

SUPPORTING INFORMATION

Figure 1:

The potential energy surface surrounding the transition state of MCO hydrolysis derived from an IRC calculation at the B3-LYP/6-31+G(d) level of theory. Relative energies have been calculated at the RMP2/6-311+G(3df,2p) and B3-LYP/6-31+G(d) levels of theory and plotted against the distance between the hydroxide nucleophile and electrophilic phosphorous.

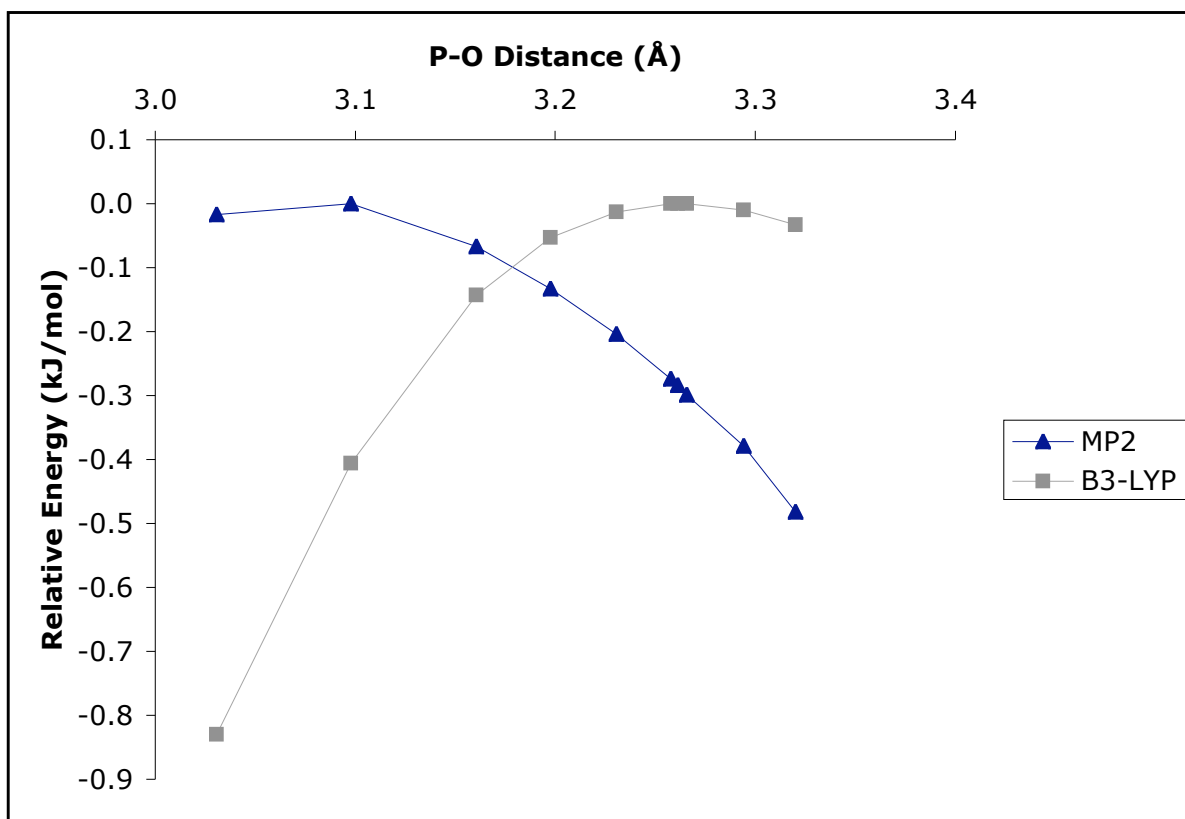


Figure 2: B3-LYP/6-31+G(d) geometries of the reactants, intermediates, transition states and products formed during the gas phase reaction of OH⁻ with MCS, MCO, MPS and MPO.

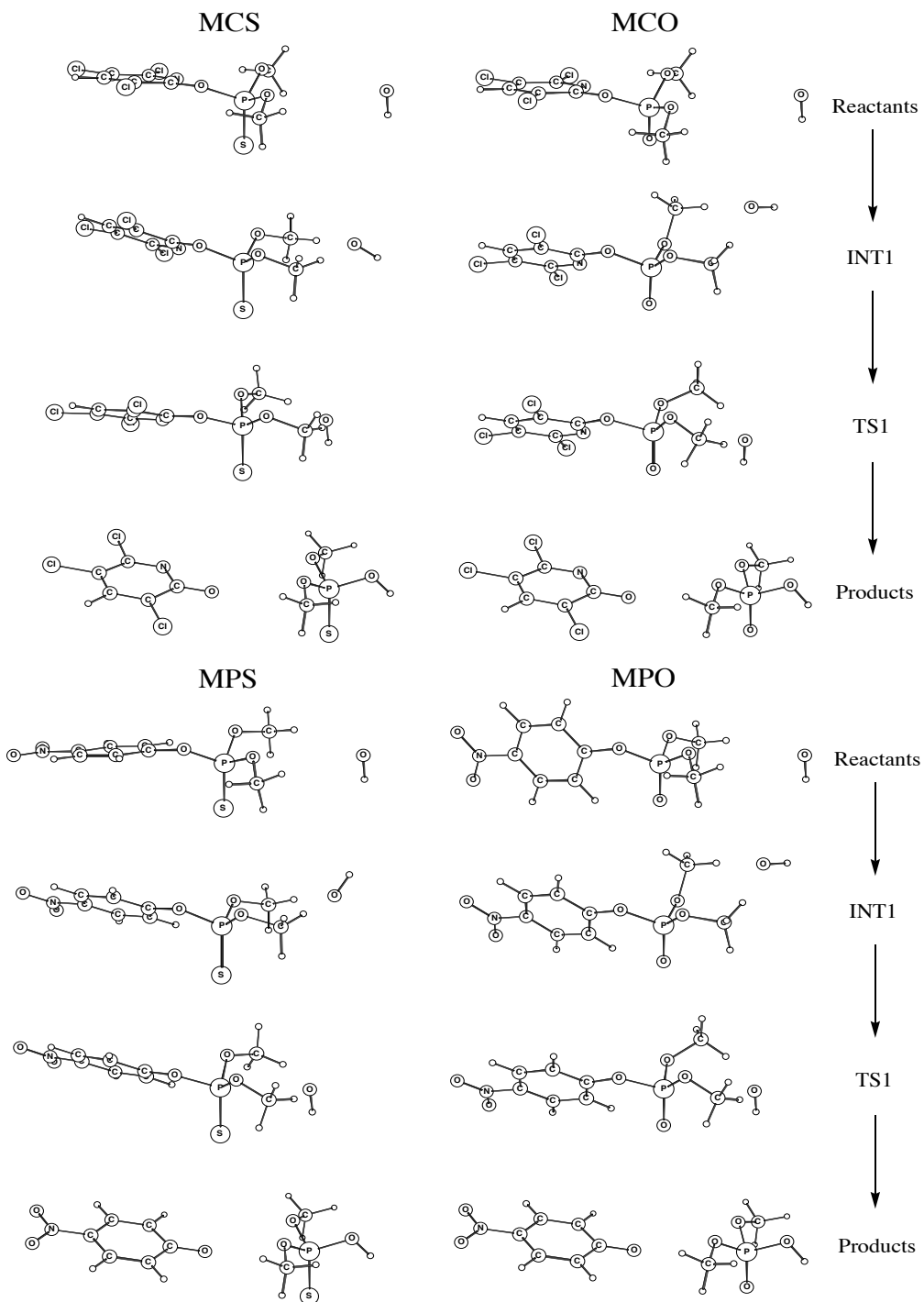


Figure 3: B3-LYP/6-31+G(d) optimised geometries of the reactants, intermediates, transition states and products formed during the gas phase reaction of OH⁻ with TMP.

