Electronic Supplementary Information for Dalton Transactions

SUPPORTING INFORMATION

The role of substrate in unmasking oxyl character in oxomanganese complexes: the key to selectivity?

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Optimised cartesian coordinates (Å) of (HO)(Porp)Mn(O) with B3LYP.

Singlet Energy = -1243.556829 au

N	1.427151000	1.467340000	-0.002295000
N	1.439534000	-1.448292000	-0.108931000
N	-1.475816000	-1.425771000	0.000094000
N	-1.433382000	1.435054000	0.012229000
C	1.242013000	2.824889000	-0.009478000
C	2.527549000	3.495135000	-0.035709000
C	3.481450000	2.518553000	-0.046301000
C	2.787692000	1.243383000	-0.028526000
C	3.420853000	0.003613000	-0.042421000
C	2.798659000	-1.243497000	-0.054988000
C	3.477228000	-2.524655000	-0.009276000
C	2.508908000	-3.489625000	-0.008597000
C	1.230062000	-2.806672000	-0.053874000
C	-0.019170000	-3.424567000	-0.039866000
C	-1.256726000	-2.787080000	-0.025276000
C	-2.534382000	-3.476346000	-0.041158000
C	-3.507544000	-2.518969000	-0.030265000
C	-2.832657000	-1.235794000	-0.005718000
C	-3.457035000	0.009166000	-0.000741000
C	-2.807365000	1.235925000	-0.002219000
C	-3.475922000	2.517056000	-0.020613000
C	-2.508570000	3.481171000	-0.021618000
C	-1.229685000	2.808328000	-0.003837000
C	-0.000683000	3.453736000	-0.004152000
H	2.664263000	4.566699000	-0.047454000
H	4.555763000	2.631810000	-0.068225000
H	4.549513000	-2.653616000	0.023821000
H	2.634180000	-4.562327000	0.025148000
H	-2.651473000	-4.550267000	-0.062147000
H	-4.579601000	-2.651873000	-0.040759000
H	-4.548424000	2.646116000	-0.033714000
H	-2.634047000	4.554085000	-0.035699000
H	-0.029692000	-4.509643000	-0.030244000
H	4.505965000	0.010399000	-0.033546000
H	-0.012006000	4.538248000	-0.012648000
H	-4.541512000	0.024333000	-0.008064000
Mn	-0.052589000	0.049532000	0.069107000

O	0.175257000	-0.178792000	1.587056000
O	0.009201000	-0.014851000	-1.747276000
H	0.652766000	-0.662106000	-2.081893000

Triplet Energy = -1243.564922 au

N	1.447970000	1.446498000	-0.033652000
N	1.430182000	-1.438260000	-0.049422000
N	-1.454796000	-1.447044000	-0.030129000
N	-1.433808000	1.434564000	0.010267000
C	1.245272000	2.806817000	-0.028687000
C	2.526992000	3.484729000	-0.029484000
C	3.490347000	2.518556000	-0.030799000
C	2.808532000	1.238746000	-0.030796000
C	3.439436000	0.000579000	-0.026211000
C	2.798777000	-1.233877000	-0.025971000
C	3.467597000	-2.513262000	-0.004638000
C	2.498783000	-3.479011000	-0.003560000
C	1.221494000	-2.806175000	-0.024211000
C	-0.014965000	-3.442947000	-0.022299000
C	-1.251188000	-2.808229000	-0.026100000
C	-2.533071000	-3.486130000	-0.023702000
C	-3.496300000	-2.519827000	-0.022668000
C	-2.814470000	-1.240183000	-0.023786000
C	-3.443483000	-0.001473000	-0.011636000
C	-2.799727000	1.230555000	-0.001134000
C	-3.471120000	2.510477000	-0.010075000
C	-2.503307000	3.475234000	-0.011250000
C	-1.225500000	2.799816000	-0.003113000
C	0.008530000	3.439678000	-0.015876000
H	2.652293000	4.557652000	-0.027154000
H	4.563669000	2.640617000	-0.029885000
H	4.540020000	-2.642016000	0.009870000
H	2.624160000	-4.551819000	0.011994000
H	-2.658402000	-4.559073000	-0.021399000
H	-4.569597000	-2.641854000	-0.019132000
H	-4.543735000	2.637696000	-0.018495000
H	-2.627151000	4.548234000	-0.020827000
H	-0.012358000	-4.527118000	-0.010529000
H	4.523605000	-0.005397000	-0.015600000
H	0.003660000	4.523851000	-0.018592000
H	-4.527637000	0.006784000	-0.013085000
Mn	-0.007910000	0.004215000	-0.034697000
O	0.074497000	-0.076197000	1.742463000
O	-0.055815000	0.049904000	-1.882101000
H	0.578251000	-0.585482000	-2.253974000

Quintet Energy = -1243.560524 au

N	1.429778000	1.422090000	0.047617000
N	1.441211000	-1.449488000	-0.155036000
N	-1.430142000	-1.428988000	0.051810000
N	-1.445121000	1.445964000	-0.104045000
C	1.227513000	2.789978000	0.043401000
C	2.505966000	3.462042000	0.070118000
C	3.471844000	2.494717000	0.067862000
C	2.797070000	1.217581000	0.039304000
C	3.438436000	-0.013840000	-0.029160000
C	2.806459000	-1.248715000	-0.105061000
C	3.481490000	-2.528929000	-0.087658000

C	2.514281000	-3.493093000	-0.086553000
C	1.236164000	-2.814067000	-0.103286000
C	-0.000556000	-3.442090000	-0.025106000
C	-1.229925000	-2.796824000	0.044198000
C	-2.509137000	-3.467685000	0.074444000
C	-3.473428000	-2.498798000	0.076610000
C	-2.797294000	-1.222468000	0.048349000
C	-3.438101000	0.009139000	-0.013252000
C	-2.805958000	1.244050000	-0.081130000
C	-3.484390000	2.525209000	-0.089013000
C	-2.518191000	3.488490000	-0.090114000
C	-1.239098000	2.806177000	-0.082969000
C	-0.002125000	3.434576000	-0.017367000
H	2.632612000	4.534744000	0.077580000
H	4.544788000	2.619528000	0.073023000
H	4.553986000	-2.655330000	-0.061030000
H	2.637337000	-4.565952000	-0.058838000
H	-2.637252000	-4.540233000	0.080591000
H	-4.546518000	-2.622052000	0.084997000
H	-4.557285000	2.650309000	-0.081886000
H	-2.640037000	4.561765000	-0.084087000
H	-0.008160000	-4.526159000	-0.005992000
H	4.522538000	-0.009579000	-0.011075000
H	0.006315000	4.518749000	-0.009352000
H	-4.522289000	0.004109000	-0.004196000
Mn	-0.005819000	0.002378000	-0.095717000
O	0.018518000	-0.016962000	1.739511000
O	-0.058057000	0.050941000	-1.933052000
H	0.582302000	-0.591456000	-2.284518000

Optimised cartesian coordinates (Å) of (HO)(Porp)Mn(O) with BLYP.

Singlet Energy = -1243. 221349 au

N	1.468743000	1.440706000	0.014057000
N	1.507682000	-1.445684000	0.006699000
N	-1.433793000	-1.463954000	-0.124784000
N	-1.418590000	1.477983000	-0.012048000
C	1.265506000	2.829643000	-0.004602000
C	2.554548000	3.502422000	-0.016393000
C	3.529568000	2.528385000	-0.009050000
C	2.857916000	1.238825000	0.007262000
C	3.506846000	-0.001103000	0.014510000
C	2.879314000	-1.256297000	0.008232000
C	3.554700000	-2.550724000	-0.009938000
C	2.571850000	-3.514712000	-0.024298000
C	1.285101000	-2.820768000	-0.017034000
C	0.034813000	-3.457906000	-0.037752000
C	-1.224666000	-2.836794000	-0.060134000
C	-2.514650000	-3.520135000	-0.012864000
C	-3.489810000	-2.545677000	-0.017884000
C	-2.807220000	-1.255429000	-0.068455000
C	-3.429454000	0.003621000	-0.056797000
C	-2.793312000	1.254537000	-0.041072000
C	-3.487932000	2.540861000	-0.061050000
C	-2.524481000	3.524264000	-0.049097000
C	-1.229834000	2.849549000	-0.019401000
C	0.025106000	3.477678000	-0.010387000
H	2.684185000	4.582253000	-0.030660000

H	4.609350000	2.659003000	-0.016231000
H	4.633726000	-2.687535000	-0.014354000
H	2.689316000	-4.596029000	-0.042490000
H	-2.643604000	-4.599658000	0.025449000
H	-4.569425000	-2.675239000	0.015515000
H	-4.569205000	2.657625000	-0.085449000
H	-2.661735000	4.603168000	-0.061963000
H	0.043559000	-4.550559000	-0.024015000
H	4.599016000	0.012221000	0.013756000
H	0.037866000	4.569829000	-0.019079000
H	-4.522168000	0.011552000	-0.048628000
Mn	0.075744000	0.046730000	0.068126000
O	-0.165116000	-0.181494000	1.618110000
O	0.022594000	-0.016269000	-1.778007000
H	-0.638414000	-0.671147000	-2.097880000

Triplet Energy = -1243.208104 au

N	1.444624000	1.477630000	-0.016018000
N	1.456506000	-1.474763000	-0.052810000
N	-1.453231000	-1.441786000	-0.061228000
N	-1.444363000	1.454346000	0.009533000
C	1.254960000	2.849106000	0.048341000
C	2.551013000	3.520031000	0.018832000
C	3.510536000	2.537247000	-0.069375000
C	2.815445000	1.251933000	-0.083931000
C	3.449021000	0.001102000	-0.123634000
C	2.827913000	-1.254951000	-0.086440000
C	3.517777000	-2.542476000	-0.038582000
C	2.551791000	-3.520439000	0.046240000
C	1.256395000	-2.845580000	0.042390000
C	0.000600000	-3.466563000	0.081078000
C	-1.243932000	-2.820733000	0.025994000
C	-2.532837000	-3.501587000	0.010152000
C	-3.508173000	-2.533044000	-0.081045000
C	-2.830790000	-1.243897000	-0.112027000
C	-3.463347000	0.006782000	-0.138326000
C	-2.823597000	1.250604000	-0.077290000
C	-3.499519000	2.540476000	-0.069223000
C	-2.528189000	3.511784000	0.024458000
C	-1.238718000	2.835537000	0.063276000
C	0.004213000	3.479865000	0.100002000
H	2.690065000	4.598011000	0.054478000
H	4.590985000	2.652509000	-0.116582000
H	4.598365000	-2.664238000	-0.061768000
H	2.687518000	-4.598238000	0.100384000
H	-2.658356000	-4.580915000	0.058011000
H	-4.587261000	-2.664112000	-0.114603000
H	-4.577907000	2.669034000	-0.125761000
H	-2.655782000	4.591369000	0.054487000
H	-0.013675000	-4.556837000	0.143736000
H	4.540845000	0.007933000	-0.157748000
H	-0.004554000	4.570992000	0.140221000
H	-4.554294000	0.012279000	-0.184474000
Mn	-0.016604000	0.031842000	0.039945000
O	0.183321000	-0.156293000	1.677351000
O	0.180377000	0.016880000	-1.850104000
H	-0.163500000	-0.837096000	-2.198019000

