

Cartesian coordinates

BLYP Structures

Structure [Fe₂^S] Small (uBLYP)

Fe	1.624959000	0.223157000	-0.4944478000
Fe	-1.672533000	0.147604000	0.5320650000
S	1.735476000	2.359334000	-1.2605340000
S	-0.330213000	0.177101000	-1.698272000
N	3.429497000	0.351734000	0.3390870000
N	2.286625000	-1.665238000	-0.9121750000
C	3.935974000	1.423810000	1.044153000
C	5.234007000	1.392818000	1.575181000
H	5.592804000	2.261497000	2.1317420000
C	6.060075000	0.268053000	1.3909960000
H	7.069958000	0.239143000	1.808173000
C	5.558752000	-0.808282000	0.6615480000
H	6.170745000	-1.697757000	0.5059940000
C	4.245378000	-0.750839000	0.1424830000
C	3.633987000	-1.838992000	-0.615741000
C	4.354398000	-2.979984000	-1.0338890000
H	5.418438000	-3.065720000	-0.8100780000
C	3.706142000	-3.983431000	-1.7498240000
H	4.248190000	-4.868655000	-2.0921330000
C	2.332774000	-3.828287000	-2.0160360000
H	1.783390000	-4.603917000	-2.554511000
C	1.642741000	-2.682707000	-1.5916770000
C	2.780027000	3.427999000	-0.1095480000
C	3.075372000	2.652478000	1.2137990000
H	3.588904000	3.337348000	1.9140490000
H	2.113224000	2.370966000	1.6706990000
C	4.081515000	3.855693000	-0.8311630000
C	1.935769000	4.679300000	0.2482020000
C	-0.378929000	-1.424157000	-2.7073860000
C	0.146967000	-2.608121000	-1.8485910000
H	-0.394640000	-2.591388000	-0.8871020000
H	-0.138179000	-3.550283000	-2.3526050000
C	0.463004000	-1.213136000	-3.9898620000
C	-1.852325000	-1.706825000	-3.0909040000
S	-1.940424000	2.336707000	1.0704410000
S	0.278763000	0.377461000	1.7290770000
N	-3.478271000	0.050139000	-0.2973690000
N	-2.177696000	-1.735687000	1.1379390000
C	-4.066623000	1.001558000	-1.1048770000
C	-5.358253000	0.815593000	-1.6193020000
H	-5.783567000	1.591591000	-2.2596920000
C	-6.095261000	-0.343460000	-1.3115090000
H	-7.100947000	-0.492074000	-1.7130830000
C	-5.511542000	-1.297243000	-0.4799610000
H	-6.054113000	-2.209039000	-0.2270090000
C	-4.204976000	-1.087502000	0.0166500000
C	-3.506705000	-2.045590000	0.8696660000
C	-4.128948000	-3.200236000	1.3942630000
H	-5.182592000	-3.393424000	1.1889150000
C	-3.397139000	-4.080825000	2.1872950000
H	-3.862824000	-4.974743000	2.6099920000
C	-2.040079000	-3.791527000	2.4236090000
H	-1.425876000	-4.470199000	3.0199150000
C	-1.449661000	-2.633315000	1.8957830000
C	-3.074327000	3.195162000	-0.1686630000
C	-3.305996000	2.270681000	-1.4063920000
H	-2.324597000	2.022748000	-1.8416600000
H	-3.873151000	2.838805000	-2.1671110000
C	-4.406179000	3.577741000	0.5224220000
C	-2.339988000	4.472208000	-0.6532870000
C	0.454478000	-1.114809000	2.8813040000
C	0.034154000	-2.408999000	2.1291730000
H	0.567231000	-2.418561000	1.1630140000
H	0.404072000	-3.278457000	2.7037230000
C	-0.411808000	-0.860441000	4.1394600000
C	1.943621000	-1.236866000	3.2870420000
H	1.002418000	4.394508000	0.7583010000
H	2.510972000	5.354105000	0.9117470000
H	1.670407000	5.243147000	-0.6609190000
H	3.842872000	4.408856000	-1.7540740000
H	4.699377000	2.988051000	-1.1120530000
H	4.688843000	4.519528000	-0.1846490000
H	-2.969570000	5.027880000	-1.3754280000
H	-2.124345000	5.142963000	0.1943830000
H	-1.385443000	4.218964000	-1.1402020000
H	-4.946750000	2.690389000	0.8885510000
H	-4.213802000	4.233278000	1.3872860000
H	-5.069557000	4.124130000	-0.1767620000

H	0.457889000	-2.129048000	-4.611630000
H	1.508360000	-0.959673000	-3.754760000
H	0.046098000	-0.389144000	-4.590431000
H	-1.910837000	-2.591151000	-3.753345000
H	-2.470901000	-1.901077000	-2.2015020000
H	-2.287096000	-0.849667000	-3.6298870000
H	-0.339413000	-1.714970000	4.8395060000
H	-0.066171000	0.043116000	4.6663050000
H	-1.471892000	-0.712026000	3.8809560000
H	2.581953000	-1.458000000	2.4182490000
H	2.301627000	-0.300400000	3.7444030000
H	2.071604000	-2.048917000	4.0275860000

Structure [Fe₂⁰⁰] Small (uBLYP)

Fe	1.695182000	0.339906000	-0.669642000
Fe	-1.705799000	0.152479000	0.4310380000
S	1.407263000	2.549132000	-0.937416000
S	-0.406696000	0.212095000	-1.7745600000
S	-1.984474000	2.317385000	1.0788290000
S	0.351605000	0.350363000	1.4783620000
N	-3.531663000	0.067094000	-0.3237540000
N	-2.219142000	-1.723061000	1.0969700000
N	3.433885000	0.434424000	0.3044560000
N	2.232708000	-1.639082000	-0.9039090000
C	3.928292000	1.462894000	1.0623420000
C	5.233707000	1.407632000	1.5891830000
H	5.598205000	2.250569000	2.1802780000
C	6.045111000	0.288334000	1.3599650000
H	7.056866000	0.235769000	1.7708930000
C	5.528305000	-0.768118000	0.6059270000
H	6.127468000	-1.663093000	0.4372900000
C	4.223806000	-0.670938000	0.0794330000
C	3.585811000	-1.771392000	-0.6740060000
C	4.299602000	-2.925096000	-1.0701420000
H	5.371587000	-2.999793000	-0.8876210000
C	3.628369000	-3.949088000	-1.7336080000
H	4.163662000	-4.843093000	-2.0648760000
C	2.252490000	-3.806788000	-1.9735770000
H	1.695329000	-4.590441000	-2.4912280000
C	1.570165000	-2.648738000	-1.5563700000
C	2.619879000	3.517816000	0.1301320000
C	3.056564000	2.667160000	1.3578040000
H	3.618751000	3.323110000	2.0478450000
H	2.148397000	2.334246000	1.8873130000
C	3.828673000	3.946019000	-0.7392370000
C	1.859235000	4.768179000	0.6438240000
C	-0.465160000	-1.425480000	-2.7193100000
C	0.072096000	-2.570095000	-1.8080380000
H	-0.462485000	-2.502273000	-0.8473280000
H	-0.221677000	-3.533431000	-2.2648340000
C	0.343809000	-1.293412000	-4.0319250000
C	-1.946385000	-1.732721000	-3.0545070000
C	-4.135177000	1.028487000	-1.1086590000
C	-5.425343000	0.835450000	-1.6234060000
H	-5.861718000	1.617202000	-2.2491710000
C	-6.148595000	-0.337104000	-1.3332490000
H	-7.150664000	-0.493514000	-1.7406640000
C	-5.558020000	-1.290732000	-0.5060510000
H	-6.091268000	-2.210094000	-0.2603890000
C	-4.254370000	-1.072467000	-0.0064850000
C	-3.554731000	-2.021524000	0.8557820000
C	-4.185192000	-3.151803000	1.4219770000
H	-5.243864000	-3.337158000	1.2358410000
C	-3.455326000	-4.012483000	2.2386800000
H	-3.927847000	-4.884209000	2.6985660000
C	-2.091958000	-3.734157000	2.4502470000
H	-1.480452000	-4.401346000	3.0621020000
C	-1.491361000	-2.605945000	1.8702020000
C	-3.171179000	3.196395000	-0.0928920000
C	-3.396457000	2.319842000	-1.3691540000
H	-2.415581000	2.106745000	-1.8239880000
H	-3.980970000	2.909270000	-2.0997410000
C	-4.501636000	3.506276000	0.6361250000
C	-2.484212000	4.516441000	-0.5304940000
C	0.512320000	-1.096997000	2.6944880000
C	0.006662000	-2.417314000	2.0486910000
H	0.505863000	-2.523002000	1.0719860000
H	0.361100000	-3.258812000	2.6723960000
C	-0.305236000	-0.726102000	3.9573080000
C	2.003171000	-1.270819000	3.0712610000

H	0.991983000	4.484142000	1.260381000
H	2.533004000	5.402428000	1.251393000
H	1.493864000	5.374474000	-0.200962000
H	3.493364000	4.574502000	-1.579764000
H	4.358451000	3.077954000	-1.161116000
H	4.546841000	4.535486000	-0.136508000
H	-3.141353000	5.083133000	-1.218419000
H	-2.276471000	5.155123000	0.343526000
H	-1.529288000	4.314807000	-1.040264000
H	-5.003906000	2.587966000	0.979065000
H	-4.315140000	4.136809000	1.520662000
H	-5.196925000	4.053545000	-0.030545000
H	0.340451000	-2.256081000	-4.579222000
H	1.383391000	-0.995902000	-3.841507000
H	-0.110085000	-0.529221000	-4.683051000
H	-2.011810000	-2.641693000	-3.682232000
H	-2.545060000	-1.898243000	-2.145829000
H	-2.397642000	-0.899600000	-3.616850000
H	-0.261410000	-1.550151000	4.694857000
H	0.103340000	0.180504000	4.431050000
H	-1.362349000	-0.531534000	3.718018000
H	2.602635000	-1.596134000	2.208190000
H	2.426214000	-0.325786000	3.447367000
H	2.106412000	-2.030807000	3.864892000
O	3.830750000	0.031490000	-2.571660000
O	2.592981000	0.466858000	-2.463431000

Structure [Fe₂⁰⁰] Small (uBLYP)

Fe	2.101245000	0.260466000	0.353673000
Fe	-2.087757000	-0.263615000	0.130470000
O	0.636891000	-0.388582000	-0.551934000
O	-0.532866000	0.408106000	-0.595019000
S	-2.705478000	-0.742567000	2.217192000
S	-1.775846000	-2.504060000	-0.016380000
S	2.455028000	0.676266000	2.513357000
S	1.805796000	2.502833000	0.239146000
N	-3.066344000	0.058956000	-1.608579000
N	3.261876000	-0.007662000	-1.286764000
N	-2.448703000	1.734583000	0.346301000
N	2.450638000	-1.745124000	0.546240000
C	2.423067000	-0.920616000	3.517351000
C	3.866005000	-1.461445000	3.680222000
C	1.339261000	2.677433000	-2.557226000
C	4.145901000	-1.744597000	-2.756299000
H	4.282287000	-2.804372000	-2.972531000
C	1.845824000	-0.566911000	4.911667000
C	2.373565000	3.048036000	-1.466975000
C	4.524431000	0.571589000	-3.265832000
H	4.946396000	1.356475000	-3.897013000
C	4.676889000	-0.778992000	-3.611281000
C	5.213631000	-1.069277000	-4.518290000
C	3.766908000	2.419837000	-1.745142000
H	4.240847000	2.967333000	-2.581435000
H	4.398573000	2.590223000	-0.852915000
C	2.542754000	4.588490000	-1.400369000
C	2.936266000	-2.304012000	-0.610941000
C	2.064238000	-3.962980000	1.412700000
H	1.712597000	-4.587197000	2.236739000
C	3.447675000	-1.340794000	-1.599319000
C	2.976203000	-3.701768000	-0.799876000
H	3.341206000	-4.125344000	-1.736169000
C	2.532812000	-4.541454000	0.224286000
H	2.550339000	-5.627391000	0.099970000
C	2.016554000	-2.562970000	1.550965000
C	1.480003000	-1.951460000	2.828025000
H	1.277027000	-2.776683000	3.535014000
H	0.507838000	-1.470018000	2.619781000
C	3.826384000	0.943428000	-2.100480000
C	-2.771541000	0.820314000	3.273068000
C	-4.218942000	1.373799000	3.296162000
C	-1.063552000	-2.631418000	-2.764056000
C	-3.762608000	1.839802000	-3.124519000
H	-3.858898000	2.905853000	-3.331718000
C	-2.354835000	0.412667000	4.709517000
C	-2.197291000	-3.006111000	-1.778620000
C	-4.117491000	-0.459845000	-3.722291000
H	-4.481855000	-1.224448000	-4.411612000
C	-4.209959000	0.899982000	-4.053201000
H	-4.639365000	1.217243000	-5.007132000
C	-3.550919000	-2.349011000	-2.165929000
H	-3.958558000	-2.874392000	-3.049930000
H	-4.259960000	-2.522391000	-1.334618000
C	-2.395928000	-4.544434000	-1.761037000
C	-2.798003000	2.331704000	-0.840879000

C	-2.153076000	3.921695000	1.318690000
H	-1.894661000	4.518524000	2.195826000
C	-3.202441000	1.401244000	-1.906738000
C	-2.809773000	3.734608000	-0.990305000
H	-3.065925000	4.188934000	-1.948128000
C	-2.480465000	4.539194000	0.102866000
H	-2.478188000	5.628479000	0.010841000
C	-2.129677000	2.517872000	1.419354000
C	-1.748260000	1.862027000	2.729991000
H	-1.621265000	2.663332000	3.480956000
H	-0.762333000	1.376364000	2.620381000
C	-3.553664000	-0.866576000	-2.497656000
H	-4.276268000	2.281458000	3.927482000
H	-4.908457000	0.624413000	3.717563000
H	-4.578376000	1.630772000	2.287932000
H	-3.023871000	-0.369609000	5.103186000
H	-1.325945000	0.021658000	4.733349000
H	-2.408214000	1.284863000	5.388201000
H	-1.482747000	-5.047383000	-1.403571000
H	-2.617459000	-4.919049000	-2.778886000
H	-3.225057000	-4.834436000	-1.095100000
H	-0.832237000	-1.556753000	-2.729572000
H	-1.340975000	-2.903542000	-3.801801000
H	-0.141816000	-3.176141000	-2.504712000
H	4.496352000	-0.720959000	4.198681000
H	3.866503000	-2.390407000	4.282499000
H	4.334431000	-1.678630000	2.708073000
H	0.814549000	-0.189215000	4.835587000
H	1.838221000	-1.460632000	5.563951000
H	2.455898000	0.209593000	5.400877000
H	1.697864000	2.990615000	-3.557839000
H	1.137046000	1.596781000	-2.575540000
H	0.383130000	3.188149000	-2.361092000
H	1.592067000	5.068208000	-1.116419000
H	3.303237000	4.877322000	-0.656505000
H	2.848026000	4.988480000	-2.386346000

