.35117211	-1.26113943	3.17229334
C	2.35117211	-1.26113943	-3.17229334
C	-2.35117211	1.26113943	-3.17229334
C	-3.29337569	-0.58493688	2.34573871
C	3.29337569	-0.58493688	-2.34573871
C	-3.29337569	0.58493688	-2.34573871
C	-3.85292706	-1.35054271	1.25748219
C	3.85292706	-1.35054271	-1.25748219
C	-3.85292706	1.35054271	-1.25748219
C	-3.83158756	-1.49795227	-1.09553079
C	3.83158756	-1.49795227	1.09553079

C	-3.83158756	1.49795227	1.09553079
C	-3.24046491	-0.87942798	-2.26158438
C	3.24046491	-0.87942798	2.26158438
C	-3.24046491	0.87942798	2.26158438
C	-2.19674215	-1.61365461	-2.97669332
C	2.19674215	-1.61365461	2.97669332
C	-2.19674215	1.61365461	2.97669332
C	-1.19173560	-0.87023124	-3.73998736
C	1.19173560	-0.87023124	3.73998736
C	-1.19173560	0.87023124	3.73998736
C	-0.47951448	-3.42222503	-2.62134166
C	0.47951448	-3.42222503	2.62134166
C	-0.47951448	3.42222503	2.62134166
C	-3.32569989	-2.72824686	-0.55967959
C	3.32569989	-2.72824686	0.55967959
C	-3.32569989	2.72824686	0.55967959
C	-2.34094503	-3.45008172	-1.25504281
C	2.34094503	-3.45008172	1.25504281
C	-2.34094503	3.45008172	1.25504281
C	-1.82388177	-2.92890684	-2.49978333
C	1.82388177	-2.92890684	2.49978333
C	-1.82388177	2.92890684	2.49978333
C	-1.83954092	-2.59039854	2.82955490
C	1.83954092	-2.59039854	-2.82955490
C	-1.83954092	2.59039854	-2.82955490
C	-2.20648417	-3.23010500	1.60210282
C	2.20648417	-3.23010500	-1.60210282
C	-2.20648417	3.23010500	-1.60210282
C	-3.28418316	-2.64326812	0.87752423
C	3.28418316	-2.64326812	-0.87752423
C	-3.28418316	2.64326812	-0.87752423
C	-0.49391600	-2.66083351	3.30905778
C	0.49391600	-2.66083351	-3.30905778
C	-0.49391600	2.66083351	-3.30905778
C	-1.31096507	-4.15384792	-0.55592820
C	1.31096507	-4.15384792	0.55592820
C	-1.31096507	4.15384792	0.55592820
C	-1.18804717	-4.01927066	0.86963362
C	1.18804717	-4.01927066	-0.86963362
C	-1.18804717	4.01927066	-0.86963362
C	-0.12234687	-4.13072827	-1.42073803
C	0.12234687	-4.13072827	1.42073803
C	-0.12234687	4.13072827	1.42073803

$C_{84}(23, D_{2d})$
Total energy -3200.88037 au

C 2.351831095 1.318975329 3.137132496
C 3.292610208 1.227270796 2.085997261
C 3.800336021 -0.081579801 1.833232602
C 3.253662004 2.218984192 1.003262451
C 1.837763419 0.167557215 3.793943301
C 3.250395064 -1.240767931 2.458498211
C 2.191606409 -1.151349533 3.393204578
C 3.298285215 -2.325462647 1.486688050
C 4.213532466 -0.465590500 0.500116221
C 3.806051657 -1.831708620 0.242935044
C 0.485021193 0.485021193 4.208289557
C 2.351831095 -1.318975329 -3.137132496
C 3.292610208 -1.227270796 -2.085997261
C 3.800336021 0.081579801 -1.833232602
C 3.253662004 -2.218984192 -1.003262451
C 1.837763419 -0.167557215 -3.793943301
C 3.250395064 1.240767931 -2.458498211
C 2.191606409 1.151349533 -3.393204578
C 3.298285215 2.325462647 -1.486688050
C 4.213532466 0.465590500 -0.500116221
C 3.806051657 1.831708620 -0.242935044
C 0.485021193 -0.485021193 -4.208289557
C 1.318975329 2.351831095 3.137132496
C 1.227270796 3.292610208 2.085997261
C -0.081579801 3.800336021 1.833232602
C 2.218984192 3.253662004 1.003262451
C 0.167557215 1.837763419 3.793943301
C -1.240767931 3.250395064 2.458498211
C -1.151349533 2.191606409 3.393204578
C -2.325462647 3.298285215 1.486688050
C -0.465590500 4.213532466 0.500116221
C -1.831708620 3.806051657 0.242935044
C -1.318975329 2.351831095 -3.137132496
C -1.227270796 3.292610208 -2.085997261
C 0.081579801 3.800336021 -1.833232602
C -2.218984192 3.253662004 -1.003262451
C -0.167557215 1.837763419 -3.793943301
C 1.240767931 3.250395064 -2.458498211
C 1.151349533 2.191606409 -3.393204578
C 2.325462647 3.298285215 -1.486688050
C 0.465590500 4.213532466 -0.500116221