Quintet Energy = -1243.190475 au

N	1.449927000	1.447396000	-0.006561000
N	1.457343000	-1.455874000	-0.132111000
N	-1.449185000	-1.450355000	0.045995000
N	-1.447491000	1.465170000	-0.079837000
C	1.247203000	2.832364000	0.043688000
C	2.538244000	3.502221000	0.100864000
C	3.510761000	2.526872000	0.076907000
C	2.835087000	1.239293000	0.007216000
C	3.468481000	-0.004807000	-0.067566000
C	2.832910000	-1.256788000	-0.114230000
C	3.514113000	-2.545849000	-0.089035000
C	2.539226000	-3.518180000	-0.054604000
C	1.251005000	-2.835319000	-0.063955000
C	0.002161000	-3.464230000	0.015070000
C	-1.247676000	-2.824449000	0.046852000
C	-2.537373000	-3.505768000	0.041245000
C	-3.508709000	-2.528822000	0.019490000
C	-2.821094000	-1.242614000	0.015067000
C	-3.456349000	0.009343000	-0.031487000
C	-2.824547000	1.256926000	-0.074961000
C	-3.509835000	2.546412000	-0.079421000
C	-2.538044000	3.520298000	-0.069617000
C	-1.247792000	2.836199000	-0.057652000
C	0.004249000	3.470069000	-0.001052000
H	2.669369000	4.580921000	0.143581000
H	4.590612000	2.653894000	0.097094000
H	4.594098000	-2.673593000	-0.082384000
H	2.665197000	-4.597712000	-0.015160000
H	-2.665899000	-4.585662000	0.041706000
H	-4.589074000	-2.651745000	0.000727000
H	-4.590200000	2.670811000	-0.080954000
H	-2.664521000	4.600378000	-0.063205000
H	-0.000693000	-4.556013000	0.047788000
H	4.560601000	-0.004446000	-0.059013000
H	0.007030000	4.561925000	0.021081000
H	-4.548619000	0.007716000	-0.035234000
Mn	0.013821000	0.021880000	-0.053134000
O	0.158475000	0.114659000	1.724786000
O	-0.168615000	-0.043566000	-1.961599000
H	0.405529000	-0.769128000	-2.296461000

Optimised cartesian coordinates (Å) of $[(H_2O)(Porp)Mn(O)]^+$ with B3LYP.

Singlet Energy = -1243.964562 au

N	1.395639000	1.391396000	-0.016428000
N	1.392406000	-1.422117000	-0.008530000
N	-1.408500000	-1.428517000	-0.040070000
N	-1.405664000	1.401386000	-0.057223000
C	1.214002000	2.772322000	0.044588000
C	2.487923000	3.440419000	0.000056000
C	3.447011000	2.473896000	-0.105136000
C	2.771772000	1.203335000	-0.108545000
C	3.415724000	-0.017707000	-0.163286000
C	2.769524000	-1.237168000	-0.099430000
C	3.442450000	-2.508576000	-0.081606000
C	2.481755000	-3.472555000	0.033506000
C	1.208862000	-2.802527000	0.069798000

C	-0.009682000	-3.451436000	0.128789000
C	-1.231747000	-2.806034000	0.067563000
C	-2.506463000	-3.471460000	0.062603000
C	-3.465769000	-2.503959000	-0.047026000
C	-2.788092000	-1.235866000	-0.094792000
C	-3.430567000	-0.012364000	-0.151312000
C	-2.786113000	1.210523000	-0.107761000
C	-3.461287000	2.480210000	-0.071764000
C	-2.500148000	3.447060000	0.027691000
C	-1.226559000	2.779797000	0.038199000
C	-0.003577000	3.423739000	0.094598000
H	2.616179000	4.511834000	0.037435000
H	4.517974000	2.595438000	-0.167652000
H	4.513303000	-2.632529000	-0.141297000
H	2.608610000	-4.543632000	0.083517000
H	-2.637766000	-4.540926000	0.132169000
H	-4.538267000	-2.624427000	-0.080814000
H	-4.533598000	2.602323000	-0.105599000
H	-2.629636000	4.517356000	0.087141000
H	-0.007514000	-4.532400000	0.198651000
H	4.496622000	-0.019015000	-0.234012000
H	0.000174000	4.505396000	0.152693000
H	-4.513214000	-0.011661000	-0.192250000
Mn	0.003541000	-0.012795000	0.296915000
O	-0.036008000	-0.006032000	1.803213000
O	0.074357000	-0.015058000	-2.077208000
H	-0.359915000	-0.822491000	-2.401232000
H	-0.477119000	0.722126000	-2.390563000

Triplet Energy = -1243.979974 au

N	1.423768000	1.423757000	-0.089528000
N	1.421439000	-1.460983000	-0.068267000
N	-1.462570000	-1.462661000	-0.001491000
N	-1.460389000	1.421704000	-0.068061000
C	1.236737000	2.775330000	-0.056990000
C	2.510975000	3.462763000	-0.031031000
C	3.479512000	2.499217000	-0.033401000
C	2.799646000	1.220327000	-0.060842000
C	3.417661000	-0.017291000	-0.046642000
C	2.774942000	-1.272833000	-0.044713000
C	3.460898000	-2.546413000	-0.002742000
C	2.496437000	-3.514635000	0.016263000
C	1.217977000	-2.835690000	-0.014449000
C	-0.019476000	-3.453954000	0.020073000
C	-1.274803000	-2.811309000	0.021100000
C	-2.550638000	-3.500567000	0.049028000
C	-3.518194000	-2.538471000	0.047699000
C	-2.837364000	-1.257998000	0.018071000
C	-3.454763000	-0.022317000	0.009569000
C	-2.811122000	1.234108000	-0.020329000
C	-3.498174000	2.507741000	0.013338000
C	-2.535208000	3.477217000	0.003471000
C	-1.256093000	2.799154000	-0.038169000
C	-0.019554000	3.417735000	-0.038416000
H	2.634852000	4.535054000	-0.007704000
H	4.551322000	2.628650000	-0.013319000
H	4.533207000	-2.670865000	0.015872000
H	2.625832000	-4.586030000	0.051895000
H	-2.673074000	-4.573047000	0.068148000

H	-4.590091000	-2.666993000	0.064160000
H	-4.570232000	2.631001000	0.046729000
H	-2.665478000	4.548898000	0.025473000
H	-0.029155000	-4.538080000	0.058287000
H	4.502135000	-0.028009000	-0.019159000
H	-0.009377000	4.502112000	-0.007385000
H	-4.539142000	-0.010400000	0.037663000
Mn	-0.022190000	-0.022386000	0.098231000
O	0.009070000	0.009230000	1.732519000
O	-0.096818000	-0.096849000	-2.172739000
H	0.752061000	-0.352762000	-2.570264000
H	-0.336637000	0.756165000	-2.571413000

Quintet Energy = -1243.980181 au

N	1.427812000	1.422655000	-0.087550000
N	1.420880000	-1.463751000	-0.070449000
N	-1.465808000	-1.461478000	-0.005413000
N	-1.458468000	1.425566000	-0.069359000
C	1.235886000	2.786548000	-0.057579000
C	2.511029000	3.466983000	-0.031028000
C	3.476519000	2.497777000	-0.031688000
C	2.791318000	1.225275000	-0.058617000
C	3.417479000	-0.024328000	-0.042226000
C	2.786759000	-1.271061000	-0.041881000
C	3.465281000	-2.546120000	0.002608000
C	2.494865000	-3.510813000	0.016062000
C	1.223036000	-2.825824000	-0.019336000
C	-0.026702000	-3.453049000	0.013044000
C	-1.272923000	-2.823260000	0.018484000
C	-2.549911000	-3.505252000	0.051327000
C	-3.514001000	-2.537439000	0.050646000
C	-2.827217000	-1.263124000	0.017478000
C	-3.452542000	-0.015154000	0.011499000
C	-2.820924000	1.232916000	-0.019835000
C	-3.501373000	2.507336000	0.014680000
C	-2.533065000	3.474147000	0.002238000
C	-1.260460000	2.791022000	-0.040962000
C	-0.011967000	3.417250000	-0.040811000
H	2.640557000	4.538677000	-0.009039000
H	4.548753000	2.623026000	-0.010341000
H	4.536841000	-2.676595000	0.025702000
H	2.619357000	-4.582707000	0.052362000
H	-2.678157000	-4.577050000	0.072440000
H	-4.586335000	-2.661384000	0.071103000
H	-4.572801000	2.635961000	0.049735000
H	-2.659431000	4.546226000	0.024944000
H	-0.026994000	-4.537581000	0.047321000
H	4.502187000	-0.026361000	-0.012270000
H	-0.009979000	4.501952000	-0.010621000
H	-4.537109000	-0.011543000	0.044506000
Mn	-0.020358000	-0.020666000	0.093827000
O	0.005828000	0.004537000	1.728507000
O	-0.098799000	-0.095201000	-2.173262000
H	0.746264000	-0.351205000	-2.578551000
H	-0.347399000	0.752710000	-2.577162000

Optimised cartesian coordinates (Å) of $[(H_2O)(Porp)Mn(O)]^+$ with BLYP.