Structure [Fe₂⁽⁰⁾²] Small (uBLYP)

Fe	1.368473000	0.401530000	0.369690000
Fe	-1.356897000	-0.402562000	0.198713000
O	-0.023414000	0.055718000	-0.594085000
O	0.029262000	-0.075322000	1.433491000
S	-2.926053000	-0.853436000	1.951857000
S	-1.038415000	-2.678081000	0.331093000
S	2.905720000	0.860485000	2.064576000
S	1.064669000	2.714647000	0.420458000
N	2.271771000	-1.493890000	0.354847000
N	-2.248908000	1.489675000	0.267108000
N	2.669157000	0.455848000	-1.417847000
N	-2.647670000	-0.455576000	-1.511722000
C	2.956056000	-0.621892000	3.250422000
C	4.422606000	-1.108585000	3.367789000
C	0.408510000	3.142327000	-2.331922000
C	3.158522000	-1.089475000	-3.230578000
H	3.238909000	-2.117464000	-3.585970000
C	2.455336000	-0.120949000	4.630533000
C	1.482863000	3.439400000	-1.260511000
C	3.280851000	1.285491000	-3.600132000
H	3.480178000	2.147316000	-4.240917000
C	3.367550000	-0.017182000	-4.104335000
H	3.612457000	-0.195621000	-5.155077000
C	2.885620000	2.917747000	-1.708167000
H	3.269196000	3.584019000	-2.503321000
H	3.573862000	2.996969000	-0.849573000
C	1.595621000	4.970320000	-1.025121000
C	2.749439000	-1.887876000	-0.859724000
C	2.838390000	-3.646538000	1.266993000
H	2.882597000	-4.303189000	2.138500000
C	2.834620000	-0.821402000	-1.885904000
C	3.242616000	-3.191702000	-1.067006000
H	3.638419000	-3.487864000	-2.039225000
C	3.259757000	-4.090228000	0.007899000
H	3.632427000	-5.109039000	-0.129167000
C	2.357400000	-2.330170000	1.426467000
C	2.001352000	-1.773603000	2.778630000
H	2.039648000	-2.588319000	3.524284000
H	0.973057000	-1.379429000	2.736089000
C	2.930089000	1.502006000	-2.248772000
C	-2.928936000	0.610656000	3.158303000
C	-4.382930000	1.127846000	3.302166000
C	-0.417287000	-3.162767000	-2.400262000
C	-3.232730000	1.085947000	-3.297289000
H	-3.339447000	2.112783000	-3.649102000
C	-2.421657000	0.084473000	4.526632000

C -1.493952000 -3.440658000 -1.325229000
C -3.354228000 -1.291608000 -3.660804000
H -3.577263000 -2.154471000 -4.292351000
C -3.466832000 0.012041000 -4.161473000
H -3.753969000 0.188405000 -5.201807000
C -2.891841000 -2.917684000 -1.775917000
H -3.279098000 -3.591263000 -2.563050000
H -3.581046000 -2.987590000 -0.916213000
C -1.611211000 -4.966239000 -1.064392000
C -2.751905000 1.885468000 -0.937691000
C -2.827840000 3.628726000 1.203783000
H -2.864270000 4.279340000 2.080171000
C -2.850473000 0.823326000 -1.965990000
C -3.263418000 3.185595000 -1.127721000
H -3.677475000 3.485287000 -2.091263000
C -3.274682000 4.075518000 -0.045794000
H -3.661248000 5.090845000 -0.169883000
C -2.326093000 2.318075000 1.344335000
C -1.952105000 1.744388000 2.683579000
H -1.954009000 2.551387000 3.438245000
H -0.937627000 1.319999000 2.617957000
C -2.945397000 -1.504989000 -2.326989000
H -4.430758000 1.951608000 4.041077000
H -5.046773000 0.320712000 3.652256000
H -4.783239000 1.499466000 2.345472000
H -3.061806000 -0.734062000 4.893834000
H -1.391473000 -0.296255000 4.447741000
H -2.437187000 0.896463000 5.279236000
H -0.665444000 -5.365728000 -0.663481000
H -1.837213000 -5.500361000 -2.006886000
H -2.409176000 -5.188665000 -0.337439000
H -0.224185000 -2.083730000 -2.497023000
H -0.733253000 -3.561137000 -3.385069000
H 0.529205000 -3.653938000 -2.125339000
H 5.074309000 -0.291139000 3.716736000
H 4.499613000 -1.939490000 4.096194000
H 4.816303000 -1.460692000 2.400828000
H 1.416874000 0.240298000 4.568330000
H 2.496081000 -0.939808000 5.374712000
H 3.083457000 0.706410000 4.998862000
H 0.725352000 3.528127000 -3.321818000
H 0.219764000 2.061506000 -2.410203000
H -0.539328000 3.635494000 -2.066011000
H 0.649600000 5.372654000 -0.627900000
H 2.395636000 5.208445000 -0.305581000
H 1.815577000 5.487911000 -1.978272000

Structure [Fe₂⁰] Small (uBLYP)

Fe 1.111857000 -1.363264000 -0.361124000
Fe -1.109557000 1.411614000 -0.150046000
O 0.025288000 0.029394000 -0.094535000
S 1.249787000 -1.646142000 -2.625491000
S -0.022889000 -3.397130000 -0.529059000
N 3.047720000 -0.568071000 -0.215103000
N 1.635297000 -1.874190000 1.596841000
C 3.638304000 0.252658000 -1.131670000
C 4.979959000 0.658798000 -0.970739000
H 5.427459000 1.317154000 -1.718315000
C 5.722550000 0.214129000 0.131471000
H 6.767764000 0.509771000 0.255920000
C 5.098924000 -0.600979000 1.083543000
H 5.648649000 -0.936618000 1.963833000
C 3.748480000 -0.958311000 0.8989550000
C 2.960107000 -1.702041000 1.907105000
C 3.490718000 -2.152295000 3.133441000
H 4.551550000 -2.032956000 3.357343000
C 2.635570000 -2.742371000 4.071081000
H 3.025350000 -3.094286000 5.030043000
C 1.271875000 -2.863283000 3.765078000
H 0.572803000 -3.301527000 4.480897000
C 0.791641000 -2.429085000 2.514007000
C 2.823737000 0.701076000 -2.320968000
H 3.388810000 1.494486000 -2.843592000
H 1.873469000 1.143280000 -1.977217000
C 2.503218000 -0.431386000 -3.349922000
C 3.774596000 -1.204489000 -3.781202000
C 1.843602000 0.233093000 -4.586314000
C -0.658935000 -2.575442000 2.124418000
H -1.006775000 -1.624962000 1.689130000
H -1.252409000 -2.775554000 3.036183000
C -0.938423000 -3.718815000 1.090480000
C -0.498367000 -5.098633000 1.642284000
C -2.460900000 -3.734940000 0.797608000
S -1.385163000 1.898795000 -2.368784000

S -0.000598000 3.466637000 -0.201994000
N -3.042468000 0.611609000 0.043716000
N -1.499647000 1.731909000 1.876063000
C -3.711942000 -0.096140000 -0.912606000
C -5.053836000 -0.482251000 -0.712412000
H -5.564127000 -1.047620000 -1.495023000
C -5.717306000 -0.135394000 0.472423000
H -6.762786000 -0.414370000 0.628876000
C -5.013184000 0.558952000 1.462902000
H -5.500297000 0.817814000 2.403839000
C -3.665178000 0.899779000 1.233377000
C -2.799108000 1.519096000 2.261022000
C -3.234816000 1.817473000 3.568410000
H -4.275380000 1.662681000 3.856338000
C -2.310571000 2.296891000 4.503245000
H -2.626379000 2.527795000 5.524194000
C -0.974273000 2.465872000 4.111748000
H -0.223274000 2.823890000 4.819548000
C -0.589851000 2.185694000 2.785860000
C -2.982101000 -0.447281000 -2.186492000
H -3.597986000 -1.176979000 -2.743665000
H -2.026284000 -0.939855000 -1.942584000
C -2.694597000 0.767389000 -3.127059000
C -3.974591000 1.590952000 -3.417829000
C -2.116167000 0.207198000 -4.452257000
C 0.825543000 2.398666000 2.308435000
H 1.152478000 1.506358000 1.751156000
H 1.482561000 2.515376000 3.190638000
C 1.011097000 3.649242000 1.383060000
C 2.510534000 3.737915000 0.997996000
C 0.579710000 4.953280000 2.100597000
H 0.967135000 0.828730000 -4.290112000
H 2.568764000 0.899125000 -5.092883000
H 1.520291000 -0.529999000 -5.313231000
H 3.519032000 -1.960406000 -4.540969000
H 4.523348000 -0.518191000 -4.224045000
H 4.242632000 -1.731375000 -2.934470000
H -0.705663000 -5.888644000 0.902726000
H 0.580614000 -5.124048000 1.861317000
H -1.050529000 -5.349076000 2.569940000
H -0.484852000 4.930726000 2.381501000
H 1.181471000 5.119409000 3.016277000
H 0.728797000 5.820192000 1.437050000
H 2.846973000 2.817584000 0.495431000
H 2.684105000 4.581622000 0.310909000
H 3.137771000 3.894917000 1.897966000
H -4.753949000 0.956599000 -3.884892000
H -4.392427000 2.039248000 -2.502316000
H -3.747272000 2.413341000 -4.115032000
H -2.883002000 -0.394909000 -4.977178000
H -1.812398000 1.027329000 -5.123329000
H -1.240104000 -0.430512000 -4.260629000
H -3.035023000 -3.969443000 1.715961000
H -2.800741000 -2.760533000 0.413310000
H -2.700601000 -4.499330000 0.041130000

B3LYP Structures

Structure [Fe₂^S]_{Ar} Small (uB3LYP)

Fe 1.606488000 0.441142000 -0.375365000
Fe -1.649265000 0.360346000 0.379643000
S 2.129737000 2.624260000 -1.099570000
S -0.386279000 0.184181000 -1.814831000
N 3.671066000 0.310040000 0.386778000
N 2.384587000 -1.679336000 -0.956375000
C 4.227956000 1.302668000 1.115366000
C 5.561363000 1.216259000 1.534306000
H 5.985896000 2.023698000 2.121724000
C 6.318917000 0.098211000 1.201700000
H 7.348241000 0.006371000 1.536465000
C 5.739508000 -0.903663000 0.430403000
H 6.310067000 -1.787908000 0.174088000
C 4.408102000 -0.758721000 0.020314000
C 3.734147000 -1.762999000 -0.841827000
C 4.475661000 -2.737110000 -1.522605000
H 5.556023000 -2.757194000 -1.453348000
C 3.811847000 -3.664919000 -2.313986000
H 4.366490000 -4.425139000 -2.856554000
C 2.426395000 -3.600181000 -2.395585000
H 1.871351000 -4.317344000 -2.991213000
C 1.731595000 -2.594750000 -1.709666000
C 3.085630000 3.467573000 0.259311000

C	3.384051000	2.501276000	1.446844000
H	3.896963000	3.075712000	2.230392000
H	2.427940000	2.164870000	1.861152000
C	4.391711000	4.035641000	-0.320452000
C	2.216878000	4.611499000	0.812823000
C	-0.425424000	-1.467720000	-2.681445000
C	0.223188000	-2.570671000	-1.801652000
H	-0.213325000	-2.494567000	-0.802588000
H	-0.083295000	-3.543956000	-2.208439000
C	0.295247000	-1.319887000	-4.030903000
C	-1.891327000	-1.863625000	-2.921754000
S	-2.334035000	2.560817000	0.885792000
S	0.344797000	0.409961000	1.827154000
N	-3.697880000	-0.007885000	-0.352694000
N	-2.261394000	-1.751537000	1.170636000
C	-4.331022000	0.862957000	-1.169965000
C	-5.650463000	0.627507000	-1.576258000
H	-6.137137000	1.338368000	-2.235829000
C	-6.315196000	-0.513191000	-1.139384000
H	-7.331462000	-0.720606000	-1.462154000
C	-5.659350000	-1.387371000	-0.279444000
H	-6.156325000	-2.288228000	0.059098000
C	-4.346688000	-1.095447000	0.112597000
C	-3.597456000	-1.959943000	1.060075000
C	-4.258987000	-2.935618000	1.817066000
H	-5.332855000	-3.054578000	1.747748000
C	-3.525262000	-3.736267000	2.681898000
H	-4.017394000	-4.495941000	3.282440000
C	-2.151410000	-3.545227000	2.761900000
H	-1.542704000	-4.161684000	3.415028000
C	-1.539494000	-2.541172000	1.999510000
C	-3.377442000	3.186113000	-0.523338000
C	-3.590828000	2.093034000	-1.615683000
H	-2.609087000	1.803506000	-2.004674000
H	-4.150811000	2.546647000	-2.444848000
C	-4.727202000	3.677029000	0.026604000
C	-2.629442000	4.354041000	-1.191437000
C	0.490257000	-1.132313000	2.867843000
C	-0.040723000	-2.373657000	2.100191000
H	0.405949000	-2.363245000	1.102466000
H	0.342466000	-3.268511000	2.608957000
C	-0.283743000	-0.900535000	4.175289000
C	1.975377000	-1.374094000	3.184412000
H	1.271867000	4.228228000	1.209528000
H	2.745389000	5.150355000	1.6141146000
H	1.980805000	5.326594000	0.018408000
H	4.171003000	4.737100000	-1.131007000
H	5.028407000	3.245397000	-0.731715000
H	4.961188000	4.575084000	0.451940000
H	-3.218213000	4.767807000	-2.024272000
H	-2.452752000	5.154816000	-0.466409000
H	-1.657446000	4.028429000	-1.574229000
H	-5.283004000	2.868733000	0.513228000
H	-4.567854000	4.462821000	0.771553000
H	-5.351343000	4.093211000	-0.779176000
H	0.301395000	-2.276108000	-4.574414000
H	1.330026000	-0.987831000	-3.903607000
H	-0.215294000	-0.577970000	-4.652344000
H	-1.947541000	-2.791864000	-3.508543000
H	-2.417385000	-2.020447000	-1.975450000
H	-2.415676000	-1.078347000	-3.475280000
H	-0.237164000	-1.791704000	4.818349000
H	0.148682000	-0.059749000	4.725914000
H	-1.335287000	-0.664918000	3.985210000
H	2.546633000	-1.578892000	2.274049000
H	2.413015000	-0.494966000	3.667993000
H	2.089058000	-2.230214000	3.865038000