C 1.831708620 3.806051657 -0.242935044
C -0.485021193 0.485021193 -4.208289557
C -1.318975329 -2.351831095 3.137132496
C -1.227270796 -3.292610208 2.085997261
C 0.081579801 -3.800336021 1.833232602
C -2.218984192 -3.253662004 1.003262451
C -0.167557215 -1.837763419 3.793943301
C 1.240767931 -3.250395064 2.458498211
C 1.151349533 -2.191606409 3.393204578
C 2.325462647 -3.298285215 1.486688050
C 0.465590500 -4.213532466 0.500116221
C 1.831708620 -3.806051657 0.242935044
C -0.485021193 -0.485021193 4.208289557
C 1.318975329 -2.351831095 -3.137132496
C 1.227270796 -3.292610208 -2.085997261
C -0.081579801 -3.800336021 -1.833232602
C 2.218984192 -3.253662004 -1.003262451
C 0.167557215 -1.837763419 -3.793943301
C -1.240767931 -3.250395064 -2.458498211
C -1.151349533 -2.191606409 -3.393204578
C -2.325462647 -3.298285215 -1.486688050
C -0.465590500 -4.213532466 -0.500116221
C -1.831708620 -3.806051657 -0.242935044
C -2.351831095 -1.318975329 3.137132496
C -3.292610208 -1.227270796 2.085997261
C -3.800336021 0.081579801 1.833232602
C -3.253662004 -2.218984192 1.003262451
C -1.837763419 -0.167557215 3.793943301
C -3.250395064 1.240767931 2.458498211
C -2.191606409 1.151349533 3.393204578
C -3.298285215 2.325462647 1.486688050
C -4.213532466 0.465590500 0.500116221
C -3.806051657 1.831708620 0.242935044
C -2.351831095 1.318975329 -3.137132496
C -3.292610208 1.227270796 -2.085997261
C -3.800336021 -0.081579801 -1.833232602
C -3.253662004 2.218984192 -1.003262451
C -1.837763419 0.167557215 -3.793943301
C -3.250395064 -1.240767931 -2.458498211
C -2.191606409 -1.151349533 -3.393204578
C -3.298285215 -2.325462647 -1.486688050
C -4.213532466 -0.465590500 -0.500116221
C -3.806051657 -1.831708620 -0.242935044