Singlet Energy = -1243.623603 au

N	1.414697000	1.402961000	-0.006363000
N	1.411696000	-1.433878000	0.003729000
N	-1.423939000	-1.444255000	-0.046098000
N	-1.421579000	1.416933000	-0.063593000
C	1.226681000	2.800517000	0.007968000
C	2.510094000	3.471517000	-0.028206000
C	3.482291000	2.496099000	-0.082681000
C	2.807915000	1.214863000	-0.070445000
C	3.455209000	-0.017544000	-0.099438000
C	2.805818000	-1.248521000	-0.059549000
C	3.478008000	-2.530772000	-0.057108000
C	2.504359000	-3.504219000	0.007219000
C	1.221893000	-2.831395000	0.034882000
C	-0.008175000	-3.483151000	0.064803000
C	-1.243582000	-2.836574000	0.028390000
C	-2.528051000	-3.505306000	0.038927000
C	-3.498060000	-2.526863000	-0.024056000
C	-2.818093000	-1.248056000	-0.066363000
C	-3.462868000	-0.012240000	-0.100775000
C	-2.816371000	1.222904000	-0.079438000
C	-3.493955000	2.503210000	-0.048133000
C	-2.522156000	3.480510000	0.005011000
C	-1.238812000	2.809719000	-0.000702000
C	-0.002374000	3.454482000	0.030133000
H	2.638269000	4.550813000	-0.015608000
H	4.561223000	2.621447000	-0.121367000
H	4.556799000	-2.658173000	-0.093044000
H	2.631150000	-4.583470000	0.032269000
H	-2.660425000	-4.582895000	0.091633000
H	-4.578186000	-2.648841000	-0.030735000
H	-4.573870000	2.627065000	-0.054654000
H	-2.652715000	4.558745000	0.048165000
H	-0.004795000	-4.573182000	0.104550000
H	4.544897000	-0.018745000	-0.146784000
H	0.002749000	4.544862000	0.058646000
H	-4.553698000	-0.011560000	-0.116506000
Mn	0.011733000	-0.013146000	0.300105000
O	-0.049390000	-0.005075000	1.844818000
O	0.081874000	-0.016359000	-2.103670000
H	-0.398709000	-0.824263000	-2.391247000
H	-0.496934000	0.729142000	-2.379099000

Triplet Energy = -1243.615996 au

N	1.410201000	1.443559000	-0.134170000
N	1.406842000	-1.475403000	-0.143358000
N	-1.474938000	-1.450512000	0.016936000
N	-1.466941000	1.420420000	-0.007229000
C	1.230655000	2.815880000	0.040416000
C	2.520092000	3.486705000	0.043816000
C	3.483072000	2.512244000	-0.116998000
C	2.792258000	1.234354000	-0.200043000
C	3.421793000	-0.017573000	-0.266008000
C	2.790393000	-1.268150000	-0.191046000
C	3.478507000	-2.544388000	-0.074537000
C	2.512661000	-3.514587000	0.095847000
C	1.223727000	-2.843983000	0.065404000
C	-0.026632000	-3.470874000	0.183042000

C	-1.272325000	-2.833215000	0.127296000
C	-2.556993000	-3.514039000	0.099438000
C	-3.529878000	-2.548732000	-0.041203000
C	-2.856315000	-1.261473000	-0.080397000
C	-3.491836000	-0.014682000	-0.146593000
C	-2.851585000	1.229793000	-0.102306000
C	-3.521810000	2.518193000	-0.082024000
C	-2.548991000	3.485085000	0.048353000
C	-1.264705000	2.806746000	0.087961000
C	-0.019938000	3.445117000	0.145287000
H	2.660928000	4.559188000	0.150347000
H	4.562171000	2.635519000	-0.160828000
H	4.557975000	-2.669255000	-0.101456000
H	2.651684000	-4.584452000	0.228170000
H	-2.683646000	-4.591728000	0.161496000
H	-4.606340000	-2.683484000	-0.106321000
H	-4.598065000	2.652948000	-0.150593000
H	-2.676140000	4.563364000	0.097695000
H	-0.030626000	-4.556003000	0.301673000
H	4.512801000	-0.018497000	-0.307978000
H	-0.024993000	4.531861000	0.247599000
H	-4.581618000	-0.012333000	-0.205513000
Mn	-0.070802000	-0.007447000	0.137391000
O	0.143070000	-0.027165000	1.753167000
O	-0.121055000	-0.033890000	-2.136947000
H	0.423562000	-0.807082000	-2.408678000
H	0.379854000	0.754144000	-2.446573000

Quintet Energy = -1243.609406 au

N	1.437894000	1.432518000	-0.088278000
N	1.430472000	-1.473769000	-0.069964000
N	-1.475547000	-1.471127000	-0.004305000
N	-1.468338000	1.435172000	-0.069117000
C	1.244855000	2.811731000	-0.056580000
C	2.531022000	3.494314000	-0.029666000
C	3.504085000	2.517656000	-0.030202000
C	2.816843000	1.234031000	-0.057430000
C	3.445501000	-0.024370000	-0.039964000
C	2.811652000	-1.279997000	-0.039853000
C	3.492419000	-2.565933000	0.005255000
C	2.514694000	-3.538326000	0.018868000
C	1.231660000	-2.851593000	-0.016932000
C	-0.026600000	-3.481266000	0.015713000
C	-1.281702000	-2.848465000	0.020477000
C	-2.569455000	-3.532275000	0.052900000
C	-3.541181000	-2.556928000	0.052229000
C	-2.852669000	-1.271756000	0.019544000
C	-3.480754000	-0.014950000	0.014183000
C	-2.846422000	1.241660000	-0.017581000
C	-3.528647000	2.527201000	0.017490000
C	-2.552721000	3.501399000	0.004717000
C	-1.269189000	2.816062000	-0.039116000
C	-0.011820000	3.445159000	-0.038767000
H	2.661626000	4.573125000	-0.008277000
H	4.583404000	2.644177000	-0.009344000
H	4.571110000	-2.697375000	0.027522000
H	2.640653000	-4.617299000	0.054546000
H	-2.698825000	-4.611189000	0.073084000
H	-4.620602000	-2.682177000	0.071775000

H	-4.607170000	2.657160000	0.052081000
H	-2.680198000	4.580585000	0.026610000
H	-0.027164000	-4.573077000	0.051032000
H	4.537469000	-0.026673000	-0.008411000
H	-0.009946000	4.537123000	-0.007025000
H	-4.572598000	-0.011439000	0.048321000
Mn	-0.020699000	-0.021070000	0.089297000
O	0.005674000	0.004459000	1.755581000
O	-0.106544000	-0.103178000	-2.205015000
H	0.754328000	-0.349439000	-2.608403000
H	-0.348642000	0.759758000	-2.606460000

Optimised cartesian coordinates (Å) of the various stationary points on the potential energy surface for the reaction of (HO)(Porp)Mn(O) with Me_2S with B3LYP.

^{1}R Energy = -1721. 550232 au

N	1.461889000	1.587641000	-0.123418000
N	1.280991000	-1.225822000	0.428445000
N	-1.563504000	-1.151078000	0.256976000
N	-1.437609000	1.689384000	-0.401555000
C	1.309949000	2.927263000	-0.408082000
C	2.618551000	3.553296000	-0.475688000
C	3.542756000	2.577759000	-0.234017000
C	2.805432000	1.347953000	-0.014734000
C	3.366670000	0.101774000	0.256275000
C	2.662382000	-1.078992000	0.448505000
C	3.274626000	-2.362541000	0.706602000
C	2.267678000	-3.276327000	0.835818000
C	1.020005000	-2.569232000	0.659145000
C	-0.236334000	-3.157443000	0.711218000
C	-1.444220000	-2.493005000	0.515915000
C	-2.757496000	-3.105032000	0.541964000
C	-3.661317000	-2.112497000	0.290130000
C	-2.909537000	-0.885519000	0.106009000
C	-3.482845000	0.349549000	-0.180170000
C	-2.804518000	1.547821000	-0.392589000
C	-3.425444000	2.837339000	-0.626928000
C	-2.415466000	3.750261000	-0.746935000
C	-1.168404000	3.026436000	-0.586752000
C	0.104351000	3.593470000	-0.612919000
H	2.788470000	4.599426000	-0.686108000
H	4.619214000	2.665376000	-0.206818000
H	4.340078000	-2.528267000	0.773887000
H	2.347393000	-4.336215000	1.029248000
H	-2.945686000	-4.153353000	0.723089000
H	-4.737346000	-2.186774000	0.226797000
H	-4.491003000	3.007790000	-0.679834000
H	-2.492648000	4.814018000	-0.920240000
H	-0.277221000	-4.223597000	0.906074000
H	4.448450000	0.043988000	0.311856000
H	0.162289000	4.660223000	-0.803641000
H	-4.566146000	0.383947000	-0.228268000
Mn	-0.038245000	0.193054000	0.143426000
O	-0.296127000	0.741575000	1.575215000
O	0.019275000	-0.071918000	-1.654584000
H	-0.503105000	0.581292000	-2.150209000
S	-2.836753000	0.886962000	3.978146000
C	-1.490048000	2.026701000	4.462671000

H	-1.133454000	1.809859000	5.474803000
H	-0.663368000	1.960655000	3.750270000
H	-1.899274000	3.040614000	4.442545000
C	-1.946794000	-0.706960000	4.101438000
H	-2.644132000	-1.493320000	3.799789000
H	-1.089628000	-0.717019000	3.423164000
H	-1.615970000	-0.897628000	5.127509000