Structure [Fe₂⁰⁰]_{AF} Small (uB3LYP)

Fe	1.657538000	0.394041000	-0.821777000
Fe	-1.700265000	0.204257000	0.610897000
S	1.282336000	2.588443000	-1.077048000
S	-0.418728000	0.229108000	-1.818324000
S	-2.061673000	2.314260000	1.356240000
S	0.324040000	0.316640000	1.694810000
N	-3.497466000	0.110929000	-0.254977000
N	-2.192215000	-1.768326000	1.075539000
N	3.397681000	0.500330000	0.238590000
N	2.201608000	-1.605815000	-0.933234000
C	3.881621000	1.562293000	0.923457000
C	5.169584000	1.532823000	1.461780000
H	5.533670000	2.393949000	2.011350000
C	5.964341000	0.399985000	1.297087000
H	6.966826000	0.363429000	1.714078000

C	5.455737000	-0.686414000	0.604750000
H	6.056065000	-1.578176000	0.480253000
C	4.160344000	-0.611581000	0.072054000
C	3.519401000	-1.749233000	-0.615803000
C	4.203424000	-2.953267000	-0.854317000
H	5.247984000	-3.054305000	-0.590145000
C	3.539949000	-3.997687000	-1.467324000
H	4.055052000	-4.930793000	-1.676951000
C	2.196794000	-3.834285000	-1.811456000
H	1.645693000	-4.638283000	-2.287068000
C	1.545414000	-2.634092000	-1.530897000
C	2.578084000	3.533994000	-0.135422000
C	3.006023000	2.768503000	1.137970000
H	3.559156000	3.463575000	1.783334000
H	2.106231000	2.460448000	1.682754000
C	3.777324000	3.837412000	-1.048197000
C	1.901278000	4.845442000	0.306255000
C	-0.416789000	-1.384111000	-2.749223000
C	0.068112000	-2.532413000	-1.838678000
H	-0.490932000	-2.467974000	-0.898872000
H	-0.219732000	-3.481466000	-2.310051000
C	0.443321000	-1.249690000	-4.015130000
C	-1.875895000	-1.675482000	-3.143717000
C	-4.065868000	1.096536000	-0.995949000
C	-5.321773000	0.913220000	-1.581601000
H	-5.744179000	1.716437000	-2.175893000
C	-6.016577000	-0.279450000	-1.400038000
H	-6.988605000	-0.432516000	-3.285378000
C	-5.442920000	-1.270302000	-0.614807000
H	-5.958052000	-2.210745000	-0.460650000
C	-4.182757000	-1.046603000	-0.049538000
C	-3.496623000	-2.040713000	0.787324000
C	-4.142026000	-3.184248000	1.272123000
H	-5.189141000	-3.357296000	1.056614000
C	-3.430860000	-4.079942000	2.056412000
H	-3.911296000	-4.968280000	2.425815000
C	-2.088875000	-3.817449000	2.317502000
H	-1.497339000	-4.505958000	2.911504000
C	-1.483311000	-2.661432000	1.814607000
C	-3.191760000	3.204336000	0.175742000
C	-3.337899000	2.400565000	-1.144293000
H	-2.339180000	2.221652000	-1.555312000
H	-3.886491000	3.015569000	-1.870419000
C	-4.557983000	3.457572000	0.834287000
C	-2.525422000	4.548012000	-0.173156000
C	0.444845000	-1.179958000	2.797415000
C	-0.005546000	-2.457910000	2.053957000
H	0.519271000	-2.485881000	1.093248000
H	0.342925000	-3.328022000	2.626639000
C	-0.395479000	-0.938168000	4.062807000
C	1.921624000	-1.357178000	3.191404000
H	1.058115000	4.648182000	0.975699000
H	2.624181000	5.488231000	0.828436000
H	1.525093000	5.397233000	-0.561649000
H	3.457425000	4.433937000	-1.908396000
H	4.234069000	2.921516000	-1.433959000
H	4.543180000	4.408982000	-0.502806000
H	-3.160226000	5.129614000	-0.858257000
H	-2.369335000	5.143809000	0.732319000
H	-1.551653000	4.387893000	-0.645663000
H	-5.051141000	2.522797000	1.119918000
H	-4.432563000	4.054834000	1.743152000
H	-5.226335000	4.009344000	0.155676000
H	0.472390000	-2.206328000	-4.557104000
H	1.466513000	-0.945942000	-3.781760000
H	0.017985000	-0.492789000	-4.681782000
H	-1.925576000	-2.579373000	-3.766590000
H	-2.506881000	-1.830706000	-2.263017000
H	-2.293145000	-0.843661000	-3.720059000
H	-0.340119000	-1.805033000	4.738172000
H	-0.024218000	-0.061139000	4.601350000
H	-1.447069000	-0.753354000	3.821731000
H	2.542623000	-1.591085000	2.321106000
H	2.308835000	-0.440131000	3.646846000
H	2.030798000	-2.172564000	3.920435000
O	4.170394000	-0.221272000	-2.515550000
O	3.040563000	0.401759000	-2.578255000

Structure [Fe₂⁰⁰]_{AF} Small (uB3LYP)

Fe	1.680315000	0.415735000	0.376647000
Fe	-2.120012000	-0.516811000	0.379606000
O	0.328702000	0.301272000	-0.880152000
O	-0.306465000	-0.743063000	-0.107048000
S	-3.399487000	-0.337733000	2.282778000

S -2.390122000 -2.738352000 0.709114000
S 2.355954000 0.404130000 2.593858000
S 1.564286000 2.683265000 0.703332000
N -2.897318000 -0.417036000 -1.664418000
N 3.318794000 0.516339000 -1.218545000
N -2.215747000 1.522878000 0.071444000
N 2.356322000 -1.587901000 0.156604000
C 2.184874000 -1.338473000 3.244293000
C 3.581253000 -1.936971000 3.487632000
C 1.317501000 3.334172000 -2.036094000
C 3.948497000 -0.830941000 -3.102847000
H 4.001358000 -1.801294000 -3.581429000
C 1.427718000 -1.243643000 4.582336000
C 2.253663000 3.490992000 -0.827768000
C 4.297383000 1.540884000 -3.141416000
H 4.643133000 2.444425000 -3.632981000
C 4.379848000 0.307082000 -3.776719000
H 4.780968000 0.229114000 -4.783415000
C 3.677243000 2.948813000 -1.139409000
H 4.194465000 3.685064000 -1.769529000
H 4.230146000 2.881084000 -0.195388000
C 2.395714000 4.983488000 -0.470593000
C 3.024336000 -1.858460000 -0.985659000
C 2.327699000 -3.914093000 0.689813000
H 2.042923000 -4.698111000 1.383163000
C 3.433593000 -0.690865000 -1.809300000
C 3.361912000 -3.168192000 -1.338655000
H 3.919956000 -3.373358000 -2.243951000
C 2.995484000 -4.209820000 -0.491264000
H 3.245647000 -5.236248000 -0.784034000
C 2.020140000 -2.581514000 0.999710000
C 1.342364000 -2.228561000 2.292762000
H 1.098888000 -3.162610000 2.815144000
H 0.394110000 -1.730027000 2.071082000
C 3.754528000 1.620241000 -1.850630000
C -3.006664000 1.295503000 3.087741000
C -4.253630000 2.195940000 3.061196000
C -1.104903000 -3.528522000 -1.678039000
C -2.606573000 1.013992000 -3.570058000
H -2.365259000 1.989242000 -3.975328000
C -2.633866000 0.989440000 4.560052000
C -2.477228000 -3.507034000 -0.988377000
C -3.147582000 -1.304884000 -3.864100000
H -3.364017000 -2.157251000 -4.499564000
C -2.852285000 -0.062265000 -4.415546000
H -2.818296000 0.068782000 -5.493463000
C -3.543139000 -2.789011000 -1.860065000
H -3.814128000 -3.459572000 -2.686593000
H -4.444303000 -2.649110000 -1.250684000
C -2.968309000 -4.948853000 -0.752775000
C -2.453966000 1.896041000 -1.207875000
C -2.126181000 3.816492000 0.721571000
H -1.977144000 4.544943000 1.510602000
C -2.647079000 0.801886000 -2.188694000
C -2.569333000 3.240341000 -1.561862000
H -2.805854000 3.524045000 -2.580264000
C -2.404382000 4.213457000 -0.578131000
H -2.494166000 5.266687000 -0.828294000
C -2.038291000 2.451374000 1.027895000
C -1.786722000 1.983752000 2.431523000
H -1.500212000 2.852060000 3.037628000
H -0.929013000 1.300432000 2.438519000
C -3.165611000 -1.460790000 -2.471660000
H -4.058470000 3.153610000 3.565619000
H -5.087398000 1.707567000 3.575589000
H -4.574296000 2.404310000 2.035726000
H -3.445585000 0.453627000 5.062494000
H -1.733670000 0.370037000 4.616359000
H -2.446438000 1.922614000 5.110109000
H -2.290249000 -5.481015000 -0.077761000
H -3.004503000 -5.499078000 -1.703567000
H -3.967901000 -4.961905000 -0.305604000
H -0.675639000 -2.526578000 -1.748923000
H -1.188116000 -3.960236000 -2.687139000
H -0.405648000 -4.144877000 -1.103819000
H 4.135644000 -1.323854000 4.205266000
H 3.505073000 -2.955102000 3.897909000
H 4.170345000 -1.979184000 2.566010000
H 0.411612000 -0.865335000 4.433299000
H 1.360640000 -2.233022000 5.057034000
H 1.943855000 -0.568132000 5.272162000
H 1.758298000 3.799489000 -2.931267000
H 1.109499000 2.283290000 -2.254731000
H 0.360576000 3.824766000 -1.835582000
H 1.429653000 5.401475000 -0.169119000

H 3.098074000 5.127923000 0.356951000
H 2.758647000 5.552328000 -1.338519000

Structure [Fe₂⁽⁰⁾²]_{AF} Small (uB3LYP)

Fe 1.271357000 0.454459000 0.509711000
Fe -1.280673000 -0.464270000 0.499231000
O -0.000560000 -0.002264000 -0.722629000
O -0.008903000 -0.007416000 1.735913000
S -2.918850000 -0.939680000 2.122412000
S -1.279906000 -2.838605000 0.295563000
S 2.898020000 0.927116000 2.145367000
S 1.273602000 2.829099000 0.312189000
N 2.366405000 -1.521978000 0.415966000
N -2.375053000 1.513043000 0.403405000
N 2.736027000 0.340388000 -1.510007000
N -2.731453000 -0.344895000 -1.529242000
C 2.926141000 -0.533423000 3.324308000
C 4.402896000 -0.926098000 3.509691000
C 0.387212000 2.985423000 -2.355952000
C 2.910142000 -1.331899000 -3.228702000
H 2.914011000 -2.378339000 -3.510687000
C 2.331936000 -0.065386000 4.664263000
C 1.571472000 3.346691000 -1.450352000
C 2.992045000 0.993614000 -3.796486000
H 3.090649000 1.794007000 -4.522912000
C 2.995348000 -0.337600000 -4.197577000
H 3.075050000 -0.599297000 -5.249121000
C 2.900725000 2.744982000 -1.981660000
H 3.223410000 3.349484000 -0.840195000
H 3.662412000 2.851549000 -1.201587000
C 1.742061000 4.877894000 -1.392905000
C 2.818263000 -1.940325000 -0.781212000
C 3.044248000 -3.593155000 1.393626000
H 3.131585000 -4.209718000 2.281936000
C 2.797517000 -0.949949000 -1.887135000
C 3.376079000 -3.212389000 -0.947751000
H 3.762970000 -3.522335000 -1.911253000
C 3.469764000 -4.056160000 0.155046000
H 3.897047000 -5.049661000 0.052060000
C 2.500519000 -2.305993000 1.502233000
C 2.085562000 -1.745096000 2.831139000
H 2.167704000 -2.534864000 3.588665000
H 1.037184000 -1.437887000 2.769920000
C 2.8595753000 1.306366000 -2.434997000
C -2.951680000 0.516899000 3.305979000
C -4.429238000 0.908951000 3.486366000
C -0.377297000 -2.988901000 -2.367422000
C -2.894964000 1.331382000 -3.245081000
H -2.897396000 2.378475000 -3.524641000
C -2.362933000 0.044345000 4.646732000
C -1.567189000 -3.351884000 -1.469889000
C -2.972718000 -0.992788000 -3.818860000
H -3.066522000 -1.791501000 -4.547767000
C -2.973660000 0.339354000 -4.216827000
H -3.046631000 0.603517000 -5.268243000
C -2.893097000 -2.748422000 -2.007635000
H -3.210986000 -3.350761000 -2.869466000
H -3.659353000 -2.856538000 -1.232268000
C -1.738604000 -4.883189000 -1.417426000
C -2.819180000 1.934125000 -0.795664000
C -3.059855000 3.581599000 1.381670000
H -3.153253000 4.195989000 2.270869000
C -2.790884000 0.946336000 -1.903721000
C -3.376327000 3.206425000 -0.962772000
H -3.757059000 3.518642000 -1.927993000
C -3.477544000 4.047434000 0.141470000
H -3.904568000 5.041011000 0.038137000
C -2.516284000 2.294403000 1.490632000
C -2.109190000 1.730479000 2.820667000
H -2.196538000 2.518298000 3.579643000
H -1.060195000 1.424316000 2.765085000
C -2.849171000 -1.308732000 -2.457280000
H -4.520140000 1.716769000 4.226917000
H -5.016225000 0.056962000 3.845432000
H -4.874758000 1.249112000 2.546335000
H -2.922645000 -0.811876000 5.037215000
H -1.318636000 -0.257290000 4.525776000
H -2.409673000 0.851767000 5.391743000
H -0.857075000 -5.357255000 -0.973743000
H -1.867608000 -5.283777000 -2.433026000
H -2.611772000 -5.165234000 -0.820160000
H -0.163292000 -1.918195000 -2.327054000
H -0.578050000 -3.274416000 -3.411340000
H 0.517077000 -3.525208000 -2.034922000