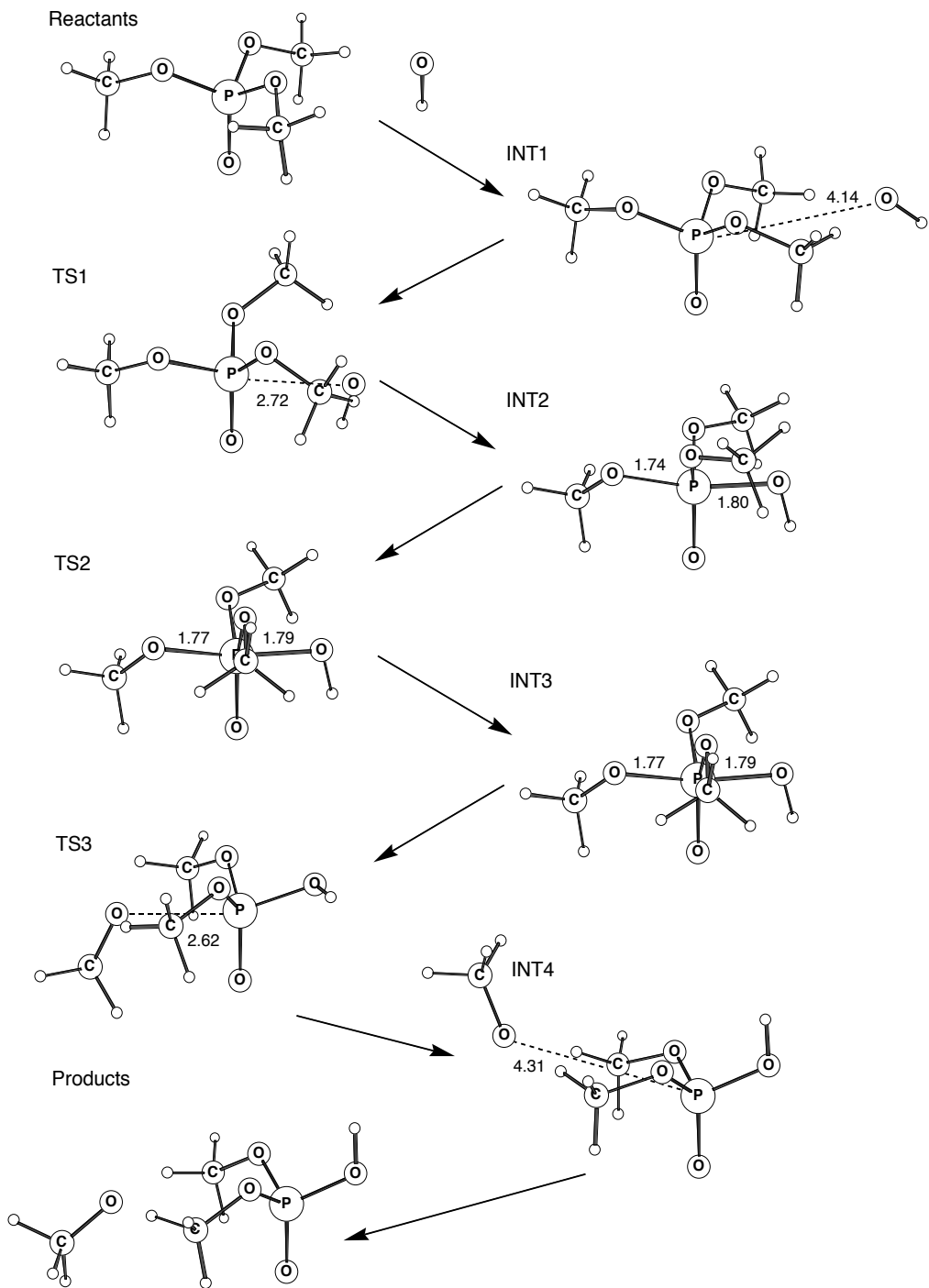


Figure 4: B3-LYP/6-31+G(d) optimized geometries of MCS, MCO, MPS and MPO with the aromatic rings sideways and upward, and the transition state between these conformations.

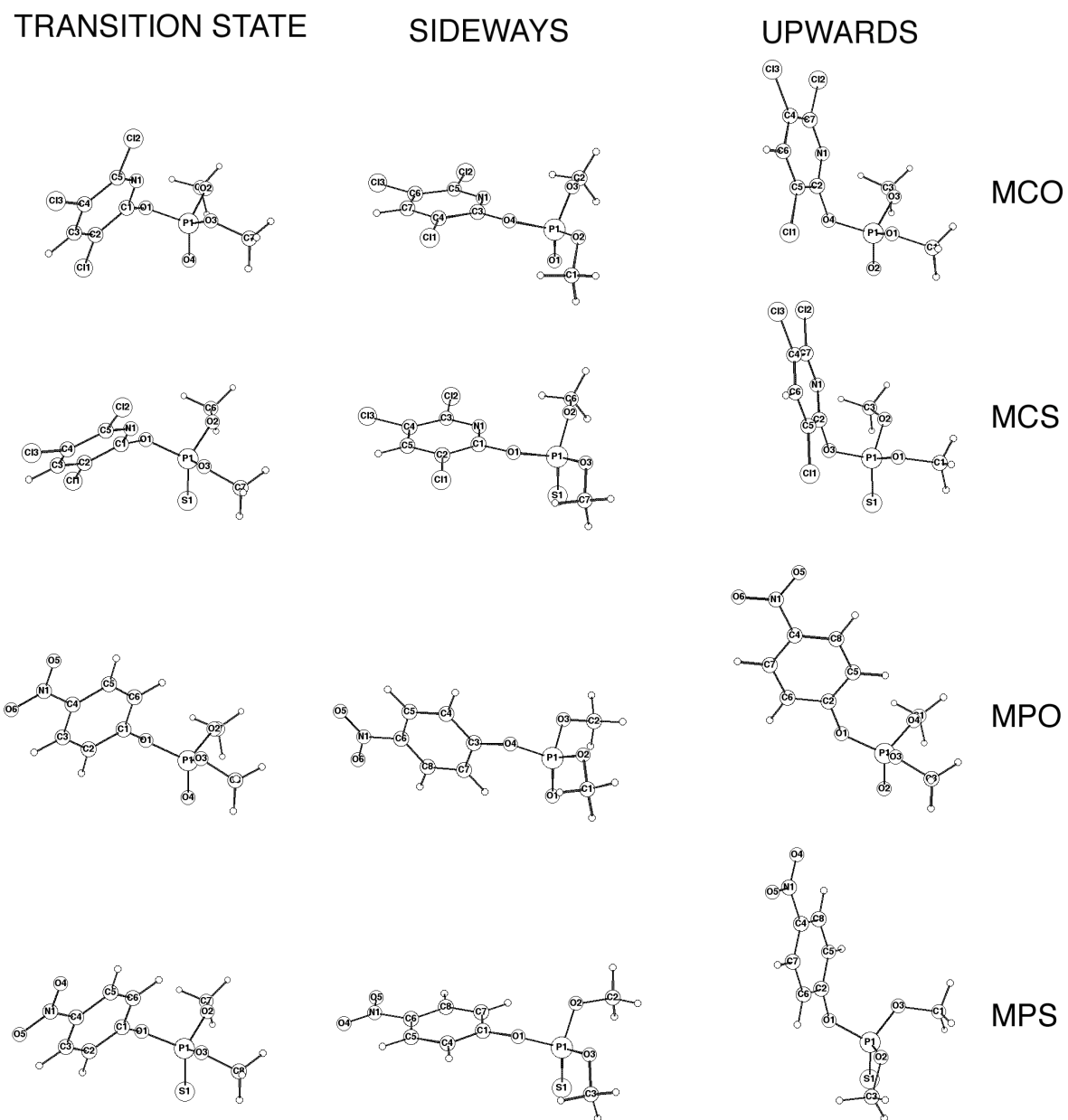
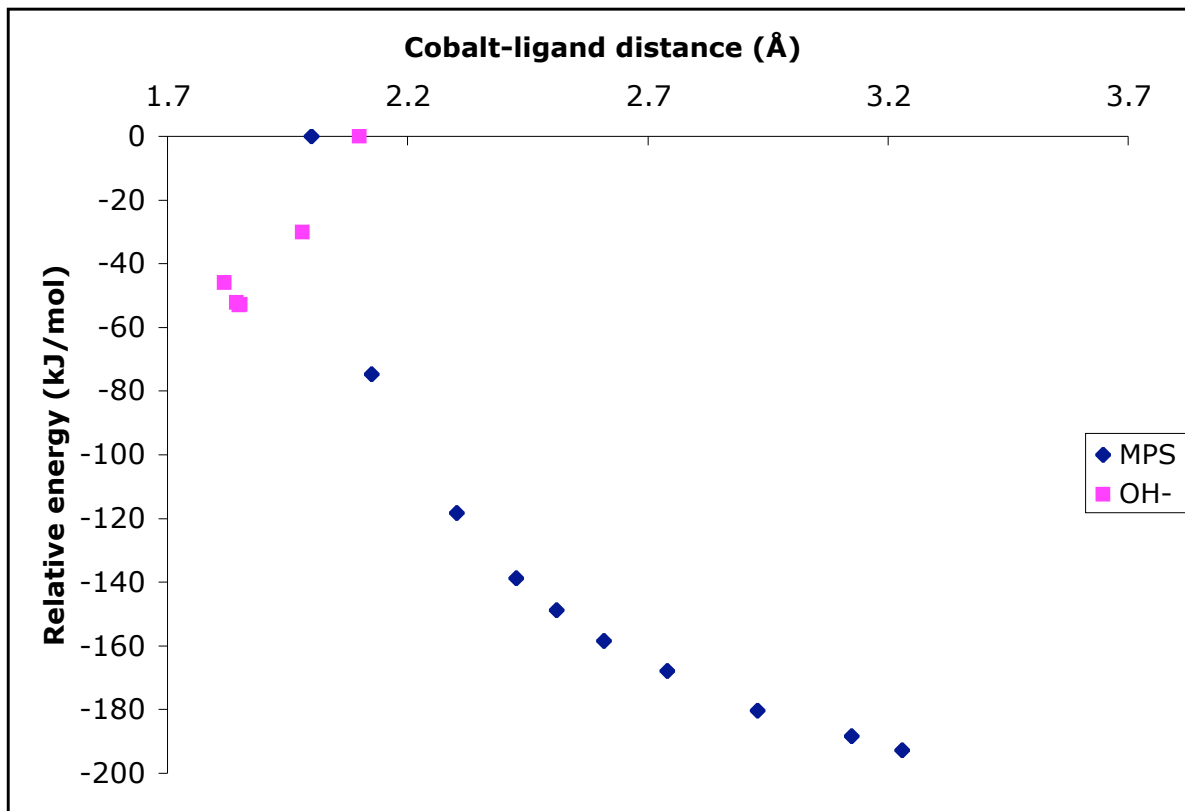


Figure 5:

The relative energy change as a function of the distance between Co^{2+} and the sulfur atom of MPS or OH^- .