C_{84}(23, D_{2d}) (4-)
Total energy -3200.65909 au

C	2.36952798	1.36124135	3.14732377
C	3.30290727	1.24098594	2.07739659
C	3.82957657	-0.06524843	1.83836614
C	3.25281739	2.21576871	0.98013774
C	1.83042867	0.18710250	3.82221827
C	3.25885074	-1.24015906	2.48220456
C	2.17835027	-1.13249909	3.39664437
C	3.29984960	-2.31493515	1.52500893
C	4.22693492	-0.46184590	0.51887616
C	3.81273649	-1.82536410	0.27564830
C	0.50201685	0.50201685	4.24254228
C	2.36952798	-1.36124135	-3.14732377
C	3.30290727	-1.24098594	-2.07739659
C	3.82957657	0.06524843	-1.83836614
C	3.25281739	-2.21576871	-0.98013774
C	1.83042867	-0.18710250	-3.82221827
C	3.25885074	1.24015906	-2.48220456
C	2.17835027	1.13249909	-3.39664437
C	3.29984960	2.31493515	-1.52500893
C	4.22693492	0.46184590	-0.51887616
C	3.81273649	1.82536410	-0.27564830
C	0.50201685	-0.50201685	-4.24254228
C	1.36124135	2.36952798	3.14732377
C	1.24098594	3.30290727	2.07739659
C	-0.06524843	3.82957657	1.83836614
C	2.21576871	3.25281739	0.98013774
C	0.18710250	1.83042867	3.82221827
C	-1.24015906	3.25885074	2.48220456
C	-1.13249909	2.17835027	3.39664437
C	-2.31493515	3.29984960	1.52500893
C	-0.46184590	4.22693492	0.51887616
C	-1.82536410	3.81273649	0.27564830
C	-1.36124135	2.36952798	-3.14732377
C	-1.24098594	3.30290727	-2.07739659
C	0.06524843	3.82957657	-1.83836614
C	-2.21576871	3.25281739	-0.98013774
C	-0.18710250	1.83042867	-3.82221827
C	1.24015906	3.25885074	-2.48220456
C	1.13249909	2.17835027	-3.39664437
C	2.31493515	3.29984960	-1.52500893
C	0.46184590	4.22693492	-0.51887616

C	1.82536410	3.81273649	-0.27564830
C	-0.50201685	0.50201685	-4.24254228
C	-1.36124135	-2.36952798	3.14732377
C	-1.24098594	-3.30290727	2.07739659
C	0.06524843	-3.82957657	1.83836614
C	-2.21576871	-3.25281739	0.98013774
C	-0.18710250	-1.83042867	3.82221827
C	1.24015906	-3.25885074	2.48220456
C	1.13249909	-2.17835027	3.39664437
C	2.31493515	-3.29984960	1.52500893
C	0.46184590	-4.22693492	0.51887616
C	1.82536410	-3.81273649	0.27564830
C	-0.50201685	-0.50201685	4.24254228
C	1.36124135	-2.36952798	-3.14732377
C	1.24098594	-3.30290727	-2.07739659
C	-0.06524843	-3.82957657	-1.83836614
C	2.21576871	-3.25281739	-0.98013774
C	0.18710250	-1.83042867	-3.82221827
C	-1.24015906	-3.25885074	-2.48220456
C	-1.13249909	-2.17835027	-3.39664437
C	-2.31493515	-3.29984960	-1.52500893
C	-0.46184590	-4.22693492	-0.51887616
C	-1.82536410	-3.81273649	-0.27564830
C	-2.36952798	-1.36124135	3.14732377
C	-3.30290727	-1.24098594	2.07739659
C	-3.82957657	0.06524843	1.83836614
C	-3.25281739	-2.21576871	0.98013774
C	-1.83042867	-0.18710250	3.82221827
C	-3.25885074	1.24015906	2.48220456
C	-2.17835027	1.13249909	3.39664437
C	-3.29984960	2.31493515	1.52500893
C	-4.22693492	0.46184590	0.51887616
C	-3.81273649	1.82536410	0.27564830
C	-2.36952798	1.36124135	-3.14732377
C	-3.30290727	1.24098594	-2.07739659
C	-3.82957657	-0.06524843	-1.83836614
C	-3.25281739	2.21576871	-0.98013774
C	-1.83042867	0.18710250	-3.82221827
C	-3.25885074	-1.24015906	-2.48220456
C	-2.17835027	-1.13249909	-3.39664437
C	-3.29984960	-2.31493515	-1.52500893
C	-4.22693492	-0.46184590	-0.51887616
C	-3.81273649	-1.82536410	-0.27564830