H	4.988111000	-0.075506000	3.874918000
H	4.490640000	-1.736993000	4.242759000
H	4.852692000	-1.262213000	2.570251000
H	1.287767000	0.235666000	4.540696000
H	2.376788000	-0.874981000	5.407029000
H	2.889422000	0.790165000	5.059376000
H	0.594072000	3.273823000	-3.397889000
H	0.173745000	1.914452000	-2.319698000
H	-0.509527000	3.520234000	-2.027452000
H	0.857760000	5.350543000	-0.953250000
H	2.611579000	5.158637000	-0.789737000
H	1.876954000	5.281141000	-2.406692000

Structure [Fe₂⁰]_{F11} Small (uB3LYP)

Fe	1.092648000	-1.373495000	-0.443173000
Fe	-1.095408000	1.443896000	-0.243357000
O	0.036070000	0.036790000	0.047242000
S	1.634789000	-1.634825000	-2.735556000
S	-0.046716000	-3.478116000	-0.495895000
N	3.223480000	-0.621371000	-0.163596000
N	1.865463000	-2.050270000	1.597407000
C	3.793275000	0.218554000	-1.048566000
C	5.160504000	0.519518000	-0.966056000
H	5.598773000	1.204805000	-1.683794000
C	5.932957000	-0.065227000	0.030425000
H	6.995489000	0.148724000	0.103014000
C	5.325512000	-0.918828000	0.947861000
H	5.908423000	-1.365163000	1.744452000
C	3.954977000	-1.166758000	0.830371000
C	3.193945000	-1.983080000	1.811127000
C	3.784105000	-2.599723000	2.919572000
H	4.854692000	-2.557761000	3.080082000
C	2.966466000	-3.263002000	3.830312000
H	3.399492000	-3.747542000	4.700838000
C	1.591190000	-3.283800000	3.621011000
H	0.925545000	-3.773031000	4.324526000
C	1.060186000	-2.667778000	2.480564000
C	2.920752000	0.811165000	-2.119041000
H	3.425239000	1.697412000	-2.525832000
H	1.978648000	1.151604000	-1.675417000
C	2.599280000	-0.141042000	-3.306365000
C	3.886154000	-0.633609000	-3.989575000
C	1.744122000	0.646647000	-4.312890000
C	-0.415191000	-2.657999000	2.190335000
H	-0.688175000	-1.661303000	1.825774000
H	-0.958113000	-2.837448000	3.128626000
C	-0.894016000	-3.710329000	1.148226000
C	-0.609015000	-5.140090000	1.638509000
C	-2.408718000	-3.522443000	0.957738000
S	-1.751381000	1.887469000	-2.474703000
S	0.004844000	3.567261000	-0.162259000
N	-3.214832000	0.660224000	0.098835000
N	-1.730633000	1.905254000	1.900311000
C	-3.857682000	-0.072184000	-0.830757000
C	-5.225837000	-0.350638000	-0.699330000
H	-5.721943000	-0.948107000	-1.456757000
C	-5.925088000	0.145022000	0.394429000
H	-6.987820000	-0.050311000	0.506024000
C	-5.242916000	0.883994000	1.357409000
H	-5.768230000	1.260482000	2.226759000
C	-3.874652000	1.112346000	1.186236000
C	-3.039846000	1.805938000	2.200466000
C	-3.545266000	2.279797000	3.415939000
H	-4.600439000	2.207694000	3.650370000
C	-2.661865000	2.835833000	4.336968000
H	-3.028512000	3.207503000	5.289613000
C	-1.306474000	2.895734000	4.028965000
H	-0.589932000	3.305343000	4.733308000
C	-0.862083000	2.423916000	2.787137000
C	-3.065654000	-0.575707000	-2.004011000
H	-3.615447000	-1.410169000	-2.458876000
H	-2.108000000	-0.974969000	-1.652743000
C	-2.791684000	0.476607000	-3.116072000
C	-4.103541000	1.060610000	-3.667270000
C	-2.023803000	-0.233898000	-4.243403000
C	0.586183000	2.469816000	2.386127000
H	0.838037000	1.523335000	1.894867000
H	1.199107000	2.556890000	3.293931000
C	0.972092000	3.637323000	1.430923000
C	2.470480000	3.502845000	1.110768000
C	0.706848000	4.999863000	2.093988000
H	0.830243000	1.026627000	-3.847328000
H	2.314241000	1.501534000	-4.705137000
H	1.463497000	0.008979000	-5.157495000

H	3.639975000	-1.274620000	-4.841731000
H	4.473116000	0.218013000	-4.364662000
H	4.514964000	-1.215614000	-3.308350000
H	-0.971005000	-5.870478000	0.908317000
H	0.462523000	-5.314263000	1.776225000
H	-1.119869000	-5.332266000	2.594192000
H	-0.353621000	5.135295000	2.328066000
H	1.286071000	5.097207000	3.024578000
H	1.003736000	5.812446000	1.423683000
H	2.685500000	2.537744000	0.642704000
H	2.786619000	4.292704000	0.422183000
H	3.071495000	3.586516000	2.028853000
H	-4.738737000	0.261641000	-4.078044000
H	-4.669103000	1.593858000	-2.896670000
H	-3.891171000	1.770215000	-4.472854000
H	-2.644897000	-1.029979000	-4.679446000
H	-1.770735000	0.474117000	-5.039149000
H	-1.098112000	-0.683337000	-3.872502000
H	-2.943467000	-3.693572000	1.904158000
H	-2.635253000	-2.510317000	0.609970000
H	-2.791655000	-4.230244000	0.215877000

Structure [Fe₂^S] , Small (uB3LYP)

Fe	1.620559000	0.174708000	-0.148427000
Fe	-1.622169000	-0.067958000	0.237982000
S	1.502057000	2.510638000	-0.603911000
S	-0.293895000	-0.176312000	-1.792328000
S	-1.861317000	2.476607000	0.638279000
S	0.201633000	-0.017494000	1.900259000
N	-3.742915000	0.125883000	-0.342328000
N	-2.646395000	-1.741344000	1.295640000
N	3.733182000	0.477618000	0.403487000
N	2.744306000	-1.562992000	-1.073264000
C	4.145076000	1.478519000	1.207984000
C	5.503229000	1.626176000	1.522696000
H	5.813380000	2.432496000	2.178774000
C	6.433572000	0.741392000	0.990780000
H	7.487466000	0.833364000	1.235696000
C	5.997911000	-0.263010000	0.130145000
H	6.709057000	-0.963434000	-0.289936000
C	4.632905000	-0.359097000	-0.155105000
C	4.086887000	-1.380775000	-1.086848000
C	4.919116000	-2.112914000	-1.940849000
H	5.985009000	-1.925262000	-1.970592000
C	4.357099000	-3.075057000	-2.771477000
H	4.982193000	-3.651399000	-3.446826000
C	2.985405000	-3.294782000	-2.712115000
H	2.518317000	-4.058919000	-3.324123000
C	2.196338000	-2.522006000	-1.852155000
C	2.531304000	3.424112000	0.666693000
C	3.119238000	2.448235000	1.729100000
H	3.590521000	3.051338000	2.515670000
H	2.292066000	1.899105000	2.190870000
C	3.646157000	4.188261000	-0.066543000
C	1.625372000	4.423218000	1.407039000
C	-0.270992000	-1.903144000	-2.519942000
C	0.717107000	-2.810866000	-1.739063000
H	0.440121000	-2.794984000	-0.681750000
H	0.559842000	-3.838862000	-2.090962000
C	0.136733000	-1.767477000	-3.995470000
C	-1.674652000	-2.521711000	-2.423458000
C	-4.205497000	1.014513000	-1.248182000
C	-5.542844000	0.975879000	-1.665294000
H	-5.893336000	1.692295000	-2.400474000
C	-6.402780000	0.019566000	-1.137359000
H	-7.436943000	-0.034317000	-1.463846000
C	-5.921696000	-0.867456000	-0.178146000
H	-6.573395000	-1.625368000	0.238956000
C	-4.582069000	-0.777335000	0.210161000
C	-3.998803000	-1.667555000	1.247868000
C	-4.805845000	-2.386110000	2.134713000
H	-5.883654000	-2.283214000	2.110970000
C	-4.202345000	-3.220824000	3.069694000
H	-4.806700000	-3.783821000	3.774474000
C	-2.816520000	-3.329545000	3.079018000
H	-2.316681000	-3.992810000	3.776712000
C	-2.053541000	-2.576344000	2.178089000
C	-2.862629000	3.185747000	-0.788967000
C	-3.262896000	2.062100000	-1.788327000
H	-2.355300000	1.581220000	-2.167579000
H	-3.749863000	2.548343000	-2.642508000
C	-4.098535000	3.855793000	-0.168803000

Marcello Gennari 4/11/y 14:23

Commentaire [1]: The following entries (in yellow) have the same title, which are the differences? AF/Fxx?

C	-2.006139000	4.225911000	-1.525747000
C	0.320066000	-1.650329000	2.814314000
C	-0.553488000	-2.742694000	2.141745000
H	-0.238663000	-2.845017000	1.099777000
H	-0.319623000	-3.695467000	2.634160000
C	-0.125478000	-1.393020000	4.262785000
C	1.780747000	-2.127989000	2.794312000
H	0.838650000	3.912461000	1.971884000
H	2.214369000	5.025240000	2.112738000
H	1.148308000	5.107359000	0.698111000
H	3.214119000	4.907894000	-0.768243000
H	4.292474000	3.516439000	-0.639946000
H	4.269930000	4.743823000	0.648322000
H	-2.596144000	4.682705000	-2.330333000
H	-1.692634000	5.022510000	-0.843896000
H	-1.108193000	3.780525000	-1.964185000
H	-4.699708000	3.156329000	0.421849000
H	-3.801284000	4.678981000	0.487104000
H	-4.736730000	4.265421000	-0.962190000
H	0.181395000	-2.757821000	-4.468827000
H	1.113318000	-1.287350000	-4.106486000
H	-0.595715000	-1.165191000	-4.540856000
H	-1.690756000	-3.509550000	-2.902983000
H	-1.988909000	-2.642483000	-1.380723000
H	-2.409739000	-1.888150000	-2.929350000
H	-0.071593000	-2.321041000	4.848352000
H	0.527872000	-0.655106000	4.737117000
H	-1.149725000	-1.011203000	4.313665000
H	2.122290000	-2.326314000	1.772759000
H	2.438485000	-1.369838000	3.230143000
H	1.890220000	-3.049934000	3.380953000
H	-0.573164000	2.653634000	0.128757000

[Fe₂^{OO}] Small (uB3LYP)

Fe	1.659248000	0.331275000	-0.668879000
Fe	-1.659938000	0.074815000	0.439159000
S	1.162665000	2.578382000	-0.754991000
S	-0.421313000	0.134531000	-1.734109000
S	-1.943042000	2.424822000	1.065758000
S	0.376501000	0.216804000	1.511302000
N	-3.518942000	0.059528000	-0.313514000
N	-2.271899000	-1.761653000	1.170861000
N	3.418823000	0.470748000	0.314646000
N	2.291562000	-1.615859000	-0.933957000
C	3.869217000	1.494733000	1.073937000
C	5.162947000	1.462921000	1.612924000
H	5.504137000	2.301369000	2.209854000
C	5.989760000	0.371195000	1.386439000
H	6.990717000	0.335901000	1.805564000
C	5.508346000	-0.683416000	0.620345000
H	6.124179000	-1.557494000	0.452566000
C	4.220591000	-0.601039000	0.087191000
C	3.626754000	-1.701747000	-0.699646000
C	4.386183000	-2.786942000	-1.148625000
H	5.454602000	-2.821968000	-0.980238000
C	3.757666000	-3.804973000	-1.849784000
H	4.327191000	-4.650074000	-2.224236000
C	2.385663000	-3.722898000	-2.063099000
H	1.862758000	-4.508793000	-2.596962000
C	1.665121000	-2.617340000	-1.598732000
C	2.490937000	3.501714000	0.167963000
C	2.983857000	2.677080000	1.377923000
H	3.555660000	3.346339000	2.032675000
H	2.114487000	2.334618000	1.949961000
C	3.636810000	3.836919000	-0.800622000
C	1.854639000	4.798723000	0.698435000
C	-0.446976000	-1.478243000	-2.674058000
C	0.166210000	-2.602049000	-1.808728000
H	-0.336690000	-2.586946000	-0.836162000
H	-0.094076000	-3.559635000	-2.277034000
C	0.306099000	-1.297820000	-4.000727000
C	-1.914275000	-1.839429000	-2.957361000
C	-4.074412000	1.027732000	-1.084686000
C	-5.383737000	0.895614000	-1.560537000
H	-5.796762000	1.676990000	-2.189166000
C	-6.140461000	-0.222054000	-1.227842000
H	-7.154174000	-0.337062000	-1.598542000
C	-5.578482000	-1.186453000	-0.400024000
H	-6.153126000	-2.060435000	-0.121234000
C	-4.266095000	-1.017971000	0.049808000
C	-3.592493000	-1.993808000	0.928057000

C	-4.261285000	-3.091092000	1.477415000
H	-5.316503000	-3.246920000	1.293439000
C	-3.557000000	-3.978550000	2.280507000
H	-4.056780000	-4.831412000	2.729305000
C	-2.199906000	-3.759909000	2.488378000
H	-1.617637000	-4.448129000	3.091139000
C	-1.567170000	-2.649697000	1.916263000
C	-3.059768000	3.234610000	-0.205617000
C	-3.283290000	2.270022000	-1.403372000
H	-2.314877000	1.995876000	-1.683274000
H	-3.828635000	2.829171000	-2.173020000
C	-4.371853000	3.578055000	0.515313000
C	-2.374928000	4.512863000	-0.713431000
C	0.490812000	-1.214568000	2.707308000
C	-0.070127000	-2.510699000	2.085005000
H	0.412142000	-2.657362000	1.112341000
H	0.253357000	-3.348420000	2.715220000
C	-0.274386000	-0.827137000	3.983789000
C	1.974163000	-1.443176000	3.039389000
H	1.071129000	4.590181000	1.434970000
H	2.617913000	5.425681000	1.178103000
H	1.413358000	5.376344000	-0.120080000
H	3.275266000	4.484009000	-1.605253000
H	4.054059000	2.938448000	-1.264149000
H	4.442801000	4.366574000	-0.2723303000
H	-3.043626000	5.033180000	-1.410268000
H	-2.155431000	5.194523000	0.114257000
H	-1.440240000	4.290024000	-1.237012000
H	-4.851623000	2.696277000	0.953472000
H	-4.192989000	4.298360000	1.319145000
H	-5.076937000	4.029951000	-0.193360000
H	0.320342000	-2.246546000	-4.554700000
H	1.333505000	-0.965100000	-3.843747000
H	-0.193010000	-0.548825000	-4.622717000
H	-1.964626000	-2.735452000	-3.589662000
H	-2.465819000	-2.041938000	-2.033698000
H	-2.417225000	-1.025287000	-3.488416000
H	-0.232876000	-1.647752000	4.712955000
H	0.169213000	0.059663000	4.445455000
H	-1.326567000	-0.604765000	3.778994000
H	2.531600000	-1.782526000	2.161634000
H	2.437306000	-0.521506000	3.404614000
H	2.072356000	-2.204363000	3.824130000
H	-0.719646000	2.664863000	0.439254000
O	3.711883000	0.341427000	-2.548626000
O	2.455058000	0.605475000	-2.441191000