Gaussian Archive Entries:

Hydroxide:

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I\I\GINC-SC126\FOpt\RB3LYP\6-31+G(d)\H1O1(1-)\MLC501\02-Aug-2004\0\#\n#  
B3LYP/6-31+G(D) SCF=TIGHT OPT=TIGHT FREQ MAXDISK=39321600\OH-6dub3-bi  
gb3\1,1\O,0,0,0,0.1083189844\H,0,0,0,-0.866551875\Version=DEC-AXP-O  
SF/1-G03RevB.03\State=1-SG\HF=-75.7966809\RMSE=5.379e-10\RMSF=3.464e-0  
8\Dipole=0,0,0,-0.7553975\PG=C*V [C*(H1O1)]\@
```

Dimethyl Phosphate:

```
I\I\GINC-SC49\FOpt\RB3LYP\6-31+G(d)\C2H7O4P1\MLC501\30-Aug-2004\0\#\n# B  
3LYP/6-31+G* OPT FREQ MAXDISK=134217728\OHO-6+dub3\0,1\O,-1.64603089  
46,0.0593171232,-0.1273674843\P,-0.1645967099,-0.0385931246,-0.0733562  
501\O,0.6856113236,1.3111939118,-0.1622319416\C,0.3893174154,2.2719557  
452,-1.1950599595\H,0.6498856595,1.8648006149,-2.1777098673\H,-0.66773  
46915,2.5518918051,-1.1667556935\H,1.0132612305,3.1401845988,-0.979498  
7478\O,0.5067014405,-0.6192082155,1.2552567837\C,0.0080566585,-1.84489  
33449,1.8268537847\H,0.2270944272,-2.6889271254,1.1643572569\H,0.54106  
40906,-1.9698691846,2.7701865655\H,-1.0680755023,-1.7730805273,2.00933  
51421\O,0.417029364,-0.9764238177,-1.2768830922\H,-0.3172788766,-1.307  
5097292,-1.8205279794\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-
```

722.7638613\RMSD=7.382e-09\RMSF=2.239e-05\Dipole=0.2500141,-0.3293539,-0.4169611\PG=C01 [X(C2H7O4P1)]\@

Dimethyl Thiophosphate:

I\GINC-SC56\FOpt\RB3LYP\6-31+G(d)\C2H7O3P1S1\MLC501\30-Aug-2004\0\#\B3LYP/6-31+G* OPT FREQ MAXDISK=134217728\OHS-6+dub3\O,1\S,-1.859086553,0.0855483031,0.0993914484P,0.0844122536,0.0713408513,-0.0213949368\O,0.7034784309,1.5408674848,-0.3905965393\O,0.7847638236,-0.9176639772,-1.0712709444\C,0.3691089221,-0.9383221036,-2.4501915526\O,0.9332017457,-0.3954416273,1.2563089417\C,0.6882677169,0.1841286572,2.551962305\H,-0.3681388564,0.0877583096,2.8200123265\H,0.9890520413,1.2367876274,2.5594247673\H,1.3067786141,-0.3831819964,3.2484859706\H,0.6378606771,0.0025158679,-2.9413266773\H,-0.708931143,-1.111108581,-2.5216468304\H,0.9141019487,-1.7645868091,-2.908243591\H,-0.0073340734,2.1959955984,-0.4922012669\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-1045.7176403\RMSD=3.218e-09\RMSF=2.899e-06\Dipole=0.3696425,0.5134713,-0.1387684\PG=C01 [X(C2H7O3P1S1)]\@

Trimethyl Phosphate reaction with hydroxide:

TMP:

I\GINC-SC105\FOpt\RB3LYP\6-31+G(d)\C3H9O4P1\CJJ506\14-Apr-2005\0\#\B3LYP/6-31+G* OPT\TMP\O,1\O,-0.013237422,-0.0072095518,1.6140353381\P,-0.0003505931,-0.0038261858,0.1285623731\O,0.9613788106,-1.0823150505,-0.5718358057\C,2.3011694827,-1.2759950755,-0.0724490221\H,2.9212702795,-0.4073153104,-0.315661467\H,2.286614865,-1.439671192,1.0087842751\H,2.6863774768,-2.1596582681,-0.5835926169\O,-1.4090059719,-0.2920519265,-0.5883668378\C,-2.2686080618,-1.331560629,-0.0754187615\H,-2.4093596814,-1.2137278974,1.0023905119\H,-3.2202336365,-1.2180958955,-0.597187829\H,-1.8404681508,-2.3146594503,-0.296260602\O,0.4645491591,1.3660602718,-0.5695215852\C,-0.034000843,2.6256453626,-0.0732011297\H,0.1133824623,2.6958146073,1.0081595341\H,0.542389737,3.3980706523,-0.5847135987\H,-1.0955545291,2.7322276483,-0.3184292\Version=Al64T-G03RevC.02\State=1-A\HF=-762.0696484\RMSD=3.314e-09\RMSF=9.031e-05\Dipole=0.0016432,0.0164628,-0.360127\PG=C01 [X(C3H9O4P1)]\@

INT1

I\GINC-SC30\FOpt\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\30-Apr-2005\0\#\B3LYP/6-31+G* OPT\TMPINT1\O,1\C,-1.6418649261,-1.7458787106,-0.1018459272\C,-0.8564657698,2.0378169517,0.0734930076\O,-0.301016134,-1.3719911937,-0.5678734867\O,0.2144479668,1.1900537405,-0.4600448227\O,1.9731875867,-0.5553872977,-0.5301250749\P,0.5400638725,-0.2453342976,0.1775334331\O,0.5513349323,-0.2793980634,1.66877025\H,-1.9340184045,-2.5683089497,-0.7604548772\H,-1.5649043166,-2.1049952727,0.9307345462\H,-2.3564859198,-0.8971846633,-0.1834836595\H,-0.6561751488,2.2290664317,1.1340619226\H,-0.7737665144,2.9688357089,-0.4950756376\H,-1.855380674,1.5691331611,-0.0716494982\O,-3.4772997604,0.6261371447,-0.3495072561\H,-4.2432056497,0.7682441383,0.230565082\C,3.0791825343,0.2760183991,-0.1782463655\H,3.9575034415,-0.1545103657,-0.6681131255\H,3.2322763334,0.2864755465,0.9076211338\H,2.9228510038,1.3002042445,-0.5373685486\Version=Al64T-G03RevC.02\State=1-A\HF=-837.9046364\RMSD=3.744e-09\RMSF=1.910e-05\Dipole=3.7428273,-0.1758144,0.3052228\PG=C01 [X(C3H10O5P1)]\@

TS1

I\GINC-SC113\FTS\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\13-Apr-2005\0

\# B3LYP/6-31+G* OPT=(TS,NOEIGENTEST,CALCF)\TMPTS1\1,1\,C,-1.93296
35402,1.5168508414,-0.7271708404\,C,-0.6859231703,-1.4039315117,1.89888
20054\O,-0.7974039716,1.2437529248,0.1228932507\O,0.3941415933,-0.8961
930587,1.0883950522\O,1.5864556531,1.0028027781,0.1411151668\,P,0.24742
44439,0.06312319,-0.2057079125\O,0.4453864056,-0.4851337735,-1.5812634
645\H,-2.5483945841,2.2276379595,-0.1646115096\H,-1.5884047163,1.98737
01523,-1.6576037151\H,-2.4468327771,0.5598248424,-0.9096896844\H,-0.26
80470248,-2.2622781218,2.4382554402\H,-0.980897511,-0.6295037162,2.620
3041275\H,-1.5142628093,-1.6800561052,1.2273644141\O,-2.0954464805,-1.
290597088,-0.4930021251\H,-1.71127459,-1.7038330935,-1.282127377\,C,2.8
631458178,0.4110832406,-0.0355128405\H,3.6063355019,1.2016201588,0.124
0901119\H,2.9753250405,0.0034931538,-1.0487307287\H,3.034466569,-0.392
1927637,0.6960746209\Version=Al64T-G03RevC.02\State=1-A\HF=-837.89552
86\RMSD=8.180e-09\RMSF=4.526e-06\Dipole=1.6762684,1.1346751,0.9614046\
PG=C01 [X(C3H10O5P1)]\@

INT2

I\GINC-SC32\FOpt\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\30-Apr-2005\
\# B3LYP/6-31+G* OPT\TMPINT2\1,1\,C,-1.8098938528,-1.9502116176,-0.
7316798153\,C,-0.5347598428,2.5030211035,-0.2680271206\O,-0.5318551147,
-1.3512382504,-0.8088746713\O,0.2078188331,1.3405019894,-0.5847176633\
O,1.5540211209,-0.5716558271,-0.467383416\,P,0.0072256942,-0.1369201421
,0.2118473297\O,0.3543369712,-0.2952127427,1.6942609503\H,-1.765544809
, -2.8252199876,-1.3964015771\H,-2.0494299271,-2.2888535888,0.284766525
2\H,-2.6071591945,-1.2757114282,-1.063447294\H,-0.0340602958,3.3309352
473,-0.7911229594\H,-1.5766450077,2.4313992761,-0.5991737038\H,-0.5303
032805,2.7135066364,0.8105772058\O,-1.70154622,0.2973256477,0.55198796
8\H,-1.7106246321,0.2786661123,1.5206260874\,C,2.6894981461,0.058165618
1,0.0640793952\H,3.570819911,-0.3819696183,-0.428709166\H,2.7709686787
, -0.0972128322,1.1505221934\H,2.6923217189,1.1446451544,-0.1337673551\