$C_{84}(23, D_{2d})$ (6-)
Total energy -3199.91345 au

C	2.36832476	1.36054811	3.16480963
C	3.29600044	1.24026682	2.08156263
C	3.82285237	-0.07191379	1.84506055
C	3.25284375	2.22525003	0.99320865
C	1.83125472	0.18289962	3.84776891
C	3.26751517	-1.24459275	2.49792033
C	2.17754342	-1.13853318	3.42625987
C	3.29660817	-2.31014032	1.52876500
C	4.22589611	-0.47373640	0.51667025
C	3.84201698	-1.83233481	0.27717876
C	0.50318386	0.50318386	4.27947062
C	2.36832476	-1.36054811	-3.16480963
C	3.29600044	-1.24026682	-2.08156263
C	3.82285237	0.07191379	-1.84506055
C	3.25284375	-2.22525003	-0.99320865
C	1.83125472	-0.18289962	-3.84776891
C	3.26751517	1.24459275	-2.49792033
C	2.17754342	1.13853318	-3.42625987
C	3.29660817	2.31014032	-1.52876500
C	4.22589611	0.47373640	-0.51667025
C	3.84201698	1.83233481	-0.27717876
C	0.50318386	-0.50318386	-4.27947062
C	1.36054811	2.36832476	3.16480963
C	1.24026682	3.29600044	2.08156263
C	-0.07191379	3.82285237	1.84506055
C	2.22525003	3.25284375	0.99320865
C	0.18289962	1.83125472	3.84776891
C	-1.24459275	3.26751517	2.49792033
C	-1.13853318	2.17754342	3.42625987
C	-2.31014032	3.29660817	1.52876500
C	-0.47373640	4.22589611	0.51667025
C	-1.83233481	3.84201698	0.27717876
C	-1.36054811	2.36832476	-3.16480963
C	-1.24026682	3.29600044	-2.08156263
C	0.07191379	3.82285237	-1.84506055
C	-2.22525003	3.25284375	-0.99320865
C	-0.18289962	1.83125472	-3.84776891
C	1.24459275	3.26751517	-2.49792033
C	1.13853318	2.17754342	-3.42625987
C	2.31014032	3.29660817	-1.52876500
C	0.47373640	4.22589611	-0.51667025

C	1.83233481	3.84201698	-0.27717876
C	-0.50318386	0.50318386	-4.27947062
C	-1.36054811	-2.36832476	3.16480963
C	-1.24026682	-3.29600044	2.08156263
C	0.07191379	-3.82285237	1.84506055
C	-2.22525003	-3.25284375	0.99320865
C	-0.18289962	-1.83125472	3.84776891
C	1.24459275	-3.26751517	2.49792033
C	1.13853318	-2.17754342	3.42625987
C	2.31014032	-3.29660817	1.52876500
C	0.47373640	-4.22589611	0.51667025
C	1.83233481	-3.84201698	0.27717876
C	-0.50318386	-0.50318386	4.27947062
C	1.36054811	-2.36832476	-3.16480963
C	1.24026682	-3.29600044	-2.08156263
C	-0.07191379	-3.82285237	-1.84506055
C	2.22525003	-3.25284375	-0.99320865
C	0.18289962	-1.83125472	-3.84776891
C	-1.24459275	-3.26751517	-2.49792033
C	-1.13853318	-2.17754342	-3.42625987
C	-2.31014032	-3.29660817	-1.52876500
C	-0.47373640	-4.22589611	-0.51667025
C	-1.83233481	-3.84201698	-0.27717876
C	-2.36832476	-1.36054811	3.16480963
C	-3.29600044	-1.24026682	2.08156263
C	-3.82285237	0.07191379	1.84506055
C	-3.25284375	-2.22525003	0.99320865
C	-1.83125472	-0.18289962	3.84776891
C	-3.26751517	1.24459275	2.49792033
C	-2.17754342	1.13853318	3.42625987
C	-3.29660817	2.31014032	1.52876500
C	-4.22589611	0.47373640	0.51667025
C	-3.84201698	1.83233481	0.27717876
C	-2.36832476	1.36054811	-3.16480963
C	-3.29600044	1.24026682	-2.08156263
C	-3.82285237	-0.07191379	-1.84506055
C	-3.25284375	2.22525003	-0.99320865
C	-1.83125472	0.18289962	-3.84776891
C	-3.26751517	-1.24459275	-2.49792033
C	-2.17754342	-1.13853318	-3.42625987
C	-3.29660817	-2.31014032	-1.52876500
C	-4.22589611	-0.47373640	-0.51667025
C	-3.84201698	-1.83233481	-0.27717876