[Fe₂^{OO}] Small (uB3LYP)

Fe	1.802097000	0.617160000	0.322705000
Fe	-1.987895000	-0.775889000	0.136953000
O	-0.063013000	0.011064000	0.390324000
O	-0.607597000	-0.817949000	1.437079000
S	-3.942756000	-1.565863000	1.682442000
S	-1.554630000	-2.811155000	-0.868044000
S	2.756290000	1.627866000	2.146394000
S	1.134213000	2.404620000	-1.036415000
N	-2.748300000	0.217913000	-1.680520000
N	3.107770000	-0.182506000	-1.270327000
N	-2.649510000	1.260024000	0.749960000
N	2.441442000	-1.384947000	0.971324000
C	2.958710000	0.341942000	3.499394000
C	4.425502000	-0.113666000	3.544501000
C	1.838760000	2.703410000	-3.697442000
C	3.482052000	-2.216187000	-2.480008000
H	3.455986000	-3.298319000	-2.523381000
C	2.591557000	1.050548000	4.816625000
C	2.430519000	2.876906000	-2.289150000
C	3.997164000	-0.092525000	-3.480768000
H	4.385137000	0.502301000	-4.300831000
C	3.915467000	-1.478437000	-3.579153000
H	4.216822000	-1.984249000	-4.491639000
C	3.717575000	2.029692000	-2.111960000
H	4.461831000	2.398696000	-2.829491000
H	4.116267000	2.212707000	-1.107407000
C	2.796119000	4.352717000	-2.050306000
C	2.790907000	-2.211493000	-0.035539000
C	2.468376000	-3.208034000	2.498588000
H	2.362459000	-3.568449000	3.516348000
C	3.105314000	-1.534907000	-1.320353000
C	2.944470000	-3.582907000	0.171971000
H	3.218799000	-4.246941000	-0.638701000
C	2.765371000	-4.084059000	1.460236000
H	2.882354000	-5.146284000	1.652833000
C	2.303908000	-1.842500000	2.226255000

C 1.984019000 -0.855976000 3.322694000
H 1.964697000 -1.409795000 4.270166000
H 0.970985000 -0.471962000 3.156409000
C 3.584052000 0.540887000 -2.302194000
C -4.097393000 -0.286429000 3.065809000
C -5.393518000 0.484027000 2.772900000
C -1.079302000 -2.697020000 -3.584658000
C -2.601739000 2.335481000 -2.790854000
H -2.472061000 3.409342000 -2.746579000
C -4.213231000 -1.053062000 4.391902000
C -2.241805000 -2.903488000 -2.599195000
C -3.015292000 0.328816000 -4.046993000
H -3.218973000 -0.180009000 -4.983147000
C -2.789775000 1.701999000 -4.015989000
H -2.792285000 2.280579000 -4.934904000
C -3.368647000 -1.865767000 -2.833092000
H -3.830496000 -2.097974000 -3.801047000
H -4.142945000 -2.017743000 -2.071572000
C -2.843149000 -4.309043000 -2.777574000
C -2.539165000 2.146465000 -0.261563000
C -2.663312000 3.045368000 2.328411000
H -2.728311000 3.372443000 3.360765000
C -2.599007000 1.561638000 -1.628473000
C -2.444048000 3.517942000 -0.017607000
H -2.320561000 4.224267000 -0.828464000
C -2.500201000 3.967178000 1.298850000
H -2.424626000 5.027929000 1.517141000
C -2.723704000 1.680042000 2.024871000
C -2.859347000 0.648406000 3.123404000
H -2.913974000 1.182740000 4.079408000
C -4.944994000 0.045087000 3.142869000
H -3.000836000 -0.400075000 -2.852027000
H -5.522903000 1.273908000 3.522357000
H -6.262471000 -0.178550000 -2.823329000
H -5.379484000 0.957331000 1.786111000
H -5.029569000 -1.780929000 4.360020000
H -3.284423000 -1.580938000 4.636373000
H -4.421148000 -0.347700000 5.205280000
H -2.092183000 -5.078405000 -2.575258000
H -3.201354000 -4.441836000 -3.807050000
H -3.685253000 -4.471181000 -2.096934000
H -0.601649000 -1.721427000 -3.451073000
H -1.442809000 -2.767509000 -4.619210000
H -0.316843000 -3.468851000 -3.442896000
H 5.085366000 0.739493000 3.728246000
H 4.573684000 -0.837535000 4.357951000
H 4.736976000 -0.581633000 2.606092000
H 1.543329000 1.367435000 4.818275000
H 2.751451000 0.375136000 5.667963000
H 3.213298000 1.938383000 4.964337000
H 2.568146000 3.011708000 -4.459392000
H 1.551154000 1.665885000 -3.894412000
H 0.947543000 3.327438000 -3.815695000
H 1.912455000 4.990360000 -2.151221000
H 3.208877000 4.501623000 -1.047902000
H 3.541197000 4.683926000 -2.786496000
H -3.142173000 -2.442097000 2.325351000

[Fe₂(O)²/SH⁺] Small (uB3LYP)

Fe 1.381826000 0.280787000 0.134249000
Fe -1.262984000 -0.493350000 0.196615000
O -0.006475000 -0.065382000 -0.981686000
O -0.020689000 -0.163560000 1.379739000
S -2.949955000 -0.866502000 2.178376000
S -0.919998000 -2.730091000 0.400469000
S 3.072596000 0.746384000 1.697641000
S 1.017800000 2.487923000 0.549630000
N 2.259639000 -1.530118000 0.095922000
N -2.263609000 1.404395000 0.206687000
N 2.580590000 0.484054000 -1.513991000
N -2.652695000 -0.606431000 -1.448606000
C 2.956038000 -0.609841000 2.984200000
C 4.404770000 -1.046989000 3.272547000
C 0.554321000 3.499687000 -1.987048000
C 3.135682000 -0.862739000 -3.426034000
H 3.245281000 -1.841809000 -3.877606000
C 2.309906000 -0.023688000 4.250415000
C 1.636731000 3.485526000 -0.895022000
C 3.302116000 1.527612000 -3.531530000
H 3.554440000 2.439431000 -4.062286000
C 3.378178000 0.291627000 -4.165567000
H 3.660980000 0.224574000 -5.211754000
C 2.963052000 2.913880000 -1.444207000
H 3.385937000 3.661820000 -2.126157000

H 3.674364000 2.807375000 -0.615563000
C 1.896220000 4.910379000 -0.374360000
C 2.695478000 -1.864488000 -1.137984000
C 2.974019000 -3.631645000 0.943977000
H 3.110768000 -4.291807000 1.793682000
C 2.762342000 -0.733052000 -2.088350000
C 3.211683000 -3.135040000 -1.397795000
H 3.559740000 -3.402506000 -2.388559000
C 3.327013000 -4.036064000 -0.340114000
H 3.731440000 -5.029110000 -0.511867000
C 2.438808000 -2.353816000 1.145537000
C 2.092599000 -1.818362000 2.504317000
H 2.200107000 -2.619494000 3.245374000
H 1.047352000 -1.498627000 2.483866000
C 2.910866000 1.600577000 -2.187762000
C -3.038484000 0.734104000 3.169689000
C -4.490678000 1.225597000 3.067696000
C -0.556811000 -3.462782000 -2.275146000
C -3.200692000 0.811421000 -3.313571000
H -3.295922000 1.806074000 -3.732018000
C -2.683715000 0.418964000 4.630194000
C -1.558959000 -3.586919000 -1.118076000
C -3.86743000 -1.566984000 -3.510924000
H -3.640960000 -2.458503000 -4.074076000
C -3.466460000 -0.309122000 -4.094997000
H -3.760031000 -0.198156000 -5.134492000
C -2.950674000 -3.049406000 -1.519393000
H -3.400661000 -3.763476000 -2.220240000
H -3.590576000 -3.025753000 -0.629726000
C -1.713550000 -5.062931000 -0.699931000
C -2.708402000 1.747994000 -1.020512000
C -2.803720000 3.580129000 1.018306000
H -2.857363000 4.269862000 1.853729000
C -2.820330000 0.629016000 -1.983494000
C -3.168226000 3.039022000 -1.291625000
H -3.533824000 3.305852000 -2.275682000
C -3.191159000 3.972567000 -0.257858000
H -3.543451000 4.983278000 -0.441266000
C -2.347444000 2.272575000 1.232562000
C -2.021954000 1.775130000 2.614917000
H -2.015830000 2.629073000 3.302530000
H -1.023768000 1.328255000 2.611483000
C -2.976892000 -1.691892000 -2.175770000
H -4.592406000 2.188416000 3.583246000
H -5.174807000 0.513685000 3.539037000
H -4.810941000 1.365292000 2.029939000
H -3.332423000 -0.363667000 5.035957000
H -1.641651000 0.096075000 4.740351000
H -2.816554000 1.318695000 5.233066000
H -0.764547000 -5.468244000 -0.334685000
H -2.026530000 -5.662093000 -1.564906000
H -2.461775000 -5.179686000 0.090551000
H -0.339029000 -2.414917000 -2.501775000
H -0.953522000 -3.945172000 -3.179534000
H 0.384261000 -3.956106000 -2.015648000
H 5.011690000 -0.201460000 3.610334000
H 4.408619000 -1.805588000 4.066743000
H 4.885796000 -1.476745000 2.387524000
H 1.298919000 0.336367000 4.038151000
H 2.249842000 -0.793822000 5.031151000
H 2.900132000 0.810823000 4.641052000
H 0.912553000 4.064573000 -2.859262000
H 0.295614000 2.486091000 -2.307268000
H -0.354934000 3.987072000 -1.623267000
H 0.992745000 5.328908000 0.080309000
H 2.690335000 4.921402000 0.379025000
H 2.194908000 5.567198000 -1.201615000
H -1.938305000 -1.423846000 2.869261000

[Fe₂(O)(OH)] Small (uB3LYP)

Fe -1.406622000 -0.220715000 0.268873000
Fe 1.464656000 0.235129000 0.335114000
S 1.317366000 2.517835000 0.429032000
S -2.782900000 -0.759556000 1.949189000
S -1.143346000 -2.538939000 -0.035058000
S 2.801220000 0.539515000 2.131799000
N 2.848148000 0.193263000 -1.328046000
O 0.035951000 0.114517000 -1.108735000
H 0.100402000 -0.774336000 -1.504609000
O -0.005509000 -0.080763000 1.324032000
N -2.760861000 -0.004002000 -1.365786000
N -2.046162000 1.730350000 0.431840000
N 2.145591000 -1.740088000 0.310159000
C -2.410947000 2.276635000 -0.746876000

C 1.991523000 3.249352000 -1.136179000
C -4.288405000 1.288765000 3.084570000
C 2.582661000 -2.154059000 -0.898563000
C 2.223684000 4.736891000 -0.797364000
C -2.139058000 -3.152701000 -1.480532000
C 2.931323000 -1.065178000 -1.836249000
C 1.023163000 3.122689000 -2.320770000
C -2.765168000 1.289208000 -1.785632000
C 3.857236000 -0.241625000 -3.892074000
H 4.234322000 -0.404353000 -4.897159000
C 2.024567000 -2.608836000 1.330273000
C -2.607574000 0.095464000 4.535048000
C 3.409469000 -1.311301000 -3.124012000
H 3.445491000 -2.319533000 -3.517623000
C 4.240984000 -1.629812000 -0.521744000
C -2.440640000 4.455594000 0.253998000
H -2.578721000 5.530246000 -1.862714000
C -3.324194000 -0.956151000 -2.134716000
C 3.364640000 2.609445000 -1.444791000
H 3.896385000 3.259499000 -2.150261000
H 3.955408000 2.581248000 -0.251744000
C 3.839809000 1.030539000 -3.336989000
H 4.219972000 1.882516000 -3.889783000
C 2.824894000 -1.030599000 3.158599000
C -1.780308000 1.754459000 2.850733000
H -1.799301000 2.488766000 3.664704000
H -0.797731000 1.272102000 2.853490000
C 2.795220000 -3.507274000 -1.166523000
H 3.144548000 -3.837780000 -2.136938000
C -2.166058000 3.859939000 -1.479294000
C -2.103125000 4.450096000 2.386468000
C -2.873169000 0.689008000 3.138136000
C -3.457942000 -2.355927000 -1.597118000
H -4.132977000 -2.90498000 -2.265042000
H -3.933526000 -2.315063000 -0.610739000
C -1.976542000 2.473618000 1.548684000
C -2.486887000 -4.615496000 -1.138323000
C -1.331036000 -3.106341000 -2.787899000
C 2.479498000 -0.589191000 4.594080000
C 1.750345000 -2.048188000 2.694208000
H 1.725209000 -2.873374000 3.415831000
H 0.768542000 -1.564758000 2.706338000
C -3.217043000 1.647331000 -3.054940000
H -3.186523000 2.679918000 -3.380840000
C 2.588871000 -4.432068000 -0.144647000
H 2.744908000 -5.491032000 -0.326897000
C 2.233905000 -3.977568000 1.119309000
H 2.122565000 -4.665714000 1.950112000
C -2.593977000 3.653348000 -0.876397000
H -2.886398000 4.091737000 -1.822961000
C -3.819759000 -0.642603000 -3.408622000
H -4.270587000 -1.426279000 -4.007690000
C -3.733445000 0.658587000 -3.887338000
H -4.093615000 0.908413000 -4.880694000
C 3.329305000 1.228691000 -2.045439000
H -4.380181000 2.109073000 3.809390000
H -4.532760000 1.678548000 2.091633000
H -5.036767000 0.531731000 3.339010000
H -1.579388000 -5.203412000 -0.966687000
H -3.106104000 -4.676912000 -0.238742000
H -3.033280000 -5.074570000 -1.972844000
H -0.420681000 -3.706309000 -2.693591000
H -1.039655000 -2.084543000 -3.055415000
H -1.917537000 -3.515456000 -3.622368000
H 3.184002000 0.167197000 4.953789000
H 1.470581000 -0.168616000 4.648589000
H 2.533677000 -1.450949000 5.272371000
H 1.290675000 5.215986000 -0.483685000
H 2.592876000 5.265505000 -1.685880000
H 2.955647000 4.856881000 0.007296000
H 1.476824000 3.540740000 -3.230544000
H 0.746498000 2.081713000 -2.504764000
H 0.105923000 3.682859000 -2.115863000
H 4.974095000 -0.906474000 3.492402000
H 4.2933357000 -2.519799000 3.763768000
H 4.540595000 -1.918656000 2.109830000
H -1.598252000 -0.321979000 4.605157000
H -3.322472000 -0.700211000 4.766532000
H -2.713004000 0.877444000 5.298431000