\Version=Al64T-G03RevC.02\State=1-A\HF=-837.9185055\RMSD=6.654e-09\RMS
F=1.758e-05\Dipole=-0.6725421,0.59894,-0.3860576\PG=C01 [X(C3H10O5P1)]
\@

TS2

I\GINC-SC9\FTS\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\02-May-2005\
\# B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\TMPTS3\1,1\,C,-2.19836
37297,-1.4352018669,-0.4306743063\,C,0.9534686694,2.4745126086,-0.47101
13198\O,-1.3064297562,-0.440473013,-0.8813994884\O,0.9372490367,1.0631
54377,-0.6146688533\O,0.8398136224,-1.275037505,-0.5138789228\,P,-0.107
7923101,0.0369812689,0.1966112814\O,0.0453697,-0.4100190771,1.65406498
72\H,-2.8966131539,-1.6346541566,-1.254365162\H,-1.6704356552,-2.36566
07226,-0.1754102487\H,-2.7734738616,-1.0989847294,0.446436803\H,1.8133
929421,2.8194358576,-1.062844386\H,0.0340195843,2.9352775622,-0.845116
9903\H,1.0913812922,2.7820730337,0.5735394401\O,-1.1608604015,1.415356
4894,0.6305354157\H,-1.1573971674,1.3625157061,1.5981841932\,C,2.084735
7047,-1.5710118444,0.0613453754\H,2.5029949617,-2.4394952063,-0.473068
9669\H,1.9944539768,-1.8156846934,1.1305096902\H,2.7983802559,-0.73318
5239,-0.0422171956\Version=Al64T-G03RevC.02\State=1-A\HF=-837.9148914
\RMSD=6.444e-09\RMSF=6.333e-06\Dipole=0.090993,0.3095611,-0.2712904\PG
=C01 [X(C3H10O5P1)]\@

TMPINT3

I\GINC-SC26\FOpt\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\02-May-2005\
\# B3LYP/6-31+G* OPT\TMPINT3\1,1\,C,2.3939446899,-1.0757186105,-0.4
319501166\,C,-2.5998428931,-0.516896921,-0.4826342848\O,1.0737251128,-0

.8659781847,-0.8806714569\O,-1.3979414735,0.2246853099,-0.618013257\O,
0.6291838583,1.3924609379,-0.5044379364\O,0.0250551514,-0.1136457156,0
.1968704975\O,0.3162490485,0.2480074219,1.6569520318\H,2.9386927393,-1
.5550968316,-1.2561230865\H,2.8898026194,-0.1273668152,-0.1784509697\H
,2.4247893157,-1.740444594,0.4457405507\H,-3.3488971809,0.0284442209,-
1.0744337882\H,-2.4962474397,-1.5382899442,-0.8617054843\H,-2.93733718
28,-0.5702696916,0.560406587\O,-0.5785489439,-1.7422248158,0.620524729
7\H,-0.5371196439,-1.7165820674,1.5883896553\C,0.212211556,2.599891317
7,0.0756024517\H,0.7236878002,3.4203219234,-0.4536501725\H,0.464719173
6,2.6492937274,1.1456330159\H,-0.8771384072,2.7554157358,-0.0298049631
\Version=Al64T-G03RevC.02\State=1-A\HF=-837.9148959\RMSD=3.887e-09\RM
SF=2.270e-05\Dipole=-0.306095,-0.0811224,-0.2752485\PG=C01 [X(C3H10O5P
1)]\@

TMPTS3

I\GINC-SC32\FTS\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\03-May-2005\O\
\# B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\tmpts3\1,1\C,2.41319
25059,-0.1646958753,-0.3498989423\C,-2.198440524,0.6269897268,-0.70835
68924\O,1.2634956967,-1.0319853152,-0.4050972229\O,-1.4121097804,-0.57
11973763,-0.6049156038\O,0.3279559008,1.5751648133,-0.8529037316\O,-0.
1331344,-0.6952198275,0.3669992522\O,-0.0664413447,0.0665245907,1.6483
443598\H,3.1708858274,-0.6522498587,-0.9742616843\H,2.1115625985,0.818
6057866,-0.7277275258\H,2.7756534953,-0.0939942621,0.6838450895\H,-3.1
784690065,0.2917493951,-1.0698961484\H,-2.3056491374,1.1019114822,0.27
18494549\H,-1.7018938417,1.3182717794,-1.3902428957\O,-0.4648438496,-2
.3070192908,0.6653886801\H,0.3623526071,-2.7334406688,0.9357486097\C,0
.2637905131,2.7327214787,-0.131712544\H,0.9117783995,3.5505870015,-0.5
473631829\H,0.563237964,2.6160133182,0.9371671942\H,-0.7681508591,3.18
88520837,-0.0908292748\Version=Al64T-G03RevC.02\State=1-A\HF=-837.899
7963\RMSD=5.359e-09\RMSF=3.292e-06\Dipole=0.2987716,-1.1980961,0.00988
57\PG=C01 [X(C3H10O5P1)]\@

TMPINT4

I\GINC-SC32\FOpt\RB3LYP\6-31+G(d)\C3H10O5P1(1-)\CJJ506\03-May-2005\O\
\# B3LYP/6-31+G* OPT\tmpint4\1,1\C,0.4926097434,-1.8459692876,0.43
76282953\C,0.4893971491,1.8483259204,0.4351595912\O,-0.5717753125,-1.3
007000038,-0.4100059924\O,-0.5729673434,1.2990604897,-0.4123846512\O,2
.8799014747,0.0029806619,0.4311242883\O,-1.4097917948,-0.0007907531,0.
0155609913\O,-1.9795365039,0.000322618,1.3870020947\H,0.6941363866,-2.
8366023617,0.0211119993\H,1.3976047054,-1.2053922433,0.3971143844\H,0.
1140305074,-1.9481127097,1.4603850664\H,0.6886400288,2.8388875826,0.01
7358504\H,0.1099493319,1.9509350812,1.457543627\H,1.3959441203,1.20995
57734,0.3958880467\O,-2.5475403914,-0.0026294732,-1.1472142503\H,-2.13
30359793,-0.0049642338,-2.0258505506\C,3.8174422659,0.0003845636,-0.55
21631848\H,4.8800906574,-0.0043280825,-0.1780436519\H,3.7726491328,0.8
914420847,-1.244359233\H,3.7655176909,-0.8886811124,-1.2464831849\Ver
sion=Al64T-G03RevC.02\State=1-A\HF=-837.9123161\RMSD=4.067e-09\RMSF=3.
467e-06\Dipole=-2.2193516,-0.0037578,-1.2211152\PG=C01 [X(C3H10O5P1)]\
\@

TMP leaving group: Methoxide

I\GINC-SC124\FOpt\RB3LYP\6-31+G(d)\C1H3O1(1-)\CJJ506\15-Apr-2005\O\
\# B3LYP/6-31+G* OPT\tmpmg\1,1\H,1.0304701249,0.,1.0363620538\C,-0.0
00023152,0.,0.5436131138\H,-0.5152596001,-0.8923803267,1.0363952517\O
,0.0000078708,0.,-0.796353905\H,-0.5152596001,0.8923803267,1.036395251
7\Version=Al64T-G03RevC.02\State=1-A\HF=-115.1115311\RMSD=4.778e-09\

RMSF=1.424e-05\Dipole=-0.0000047,0.,0.9968462\PG=CS [SG(C1H1O1),X(H2)]
\@

Dimethoate reaction with hydroxide:

Dimethoate

I\GINC-SC107\FOpt\RB3LYP\6-31+G(d)\C5H12N1O3P1S2\CJJ506\07-Apr-2005\
0\# B3LYP/6-31+G* OPT\dimethoate\0,1\S,1.2075810947,-0.102363117,1.
9162150786\P,1.4326378594,-0.0048415735,-0.0163796613\O,2.1147245624,1
.3524941089,-0.5961666199\S,-0.3059570034,-0.1464915418,-1.2227345202\
O,2.3870989297,-1.1115131307,-0.700871426\C,3.7300371487,-1.3356696664
,-0.2136858118\C,1.7345645109,2.6570389396,-0.1181953714\H,4.353511463
2,-0.4604357582,-0.4177807142\H,4.0999798589,-2.1987129829,-0.76856335
5\H,3.7140823962,-1.5525263188,0.858273545\H,0.7040798179,2.8816548414
,-0.4128659233\H,2.418568426,3.35786683,-0.5990913191\H,1.834481086,2.
7106016656,0.9695810877\C,-1.4192344072,-1.2311655645,-0.222158958\H,-
1.4909319866,-2.2035935375,-0.7117231239\C,-2.8473140997,-0.7136071936
,-0.012538541\H,-0.9648071823,-1.3707577258,0.7654640288\O,-3.73675667
39,-1.5237189464,0.2362514532\N,-3.0539995285,0.6239922999,-0.06766687
6\H,-2.2657976862,1.2286946736,-0.255465113\C,-4.3602807477,1.20472106
63,0.2089531834\H,-5.1261060821,0.7138303473,-0.3984685522\H,-4.632126
1678,1.0850881489,1.2640433273\H,-4.3296595721,2.2686401169,-0.0376840
361\Version=Al64T-G03RevC.02\State=1-A\HF=-1616.0015276\RMSD=4.595e-0
9\RMSF=8.082e-06\Dipole=1.1069385,1.5466524,-0.4534151\PG=C01 [X(C5H12
N1O3P1S2)]\@

Dimethoate INT1

I\GINC-SC117\FOpt\RB3LYP\6-31+G(d)\C5H13N1O4P1S2(1-)\CJJ506\07-Apr-2
005\0\# B3LYP/6-31+G* OPT\dmoint1\1,1\S,0.3728726485,1.8038374048,0