^{3}R Energy = -1721.562297 au

N	1.353523000	1.570256000	-0.037659000
N	1.293893000	-1.289595000	0.352809000
N	-1.563562000	-1.284372000	-0.056052000
N	-1.524839000	1.593443000	-0.235231000
C	1.170378000	2.926809000	-0.184876000
C	2.457245000	3.590457000	-0.145252000
C	3.402653000	2.622362000	0.036674000
C	2.705487000	1.354833000	0.112487000
C	3.314273000	0.123938000	0.326988000
C	2.656951000	-1.096228000	0.434231000
C	3.307972000	-2.372861000	0.635129000
C	2.329150000	-3.325560000	0.660027000
C	1.066020000	-2.644685000	0.472534000
C	-0.172665000	-3.271712000	0.395191000
C	-1.387689000	-2.637454000	0.161742000
C	-2.674573000	-3.297286000	0.130596000
C	-3.618563000	-2.331662000	-0.079052000
C	-2.922259000	-1.067696000	-0.177638000
C	-3.535217000	0.169994000	-0.337305000
C	-2.882933000	1.396776000	-0.366990000
C	-3.533554000	2.674699000	-0.563564000
C	-2.556759000	3.628258000	-0.560491000
C	-1.295005000	2.946838000	-0.362895000
C	-0.053002000	3.569448000	-0.335030000
H	2.599478000	4.656830000	-0.242730000
H	4.473568000	2.737861000	0.118611000
H	4.375265000	-2.506195000	0.735183000
H	2.436302000	-4.393343000	0.783665000
H	-2.821185000	-4.359417000	0.262707000
H	-4.690190000	-2.447341000	-0.151484000
H	-4.598497000	2.805964000	-0.687059000
H	-2.662088000	4.696221000	-0.683262000
H	-0.192617000	-4.347708000	0.527868000
H	4.394573000	0.114276000	0.419377000
H	-0.036964000	4.647897000	-0.445900000
H	-4.614928000	0.180255000	-0.435271000
Mn	-0.106546000	0.154435000	-0.001626000
O	-0.285525000	0.308712000	1.759201000
O	0.126475000	-0.001695000	-1.824141000
H	-0.463572000	-0.694381000	-2.166528000
S	-2.486119000	1.794444000	4.039547000
C	-0.774954000	2.336547000	4.402867000
H	-0.518738000	2.154231000	5.451670000
H	-0.072578000	1.819702000	3.744383000
H	-0.726432000	3.411788000	4.208870000
C	-2.317878000	0.006935000	4.397171000
H	-3.293355000	-0.454089000	4.218144000
H	-1.579986000	-0.437442000	3.724632000
H	-2.033622000	-0.160601000	5.441171000

^{5}R Energy = -1721.555707 au

N	1.310342000	1.561342000	-0.032875000
N	1.263221000	-1.288014000	0.377792000
N	-1.566713000	-1.339884000	-0.149422000
N	-1.561957000	1.536330000	-0.214980000
C	1.111543000	2.915693000	-0.173355000
C	2.387252000	3.600049000	-0.103480000
C	3.341280000	2.646662000	0.104573000
C	2.659027000	1.369197000	0.163010000
C	3.272119000	0.149602000	0.420403000
C	2.622272000	-1.074991000	0.518327000
C	3.284024000	-2.340257000	0.737455000
C	2.322225000	-3.311240000	0.703760000
C	1.058833000	-2.652740000	0.464236000
C	-0.156968000	-3.308032000	0.306081000
C	-1.373897000	-2.695079000	0.034317000
C	-2.648487000	-3.376531000	-0.038531000
C	-3.605688000	-2.420118000	-0.225690000
C	-2.928046000	-1.142362000	-0.271255000
C	-3.558614000	0.091828000	-0.370455000
C	-2.921503000	1.326659000	-0.343702000
C	-3.589702000	2.598522000	-0.499261000
C	-2.624636000	3.565380000	-0.486086000
C	-1.353624000	2.898291000	-0.320234000
C	-0.121761000	3.540686000	-0.307942000
H	2.514707000	4.669046000	-0.192127000
H	4.407285000	2.777836000	0.219951000
H	4.348049000	-2.456657000	0.882879000
H	2.443981000	-4.378648000	0.816467000
H	-2.778612000	-4.444347000	0.060702000
H	-4.674817000	-2.549598000	-0.310492000
H	-4.657249000	2.718830000	-0.610913000
H	-2.745753000	4.634164000	-0.584140000
H	-0.156375000	-4.386831000	0.415037000
H	4.348050000	0.151305000	0.554563000
H	-0.125516000	4.620604000	-0.404198000
H	-4.638342000	0.093121000	-0.469053000
Mn	-0.129064000	0.118782000	-0.056090000
O	-0.357923000	0.260324000	1.764244000
O	0.132827000	-0.000624000	-1.871134000
H	-0.480773000	-0.661034000	-2.236840000
S	-2.222129000	2.098543000	4.087106000
C	-0.429533000	2.288567000	4.407881000
H	-0.184457000	2.028688000	5.442929000
H	0.136823000	1.664005000	3.712630000
H	-0.177814000	3.339349000	4.238422000
C	-2.393064000	0.300621000	4.388695000
H	-3.439426000	0.038140000	4.208389000
H	-1.756201000	-0.250696000	3.692528000
H	-2.138408000	0.048403000	5.423319000

^{3}I Energy = -1721.565504 au

N	1.348225000	1.649470000	0.009382000
N	1.208646000	-1.217773000	0.382354000
N	-1.670528000	-1.103198000	0.196892000
N	-1.528160000	1.736448000	-0.253271000
C	1.204432000	3.004463000	-0.163366000
C	2.514411000	3.629977000	-0.172859000

C	3.433246000	2.633680000	-0.014576000
C	2.694618000	1.389124000	0.102225000
C	3.268504000	0.137091000	0.298522000
C	2.577132000	-1.061702000	0.449007000
C	3.190088000	-2.340978000	0.742792000
C	2.179567000	-3.251488000	0.873300000
C	0.936289000	-2.542088000	0.652267000
C	-0.331160000	-3.115953000	0.687493000
C	-1.531048000	-2.450447000	0.453298000
C	-2.832391000	-3.086192000	0.392090000
C	-3.739593000	-2.114440000	0.077879000
C	-3.006418000	-0.870928000	-0.046114000
C	-3.572990000	0.364315000	-0.341693000
C	-2.884502000	1.569826000	-0.427343000
C	-3.495315000	2.857721000	-0.685692000
C	-2.495876000	3.788301000	-0.660719000
C	-1.259503000	3.080038000	-0.396910000
C	-0.002302000	3.673688000	-0.337840000
H	2.687898000	4.689263000	-0.296032000
H	4.510091000	2.713741000	0.022278000
H	4.253895000	-2.502919000	0.840357000
H	2.253238000	-4.306423000	1.094993000
H	-3.008148000	-4.139990000	0.553868000
H	-4.806257000	-2.213734000	-0.062358000
H	-4.550269000	3.011549000	-0.860757000
H	-2.569424000	4.854916000	-0.816646000
H	-0.387097000	-4.180670000	0.887475000
H	4.350344000	0.093922000	0.364591000
H	0.042299000	4.749075000	-0.472634000
H	-4.644711000	0.392571000	-0.505038000
Mn	-0.174471000	0.277144000	0.116336000
O	-0.166895000	0.536147000	1.850116000
O	-0.035858000	0.041334000	-1.733685000
H	0.474857000	-0.764396000	-1.916283000
S	-2.140790000	0.658556000	3.185390000
C	-1.325019000	2.043785000	4.037897000
H	-1.628751000	2.095358000	5.087614000
H	-0.243170000	1.922399000	3.946775000
H	-1.622942000	2.961624000	3.525854000
C	-1.484303000	-0.740984000	4.146713000
H	-1.885839000	-1.656059000	3.705405000
H	-0.395759000	-0.749865000	4.054563000
H	-1.789065000	-0.676467000	5.195467000

^{3}TS Energy = -1721.562323 au

N	1.329118000	1.649911000	0.044755000
N	1.167106000	-1.204115000	0.523614000
N	-1.692094000	-1.081141000	0.149879000
N	-1.556940000	1.749344000	-0.265323000
C	1.197462000	2.994400000	-0.194603000
C	2.508708000	3.619192000	-0.170233000
C	3.415202000	2.631291000	0.082833000
C	2.666661000	1.393639000	0.218826000
C	3.225963000	0.148012000	0.489156000
C	2.529152000	-1.048286000	0.629570000
C	3.140482000	-2.335744000	0.908446000
C	2.131756000	-3.253442000	0.963551000
C	0.894546000	-2.534952000	0.715667000
C	-0.372763000	-3.110652000	0.666249000

C	-1.561616000	-2.438502000	0.397459000
C	-2.864025000	-3.064767000	0.330502000
C	-3.771745000	-2.083852000	0.042746000
C	-3.039003000	-0.842127000	-0.067786000
C	-3.609010000	0.397358000	-0.340574000
C	-2.914983000	1.600553000	-0.435492000
C	-3.508674000	2.887071000	-0.740065000
C	-2.492789000	3.800034000	-0.759439000
C	-1.267061000	3.082151000	-0.469260000
C	-0.002157000	3.660871000	-0.428159000
H	2.691243000	4.671639000	-0.333235000
H	4.489216000	2.712160000	0.169046000
H	4.201447000	-2.496945000	1.034897000
H	2.200713000	-4.316810000	1.142939000
H	-3.044512000	-4.119718000	0.479936000
H	-4.840446000	-2.178177000	-0.085865000
H	-4.561453000	3.051130000	-0.919819000
H	-2.549150000	4.860316000	-0.960359000
H	-0.439108000	-4.180630000	0.833527000
H	4.304619000	0.105415000	0.598103000
H	0.055035000	4.728854000	-0.611245000
H	-4.682069000	0.426836000	-0.495541000
Mn	-0.190251000	0.287803000	0.138666000
O	-0.212758000	0.628267000	1.885851000
O	0.139286000	0.049834000	-1.686286000
H	-0.601671000	-0.460206000	-2.054317000
S	-1.869699000	0.479216000	3.074543000
C	-1.372897000	1.965305000	3.990837000
H	-1.794700000	1.963269000	4.999907000
H	-0.281493000	2.004757000	4.017353000
H	-1.747448000	2.827811000	3.435590000
C	-1.109797000	-0.815654000	4.096410000
H	-1.270978000	-1.765244000	3.581836000
H	-0.036291000	-0.623093000	4.157208000
H	-1.563322000	-0.849499000	5.091135000

^{3}P Energy = -1721.605478 au

N	1.345704000	1.667997000	-0.037073000
N	1.172082000	-1.153470000	0.539779000
N	-1.687550000	-1.052215000	0.183659000
N	-1.531657000	1.781650000	-0.287350000
C	1.222124000	3.011372000	-0.302719000
C	2.536828000	3.633840000	-0.305064000
C	3.441292000	2.649876000	-0.037541000
C	2.686967000	1.417954000	0.132281000
C	3.242742000	0.179004000	0.435514000
C	2.539691000	-1.009444000	0.619704000
C	3.146159000	-2.291979000	0.917223000
C	2.132047000	-3.203506000	1.002140000
C	0.896915000	-2.485606000	0.754650000
C	-0.370873000	-3.066175000	0.724539000
C	-1.566185000	-2.404497000	0.450466000
C	-2.873688000	-3.029509000	0.406926000
C	-3.777480000	-2.049295000	0.107709000
C	-3.034079000	-0.812980000	-0.031396000
C	-3.592917000	0.428711000	-0.320758000
C	-2.894325000	1.629268000	-0.443181000
C	-3.491195000	2.908026000	-0.769204000
C	-2.474757000	3.820866000	-0.822792000