[Fe₂(O)] Small (uB3LYP)

Fe 1.112332000 -1.560292000 -0.308002000
Fe -1.031567000 1.606424000 -0.087712000
O 0.012878000 -0.042064000 0.421573000

S 1.005668000 -1.348632000 -2.549507000
S -0.057402000 -3.476818000 -0.789181000
N 3.100719000 -0.863721000 -0.077588000
N 1.614317000 -2.318160000 1.591611000
C 3.752266000 -0.045346000 -0.929853000
C 5.118058000 0.221607000 -0.753255000
H 5.622615000 0.880383000 -1.451364000
C 5.806626000 -0.358780000 0.303115000
H 6.867012000 -0.171430000 0.442611000
C 5.115315000 -1.177323000 1.193144000
H 5.633777000 -1.624727000 2.031660000
C 3.754039000 -1.401554000 0.984929000
C 2.924103000 -2.197009000 1.920706000
C 3.428437000 -2.765130000 3.093111000
H 4.475891000 -2.674844000 3.351364000
C 2.560417000 -3.447990000 3.941010000
H 2.931887000 -3.893123000 4.859040000
C 1.216810000 -3.550538000 3.598275000
H 0.515458000 -4.074855000 4.238254000
C 0.764666000 -2.981881000 2.402066000
C 2.990558000 0.600928000 -2.053702000
H 3.660378000 1.324283000 -2.534400000
H 2.154444000 1.173664000 -1.635783000
C 2.464095000 -0.355560000 -3.150030000
C 3.560320000 -1.305914000 -3.658257000
C 1.932791000 0.505166000 -4.313671000
C -0.663444000 -3.111744000 1.955961000
H -1.042331000 -2.128552000 1.654611000
H -1.266472000 -3.458857000 2.804332000
C -0.868300000 -4.099201000 0.776012000
C -0.306856000 -5.494049000 1.099021000
C -2.379477000 -4.197967000 0.498784000
S -1.604115000 2.176923000 -2.223204000
S 0.563402000 3.187532000 -0.480282000
N -2.901206000 0.705254000 0.192842000
N -1.490499000 2.201093000 1.919242000
C -3.487039000 -0.136747000 -0.682168000
C -4.710940000 -0.746776000 -0.370818000
H -5.161672000 -1.424142000 -1.087720000
C -5.331514000 -0.471870000 0.840696000
H -6.279230000 -0.936478000 1.095437000
C -4.722090000 0.412530000 1.727913000
H -5.186017000 0.630907000 2.681448000
C -3.500427000 0.988581000 1.375538000
C -2.767265000 1.910136000 2.275856000
C -3.337367000 2.439547000 3.436293000
H -4.369427000 2.235420000 3.692368000
C -2.561576000 3.251010000 4.258540000
H -2.984625000 3.678139000 5.162730000
C -1.238906000 3.499144000 3.910363000
H -0.603250000 4.110828000 4.541279000
C -0.720677000 2.962896000 2.725166000
C -2.819852000 -0.366926000 -2.005971000
H -3.369183000 -1.151843000 -2.539432000
H -1.799493000 -0.737266000 -1.856831000
C -2.777147000 0.892888000 -2.908171000
C -4.167773000 1.527026000 -3.079725000
C -2.220722000 0.474554000 -4.282200000
C 0.716389000 3.209836000 2.342434000
H 1.220214000 2.249994000 2.174425000
H 1.210328000 3.685608000 3.198766000
C 0.942395000 4.103618000 1.096759000
C 2.443613000 4.446849000 1.027201000
C 0.115272000 5.397018000 1.167185000
H 1.178662000 1.219900000 -3.971175000
H 2.761298000 1.063018000 -4.769884000
H 1.486542000 -0.124418000 -5.090184000
H 3.175760000 -1.933460000 -4.467476000
H 4.412500000 -0.733040000 -4.049720000
H 3.925004000 -1.971815000 -2.869448000
H -0.493012000 -6.179064000 0.266478000
H 0.773630000 -5.470552000 1.270184000
H -0.792960000 -5.910681000 1.992526000
H -0.960309000 5.195174000 1.160567000
H 0.356173000 5.963899000 2.077565000
H 0.335069000 6.032597000 0.304719000
H 3.060530000 3.541942000 1.027932000
H 2.669701000 5.011657000 0.117682000
H 2.730154000 5.064529000 1.888833000
H -4.868978000 0.801257000 -3.514441000
H -4.581071000 1.881532000 -2.130207000
H -4.112123000 2.385210000 -3.756127000
H -2.920843000 -0.215226000 -4.772524000
H -2.096759000 1.346266000 -4.932516000
H -1.254243000 -0.026009000 -4.181091000

H	-2.898959000	-4.629605000	1.365597000
H	-2.809757000	-3.213063000	0.290432000
H	-2.572071000	-4.841393000	-0.364964000
H	0.236654000	0.051850000	1.361638000

Large uB3LYP Models

Structure [Fe₂^{5J}]_{AF} Large (uB3LYP)

Fe	1.628652000	0.366597000	-0.410061000
Fe	-1.731412000	0.320942000	0.451202000
S	2.198497000	2.543747000	-1.188962000
S	-0.457159000	0.421569000	-1.732928000
S	-2.438666000	2.491527000	1.094207000
S	0.347682000	0.434930000	1.796501000
N	-3.771269000	-0.096617000	-0.208649000
N	-2.205220000	-1.811317000	1.218964000
N	3.693445000	0.082840000	0.263462000
N	2.170046000	-1.746153000	-1.067499000
C	4.397298000	1.079368000	0.833017000
C	5.782040000	0.968414000	1.016025000
H	6.325525000	1.787403000	1.473024000
C	6.439143000	-0.170913000	0.572179000
H	7.514763000	-0.269439000	0.686645000
C	5.704568000	-1.180961000	-0.042690000
H	6.214005000	-2.058114000	-0.421347000
C	4.320605000	-1.027861000	-0.176530000
C	3.470777000	-2.057952000	-0.834366000
C	4.004518000	-3.296717000	-1.210119000
H	5.032538000	-3.549242000	-0.985466000
C	3.198304000	-4.209490000	-1.876264000
H	3.595842000	-5.171515000	-2.186995000
C	1.877909000	-3.869919000	-2.137153000
H	1.224609000	-4.555343000	-2.665380000
C	1.375788000	-2.632952000	-1.708328000
C	3.413300000	3.309882000	0.019783000
C	3.656109000	2.327392000	1.218615000
H	4.231452000	2.852267000	1.990997000
H	2.692225000	2.045637000	1.648673000
C	-0.485026000	-1.120386000	-2.807560000
C	-0.097373000	-2.358043000	-1.939748000
H	-0.612228000	-2.277355000	-0.976753000
H	-0.487999000	-3.255656000	-2.429817000
C	-4.484229000	0.794611000	-0.928232000
C	-5.819051000	0.541084000	-1.264438000
H	-6.371204000	1.278358000	-1.835825000
C	-6.419034000	-0.640477000	-0.848582000
H	-7.450596000	-0.859589000	-1.108567000
C	-5.681959000	-1.538339000	-0.084489000
H	-6.136690000	-2.465426000	0.241605000
C	-4.354506000	-1.229471000	0.235703000
C	-3.525193000	-2.109482000	1.097855000
C	-4.101296000	-3.188313000	1.781132000
H	-5.161074000	-3.391443000	1.699864000
C	-3.305591000	-3.984921000	2.591502000
H	-3.734426000	-4.821223000	3.136002000
C	-1.954085000	-3.685489000	2.697279000
H	-1.302041000	-4.283208000	3.324058000
C	-1.424803000	-2.589033000	2.004402000
C	-3.680521000	3.118983000	-0.162683000
C	-3.816314000	2.080155000	-1.330365000
H	-2.823368000	1.854253000	-1.726451000
H	-4.401470000	2.535731000	-2.137369000
C	0.491560000	-1.054373000	2.926976000
C	0.061612000	-2.328984000	2.133337000
H	0.523919000	-2.290428000	1.142567000
H	0.472364000	-3.204900000	2.645974000
C	2.744376000	4.607298000	0.507128000
C	2.095671000	4.718440000	1.743966000
C	2.746032000	5.732540000	-0.335883000
C	1.477371000	5.911760000	2.128380000
C	2.130199000	6.921310000	0.044869000
C	1.492826000	7.019727000	1.284439000
H	2.041698000	3.872045000	2.419365000
H	3.232282000	5.668327000	-1.304511000
H	0.975342000	5.964113000	3.091044000
H	2.146034000	7.773044000	-0.630767000
H	1.008447000	7.945778000	1.582813000
C	4.785793000	3.630308000	-0.614489000
C	5.691148000	4.435708000	0.101367000
C	5.203979000	3.111792000	-1.844796000
C	6.968040000	4.703066000	-0.390530000
C	6.483035000	3.381035000	-2.342802000
C	7.372501000	4.173886000	-1.619355000

H	5.383199000	4.874628000	1.046805000
H	4.510707000	2.503438000	-2.415819000
H	7.643697000	5.334567000	0.181600000
H	6.778086000	2.971043000	-3.305994000
H	8.364653000	4.386930000	-2.009452000
C	-1.921173000	-1.245163000	-3.347880000
C	-2.347696000	-0.337711000	-4.335280000
C	-2.834798000	-2.215945000	-2.918236000
C	-3.627201000	-0.407472000	-4.878053000
C	-4.121019000	-2.291070000	-3.465135000
C	-4.523708000	-1.391734000	-4.448780000
H	-1.658194000	0.425711000	-4.682065000
H	-2.563417000	-2.928140000	-2.146291000
H	-3.923386000	0.303922000	-5.644829000
H	-4.804827000	-3.060282000	-3.115042000
H	-5.519976000	-1.454327000	-4.878633000
C	0.490699000	-1.037393000	-4.005074000
C	0.435677000	-2.057379000	-4.973163000
C	1.448843000	-0.030729000	-4.165154000
C	1.315941000	-2.078523000	-6.053108000
C	2.331790000	-0.049289000	-5.250934000
C	2.274116000	-1.071176000	-6.196465000
H	-0.320926000	-2.833996000	-4.892587000
H	1.509652000	0.779652000	-3.447990000
H	1.246775000	-2.876694000	-6.788319000
H	3.060698000	0.750739000	-5.352181000
H	2.958470000	-1.080333000	-7.040910000
C	1.964118000	-1.134566000	3.366703000
C	2.456224000	-0.150606000	4.244031000
C	2.847594000	-2.139102000	2.952560000
C	3.773384000	-0.174847000	4.691876000
C	4.172278000	-2.168309000	3.404664000
C	4.642361000	-1.189583000	4.275972000
H	1.788542000	0.637211000	4.579050000
H	2.522763000	-2.915044000	2.267687000
H	4.121718000	0.596133000	5.374466000
H	4.832324000	-2.965100000	3.070602000
H	5.668924000	-1.215227000	4.631745000
C	-0.402355000	-0.926272000	4.182891000
C	-0.226201000	-1.858172000	5.222088000
C	-1.410685000	0.034025000	4.323572000
C	-1.037013000	-1.838780000	6.355568000
C	-2.222209000	0.056874000	5.463096000
C	-2.043858000	-0.877963000	6.481146000
H	0.568716000	-2.596444000	5.152400000
H	-1.563352000	0.776994000	3.548896000
H	-0.874628000	-2.567977000	7.145643000
H	-2.991480000	0.820018000	5.548688000
H	-2.673292000	-0.854731000	7.366983000
C	-5.090937000	3.342090000	0.429161000
C	-6.046103000	4.035483000	-0.337277000
C	-5.491701000	2.835606000	1.670159000
C	-7.352961000	4.207345000	0.117124000
C	-6.801140000	3.008927000	2.130264000
C	-7.738946000	3.692024000	1.357615000
H	-5.755069000	4.463439000	-1.292989000
H	-4.761585000	2.313135000	2.278795000
H	-8.067532000	4.753772000	-0.494008000
H	-7.082204000	2.611419000	3.102869000
H	-8.755129000	3.830999000	1.718221000
C	-3.107590000	4.448315000	-0.685138000
C	-3.249675000	5.609131000	0.094935000
C	-2.409937000	4.555426000	-1.895715000
C	-2.725101000	6.829051000	-0.323431000
C	-1.883712000	5.779369000	-2.317786000
C	-2.040646000	6.923046000	-1.537908000
H	-3.775053000	5.549441000	1.043115000
H	-2.246853000	3.683695000	-2.519247000
H	-2.850331000	7.709026000	0.302933000
H	-1.341358000	5.828587000	-3.258506000
H	-1.629150000	7.874025000	-1.866142000

Structure [Fe₂^{00J}]_{AF} Large (uB3LYP)

Fe	1.693165000	0.516157000	-0.823604000
Fe	-1.763431000	0.262944000	0.356622000
S	1.863530000	2.900413000	-0.700661000
S	-0.486465000	-0.101088000	-1.914648000
S	-1.927269000	2.510568000	0.690511000
S	0.289217000	0.509826000	1.459397000
N	-3.636838000	0.131633000	-0.323985000
N	-2.240998000	-1.626386000	1.061155000
N	3.716773000	0.265646000	0.147947000
N	2.466934000	-1.763480000	-1.243230000