.2681767931\P,0.8570942691,-0.0618046897,-0.1797646539\O,1.8502697093,
-0.2508841752,-1.4143076618\S,-0.6821182731,-1.300638345,-0.9701743259
\O,1.3255597374,-0.9330233018,1.079810148\C,2.2963816105,-0.4525788977
,2.0831247481\C,3.092851227,0.5283470771,-1.582535338\H,2.2546587252,-
1.2122945992,2.8682725212\H,1.9471005073,0.5098192984,2.4710156256\H,2
.8357780645,1.5925475539,-1.5700969905\H,3.4449979055,0.2399779686,-2.
5761897653\H,3.8288088523,0.260553918,-0.7879435686\C,-1.8957481641,-1
.3065398285,0.4290226754\H,-2.2211225034,-2.3404889848,0.5538463478\C,
-3.1466299307,-0.4620420121,0.1800003864\H,-1.3770886837,-0.992072836,
1.3398761625\O,-4.2576321167,-0.990474943,0.0644047709\N,-2.9565063025
,0.8765274279,0.12842096\H,-2.003514912,1.2418728447,0.1583690797\C,-4
.0455308408,1.7882161314,-0.1689028112\H,-4.4405090224,1.6271584898,-1
.1804836205\H,-4.8686931878,1.6482989265,0.5400741654\H,-3.6700383774,
2.8116710023,-0.089541891\H,3.3121721936,-0.3812840491,1.6273750603\O,
4.8750037529,-0.0875077834,0.6903479148\H,5.5909584383,-0.7428593327,0
.6686111474\Version=Al64T-G03RevC.02\State=1-A\HF=-1691.8512715\RMSD=
6.557e-09\RMSF=1.331e-05\Dipole=-3.8834368,0.2050459,-0.4196464\PG=C01
[X(C5H13N1O4P1S2)]\@

Dimethoate TS1

I\GINC-SC99\FTS\RB3LYP\6-31+G(d)\C5H13N1O4P1S2(1-)\CJJ506\17-Nov-200
4\0\# B3LYP/6-31+G* OPT=(TS,NOEIGENTEST) IOP(1/8=10)\dmots1\1,1\S,-0.
4650220937,1.34784363,-1.2008133354\P,-1.0578041565,0.1143825084,0.224
1581582\O,-1.915512977,0.7021954808,1.4592160713\S,0.5205544265,-0.455
531657,1.5996667933\O,-1.435898209,-1.3923114878,-0.2258280406\C,-2.00
28332386,-1.6924940766,-1.5369089825\C,-2.7206896599,1.9100091111,1.33
34477546\H,-2.3375340907,-2.7315955241,-1.4583235771\H,-1.2111067337,-

1.6058611495,-2.2897153989\H,-2.0512614621,2.7748912196,1.2684734258\H
,-3.2998921368,1.9510832342,2.2609051876\H,-3.3560379946,1.7837535154,
0.4412769648\C,1.6317551176,-1.503860599,0.5626434858\H,1.9390197275,-
2.3502851608,1.1799420177\C,2.9124390167,-0.8300778591,0.0670902403\H,
1.0468901809,-1.8900423956,-0.2785140968\O,4.0237651757,-1.3073612697,
0.3314113448\N,2.7509510333,0.2726979003,-0.6979961007\H,1.8108643026,
0.6519105733,-0.8377231983\C,3.8844846565,1.0186195533,-1.2078015976\H
,4.4708419724,1.4674390467,-0.394902834\H,4.5523172291,0.3656353563,-1
.7811511349\H,3.5089913701,1.8130563408,-1.8583940381\H,-2.8329659035,
-0.9829608247,-1.7037156445\O,-3.7217914791,0.436934042,-0.8632867057\H,
-4.3536741101,-0.0774696282,-0.3291394299\Version=DEC-AXP-OSF/1-G98
RevA.11.3\HF=-1691.8440126\RMSD=2.630e-09\RMSF=6.488e-06\Dipole=1.8055
737,-0.2965522,0.4199406\PG=C01 [X(C5H13N1O4P1S2)]\@

Dimethoate INT2

I\GINC-SC160FOpt\RB3LYP\6-31+G(d)\C5H13N1O4P1S2(1-)\CJJ506\06-Nov-2
0040\# B3LYP/6-31+G* OPT\dmoint2\1,1\N,-0.4456003668,1.4085420163,-1.
2501270658P,-1.3433023978,0.149507275,0.0592918048\O,-1.8925656934,0.
7297239634,1.5618717299\N,0.3813757813,-0.4601438357,1.4667159157\O,-1
.3936485511,-1.5027353338,-0.33855792\C,-1.9379818975,-1.9270151279,-1
.591565218\C,-2.6783700617,1.9200343599,1.6309943364\H,-3.0270917877,-
2.04676707,-1.5421160191\H,-1.4756075296,-2.8993775684,-1.8012832474\H
,-2.3508212908,2.6556844833,0.8878094183\H,-2.5253613039,2.3204907734,
2.6399428151\H,-3.7452275913,1.7130610327,1.4791758882\C,1.5296124256,
-1.4813281649,0.4468294672\H,1.7962964718,-2.3764049135,1.0144297081\C
,2.8401959478,-0.80560259,0.0496407251\H,0.9875041153,-1.7959567528,-0
.4507995716\O,3.9402650408,-1.3225934392,0.3016164238\N,2.7220070689,0
.3600921259,-0.626288653\H,1.7869922997,0.7630576297,-0.75256308\C,3.8
787556143,1.1258704071,-1.0365339122\H,4.4377005858,1.514998532,-0.173
4741277\H,4.5671518766,0.5076495256,-1.6252795138\H,3.537420265,1.9672
71155,-1.6469651194\H,-1.6943476289,-1.2198192212,-2.3919677269\O,-2.9
526670142,0.3613040388,-0.5934812239\H,-3.5758710561,-0.1588596399,-0.
0554719943\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-1691.8799978\RMSD=8
.514e-09\RMSF=6.183e-06\Dipole=-1.3675205,-0.018534,-0.3485259\PG=C01
[X(C5H13N1O4P1S2)]\@

Dimethoate TS2

I\GINC-SC82FTS\RB3LYP\6-31+G(d)\C5H13N1O4P1S2(1-)\CJJ506\23-Feb-200
5\# B3LYP/6-31+G* OPT=(TS,NOEIGENTEST,MAXCYC=200,CALCFC) IOP(1/8=10
)\Reactant\1,1\N,-0.4244390357,-0.7566578895,1.6759061698\N,-1.4482
001991,-0.0743908469,0.0628231323\O,-2.0046011729,-1.000850923,-1.2648
853206\N,0.3416039769,0.2651251618,-1.4454179414\O,-1.70754144,1.56583
46262,-0.1386236903\C,-2.4942911862,2.3068362914,0.8023613645\C,-1.687
7217179,-2.3909107642,-1.2793673451\H,-3.5658989317,2.1413726097,0.652
38752\H,-2.2496799829,3.3585292418,0.6152639511\H,-0.6019632835,-2.543
7621146,-1.2716116575\H,-2.1050349375,-2.7894928854,-2.2110149438\H,-2
.1343912261,-2.9104945573,-0.4207165397\C,1.5566727927,1.3283865297,-0
.5496084825\H,1.7911337026,2.1953363033,-1.1719588743\C,2.8724152186,0
.6273309788,-0.230645136\H,1.0815689074,1.6730503655,0.3756204272\O,3.
9417551999,0.9440052016,-0.7722697284\N,2.788185675,-0.3495350591,0.70
65303514\H,1.8496657377,-0.6142775616,1.0238240441\C,3.9151082009,-1.1
959890735,1.0327756907\H,4.2036006983,-1.842117512,0.1903629524\H,4.78
77843069,-0.5888227406,1.2990605178\H,3.6423170022,-1.8263296908,1.884
9042546\H,-2.2350344725,2.0429927445,1.8334283992\O,-3.0121314106,-0.3
182264754,0.7892010568\H,-3.6459525792,-0.4488756505,0.0641037605\Ver
sion=Al64T-G03RevC.02\State=1-A\HF=-1691.8788506\RMSD=4.466e-09\RMSF=3

.881e-06\Dipole=-1.1380688,-0.3708369,0.2765764\PG=C01 [X(C5H13N1O4P1S2)]\@

Dimethoate LEAVING GROUP

I\GINC-SC117FOpt\RB3LYP\6-31+G(d)\C3H6N1O1S1(1-)\CJJ506\06-Apr-2005
\#\ B3LYP/6-31+G* OPT\thio\1,1\S,-2.1019651515,-0.5377192044,0.0
000307935\C,-0.967541581,0.9195780054,0.0000271642\H,-1.1466803127,1.5
574421539,0.8765693925\H,-1.1466760659,1.5574431223,-0.8765151798\C,0.
5438432145,0.6523339564,0.0000461557\O,1.3756176325,1.5783631848,0.000
096996\N,0.8829349485,-0.6570126502,-0.0001080084\C,2.2365637921,-1.14
7081625,-0.0000966834\H,0.0644823031,-1.2826091308,-0.0001566941\H,2.4
427783888,-1.7593607672,-0.891037418\H,2.442583376,-1.7597930732,0.890
5895337\H,2.9122764828,-0.2864139816,0.000177942\Version=Al64T-G03Rev
C.02\State=1-AHF=-646.1760779\RMSD=7.655e-09\RMSF=5.711e-05\Dipole=2.
3342697,-0.4481087,-0.0001225\PG=C01 [X(C3H6N1O1S1)]\@

MCO, MCS reactions with hydroxide:

MCO

I\GINC-SC14FOpt\RB3LYP\6-31+G(d)\C7H7Cl3N1O4P1\MLC501\02-Aug-2004\0
\#\ B3LYP/6-31+G(D) OPT=TIGHT FREQ MAXDISK=402653184\mco-cis-6+dub3\