C	-1.247460000	3.108547000	-0.532853000
C	0.023541000	3.680708000	-0.529389000
H	2.720891000	4.682392000	-0.490856000
H	4.516109000	2.728988000	0.041335000
H	4.207513000	-2.458094000	1.034350000
H	2.199035000	-4.263780000	1.200554000
H	-3.058933000	-4.080786000	0.576683000
H	-4.847645000	-2.140361000	-0.013008000
H	-4.545808000	3.069334000	-0.941610000
H	-2.534624000	4.875984000	-1.049001000
H	-0.428747000	-4.134320000	0.908496000
H	4.322502000	0.132168000	0.533471000
H	0.083714000	4.744132000	-0.737930000
H	-4.666991000	0.464969000	-0.471355000
Mn	-0.156007000	0.306364000	0.030466000
O	-0.234088000	0.773248000	2.135859000
O	0.064833000	-0.005547000	-1.762876000
H	-0.682457000	-0.556865000	-2.052852000
S	-1.527696000	0.555094000	2.944643000
C	-1.429039000	1.833988000	4.242756000
H	-2.229125000	1.687576000	4.973917000
H	-0.447078000	1.785615000	4.720424000
H	-1.548583000	2.800288000	3.748648000
C	-1.202644000	-0.903818000	3.997505000
H	-1.123621000	-1.762786000	3.327918000
H	-0.258536000	-0.764925000	4.530868000
H	-2.032028000	-1.048873000	4.696005000

^{5}P Energy = -1721.614932

N	1.184660000	1.652691000	0.196375000
N	1.346239000	-1.310101000	0.451016000
N	-1.588777000	-1.374345000	0.058956000
N	-1.764786000	1.596767000	-0.036657000
C	0.932989000	2.992966000	-0.009254000
C	2.198115000	3.707855000	0.008261000
C	3.186695000	2.782537000	0.214834000
C	2.547774000	1.481447000	0.322713000
C	3.222509000	0.262640000	0.511767000
C	2.677755000	-1.030288000	0.567417000
C	3.409446000	-2.284256000	0.731063000
C	2.484356000	-3.292562000	0.698121000
C	1.178837000	-2.664214000	0.512882000
C	-0.062879000	-3.309000000	0.400705000
C	-1.325300000	-2.722168000	0.204203000
C	-2.584491000	-3.443282000	0.145764000
C	-3.580625000	-2.517451000	-0.022780000
C	-2.952966000	-1.208605000	-0.071016000
C	-3.633768000	0.013884000	-0.217624000
C	-3.090333000	1.309504000	-0.243951000
C	-3.798885000	2.548238000	-0.542576000
C	-2.865555000	3.552092000	-0.546440000
C	-1.578260000	2.939486000	-0.244889000
C	-0.329584000	3.579660000	-0.203646000
H	2.307614000	4.774967000	-0.125962000
H	4.252132000	2.954871000	0.277365000
H	4.480678000	-2.372304000	0.848012000
H	2.660552000	-4.355944000	0.782239000
H	-2.685752000	-4.516425000	0.228026000
H	-4.643759000	-2.696399000	-0.103212000

H	-4.857498000	2.629001000	-0.747607000
H	-3.025080000	4.601632000	-0.751764000
H	-0.054377000	-4.392473000	0.479015000
H	4.303150000	0.333127000	0.600036000
H	-0.331243000	4.652692000	-0.373147000
H	-4.708566000	-0.060481000	-0.358709000
Mn	-0.182153000	0.120454000	0.012147000
O	-0.385381000	0.142106000	2.147516000
O	0.013454000	0.052685000	-1.789211000
H	-0.578365000	-0.643662000	-2.122392000
S	-0.755783000	1.451711000	2.879024000
C	0.155528000	1.301783000	4.452155000
H	-0.135255000	2.108577000	5.131095000
H	-0.047134000	0.323537000	4.895122000
H	1.217650000	1.382150000	4.212093000
C	-2.441218000	1.171001000	3.523546000
H	-3.102527000	1.124083000	2.656336000
H	-2.471043000	0.220913000	4.063233000
H	-2.731979000	2.001791000	4.173237000

Optimised cartesian coordinates (Å) of the various stationary points on the potential energy surface for the reaction of (HO)(Porp)Mn(O) with Me_2S with BLYP.

^{1}R Energy = -1721.133779 au

N	1.156541000	1.754643000	-0.024828000
N	1.139987000	-1.155187000	0.413361000
N	-1.756835000	-1.178585000	-0.063030000
N	-1.656533000	1.695734000	-0.557283000
C	1.001491000	3.108442000	-0.297517000
C	2.295013000	3.775693000	-0.212909000
C	3.226445000	2.812023000	0.104215000
C	2.515924000	1.542218000	0.220245000
C	3.122652000	0.318534000	0.537515000
C	2.487499000	-0.929677000	0.652852000
C	3.125947000	-2.179846000	1.056381000
C	2.142444000	-3.145568000	1.080114000
C	0.892917000	-2.497421000	0.688962000
C	-0.358983000	-3.127850000	0.593764000
C	-1.576593000	-2.523584000	0.240923000
C	-2.856330000	-3.221412000	0.112883000
C	-3.791687000	-2.285497000	-0.268364000
C	-3.092990000	-1.005540000	-0.372251000
C	-3.672101000	0.223222000	-0.729101000
C	-3.014223000	1.455873000	-0.818476000
C	-3.657008000	2.707998000	-1.190335000
C	-2.695093000	3.693672000	-1.154359000
C	-1.443831000	3.063183000	-0.762817000
C	-0.215360000	3.720782000	-0.628501000
H	2.455865000	4.837848000	-0.383274000
H	4.298169000	2.933202000	0.246062000
H	4.182321000	-2.290024000	1.291814000
H	2.240319000	-4.198199000	1.337124000
H	-3.001177000	-4.285329000	0.288199000
H	-4.851522000	-2.432790000	-0.464156000
H	-4.710398000	2.806384000	-1.442878000
H	-2.809232000	4.752805000	-1.373779000
H	-0.388199000	-4.197393000	0.816237000
H	4.198693000	0.342462000	0.726652000

H	-0.200940000	4.795921000	-0.819562000
H	-4.740548000	0.221056000	-0.957121000
Mn	-0.314552000	0.356682000	0.020356000
O	-0.507964000	0.358923000	1.596978000
O	0.031190000	-0.084233000	-1.741569000
H	0.467121000	-0.961614000	-1.825728000
S	-1.779837000	1.507870000	4.648577000
C	0.062218000	1.691540000	4.658660000
H	0.499747000	1.246053000	5.567045000
H	0.492598000	1.226052000	3.759211000
H	0.278149000	2.770886000	4.647413000
C	-1.904998000	-0.339819000	4.663764000
H	-2.976877000	-0.589577000	4.642520000
H	-1.417150000	-0.758160000	3.770884000
H	-1.455477000	-0.759509000	5.578565000

^{3}R Energy = -1721.122480 au

N	1.165159000	1.702194000	0.021670000
N	1.111526000	-1.209034000	0.464706000
N	-1.735631000	-1.213875000	-0.144557000
N	-1.678085000	1.665160000	-0.525581000
C	0.997914000	3.062787000	-0.191020000
C	2.288716000	3.733284000	-0.069834000
C	3.223039000	2.762138000	0.211119000
C	2.516059000	1.485298000	0.273661000
C	3.114552000	0.251537000	0.567993000
C	2.467459000	-0.987753000	0.671688000
C	3.106621000	-2.249872000	1.037286000
C	2.123151000	-3.213720000	1.059407000
C	0.869140000	-2.556178000	0.700799000
C	-0.379405000	-3.180696000	0.572563000
C	-1.576644000	-2.562978000	0.180599000
C	-2.854922000	-3.246312000	0.023670000
C	-3.775468000	-2.306086000	-0.384435000
C	-3.075858000	-1.031318000	-0.476512000
C	-3.665100000	0.196178000	-0.810331000
C	-3.019993000	1.438906000	-0.831367000
C	-3.654745000	2.706984000	-1.167822000
C	-2.693136000	3.686258000	-1.062926000
C	-1.450536000	3.034201000	-0.668530000
C	-0.220752000	3.682974000	-0.499794000
H	2.443407000	4.802668000	-0.193643000
H	4.293182000	2.881081000	0.365020000
H	4.167630000	-2.365755000	1.247008000
H	2.222791000	-4.272805000	1.286482000
H	-3.011013000	-4.307836000	0.202449000
H	-4.832378000	-2.446715000	-0.599011000
H	-4.700706000	2.815994000	-1.444852000
H	-2.796490000	4.754134000	-1.240957000
H	-0.423760000	-4.251354000	0.784001000
H	4.191331000	0.261155000	0.751658000
H	-0.206817000	4.764706000	-0.648202000
H	-4.728355000	0.185924000	-1.058904000
Mn	-0.311560000	0.272487000	0.015478000
O	-0.497793000	0.379234000	1.672949000
O	0.227656000	-0.032419000	-1.783037000
H	-0.114730000	-0.908993000	-2.070903000
S	-1.845849000	1.504875000	4.700436000
C	-0.066092000	1.993413000	4.556764000

H	0.506071000	1.658187000	5.437279000
H	0.352766000	1.565412000	3.633884000
H	-0.035059000	3.092304000	4.501620000
C	-1.656765000	-0.336160000	4.703381000
H	-2.668726000	-0.765966000	4.756529000
H	-1.170234000	-0.650213000	3.767785000
H	-1.074757000	-0.670544000	5.577774000