C	4.260379000	1.165044000	0.993080000	C	0.883338000	-0.588630000	-6.200841000
C	5.608011000	1.072550000	1.371335000	C	0.823752000	-1.764112000	-6.945851000
H	6.022331000	1.822077000	2.035493000	H	-0.546361000	-3.796318000	-4.594624000
C	6.390256000	0.032231000	0.892545000	H	0.486701000	0.359355000	-4.309434000
H	7.431727000	-0.060190000	1.187315000	H	0.239315000	-3.843639000	-6.922821000
C	5.813271000	-0.902337000	0.039367000	H	1.265307000	0.324741000	-6.649552000
H	6.390215000	-1.748145000	-0.314804000	H	1.158791000	-1.779592000	-7.979721000
C	4.472720000	-0.747205000	-0.328041000	C	1.861632000	-0.997636000	3.155353000
C	3.818740000	-1.709386000	-1.255571000	C	2.281956000	-0.076719000	4.132043000
C	4.585801000	-2.507648000	-2.112227000	C	2.793639000	-1.944731000	2.709858000
H	5.664182000	-2.410704000	-2.140328000	C	3.573066000	-0.112689000	4.653454000
C	3.940173000	-3.400158000	-2.959064000	C	4.087983000	-1.988778000	3.237530000
H	4.510105000	-4.023116000	-3.642532000	C	4.484224000	-1.077115000	4.213763000
C	2.554803000	-3.478357000	-2.916962000	H	1.577632000	0.663855000	4.497947000
H	2.018297000	-4.167702000	-3.558548000	H	2.525949000	-2.661256000	1.941295000
C	1.837370000	-2.639352000	-2.051668000	H	3.863679000	0.607023000	5.414587000
C	3.096584000	3.453672000	0.588879000	H	4.784467000	-2.742667000	2.879420000
C	3.403320000	2.268794000	1.558297000	H	5.487734000	-1.116370000	4.629213000
H	3.923346000	2.670643000	2.435272000	C	-0.528618000	-0.779528000	3.873657000
H	2.459067000	1.841016000	1.898586000	C	-0.454267000	-1.748671000	4.891476000
C	-0.535200000	-1.768744000	-2.789275000	C	-1.459791000	0.254820000	4.018825000
C	0.333351000	-2.783608000	-1.982299000	C	-1.290870000	-1.696513000	6.004240000
H	0.017368000	-2.740869000	-0.939196000	C	-2.298960000	0.309997000	5.138099000
H	0.107855000	-3.791889000	-2.346731000	C	-2.223650000	-0.663420000	6.132021000
C	-4.257949000	1.049434000	-1.102505000	H	0.283675000	-2.543982000	4.821988000
C	-5.616532000	0.931978000	-1.406814000	H	-1.532741000	1.028046000	3.262258000
H	-6.084295000	1.696468000	-2.016759000	H	-1.208308000	-2.457914000	6.776108000
C	-6.354435000	-0.134541000	-0.905707000	H	-3.008612000	1.128741000	5.226813000
H	-7.414565000	-0.227469000	-1.121746000	H	-2.874849000	-0.615714000	7.001009000
C	-5.707082000	-1.084122000	-0.127206000	C	-4.471495000	3.717248000	0.132662000
H	-6.255976000	-1.932894000	0.260707000	C	-5.349220000	4.527763000	-0.610486000
C	-4.342757000	-0.934025000	0.138924000	C	-4.878788000	3.308173000	-0.17236000
C	-3.564694000	-1.911544000	0.911970000	C	-6.591121000	4.905245000	-0.101815000
C	-4.136297000	-3.072886000	1.443618000	C	-6.122287000	3.688661000	1.922032000
H	-5.193132000	-3.272802000	1.321193000	C	-6.985723000	4.485160000	1.171373000
C	-3.331795000	-3.972471000	2.125787000	H	-5.046618000	4.882036000	-1.592509000
H	-3.751647000	-4.880753000	2.548091000	H	-4.204590000	2.696666000	1.997255000
C	-1.977302000	-3.685632000	2.259340000	H	-7.247043000	5.536677000	-0.696568000
H	-1.318327000	-4.365360000	2.788178000	H	-6.410196000	3.362701000	2.918954000
C	-1.451687000	-2.504140000	1.726476000	H	-7.950374000	4.783948000	1.574027000
C	-3.141322000	3.271229000	-0.515762000	C	-2.422741000	4.491036000	-1.116169000
C	-3.462551000	2.214316000	-1.613887000	C	-2.228033000	5.624675000	-0.308192000
H	-2.524555000	1.846428000	-2.039581000	C	-1.935437000	4.530616000	-2.428788000
H	-4.036796000	2.692044000	-2.416307000	C	-1.573664000	6.752701000	-0.793552000
C	0.408876000	-0.939391000	2.651628000	C	-1.281340000	5.664846000	-2.920016000
C	0.026215000	-2.241466000	1.893287000	C	-1.098357000	6.781251000	-2.107657000
H	0.516523000	-2.214398000	0.915596000	H	-2.588157000	5.611960000	0.715978000
H	0.432940000	-3.103067000	2.433318000	H	-2.046534000	3.675588000	-3.086503000
C	2.407580000	4.608431000	1.337265000	H	-1.428996000	7.609769000	-0.141046000
C	1.776483000	4.443592000	2.577985000	H	-0.911439000	5.665590000	-3.942340000
C	2.371134000	5.882686000	0.745738000	H	-0.586943000	7.661250000	-2.489260000
C	1.146793000	5.516768000	3.212971000	O	2.633516000	0.629939000	-2.448189000
C	1.740789000	6.953026000	1.376049000	O	2.392478000	1.397969000	-3.405555000
C	1.128447000	6.777875000	2.619251000				
H	1.749829000	3.471449000	3.056642000				
H	2.841913000	6.033152000	-0.220677000				
H	0.664971000	5.358513000	4.174653000				
H	1.730353000	7.927326000	0.893690000				
H	0.639407000	7.612502000	3.115196000				
C	4.438350000	3.932524000	-0.012771000				
C	5.348803000	4.608248000	0.820498000				
C	4.826309000	3.669380000	-1.330684000				
C	6.604171000	4.997239000	0.354900000				
C	6.084010000	4.060875000	-1.801013000				
C	6.979894000	4.722952000	-0.962989000				
H	5.062035000	4.848870000	1.840948000				
H	4.127779000	3.166627000	-1.989989000				
H	7.285184000	5.523986000	1.019317000				
H	6.356437000	3.849969000	-2.832516000				
H	7.955317000	5.030699000	-1.331479000				
C	-2.009712000	-2.220730000	-2.822844000				
C	-2.912851000	-1.504608000	-3.629779000				
C	-2.494303000	-3.349617000	-2.149483000				
C	-4.238178000	-1.905681000	-3.765128000				
C	-3.825267000	-3.760966000	-2.290557000				
C	-4.703174000	-3.045118000	-3.099630000				
H	-2.557739000	-0.631859000	-4.168861000				
H	-1.844361000	-3.933744000	-1.507712000				
H	-4.908159000	-1.335365000	-4.403400000				
H	-4.165741000	-4.649656000	-1.764516000				
H	-5.733972000	-3.368915000	-3.217499000				
C	-0.043241000	-1.718888000	-4.255865000				
C	-0.118681000	-2.894876000	-5.026774000				
C	0.450007000	-0.565467000	-4.870511000				
C	0.313147000	-2.921549000	-6.351244000				

Structure [Fe₂⁰⁰]_{AF} Large (uB3LYP)

Fe	1.875855000	0.784420000	0.645371000
Fe	-2.092987000	-0.632986000	0.647227000
O	0.027120000	0.424168000	0.708898000
O	-0.532483000	-0.436960000	1.694965000
S	-3.813838000	-1.431261000	2.026250000
S	-1.363563000	-2.551264000	-0.503002000
S	3.072650000	1.323457000	2.557527000
S	1.436118000	2.866562000	-0.414828000
N	-2.687086000	0.350633000	-1.260773000
N	3.001624000	0.098863000	-1.132013000
N	-2.639644000	1.440011000	1.141250000
N	2.282129000	-1.364065000	0.915402000
C	3.160152000	-0.200464000	3.670099000
C	2.894849000	-1.690785000	-2.717431000
H	2.632717000	-2.713924000	-2.957836000
C	2.784751000	3.377078000	-1.610103000
C	3.708297000	0.479077000	-3.374726000
H	4.113473000	1.158743000	-4.116344000
C	3.359039000	-0.827511000	-3.707237000
H	3.466242000	-1.181595000	-4.728333000
C	3.914915000	2.303415000	-1.605289000
H	4.729668000	2.655026000	-2.249765000
H	4.305366000	2.209693000	-0.587721000

C	2.449904000	-2.044225000	-0.235563000
C	2.152910000	-3.407166000	2.121708000
H	2.053548000	-3.918070000	3.073231000
C	2.758184000	-1.200163000	-1.417070000
C	2.438671000	-3.438189000	-0.265458000
H	2.557529000	-3.978641000	-1.196755000
C	2.276287000	-4.123317000	0.936753000
H	2.261498000	-5.209145000	0.947818000
C	2.151116000	-2.005849000	2.084923000
C	1.995760000	-1.188101000	3.343592000
H	1.898038000	-1.888468000	4.180398000
H	1.054335000	-0.635890000	3.263604000
C	3.510517000	0.924474000	-2.063182000
C	-4.124989000	-0.130487000	3.358983000
C	-2.600002000	2.460010000	-2.399759000
H	-2.478002000	3.535315000	-2.367262000
C	-2.341741000	-2.912982000	-2.048260000
C	-3.046402000	0.439506000	-3.614702000
H	-3.300095000	-0.076646000	-0.534792000
C	-2.840716000	1.815104000	-3.60831000
H	-2.901817000	2.386425000	-4.530186000
C	-3.342684000	-1.750825000	-2.378963000
H	-3.819976000	-1.988836000	-3.336798000
H	-4.127245000	-1.827866000	-1.617773000
C	-2.504467000	2.308885000	0.123999000
C	-2.685069000	3.231568000	2.700667000
H	-2.776953000	3.566785000	3.728083000
C	-2.557754000	1.697136000	-1.229690000
C	-2.408644000	3.682587000	0.353875000
H	-2.262145000	4.381641000	-0.460031000
C	-2.492502000	4.141412000	1.666534000
H	-2.415472000	5.203908000	1.877169000
C	-2.744593000	1.862711000	2.408119000
C	-2.896948000	0.827816000	3.495386000
H	-2.977182000	1.356766000	4.451191000
H	-1.976699000	0.235365000	3.518558000
C	-2.950379000	-0.285966000	-2.418227000
C	-5.380316000	0.729123000	3.097304000
C	-6.064788000	0.749502000	1.877673000
C	-5.837241000	1.575282000	4.124135000
C	-7.165124000	1.591236000	1.685054000
C	-6.931086000	2.417659000	3.933683000
C	-7.602014000	2.431022000	2.707924000
H	-5.736159000	0.093015000	1.019799000
H	-5.341641000	1.560777000	5.091402000
H	-7.682879000	1.581689000	0.728866000
H	-7.264455000	3.058212000	4.746494000
H	-8.458927000	3.082701000	2.557987000
C	-4.309139000	-0.960328000	4.643619000
C	-3.292962000	-1.130546000	5.593923000
C	-5.531953000	-1.616987000	4.866087000
C	-3.493172000	-1.919498000	6.730327000
C	-5.732488000	-2.405915000	5.995746000
C	-4.712931000	-2.560150000	6.938939000
H	-2.326609000	-0.657506000	5.457281000
H	-6.331464000	-1.508154000	4.139903000
H	-2.687042000	-2.030845000	7.451290000
H	-6.689289000	-2.901392000	6.140131000
H	-4.868654000	-3.173159000	7.822757000
C	4.495548000	-0.964612000	3.548923000
C	4.802574000	-1.933666000	4.521115000
C	5.391144000	-0.792725000	2.488185000
C	5.960766000	-2.704045000	4.432553000
C	6.555427000	-1.562133000	2.398614000
C	6.846129000	-2.521562000	3.367112000
H	4.134928000	-2.074280000	5.366976000
H	5.173808000	-0.044764000	1.733994000
H	6.175374000	-3.442261000	5.201359000
H	7.237595000	-1.402941000	1.566846000
H	7.753151000	-3.116594000	3.298555000
C	3.001661000	0.375457000	5.089725000
C	1.803588000	0.305089000	5.813264000
C	4.089614000	1.038700000	5.683884000
C	1.697772000	0.869018000	7.088283000
C	3.985285000	1.603585000	6.952112000
C	2.786343000	1.519533000	7.665366000
H	0.933053000	-0.184640000	5.390880000
H	5.025778000	1.113294000	5.139216000
H	0.756458000	0.796047000	7.627427000
H	4.843788000	2.110770000	7.385085000
H	2.703875000	1.957275000	8.656705000
C	-3.264954000	-4.147816000	-1.873783000
C	-3.766601000	-4.792109000	-3.017670000
C	-3.699009000	-4.593899000	-0.619761000
C	-4.667431000	-5.851603000	-2.911563000

C	-4.601562000	-5.655509000	-0.512367000
C	-5.089090000	-6.290053000	-1.654526000
H	-3.439884000	-4.470628000	-4.003087000
H	-3.325564000	-4.110650000	0.276514000
H	-5.035968000	-6.336088000	-3.812451000
H	-4.920462000	-5.983626000	0.473568000
H	-5.788442000	-7.117670000	-1.568144000
C	-1.287004000	-3.208953000	-3.127251000
C	-0.559681000	-4.412480000	-3.041623000
C	-0.986216000	-2.347461000	-4.187958000
C	0.414722000	-4.739923000	-3.980171000
C	-0.007547000	-2.671889000	-5.135124000
C	0.696348000	-3.869991000	-5.040716000
H	-0.773644000	-5.098353000	-2.228129000
H	-1.504536000	-1.403426000	-4.287265000
H	0.945932000	-5.684993000	-3.894328000
H	0.192927000	-1.981904000	-5.951233000
H	1.444947000	-4.131606000	-5.784378000
C	2.272941000	3.504593000	-3.062270000
C	3.046382000	4.220633000	-3.993642000
C	1.120521000	2.858861000	-3.525149000
C	2.679605000	4.289746000	-5.337473000
C	0.750927000	2.927770000	-4.871678000
C	1.525666000	3.641675000	-5.784936000
H	3.939454000	4.741226000	-3.659459000
H	0.509895000	2.302537000	-2.822407000
H	3.293445000	4.856235000	-6.033314000
H	-0.148589000	2.414584000	-5.203214000
H	1.235194000	3.696902000	-6.830951000
C	3.301501000	4.735520000	-1.105307000
C	2.467913000	5.861864000	-1.228038000
C	4.557157000	4.913461000	-0.511027000
C	2.871901000	7.112853000	-0.772515000
C	4.965499000	6.170370000	-0.051943000
C	4.127723000	7.275169000	-0.179310000
H	1.489399000	5.746168000	-1.684496000
H	5.237172000	4.077864000	-0.388732000
H	2.204946000	7.964656000	-0.879786000
H	5.944674000	6.276591000	0.407812000
H	4.445339000	8.250960000	0.178285000