0,1\O,2.2463552835,-0.9812421832,1.5737042664\P,2.4169951611,-0.568429
9214,0.1641953442\O,3.7754698976,0.1502590932,-0.2597950577\C,4.267585
5691,1.2741164419,0.504674148\H,3.6159246139,2.1401701213,0.3577404805
\H,4.3282325394,1.0159993765,1.5655624778\H,5.2626411333,1.4837455975,
0.1107568353\O,2.3275143939,-1.6829029748,-0.9663377466\C,1.8327740973
, -3.0129110703,-0.6653525501\H,0.7538048891,-2.9754560639,-0.506086299
7\H,2.0731211798,-3.6119456578,-1.5443507596\H,2.3330449715,-3.4126225
588,0.2195133119\O,1.3608093376,0.631470096,-0.3035377786\C,0.01645468
08,0.5472948938,-0.1712511912\C,-0.7354074491,1.7354884384,-0.16684541
12\N,-0.5554269726,-0.6436713989,-0.0813498622\C1,0.0327024639,3.29252
28654,-0.2878229592\C,-1.8715855835,-0.7459225683,0.0267074645\C1,-2.5
170959213,-2.362804725,0.142668862\C,-2.7125287792,0.3740367149,0.0408
274955\C1,-4.4431852193,0.251848808,0.1778041128\C,-2.1165422829,1.634
0795513,-0.0607230444\H,-2.7305632463,2.5278530167,-0.0521583751\Vers
ion=DEC-AXP-OSF/1-G03RevB.03\State=1-AHF=-2348.6365905\RMSD=7.874e-09
\RMSF=3.429e-06\Dipole=0.0365897,0.5870058,-0.4244569\PG=C01 [X(C7H7Cl
3N1O4P1)]\@

MCOINT1

I\GINC-SC96FOpt\RB3LYP\6-31+G(d)\C7H8Cl3N1O5P1(1-)\CJJ506\09-Apr-20
05\#\ B3LYP/6-31+G* OPT\mcoint1\1,1\C,0.4852876083,0.5454104619,0.074
457883\C,-4.505164776,0.8263079332,-1.001643121\C,1.3922920187,1.55316
25341,0.4786146332\C,-2.8284206139,-1.2873961222,1.4687539498\C,2.7405
157413,1.2414209691,0.5619433095\C,3.1714786819,-0.0496992718,0.243371
3245\C,2.1989946338,-0.9765256823,-0.1456141801\N,0.9165242931,-0.6770
981836,-0.2173204926\C1,4.8761458364,-0.4336839333,0.3454636207\O,-3.1
29441173,1.0115588665,-0.5055362571\O,-2.2076851143,-1.336361878,0.133
9642503\O,-0.8110572211,0.8511396141,0.0183103797\P,-1.9992487775,-0.0
635357033,-0.7776964098\O,-1.6268324774,-0.3763423879,-2.1759858232\H,
-4.9400804737,1.8272892096,-0.953563847\H,-4.4636990662,0.4917775235,-
2.0442132184\H,-5.0541012541,0.1195051284,-0.3394656373\C1,0.835818592
,3.1601529658,0.8673489945\H,-2.5401477443,-2.2359841483,1.9292499624\
H,-2.397123261,-0.4562152849,2.0382078071\H,-3.9356688061,-1.203610958
,1.3680132365\H,3.4575646512,1.9949941933,0.8684197134\C1,2.6407281499
, -2.6225311314,-0.5589268295\O,-5.7371292493,-0.911722262,1.0470109409

\H,-6.3821941481,-1.6342377012,0.9825725044\Version=A164T-G03RevC.02\
State=1-A\HF=-2424.4784834\RMSE=8.911e-09\RMSF=1.099e-05\Dipole=6.5954
904,1.4006293,0.0333778\PG=C01 [X(C7H8C13N1O5P1)]\@

MCOTS1

I\INGINC-SC39\Freq\RB3LYP\6-31+G(d)\C7H8C13N1O5P1(1-)\MLC501\28-Oct-20
04\0\# B3LYP/6-31+G* OPT=(TS,CALL,NOEIGENTEST,MAXCYC=200) IOP(1/8=
10) MAXDISK=402653184 GEOM=CHECK GUESS=READ\TS_mco_oh-6+dub3\1,1\C,
0.4689014332,0.6231132882,0.0495622967\C,-4.3949476468,1.1685448301,-0
.8373388613\C,1.4367618141,1.6585956629,0.0840390993\C,-3.1334578623,-
1.5181989775,1.8637747089\C,2.7806762562,1.3254742661,0.0454206216\C,3
.1555762707,-0.019643561,-0.030405208\C,2.1312616567,-0.9705692513,-0.
062050013\N,0.8541881544,-0.6496856563,-0.0206768069\C1,4.8572460438,-
0.4342374059,-0.0806988779\O,-3.2378087144,1.0311156642,0.0494086692\O
,-2.0007967081,-0.9642519316,1.1157780789\O,-0.8117301926,0.9585069211
,0.1059089958\P,-2.1397791944,-0.091080679,-0.20297594\O,-1.9825098646
,-0.6774006715,-1.5519909552\H,-4.9856886811,1.9708701867,-0.386501714
2\H,-4.0469869882,1.4707290962,-1.8313617075\H,-4.9208737577,0.1915426
051,-0.8434305828\C1,0.9521993086,3.3350795634,0.1757512901\H,-2.73972
05027,-2.4265270498,2.3291315091\H,-3.4027679475,-0.7892096001,2.63691
41586\H,-3.9754854028,-1.7222570009,1.1631749131\H,3.5378628984,2.1014
790765,0.0710557192\C1,2.5030662562,-2.6852779575,-0.1531711852\O,-5.0
329992325,-1.5928020382,-0.2959319859\H,-4.803539962,-2.192450033,-1.0
249846933\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-2424.4761836
\RMSE=4.002e-09\RMSF=2.304e-06

MCS

I\INGINC-SC74\Fopt\RB3LYP\6-31+G(d)\C7H7C13N1O3P1S1\MLC501\30-Aug-2004
\0\# B3LYP/6-31+G* OPT FREQ MAXDISK=134217728\mcs-cis-6+dub3\0,1\S,
2.3356886078,-1.0226465297,1.7989545357\P,2.3400513837,-0.4427483232,-
0.0450584517\O,1.2006023544,0.728060243,-0.4124491929\C,-0.1343934967,
0.5999178712,-0.2378730635\C,-0.9135423063,1.7666301989,-0.1394470757\N,
-0.6745300758,-0.6087489727,-0.1951526009\C1,-0.1870620722,3.3468793
18,-0.1992421557\C,-1.98348705,-0.7496117256,-0.0483122476\C1,-2.58681
8606,-2.3862860311,-0.0006462569\C,-2.8494594874,0.3459917745,0.057522
247\C1,-4.5708932121,0.1727169953,0.2461127685\C,-2.2872545024,1.62457
31728,0.0074337607\H,-2.9214232515,2.5005200476,0.087589071\O,2.200221
7453,-1.5245147919,-1.210826034\C,1.7396829807,-2.8781626442,-0.987365
3219\O,3.6170553834,0.3452396365,-0.6031034285\C,4.1267791522,1.512682
5575,0.0762603187\H,4.3145902904,1.2871475289,1.1300213705\H,3.4177835
092,2.3399196373,-0.0175365586\H,5.0613043596,1.7585600924,-0.42924353
38\H,0.665809631,-2.8732259803,-0.7927967841\H,2.2772357466,-3.3282668
303,-0.1495209514\H,1.9627902939,-3.4085250934,-1.9139367148\Version=
DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-2671.5896612\RMSE=6.726e-09\RMS
F=4.604e-05\Dipole=-0.0871899,0.5814402,-0.4296467\PG=C01 [X(C7H7C13N1
O3P1S1)]\@

MCSINT1

I\INGINC-SC119\Fopt\RB3LYP\6-31+G(d)\C7H8C13N1O4P1S1(1-)\CJJ506\04-Apr
-2005\0\# B3LYP/6-31+G* OPT\mcs\1,1\C,-0.5961584999,0.7164735096,-
0.0848604624\C,4.4944406401,1.0101801324,0.2825461869\C,-1.5446571724,
1.749228604,-0.274151465\C,2.5738362918,-2.219218097,-1.0843405299\C,-
2.8904868051,1.419144984,-0.3068547685\C,-3.2777779329,0.0851733178,-0
.1482396177\C,-2.2662491165,-0.8619479253,0.0379191705\N,-0.9865545917
,-0.5438459298,0.0643109961\C1,-4.9789693874,-0.3240435751,-0.19042154
74\O,3.0663594139,1.1707388626,-0.0372838316\O,1.8574956094,-0.9378813

891,-0.9687190957\O,0.6943227533,1.0548184391,-0.0671153006\P,1.998817
6026,0.0349890828,0.2783858398\S,1.9994126264,-0.7271935733,2.06810509
15\H,4.9442042111,1.9409217839,-0.0718075355\H,4.5934918181,0.93475879
11,1.37081924\H,4.9213025471,0.1195173129,-0.2355226898\Cl,-1.04246686
26,3.4085860097,-0.4679882423\H,2.288927657,-2.8482012524,-0.234451576
2\H,2.1895569365,-2.6472506747,-2.0134124111\H,3.6729001294,-2.0391181
261,-1.127729478\H,-3.6388044554,2.1901249761,-0.453768358\Cl,-2.65282
02532,-2.5601514721,0.2474463358\O,5.4230854811,-1.4211880786,-1.14103
87203\H,6.1360072999,-1.9743265595,-0.7822500064\Version=Al64T-G03Rev