^{5}R Energy = -1721.107790 au

N	1.161743000	1.735232000	0.010135000
N	1.090990000	-1.118162000	0.629121000
N	-1.726826000	-1.195636000	-0.105332000
N	-1.682741000	1.678776000	-0.555266000
C	0.991700000	3.082468000	-0.273654000
C	2.272355000	3.773064000	-0.150829000
C	3.205473000	2.830545000	0.216611000
C	2.506779000	1.552808000	0.322679000
C	3.096194000	0.341393000	0.705170000
C	2.444709000	-0.895413000	0.838488000
C	3.092663000	-2.149802000	1.209675000
C	2.117966000	-3.122934000	1.210305000
C	0.865471000	-2.472782000	0.836159000
C	-0.367853000	-3.124751000	0.675748000
C	-1.565132000	-2.537783000	0.243366000
C	-2.840208000	-3.231371000	0.102224000
C	-3.765727000	-2.299442000	-0.313326000
C	-3.068918000	-1.023243000	-0.426151000
C	-3.669506000	0.200725000	-0.764098000
C	-3.037224000	1.448449000	-0.805442000
C	-3.685651000	2.710986000	-1.140425000
C	-2.720899000	3.691492000	-1.093187000
C	-1.464350000	3.046257000	-0.731102000
C	-0.227391000	3.689935000	-0.614554000
H	2.419921000	4.836424000	-0.325072000
H	4.267697000	2.970355000	0.403937000
H	4.152560000	-2.256453000	1.429223000
H	2.223038000	-4.183305000	1.428434000
H	-2.992974000	-4.289568000	0.302257000
H	-4.823839000	-2.445795000	-0.518239000
H	-4.740809000	2.815636000	-1.382245000
H	-2.832022000	4.755332000	-1.289851000
H	-0.393894000	-4.194152000	0.897467000
H	4.168021000	0.358903000	0.915698000
H	-0.209178000	4.765435000	-0.804086000
H	-4.736973000	0.180175000	-0.994805000
Mn	-0.301604000	0.298725000	0.008642000
O	-0.773867000	0.664265000	1.678988000
O	0.261064000	-0.115843000	-1.792452000
H	-0.221931000	-0.921338000	-2.085117000
S	-1.530927000	1.395445000	5.016987000
C	0.217583000	1.620883000	4.478359000
H	0.889873000	0.942085000	5.028413000
H	0.263208000	1.413783000	3.393020000
H	0.498918000	2.664626000	4.683445000
C	-1.795574000	-0.332134000	4.432918000
H	-2.847818000	-0.592137000	4.621894000
H	-1.578896000	-0.354453000	3.348343000
H	-1.138385000	-1.034820000	4.970968000

^{3}I Energy = -1721.123674 au

N	1.338096000	1.674255000	-0.002201000
N	1.189999000	-1.237001000	0.385775000
N	-1.700435000	-1.113124000	0.125988000
N	-1.551937000	1.751710000	-0.314990000
C	1.201519000	3.042743000	-0.172967000
C	2.524630000	3.665075000	-0.164383000
C	3.444209000	2.655293000	0.004117000
C	2.695348000	1.403201000	0.110928000
C	3.262760000	0.137994000	0.320130000
C	2.570473000	-1.073574000	0.468680000
C	3.185847000	-2.360680000	0.778067000
C	2.168222000	-3.281493000	0.902049000
C	0.915898000	-2.572739000	0.660617000
C	-0.365330000	-3.144028000	0.671202000
C	-1.568111000	-2.473871000	0.403335000
C	-2.878789000	-3.109315000	0.317906000
C	-3.785607000	-2.131197000	-0.025777000
C	-3.046708000	-0.879683000	-0.144017000
C	-3.608828000	0.366317000	-0.452458000
C	-2.918442000	1.583692000	-0.522658000
C	-3.527129000	2.881164000	-0.792837000
C	-2.521935000	3.820838000	-0.740632000
C	-1.280368000	3.111795000	-0.449068000
C	-0.015501000	3.711218000	-0.365133000
H	2.707306000	4.730625000	-0.285075000
H	4.528204000	2.731759000	0.054057000
H	4.256083000	-2.521606000	0.888319000
H	2.244236000	-4.342699000	1.129025000
H	-3.061584000	-4.168506000	0.485820000
H	-4.856670000	-2.231874000	-0.186628000
H	-4.585049000	3.035712000	-0.992962000
H	-2.594835000	4.894949000	-0.896560000
H	-0.430842000	-4.214840000	0.877093000
H	4.351395000	0.094249000	0.400879000
H	0.027198000	4.794664000	-0.497479000
H	-4.684720000	0.393885000	-0.637782000
Mn	-0.203661000	0.282320000	0.106043000
O	-0.191350000	0.532811000	1.791052000
O	0.064117000	0.048319000	-1.763660000
H	0.426670000	-0.851915000	-1.918808000
S	-2.199105000	0.618071000	3.441467000
C	-1.307312000	2.057517000	4.170070000
H	-1.431737000	2.086531000	5.264282000
H	-0.244729000	1.991276000	3.893974000
H	-1.740779000	2.965952000	3.726576000
C	-1.341807000	-0.761568000	4.314571000
H	-1.773326000	-1.700202000	3.937435000
H	-0.271885000	-0.729410000	4.062374000
H	-1.494473000	-0.695783000	5.403624000

^{3}TS Energy = -1721.122458 au

N	1.327158000	1.666851000	0.039119000
N	1.165325000	-1.220796000	0.516243000
N	-1.710615000	-1.093801000	0.132397000
N	-1.581548000	1.758499000	-0.278018000
C	1.196308000	3.024682000	-0.206371000
C	2.517051000	3.652643000	-0.172007000

C	3.429717000	2.657210000	0.092118000
C	2.677747000	1.409356000	0.226449000
C	3.236530000	0.152629000	0.501891000
C	2.540416000	-1.057649000	0.636008000
C	3.157539000	-2.353232000	0.917821000
C	2.144403000	-3.283940000	0.962741000
C	0.896276000	-2.567318000	0.706124000
C	-0.381330000	-3.144702000	0.648125000
C	-1.579874000	-2.468631000	0.375977000
C	-2.890702000	-3.098086000	0.300671000
C	-3.807049000	-2.108749000	0.013899000
C	-3.073459000	-0.856158000	-0.090843000
C	-3.647035000	0.392995000	-0.366011000
C	-2.953114000	1.608088000	-0.460379000
C	-3.547762000	2.901591000	-0.778971000
C	-2.523616000	3.822545000	-0.798828000
C	-1.289610000	3.105118000	-0.493777000
C	-0.014942000	3.688605000	-0.449619000
H	2.702853000	4.711896000	-0.336516000
H	4.510441000	2.740366000	0.185277000
H	4.225477000	-2.512145000	1.051885000
H	2.218836000	-4.354800000	1.140193000
H	-3.072178000	-4.161233000	0.444482000
H	-4.882553000	-2.205851000	-0.118350000
H	-4.606510000	3.065861000	-0.967819000
H	-2.580640000	4.888541000	-1.009076000
H	-0.449470000	-4.222779000	0.812458000
H	4.322005000	0.111598000	0.620541000
H	0.040125000	4.763272000	-0.639809000
H	-4.726746000	0.419374000	-0.528922000
Mn	-0.202559000	0.288196000	0.128902000
O	-0.186292000	0.628354000	1.897571000
O	0.160724000	0.062670000	-1.717165000
H	-0.547446000	-0.525522000	-2.064601000
S	-1.823857000	0.515819000	3.107596000
C	-1.301173000	1.996001000	4.064101000
H	-1.741314000	1.985768000	5.073490000
H	-0.202226000	2.009408000	4.105641000
H	-1.654735000	2.876515000	3.509287000
C	-1.111796000	-0.822906000	4.149373000
H	-1.279323000	-1.764991000	3.608695000
H	-0.030183000	-0.649801000	4.246709000
H	-1.602457000	-0.858474000	5.134736000

^{3}P Energy = -1721. 141503 au

N	1.342094000	1.666793000	-0.053351000
N	1.173382000	-1.161641000	0.535261000
N	-1.693773000	-1.047671000	0.155669000
N	-1.544956000	1.795818000	-0.317205000
C	1.223308000	3.033131000	-0.313950000
C	2.548175000	3.654183000	-0.303356000
C	3.458187000	2.661556000	-0.035882000
C	2.703669000	1.417965000	0.124354000
C	3.265078000	0.175505000	0.430136000
C	2.557902000	-1.022370000	0.618996000
C	3.160199000	-2.309988000	0.928958000
C	2.133442000	-3.227645000	1.019211000
C	0.894727000	-2.509196000	0.761653000
C	-0.385448000	-3.087517000	0.728113000

C	-1.580790000	-2.418718000	0.440136000
C	-2.899806000	-3.039978000	0.396394000
C	-3.806771000	-2.054088000	0.081033000
C	-3.060230000	-0.810129000	-0.069030000
C	-3.623992000	0.434191000	-0.367552000
C	-2.923304000	1.646029000	-0.485563000
C	-3.517772000	2.932570000	-0.810393000
C	-2.490461000	3.854377000	-0.853375000
C	-1.259114000	3.140081000	-0.558798000
C	0.023842000	3.711534000	-0.544689000
H	2.733771000	4.711446000	-0.480969000
H	4.539666000	2.740951000	0.051810000
H	4.227770000	-2.479176000	1.052558000
H	2.198689000	-4.293587000	1.227718000
H	-3.089226000	-4.095959000	0.578901000
H	-4.884131000	-2.144021000	-0.042213000
H	-4.578384000	3.096934000	-0.988831000
H	-2.549799000	4.917885000	-1.075503000
H	-0.450393000	-4.161147000	0.921494000
H	4.351865000	0.131058000	0.532899000
H	0.089613000	4.783323000	-0.747264000
H	-4.704819000	0.467469000	-0.523654000
Mn	-0.162202000	0.308283000	0.009285000
O	-0.230856000	0.802357000	2.140391000
O	0.064091000	-0.010814000	-1.797801000
H	-0.677458000	-0.602620000	-2.064013000
S	-1.523485000	0.537997000	2.978924000
C	-1.441588000	1.836515000	4.302167000
H	-2.230399000	1.656029000	5.048959000
H	-0.443191000	1.813926000	4.763718000
H	-1.602870000	2.803791000	3.806143000
C	-1.137404000	-0.931850000	4.054776000
H	-1.043057000	-1.792637000	3.378228000
H	-0.185856000	-0.758603000	4.579408000
H	-1.963068000	-1.093211000	4.765778000