Structure [Fe₂^{(O)2}]_{AF} Large (uB3LYP)

Fe	1.198382000	0.343685000	0.625633000
Fe	-1.604844000	-0.310732000	0.317186000
O	0.109802000	0.514046000	-0.762207000
O	-0.178787000	-0.127012000	1.588727000
S	-3.420454000	-0.743052000	1.837759000
S	-1.220551000	-2.568468000	-0.271922000
S	2.691977000	0.665157000	2.407722000
S	0.975242000	2.813434000	0.088974000
N	-2.643292000	0.101295000	-1.709561000
N	2.863016000	0.275819000	-1.100866000
N	-2.346158000	1.773216000	0.329050000
N	2.065112000	-1.672888000	0.440820000
C	2.879346000	-0.990209000	3.302673000
C	3.058873000	-1.082027000	-3.066045000
H	2.920755000	-2.039779000	-3.554672000
C	2.379078000	3.571946000	-0.884790000
C	3.718895000	1.230474000	-3.113221000
H	4.121073000	2.096024000	-3.628957000
C	3.534193000	0.019710000	-3.774459000
H	3.777512000	-0.072001000	-4.829357000
C	3.583465000	2.588181000	-0.958646000
H	4.431860000	3.133438000	-1.390446000
H	3.851812000	2.278212000	0.054566000
C	2.435420000	-2.046546000	-0.796913000
C	2.249335000	-3.913870000	1.203268000
H	2.212059000	-4.620907000	2.024903000
C	2.756863000	-0.921854000	-1.711362000
C	2.650360000	-3.388648000	-1.110231000
H	2.925547000	-3.692561000	-2.112869000
C	2.524389000	-4.333788000	-0.093319000
H	2.679134000	-5.387023000	-0.308289000
C	2.022354000	-2.553578000	1.449569000
C	1.788547000	-2.013326000	2.836575000
H	1.788093000	-2.854786000	3.537642000
H	0.805513000	-1.533944000	2.865231000
C	3.361209000	1.328278000	-1.761643000
C	-3.620107000	0.748471000	2.966699000
C	-2.651526000	1.850030000	-3.354187000

H	-2.556322000	2.901098000	-3.598633000
C	-2.236412000	-3.262664000	-1.672243000
C	-3.033056000	-0.426800000	-4.004072000
H	-3.262801000	-1.175491000	-4.755293000
C	-2.872512000	0.908933000	-4.355208000
H	-2.950828000	1.219555000	-5.393460000
C	-3.264470000	-2.219776000	-2.233316000
H	-3.775960000	-2.695576000	-3.077880000
H	-4.012386000	-2.103931000	-1.441258000
C	-2.523964000	2.346601000	-0.876092000
C	-2.732116000	3.864460000	1.400275000
H	-2.841053000	4.426374000	2.321190000
C	-2.567035000	1.411356000	-2.029103000
C	-2.773222000	3.715197000	-0.996482000
H	-2.925742000	4.173438000	-1.966279000
C	-2.854670000	4.483876000	0.162870000
H	-3.045366000	5.551234000	0.097649000
C	-2.485897000	2.485532000	1.458097000
C	-2.426430000	1.744518000	2.766610000
H	-2.444921000	2.479732000	3.578487000
H	-1.483612000	1.191323000	2.824590000
C	-2.905351000	-0.811641000	-2.660083000
C	-4.935887000	1.521543000	2.723627000
C	-5.714011000	1.368643000	1.570723000
C	-5.346367000	2.473300000	3.674471000
C	-6.862551000	2.140917000	1.370681000
C	-6.489593000	3.246253000	3.476410000
C	-7.255927000	3.083667000	2.319314000
H	-5.417706000	0.630470000	0.833006000
H	-4.772666000	2.597037000	4.589193000
H	-7.453002000	1.995773000	0.469018000
H	-6.786618000	3.970126000	4.231521000
H	-8.151591000	3.680180000	2.165388000
C	-3.611902000	0.165890000	4.390776000
C	-2.525356000	0.291770000	5.266789000
C	-4.741715000	-0.540309000	4.842034000
C	-2.572624000	-0.256480000	6.552881000
C	-4.786180000	-1.093441000	6.118493000
C	-3.699839000	-0.950502000	6.986701000
H	-1.624578000	0.812888000	4.962359000
H	-5.593361000	-0.654747000	4.178389000
H	-1.719884000	-0.127878000	7.214353000
H	-5.673551000	-1.634265000	6.438022000
H	-3.734781000	-1.374858000	7.986793000
C	4.267949000	-1.627713000	3.070265000
C	4.695420000	-2.649919000	3.936160000
C	5.095100000	-1.293184000	1.991728000
C	5.906289000	-3.310528000	3.731984000
C	6.310664000	-1.952412000	1.786437000
C	6.723382000	-2.963135000	2.653477000
H	4.079705000	-2.921182000	4.789345000
H	4.780309000	-0.508090000	1.313096000
H	6.214132000	-4.092811000	4.421511000
H	6.936698000	-1.668132000	0.943758000
H	7.670870000	-3.472074000	2.495737000
C	2.701513000	-0.632614000	4.788144000
C	1.548151000	-0.946717000	5.519679000
C	3.731615000	0.060502000	5.449134000
C	1.436577000	-0.594850000	6.868596000
C	3.616782000	0.420396000	6.789089000
C	2.466668000	0.089338000	7.510782000
H	0.718423000	-1.464062000	5.051240000
H	4.633151000	0.316717000	4.900909000
H	0.537579000	-0.868359000	7.414701000
H	4.429830000	0.956521000	7.272231000
H	2.377325000	0.361304000	8.559282000
C	-3.150560000	-4.419928000	-1.189730000
C	-3.729580000	-5.275586000	-2.143544000
C	-3.513232000	-4.587029000	0.151759000
C	-4.629815000	-6.272011000	-1.767918000
C	-4.416065000	-5.585144000	0.529641000
C	-4.976895000	-6.432934000	-0.424599000
H	-3.463442000	-5.170961000	-3.192121000
H	-3.087762000	-3.930907000	0.903485000
H	-5.057701000	-6.923378000	-2.526096000
H	-4.678900000	-5.693409000	1.578777000
H	-5.676884000	-7.209764000	-0.127793000
C	-1.195619000	-3.777026000	-2.682349000
C	-0.623633000	-5.050474000	-2.501499000
C	-0.721968000	-3.005755000	-3.753107000
C	0.352319000	-5.539946000	-3.367514000
C	0.253114000	-3.494760000	-4.627467000
C	0.794093000	-4.767395000	-4.445232000
H	-0.953559000	-5.665485000	-1.671219000
H	-1.094402000	-2.001968000	-3.907139000

H	0.762259000	-6.533753000	-3.203884000
H	0.582971000	-2.873894000	-5.457418000
H	1.542129000	-5.154373000	-5.132705000
C	1.957063000	3.943618000	-2.316499000
C	2.654385000	4.952881000	-3.000824000
C	0.972327000	3.228175000	-3.010709000
C	2.366174000	5.248683000	-4.333884000
C	0.684959000	3.524597000	-4.345611000
C	1.375346000	4.536586000	-5.013048000
H	3.423444000	5.520370000	-2.484678000
H	0.442187000	2.423987000	-2.509550000
H	2.915472000	6.039219000	-4.838841000
H	-0.078908000	2.950392000	-4.864025000
H	1.147739000	4.767346000	-6.050529000
C	2.704952000	4.813433000	-0.036476000
C	1.825166000	5.912939000	-0.065706000
C	3.823313000	4.887754000	0.807039000
C	2.063282000	7.045653000	0.706770000
C	4.062796000	6.025844000	1.581351000
C	3.187067000	7.109031000	1.535680000
H	0.948329000	5.871955000	-0.704094000
H	4.520198000	4.060980000	0.875965000
H	1.369283000	7.880952000	0.662923000
H	4.938160000	6.057346000	2.224387000
H	3.374089000	7.992108000	2.140537000

Structure [Fe₂⁰]_{Ar} Large (uB3LYP)

Fe	1.005690000	-1.396271000	-0.711041000
Fe	-1.011372000	1.463476000	-0.522348000
O	0.012959000	0.021242000	-0.261218000
S	0.434837000	-2.228812000	-2.861192000
S	0.243827000	-3.520333000	0.111581000
N	3.007778000	-0.595208000	-1.441946000
N	2.348289000	-1.321616000	1.077914000
C	3.239345000	-0.117641000	-2.681897000
C	4.390710000	0.638090000	-2.953570000
H	4.546705000	1.019504000	-3.956519000
C	5.308917000	0.896076000	-1.947099000
H	6.191525000	1.498207000	-2.141747000
C	5.081496000	0.364054000	-0.682818000
H	5.771461000	0.559568000	0.128478000
C	3.924804000	-0.386908000	-0.467429000
C	3.628375000	-0.967952000	0.864309000
C	4.602794000	-1.127134000	1.856299000
H	5.640813000	-0.888133000	1.658716000
C	4.217160000	-1.620032000	3.099407000
H	4.954293000	-1.763268000	3.884213000
C	2.877691000	-1.921932000	3.325837000
H	2.541652000	-2.298652000	4.285491000
C	1.953491000	-1.765333000	2.286178000
C	2.275413000	-0.380606000	-3.815847000
H	2.768883000	-0.018974000	-4.723896000
H	1.378007000	0.234556000	-3.674968000
C	1.854027000	-1.867683000	-4.021950000
C	0.488422000	-2.053907000	2.485284000
H	-0.085129000	-1.283284000	1.963039000
H	0.270383000	-1.978553000	3.557304000
C	0.021566000	-3.451055000	1.972879000
S	-0.603114000	2.458177000	-2.638558000
S	-0.175470000	3.509539000	0.415391000
N	-3.079708000	0.738277000	-1.164553000
N	-2.200099000	1.217367000	1.353028000
C	-3.427097000	0.390361000	-2.420894000
C	-4.592714000	-0.354858000	-2.660294000
H	-4.841883000	-0.631117000	-3.678849000
C	-5.406363000	-0.736853000	-1.604704000
H	-6.296973000	-1.333769000	-1.777659000
C	-5.063748000	-0.334365000	-0.318815000
H	-5.669855000	-0.626969000	0.529425000
C	-3.899850000	0.414370000	-0.136382000
C	-3.491700000	0.868604000	1.214729000
C	-4.379509000	0.920638000	2.295471000
H	-5.429816000	0.691116000	2.162394000
C	-3.891492000	1.293372000	3.544364000

H	-4.559866000	1.350491000	4.398654000	H	-2.382068000	4.117492000	-1.568518000
C	-2.538887000	1.587703000	3.685772000	H	-6.498052000	3.883793000	-4.323859000
H	-2.124185000	1.871170000	4.646703000	H	-4.331915000	5.516019000	-0.985339000
C	-1.706129000	1.547966000	2.561090000	H	-6.414948000	5.402539000	-2.347584000
C	-2.586716000	0.787234000	-3.614109000	C	-1.701902000	2.678695000	-5.103128000
H	-3.190025000	0.551161000	-4.496543000	C	-1.531148000	1.764045000	-6.150092000
H	-1.697745000	0.146354000	-3.657315000	C	-1.451913000	4.037327000	-5.368882000
C	-2.144057000	2.278852000	-3.680756000	C	-1.145930000	2.196813000	-7.424553000
C	-0.231882000	1.839912000	2.663766000	C	-1.056883000	4.466157000	-6.632219000
H	0.302781000	1.129583000	2.027119000	C	-0.907298000	3.545830000	-7.473837000
H	0.075873000	1.673480000	3.702943000	H	-1.684926000	0.702202000	-5.993210000
C	0.179679000	3.284587000	2.243834000	H	-1.570939000	4.762313000	-4.569823000
C	-1.476611000	-3.669565000	2.246025000	H	-1.042150000	1.468384000	-8.224419000
C	-2.035462000	-4.927903000	1.956701000	H	-0.871333000	5.523109000	-6.805823000
C	-2.323165000	-2.684970000	2.770912000	H	-0.609750000	3.878597000	-8.664802000
C	-3.383518000	-5.188921000	2.179027000				
C	-3.679610000	-2.946527000	2.998877000				
C	-4.217543000	-4.196502000	2.704748000				
H	-1.398069000	-5.705498000	1.547092000				
H	-1.943363000	-1.698281000	3.012246000				
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H	-4.308573000	-2.162436000	3.413751000				
H	-5.269939000	-4.400782000	2.884586000				
C	0.841600000	-4.534985000	2.711465000				
C	0.581394000	-4.762213000	4.075455000				
C	1.870262000	-5.267892000	2.109209000				
C	1.328353000	-5.681157000	4.811305000				
C	2.617302000	-6.194299000	2.843968000				
C	2.354209000	-6.404072000	4.196576000				
H	-0.228802000	-4.225713000	4.562650000				
H	2.075712000	-5.117669000	1.055042000				
H	1.101186000	-5.840175000	5.862667000				
H	3.405385000	-6.756348000	2.348747000				
H	2.933491000	-7.127064000	4.765073000				
C	1.691054000	3.504005000	2.425221000				
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C	2.213292000	4.793407000	2.215473000				
C	3.952641000	2.751128000	2.936588000				
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H	2.235047000	1.477652000	2.962132000				
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H	3.944620000	6.062216000	2.188648000				
H	5.514775000	4.236988000	2.841171000				
C	-0.600450000	4.284224000	3.128645000				
C	-1.701977000	5.017001000	2.672485000				
C	-0.231262000	4.420560000	4.479348000				
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H	-1.991877000	4.934535000	1.630663000				
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H	-0.631243000	5.343260000	6.380697000				
H	-2.593753000	6.632215000	5.541968000				
C	3.085135000	-2.784489000	-3.842375000				
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C	4.159138000	-2.639582000	-4.739002000				
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C	5.310271000	-3.416056000	-4.619420000				
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H	2.373977000	-3.883677000	-2.139194000				
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H	6.124245000	-3.284650000	-5.328274000				
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C	1.268947000	-2.100101000	-5.428659000				
C	1.063121000	-3.422391000	-5.861651000				
C	0.915182000	-1.062017000	-6.300084000				
C	0.535194000	-3.697048000	-7.119680000				
C	0.394711000	-1.338100000	-7.569508000				
C	0.202525000	-2.652781000	-7.987263000				
H	1.323238000	-4.242247000	-5.199550000				
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C	-4.496407000	3.152290000	-4.037021000				
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