C.02\State=1-A\HF=-2747.432285\RMSD=4.403e-09\RMSF=1.729e-05\Dipole=-6
.274405,1.7460362,0.6924199\PG=C01 [X(C7H8Cl3N1O4P1S1)]\@

MCSTS1

I\GINC-SC160\FTS\RB3LYP\6-31+G(d)\C7H8Cl3N1O4P1S1(1-)\CJJ506\14-Nov-
2004\0\# B3LYP/6-31+G* OPT=(TS,NOEIGENTEST,MAXCYC=200) IOP(1/8=10)\VT
S_mcs_oh-6+dub3\1,1\Cl,-0.5668048702,0.690673429,-0.0104615709\C,4.39
77200871,1.4350670378,0.5481790671\C,-1.5858994897,1.6759131023,0.0288
284113\C,2.4234573722,-1.9127474,-1.585994387\C,-2.9099548731,1.277831
5505,-0.0524542735\C,-3.2150426744,-0.0821975819,-0.1677393607\C,-2.14
42563592,-0.9795371072,-0.1961397313\N,-0.8853012836,-0.5973867886,-0.
1214197957\Cl,-4.89202102,-0.5793164625,-0.2687412536\O,3.03121685,1.3
793243218,0.0346930215\O,1.8950954195,-0.5955241348,-1.2388613669\O,0.
6926623483,1.0995451698,0.0632746652\N,2.089996043,0.1007076655,0.1813
991169\S,2.0897136349,-0.9255769512,1.8353260764\H,4.8133389154,2.3433
54275,0.1022253279\H,4.353514057,1.5392157618,1.6384545214\H,4.9208397
9,0.5074843145,0.2318300393\Cl,-1.1890373583,3.3707197702,0.1730289578
\H,1.8297107274,-2.6711632538,-1.0641955894\H,2.2625614115,-1.98909985
94,-2.6652217814\H,3.4951467341,-1.9311080254,-1.2999962631\H,-3.70532
20334,2.0145659424,-0.0260439612\Cl,-2.4273738968,-2.7083068444,-0.341
1056805\O,4.9589937822,-1.2091378835,-0.4192207629\H,5.0662468988,-1.7
692432441,0.3681945102\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-2747.43
07288\RMSD=6.416e-09\RMSF=1.579e-05\Dipole=-5.4084007,1.4935932,0.0334
583\PG=C01 [X(C7H8Cl3N1O4P1S1)]\@

MCO, MCS LEAVING GROUP

I\GINC-SC66\FOpt\RB3LYP\6-31+G(d)\C5H1Cl3N1O1(1-)\MLC501\30-Aug-2004
\0\# B3LYP/6-31+G* OPT FREQ MAXDISK=134217728\mc--6+dub3\1,1\O,3.0
006257881,0.1639395084,-0.2329667669\C,1.7631841599,0.1055028764,-0.13
71529298\C,0.8879513217,1.2736368933,-0.1160691533\N,1.0890383165,-1.1
130844116,-0.0391038113\Cl,1.6236490374,2.8783651419,-0.2333706202\C,-
0.2071726404,-1.1863543683,0.0615049248\Cl,-0.8946814585,-2.8494805847
0,1.775614996\C,-1.0792843595,-0.0959816913,0.0851200498\Cl,-2.8369680
981,-0.2172312582,0.2221607733\C,-0.480067923,1.1728173208,-0.00904039
56\H,-1.0999290474,2.064242544,0.0033077438\Version=DEC-AXP-OSF/1-G03
RevB.03\State=1-A\HF=-1701.7837839\RMSD=5.041e-09\RMSF=2.053e-05\Dipol
e=-2.2663328,0.6463739,0.1461391\PG=C01 [X(C5H1Cl3N1O1)]\@

MPO, MPS Reaction with hydroxide

MPS

I\GINC-SC160\FOpt\RB3LYP\6-31+G(d)\C8H10N1O5P1S1\MLC501\31-Aug-2004\
0\# B3LYP/6-31+G* OPT FREQ MAXDISK=268435456\ps-cis-6+dub3\0,1\S,-2
.1485858394,0.1511716959,1.942770399\N,-2.2012148471,0.0573064055,0.01
04513268\O,-0.9193712499,-0.6422489615,-0.7287065419\C,0.4181685387,-0
.4077115239,-0.4784963179\O,-2.2812755502,1.4369709936,-0.8114150961\C
,-3.3080290798,2.4129574707,-0.5238469118\O,-3.3966667328,-0.779818298

3,-0.6623160762\C,-3.815928107,-2.0618136142,-0.1475432213\H,-4.026440
6085,-1.9910054122,0.9230728668\H,-3.0408512268,-2.8110686914,-0.33384
98801\H,-4.7219783694,-2.316837797,-0.6984928457\H,-3.3039060111,2.665
4346417,0.5404298602\H,-4.28583131,2.0229773972,-0.8205817917\H,-3.056
6127442,3.2887864333,-1.123055172\C,1.272772504,-1.5049911326,-0.62736
55283\C,2.6409009047,-1.3423104076,-0.4406946294\C,3.130676039,-0.0790
124212,-0.1019758202\C,0.9150213983,0.856887071,-0.1465315717\C,2.2840
856871,1.0200190456,0.047324953\H,0.8545556473,-2.4713834475,-0.888675
3815\H,3.3255143774,-2.1749828043,-0.5486833451\N,4.5742390066,0.09727
97966,0.1006657606\H,0.2435365337,1.7015738011,-0.0474633681\H,2.69848
12543,1.9866178811,0.3076595486\O,5.2994137876,-0.8902217012,-0.039425
4438\O,4.9808307753,1.2223728774,0.399195306\Version=DEC-AXP-OSF/1-GO
3RevB.03\State=1-A\HF=-1481.280169\RMSD=4.713e-09\RMSF=9.509e-06\Dipol
e=-2.5882453,-0.226436,-0.7261377\PG=C01 [X(C8H10N1O5P1S1)]\@

MPSINT1

1\GINC-SC30\Freq\RB3LYP\6-31+G(d)\C8H11N1O6P1S1(1-)\CJJ506\26-Apr-20
05\O\# B3LYP/6-31+G* OPT\mps\1,1\C,0.8377748829,-0.6039453586,-0.2
991867675\C,-4.2370096956,-1.4324609443,-0.0431020302\C,1.8106336052,-
1.5176506881,-0.7458363191\C,-2.7697473192,2.1194595326,-0.418729782\C
,3.1567505406,-1.189628615,-0.6982261822\C,3.534998402,0.0613754877,-0
.1949631613\C,2.5782417406,0.9777999266,0.2532745063\C,1.228333298,0.6
506476211,0.200954714\N,4.9459379533,0.412444276,-0.139549026\O,-2.805
3984794,-1.3789435091,-0.3918963975\O,-1.7963543182,1.0293819936,-0.62
40200938\O,-0.4455086017,-1.0270209756,-0.406138858\O,5.2582717576,1.5
23859347,0.3074701937\O,5.7729919378,-0.4172936422,-0.5429921902\O,-1.
8093104078,-0.3155564407,0.2337414867\O,-1.805500884,-0.108102217,2.17
40576546\H,-4.5760984289,-2.3717368834,-0.4869795012\H,-4.3277522299,-
1.4797093107,1.046950201\H,-4.7683071584,-0.5533418752,-0.4762217906\H
,1.4803764524,-2.4788013472,-1.1263335333\H,-2.7366589993,2.4178645847
,0.63443544\H,-2.3921834147,2.9278077367,-1.0501482132\H,-3.7886720873
,1.7915707255,-0.7329807552\H,3.9153405681,-1.8836655183,-1.0399032706
\H,2.8973395226,1.9397168531,0.6366152069\H,0.4829827949,1.3573811058,
0.5417946385\O,-5.4479007689,1.0639503292,-1.0530544871\H,-5.908927373
8,1.1637359635,-1.9014852193\Version=Al64T-G03RevC.02\State=1-A\HF=-1
557.1321616\RMSD=8.190e-09\RMSF=1.001e-05\Dipole=4.008058,-1.251928,0.
0178404\PG=C01 [X(C8H11N1O6P1S1)]\@

MPSTS

1\GINC-SC160\Freq\RB3LYP\6-31+G(d)\C8H11N1O6P1S1(1-)\MLC501\09-Dec-2
004\O\# B3LYP/6-31+G* OPT=(TS,CALL,NOEIGENTEST,MAXCYC=200) IOP(1/8
=10) MAXDISK=402653184\TS_ps_oh-6+dub3\1,1\C,-0.7617609586,0.662829
44,-0.1256379475\C,4.1580529004,1.7703549713,0.1841575471\C,-1.7580983
858,1.6322964374,-0.3699568917\C,2.4077590903,-2.0002318691,-1.3835634
775\C,-3.0997572018,1.2891316892,-0.3552436385\C,-3.4616223629,-0.0382
205916,-0.0875136197\C,-2.4866185898,-1.0115876485,0.1600884525\C,-1.1
408975556,-0.668660729,0.1396908187\N,-4.8653369245,-0.4059144731,-0.0
660904953\O,2.8245965376,1.4958126397,-0.3427742237\O,1.6975291388,-0.
7430196243,-1.1571514878\O,0.5033795665,1.1182918625,-0.1624690958\O,-
5.1638025934,-1.5845313982,0.1728520797\O,-5.7086847496,0.4758961024,-
0.2879518179\O,1.9396224935,0.2419698235,0.0824550958\O,2.0303933469,-
0.4761601453,1.8962938821\H,4.5133129323,2.6129618447,-0.4158847695\H,
4.063555962,2.0697960174,1.2340733208\H,4.7615157878,0.8494132825,0.05
53623236\H,-1.4425340389,2.6509302818,-0.5719840033\H,1.9346004384,-2.
7762261154,-0.7693420972\H,2.2463639092,-2.2156231918,-2.4437646342\H,
3.4761716509,-1.8488120076,-1.1154971501\H,-3.8695620502,2.0276014405,