^{5}P Energy = -1721.135082 au

N	1.393792000	1.722051000	-0.076757000
N	1.167649000	-1.149434000	0.413521000
N	-1.748265000	-1.086403000	0.140884000
N	-1.503875000	1.766745000	-0.465790000
C	1.266084000	3.078859000	-0.333097000
C	2.581993000	3.712218000	-0.262878000
C	3.492120000	2.718494000	0.030018000
C	2.739618000	1.470013000	0.142027000
C	3.272318000	0.199851000	0.417636000
C	2.550667000	-0.999940000	0.541816000
C	3.143358000	-2.291376000	0.870494000
C	2.117060000	-3.207071000	0.945175000
C	0.875970000	-2.493848000	0.662284000
C	-0.401116000	-3.084181000	0.680618000
C	-1.627749000	-2.437642000	0.441253000
C	-2.951452000	-3.056449000	0.439609000
C	-3.859492000	-2.065482000	0.121795000
C	-3.098087000	-0.833760000	-0.070394000
C	-3.617262000	0.423359000	-0.427175000
C	-2.886342000	1.611261000	-0.608880000
C	-3.479307000	2.901689000	-0.942790000
C	-2.456413000	3.823090000	-0.994785000

C	-1.217206000	3.114593000	-0.695820000
C	0.050728000	3.718156000	-0.628543000
H	2.773222000	4.771347000	-0.422764000
H	4.568965000	2.810568000	0.155586000
H	4.206628000	-2.458932000	1.028348000
H	2.178592000	-4.268661000	1.175465000
H	-3.150832000	-4.106789000	0.643526000
H	-4.939349000	-2.154738000	0.020152000
H	-4.542094000	3.067351000	-1.106433000
H	-2.520831000	4.887479000	-1.210552000
H	-0.438173000	-4.155261000	0.895322000
H	4.353958000	0.134760000	0.558453000
H	0.090307000	4.791847000	-0.827975000
H	-4.698030000	0.490363000	-0.574946000
Mn	-0.129286000	0.284652000	-0.219669000
O	-0.281930000	0.861179000	2.312135000
O	0.019721000	-0.128505000	-2.093009000
H	-0.620894000	-0.830402000	-2.343199000
S	-1.528057000	0.586996000	3.179217000
C	-1.461015000	1.832325000	4.570483000
H	-2.254769000	1.618163000	5.303663000
H	-0.466311000	1.794523000	5.040066000
H	-1.621750000	2.820841000	4.117090000
C	-1.140498000	-0.914457000	4.224302000
H	-1.057916000	-1.761853000	3.529360000
H	-0.181749000	-0.759842000	4.742643000
H	-1.957828000	-1.088618000	4.942195000

Optimised cartesian coordinates (Å) of the various stationary points on the potential energy surface for the reaction of $[(H_2O)(Porp)Mn(O)]^+$ with Me_2S with B3LYP.

^{5}**R$_1$** Energy = -1721.985415 au

N	1.768187000	2.126894000	0.579004000
N	1.798683000	-0.740379000	0.696190000
N	-1.075846000	-0.776505000	0.494357000
N	-1.103708000	2.084692000	0.363974000
C	1.565233000	3.480199000	0.371175000
C	2.827649000	4.180241000	0.478211000
C	3.777892000	3.245457000	0.784562000
C	3.103747000	1.966283000	0.840899000
C	3.727103000	0.735171000	1.093310000
C	3.130233000	-0.527250000	0.959881000
C	3.823219000	-1.790822000	1.062652000
C	2.890660000	-2.773309000	0.863344000
C	1.619747000	-2.114830000	0.662063000
C	0.391694000	-2.757637000	0.542224000
C	-0.861209000	-2.139489000	0.498901000
C	-2.127250000	-2.836265000	0.504997000
C	-3.107418000	-1.881678000	0.530423000
C	-2.444850000	-0.597878000	0.522183000
C	-3.090618000	0.639295000	0.494990000
C	-2.469943000	1.882249000	0.397763000
C	-3.155480000	3.147143000	0.250027000
C	-2.191970000	4.108030000	0.115891000
C	-0.913417000	3.437041000	0.201059000
C	0.328624000	4.080387000	0.172022000
H	2.956352000	5.244065000	0.344174000
H	4.835896000	3.394704000	0.941467000

H	4.880908000	-1.902911000	1.249974000
H	3.038225000	-3.843191000	0.864713000
H	-2.241227000	-3.910096000	0.501346000
H	-4.177738000	-2.024056000	0.545423000
H	-4.228200000	3.270286000	0.238764000
H	-2.323034000	5.171198000	-0.019929000
H	0.402646000	-3.842421000	0.536135000
H	4.790264000	0.755943000	1.302910000
H	0.319523000	5.155312000	0.026765000
H	-4.175005000	0.629376000	0.518175000
Mn	0.337193000	0.687555000	0.703876000
O	0.261316000	0.754250000	2.345898000
O	0.497405000	0.646646000	-1.561860000
H	1.226889000	0.065074000	-1.836008000
H	-0.308620000	0.265007000	-1.949101000
S	3.236926000	0.893408000	4.183391000
C	2.113240000	2.314020000	4.373280000
C	2.119114000	-0.496902000	4.550045000
H	2.686267000	-1.420478000	4.415239000
H	1.267801000	-0.461818000	3.863676000
H	1.772999000	-0.433926000	5.586371000
H	2.673130000	3.214404000	4.111075000
H	1.776978000	2.387514000	5.412162000
H	1.255845000	2.184958000	3.705982000

^3R_I Energy = -1721.985236 au

N	1.766584000	2.127191000	0.576679000
N	1.798105000	-0.737973000	0.692552000
N	-1.075958000	-0.774033000	0.495697000
N	-1.103778000	2.085151000	0.368722000
C	1.566192000	3.477496000	0.350921000
C	2.828289000	4.177695000	0.459255000
C	3.775145000	3.246029000	0.786028000
C	3.099862000	1.968011000	0.851208000
C	3.720603000	0.737709000	1.114497000
C	3.125993000	-0.525583000	0.971255000
C	3.820085000	-1.789068000	1.067198000
C	2.891382000	-2.770777000	0.846112000
C	1.621105000	-2.112002000	0.640788000
C	0.393702000	-2.754243000	0.511423000
C	-0.860263000	-2.136517000	0.479841000
C	-2.125969000	-2.833937000	0.489199000
C	-3.106309000	-1.880254000	0.538935000
C	-2.444421000	-0.596080000	0.539425000
C	-3.089880000	0.641615000	0.524032000
C	-2.469419000	1.884269000	0.416227000
C	-3.154872000	3.147948000	0.257829000
C	-2.191581000	4.105624000	0.100080000
C	-0.912871000	3.434746000	0.184050000
C	0.329757000	4.076287000	0.143184000
H	2.959336000	5.239608000	0.312935000
H	4.831892000	3.396735000	0.949862000
H	4.876028000	-1.901811000	1.263725000
H	3.041078000	-3.840319000	0.836178000
H	-2.239738000	-3.907664000	0.472132000
H	-4.176317000	-2.023648000	0.563367000
H	-4.227504000	3.272273000	0.254130000
H	-2.323011000	5.166796000	-0.050230000
H	0.405307000	-3.838899000	0.493353000

H	4.782192000	0.758776000	1.331768000
H	0.321444000	5.149457000	-0.014604000
H	-4.174017000	0.632285000	0.557316000
Mn	0.336440000	0.689689000	0.702474000
O	0.266696000	0.751531000	2.343713000
O	0.493818000	0.648720000	-1.559951000
H	1.232229000	0.077580000	-1.831934000
H	-0.306394000	0.253609000	-1.945647000
S	3.234324000	0.888990000	4.194196000
C	2.112304000	2.311859000	4.381683000
C	2.119197000	-0.501335000	4.574240000
H	2.686511000	-1.424540000	4.437079000
H	1.262357000	-0.471069000	3.895689000
H	1.783852000	-0.435723000	5.613902000
H	2.674619000	3.210598000	4.118844000
H	1.776689000	2.387285000	5.420600000
H	1.255239000	2.184879000	3.714088000

^{3}R$_2$ Energy = -1721.977027 au

N	1.819287000	2.049970000	0.383219000
N	1.841731000	-0.804041000	0.501270000
N	-0.994264000	-0.835388000	0.324537000
N	-1.016525000	2.029885000	0.218138000
C	1.611421000	3.419140000	0.474430000
C	2.884228000	4.098563000	0.474454000
C	3.855161000	3.141070000	0.377688000
C	3.192382000	1.859857000	0.342059000
C	3.839719000	0.632696000	0.332331000
C	3.210847000	-0.599691000	0.435672000
C	3.892210000	-1.866078000	0.562075000
C	2.935182000	-2.826153000	0.735030000
C	1.652990000	-2.164514000	0.691773000
C	0.423945000	-2.807669000	0.750972000
C	-0.805519000	-2.190013000	0.568731000
C	-2.078229000	-2.867236000	0.533917000
C	-3.034046000	-1.923361000	0.279180000
C	-2.363529000	-0.649900000	0.177954000
C	-3.002531000	0.573481000	0.026224000
C	-2.381447000	1.814264000	0.082530000
C	-3.070948000	3.082106000	0.081032000
C	-2.129295000	4.056750000	0.260452000
C	-0.847258000	3.401778000	0.351003000
C	0.373686000	4.048485000	0.483611000
H	3.005294000	5.170673000	0.521616000
H	4.925861000	3.276312000	0.340021000
H	4.964478000	-1.989312000	0.528009000
H	3.070615000	-3.890092000	0.861089000
H	-2.210622000	-3.929419000	0.676740000
H	-4.100510000	-2.062440000	0.181855000
H	-4.139039000	3.197436000	-0.028757000
H	-2.276657000	5.125039000	0.317191000
H	0.427097000	-3.879827000	0.908953000
H	4.922719000	0.639686000	0.295406000
H	0.362610000	5.129721000	0.557059000
H	-4.081201000	0.561381000	-0.078703000
Mn	0.415899000	0.617869000	0.545924000
O	0.266708000	0.677251000	2.195861000
O	0.565363000	0.522012000	-1.701977000
H	0.035096000	-0.235344000	-2.006195000

H	0.145258000	1.314670000	-2.078922000
S	2.853300000	1.109864000	4.513702000
C	1.802019000	2.496638000	5.061625000
C	2.026418000	-0.284097000	5.351511000
H	2.573660000	-1.193623000	5.094615000
H	0.993177000	-0.373635000	5.005458000
H	2.047083000	-0.146766000	6.436527000
H	2.203670000	3.409378000	4.616405000
H	1.824377000	2.588589000	6.151341000
H	0.774180000	2.348998000	4.719410000

^{3}I Energy = -1721.997041 au

N	1.938616000	2.081411000	0.472749000
N	1.960183000	-0.772379000	0.609377000
N	-0.888094000	-0.806663000	0.528520000
N	-0.909409000	2.067232000	0.386693000
C	1.732884000	3.454260000	0.499327000
C	3.005441000	4.132676000	0.425155000
C	3.973080000	3.171293000	0.337626000
C	3.309427000	1.889975000	0.377369000
C	3.954918000	0.660884000	0.370369000
C	3.328315000	-0.571033000	0.501778000
C	4.010926000	-1.839758000	0.596455000
C	3.056772000	-2.801067000	0.779394000
C	1.774224000	-2.137231000	0.779157000
C	0.546435000	-2.781866000	0.862412000
C	-0.690764000	-2.162848000	0.736475000
C	-1.965809000	-2.841122000	0.753999000
C	-2.930747000	-1.891449000	0.568289000
C	-2.259901000	-0.617152000	0.451558000
C	-2.902679000	0.609206000	0.333818000
C	-2.278664000	1.850724000	0.335602000
C	-2.968590000	3.120068000	0.335005000
C	-2.017704000	4.097606000	0.424152000
C	-0.732460000	3.440087000	0.463800000
C	0.495839000	4.086546000	0.522317000
H	3.127627000	5.205760000	0.419488000
H	5.041593000	3.304420000	0.255151000
H	5.081624000	-1.964830000	0.531401000
H	3.194223000	-3.867087000	0.885030000
H	-2.092627000	-3.905743000	0.883718000
H	-4.001246000	-2.026612000	0.522881000
H	-4.041227000	3.234244000	0.282786000
H	-2.160532000	5.167721000	0.452561000
H	0.555953000	-3.857297000	0.997871000
H	5.035836000	0.665339000	0.291728000
H	0.489946000	5.170215000	0.548707000
H	-3.985651000	0.598743000	0.286880000
Mn	0.537859000	0.652122000	0.683324000
O	0.401991000	0.727784000	2.351794000
O	0.578463000	0.547975000	-1.557981000
H	0.094969000	-0.255939000	-1.818187000
H	0.043929000	1.295079000	-1.880474000
S	2.175277000	0.946708000	3.755445000
C	1.344868000	2.366502000	4.528754000
C	1.514963000	-0.423694000	4.749903000
H	1.946449000	-1.349464000	4.364662000
H	0.428234000	-0.454426000	4.641830000
H	1.795392000	-0.298390000	5.799140000

H	1.627229000	3.258670000	3.966840000
H	1.665609000	2.470782000	5.568720000
H	0.263059000	2.226988000	4.470677000

^{3}TS Energy = -1721.996162 au

N	1.957401000	2.098642000	0.472958000
N	1.985107000	-0.753618000	0.638151000
N	-0.866524000	-0.798244000	0.563089000
N	-0.894952000	2.078704000	0.394295000
C	1.747797000	3.471443000	0.473187000
C	3.018479000	4.152434000	0.383537000
C	3.988946000	3.192698000	0.311247000
C	3.328766000	1.910256000	0.373888000
C	3.976438000	0.681808000	0.377608000
C	3.353032000	-0.551054000	0.519297000
C	4.038212000	-1.818576000	0.610097000
C	3.086422000	-2.781919000	0.795426000
C	1.802429000	-2.120412000	0.802591000
C	0.575771000	-2.767836000	0.890279000
C	-0.664944000	-2.152597000	0.771130000
C	-1.939153000	-2.833619000	0.805025000
C	-2.907498000	-1.885806000	0.628663000
C	-2.239015000	-0.610714000	0.499529000
C	-2.884288000	0.614614000	0.378370000
C	-2.263650000	1.858322000	0.359373000
C	-2.957105000	3.126445000	0.346331000
C	-2.007405000	4.107007000	0.408970000
C	-0.719966000	3.451749000	0.446420000
C	0.508623000	4.100753000	0.488141000
H	3.137661000	5.225620000	0.358583000
H	5.056831000	3.327812000	0.223731000
H	5.108776000	-1.942149000	0.539894000
H	3.226665000	-3.847898000	0.898339000
H	-2.063059000	-3.898070000	0.939275000
H	-3.978257000	-2.022724000	0.595708000
H	-4.030466000	3.237770000	0.303223000
H	-2.152199000	5.177192000	0.421825000
H	0.589000000	-3.843571000	1.023996000
H	5.056913000	0.687393000	0.292245000
H	0.500746000	5.184800000	0.495250000
H	-3.967762000	0.601728000	0.342308000
Mn	0.560166000	0.666243000	0.678560000
O	0.400642000	0.765559000	2.363601000
O	0.569345000	0.543694000	-1.528922000
H	0.070918000	-0.258613000	-1.766533000
H	0.030725000	1.292179000	-1.842626000
S	2.027180000	0.877134000	3.652599000
C	1.315985000	2.312474000	4.507472000
C	1.387518000	-0.489141000	4.662924000
H	1.711360000	-1.420801000	4.195464000
H	0.296100000	-0.445502000	4.674403000
H	1.789458000	-0.426712000	5.677643000
H	1.584273000	3.201017000	3.933157000
H	1.725762000	2.388870000	5.518073000
H	0.228849000	2.210177000	4.536248000

^{3}P Energy = -1722.037564 au

N	1.956185000	2.120831000	0.459780000

N	1.986393000	-0.735675000	0.684242000
N	-0.876281000	-0.775793000	0.592425000
N	-0.905812000	2.090053000	0.385809000
C	1.747105000	3.490697000	0.386132000
C	3.017306000	4.174384000	0.303661000
C	3.992527000	3.215020000	0.311686000
C	3.330330000	1.934998000	0.410889000
C	3.979437000	0.705426000	0.467273000
C	3.356543000	-0.531908000	0.598556000
C	4.044181000	-1.799275000	0.682010000
C	3.088536000	-2.769254000	0.816348000
C	1.804710000	-2.106406000	0.805134000
C	0.573122000	-2.753794000	0.869505000
C	-0.670365000	-2.136410000	0.770121000
C	-1.942138000	-2.820351000	0.819478000
C	-2.916211000	-1.869992000	0.682083000
C	-2.251167000	-0.593677000	0.552999000
C	-2.898738000	0.632746000	0.435587000
C	-2.276088000	1.876223000	0.376123000
C	-2.967504000	3.144073000	0.321380000
C	-2.013225000	4.123841000	0.316265000
C	-0.727705000	3.465671000	0.361801000
C	0.502971000	4.115858000	0.362140000
H	3.136632000	5.245741000	0.233754000
H	5.062406000	3.351604000	0.252063000
H	5.116390000	-1.922198000	0.635818000
H	3.229612000	-3.837157000	0.898102000
H	-2.063985000	-3.886752000	0.941033000
H	-3.987264000	-2.009720000	0.673459000
H	-4.041215000	3.259151000	0.296163000
H	-2.156630000	5.193930000	0.282520000
H	0.584638000	-3.832757000	0.978873000
H	5.062331000	0.712581000	0.410010000
H	0.492518000	5.199352000	0.316522000
H	-3.982957000	0.620437000	0.416832000
Mn	0.538994000	0.681825000	0.608094000
O	0.392492000	0.833633000	2.523647000
O	0.571360000	0.520542000	-1.455858000
H	0.002432000	-0.247281000	-1.655135000
H	0.097496000	1.305622000	-1.789391000
S	1.681426000	0.853781000	3.432546000
C	1.313410000	2.224044000	4.566458000
C	1.406709000	-0.559426000	4.541258000
H	1.498323000	-1.462786000	3.935130000
H	0.405323000	-0.497844000	4.973209000
H	2.171969000	-0.558004000	5.322556000
H	1.366650000	3.146645000	3.985292000
H	2.063569000	2.244032000	5.361882000
H	0.309311000	2.098679000	4.977783000

^{5}P Energy = -1722.063322 au

N	2.004830000	2.049632000	0.482535000
N	1.999226000	-0.821348000	0.489578000
N	-0.869777000	-0.817812000	0.535665000
N	-0.866499000	2.053036000	0.453260000
C	1.806860000	3.422560000	0.457218000
C	3.083271000	4.092298000	0.372278000
C	4.046773000	3.122764000	0.325360000
C	3.373813000	1.847128000	0.388516000

C	4.008396000	0.610246000	0.365652000
C	3.371096000	-0.624528000	0.422453000
C	4.042062000	-1.902414000	0.437915000
C	3.075831000	-2.867234000	0.522655000
C	1.799712000	-2.193346000	0.553109000
C	0.563199000	-2.827531000	0.612338000
C	-0.672159000	-2.188907000	0.598994000
C	-1.950606000	-2.859599000	0.626113000
C	-2.916209000	-1.892410000	0.578775000
C	-2.241544000	-0.616821000	0.527404000
C	-2.877735000	0.619207000	0.488675000
C	-2.239968000	1.854655000	0.467563000
C	-2.911149000	3.132644000	0.475252000
C	-1.943173000	4.099112000	0.483557000
C	-0.666167000	3.425846000	0.475597000
C	0.571160000	4.061687000	0.477214000
H	3.213093000	5.163972000	0.337390000
H	5.116614000	3.248842000	0.247987000
H	5.112989000	-2.033701000	0.389475000
H	3.204785000	-3.939094000	0.554739000
H	-2.080959000	-3.930742000	0.671657000
H	-3.988665000	-2.019701000	0.580625000
H	-3.983314000	3.262576000	0.478459000
H	-2.071687000	5.171466000	0.491545000
H	0.562035000	-3.910671000	0.657236000
H	5.090480000	0.608090000	0.301071000
H	0.572358000	5.145810000	0.468045000
H	-3.961749000	0.620012000	0.492564000
Mn	0.566975000	0.616113000	0.563402000
O	0.467499000	0.624081000	2.772278000
O	0.585052000	0.625949000	-1.827959000
H	0.501007000	-0.260531000	-2.216520000
H	-0.170604000	1.135307000	-2.165331000
S	1.602638000	0.976979000	3.763399000
C	1.007404000	2.454340000	4.651473000
C	1.420677000	-0.241874000	5.105502000
H	1.688500000	-1.218104000	4.696402000
H	0.381968000	-0.255862000	5.444785000
H	2.096760000	0.011933000	5.926673000
H	0.977843000	3.273635000	3.930221000
H	1.699969000	2.700072000	5.461388000
H	0.003143000	2.267200000	5.039863000