-0.5455779095\H,-2.791372972,-2.0305306549,0.3679883528\H,-0.387286620
3,-1.418452176,0.3400488439\O,4.8313626176,-0.9523404699,-0.3181228987
\H,4.9545767618,-1.3869855321,0.5424947321\\Version=DEC-AXP-OSF/1-G03R
evB.03\State=1-A\HF=-1557.1297614\RMSD=3.730e-09\RMSF=1.471e-05\

MPO

I\GINC-SC160\FOpt\RB3LYP\6-31+G(d)\C8H10N1O6P1\MLC501\01-Oct-2004\O
\# B3LYP/6-31+G* OPT FREQ MAXDISK=268435456\po-cis-6+dub3\0,1\O,-2.3
043922204,0.6962078071,1.4856733327\P,-2.3414250745,0.105781075,0.1259
026936\O,-3.5675305832,-0.8710633246,-0.1869348294\C,-4.0125949117,-1.
8219937933,0.8085598053\H,-3.2866237864,-2.6360537825,0.8951383795\H,-
4.14774822,-1.3275922348,1.7738883439\H,-4.9637957701,-2.2100087295,0.
4425550716\O,-2.3614158517,1.1207142287,-1.1072029125\C,-3.1934497293,
2.3037761607,-1.0600367535\H,-3.0315649644,2.8458456864,-0.124861014\H
,-2.8871362004,2.9133261273,-1.9107394292\H,-4.2458524447,2.0225046957
,-1.1614385611\O,-1.0835670966,-0.8443937718,-0.278247582\C,0.25836951
68,-0.5275768021,-0.1472869865\C,1.1119154369,-1.1143880152,-1.0877357
123\C,2.4818112677,-0.8909703783,-1.0072574295\C,2.9740068013,-0.07837
22127,0.0165765689\C,0.755110365,0.2795595076,0.8825325337\C,2.1275317
592,0.5074664618,0.9583970863\H,0.6898973747,-1.7362935803,-1.87023484
62\H,3.1656458799,-1.3310935079,-1.7231002449\N,4.4198084755,0.1634749
057,0.1044960079\H,0.0786739645,0.7129665699,1.6105370566\H,2.54414438
37,1.1272656765,1.7434662869\O,5.1448997964,-0.3725354415,-0.736848317
5\O,4.8283651476,0.8889563825,1.0138455367\\Version=DEC-AXP-OSF/1-G03R
evB.03\State=1-A\HF=-1158.3279654\RMSD=7.575e-09\RMSF=1.075e-05\Dipole
=-2.5426928,-0.362293,-0.4934357\PG=C01 [X(C8H10N1O6P1)]\@

MPOINT1

I\GINC-SC56\FOpt\RB3LYP\6-31+G(d)\C8H11N1O7P1(1-)\MLC501\30-Aug-2004
\O\# B3LYP/6-31+G* OPT FREQ MAXDISK=268435456\po_oh_comp-6+dub3\1,
1\C,-0.6649735371,-0.0086626231,0.5639104848\C,4.4046719983,-0.7604045
647,0.9617952968\C,-1.5205931336,0.7816389839,1.3550427155\C,2.5661975
515,1.688459119,-1.1006677463\C,-2.8797400961,0.8299623589,1.086408892
5\C,-3.3902351579,0.0826893239,0.017076634\C,-2.5510101648,-0.70838588
36,-0.7749539325\C,-1.1885408966,-0.7599694084,-0.5050050134\N,-4.8148
95657,0.1294671943,-0.2708185506\O,2.9954126733,-0.3638507672,1.143808
1607\O,2.056562393,0.3098507659,-1.203905206\O,0.6429454142,0.01060760
38,0.9179096687\O,-5.24583419,-0.5388861843,-1.2202181132\O,-5.5360401
409,0.836376357,0.4477701621\P,1.9029118662,-0.6586424609,0.0414372042
\O,1.6441906457,-2.0615829921,-0.3696196892\H,4.8192022789,-0.73101656
9,1.9718699481\H,4.4361518502,-1.7860316872,0.5783246011\H,4.915211842
7,-0.0295644293,0.2943138169\H,-1.0898909576,1.3504185818,2.1729443182
\H,2.256311885,2.1581817025,-2.0377708118\H,2.0790802729,2.1916164606,
-0.2579335258\H,3.6763667557,1.6684209515,-1.0009390435\H,-3.548319517
2,1.4362708765,1.6858797904\H,-2.9722148942,-1.2806230819,-1.593134204
3\H,-0.5310956595,-1.3864612022,-1.0965637319\O,5.481669292,1.43899326
47,-0.6767202478\H,6.1538796697,1.458126732,-1.3766612366\\Version=DEC
-AXP-OSF/1-G03RevB.03\State=1-A\HF=-1234.1786419\RMSD=6.515e-09\RMSF=9
.989e-06\Dipole=-3.9383669,-0.6288192,0.9483684\PG=C01 [X(C8H11N1O7P1)
]\@

MPOTS

I\GINC-SC31\Freq\RB3LYP\6-31+G(d)\C8H11N1O7P1(1-)\MLC501\15-Oct-2004
\O\# B3LYP/6-31+G* FREQ MAXDISK=402653184\TS_po_oh-6+dub3f\1,1\C,0
.6612511606,0.6247850292,0.0910750146\C,-4.2123778394,1.4768180292,-0.
7066049854\C,1.6317051606,1.5381290292,0.5556330146\C,-3.0290728394,-1

.3771749708,1.8062380146\C,2.9801731606,1.2262840292,0.4993050146\C,3.3739901606,-0.0115399708,-0.0272819854\C,2.4236741606,-0.9273659708,-0.4959049854\C,1.0720331606,-0.6152929708,-0.4404709854\N,4.7845631606,-0.3454799708,-0.0877459854\O,-3.0370498394,1.2398970292,0.1388980146\O,-1.8888718394,-0.9246229708,1.0034880146\O,-0.6183358394,1.0273500292,0.1925150146\O,5.1119701606,-1.4452789708,-0.5553079854\O,5.6053691606,0.4847330292,0.3314400146\P,-1.9875888394,0.1028620292,-0.2082959854\O,-1.8511678394,-0.4005489708,-1.5962699854\H,-4.7486308394,2.283820292,-0.2002399854\H,-3.8734088394,1.8104420292,-1.6933079854\H,-4.7838858394,0.5259840292,-0.7455809854\H,1.2926151606,2.4868530292,0.9595850146\H,-2.6640428394,-2.2730409708,2.3165190146\H,-3.2556758394,-0.5960219708,2.5407580146\H,-3.8867678394,-1.5724839708,1.1261090146\H,3.7313601606,1.9207760292,0.8565990146\H,2.7529771606,-1.8761609708,-0.9030249854\H,0.3324321606,-1.3099459708,-0.8197049854\O,-4.9582098394,-1.2671949708,-0.3036669854\H,-4.8929728394,-1.8473189708,-1.0797469854\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-1234.176079\RMSD=4.145e-09\RMSF=1.534e-04

MPO, MPS Leaving Group

I\GINC-SC76\FOpt\RB3LYP\6-31+G(d)\C6H4N1O3(1-)\MLC501\30-Aug-2004\O\# B3LYP/6-31+G* OPT FREQ MAXDISK=134217728\p--6+dub3\--1,1\O,3.4447062038,0.1658852609,0.3869725526\C,2.1941664798,0.1055621977,0.2464360171\C,1.2872418802,1.0705619368,0.8555664956\C,-0.0763142577,1.0018785045,0.7002632798\C,-0.6624397012,-0.0318900906,-0.0744095385\C,1.5402997043,-0.9344325331,-0.5380480199\C,0.1759469882,-0.9970181923,-0.6891083148\H,1.7389168557,1.8626696975,1.4493321927\H,-0.7308326965,1.7328429822,1.1642165069\N,-2.0616225619,-0.0992531514,-0.2315563725\H,2.1851555663,-1.6737318137,-1.0088126341\H,-0.2871944301,-1.7817702919,-1.2786964902\O,-2.7871215278,0.7665539461,0.3219090625\O,-2.5610964164,-1.0240903886,-0.9225496755\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-511.475078\RMSD=9.679e-09\RMSF=3.311e-05\Dipole=-0.3394706,-0.0163522,-0.0382799\PG=C01 [X(C6H4N1O3)]\@

Diethyl benzylphosphonate Ring 'sideways':

I\GINC-SC113\FOpt\RB3LYP\6-31+G(d)\C12H19O3P1\CJJ506\25-Mar-2005\O\# B3LYP/6-31+G* OPT\debpside\O,1\C,-0.9521422288,1.2399589039,-0.5238631892\C,-1.6275595384,0.7972329509,-1.668270499\C,-3.0183280373,0.8908284802,-1.7570115423\C,-3.7804657925,1.4272254935,-0.7106776644\C,-3.0995710469,1.8643123286,0.4354307429\C,-1.7104740536,1.7720211645,0.5283573302\C,0.5553593825,1.151746581,-0.4235213792\C,-5.2848881881,1.5420705076,-0.8106034643\C,3.7200767301,-0.6137132722,-1.022034127\C,5.116850011,-0.774587946,-0.4488296402\C,0.8847210198,-2.0710362745,2.0384261596\C,0.1354276725,-2.0527945947,3.3580750299\P,1.2031893769,-0.5294274505,-0.1056405059\O,2.8121853954,-0.3261928941,0.0710803576\O,0.7322996911,-0.7675974419,1.4185101646\O,0.841118429,-1.5804508113,-1.0991563632\H,-1.0648876901,0.3603244256,-2.4894190338\H,-3.5179295934,0.537851644,-2.6568659971\H,-3.6623624244,2.283970013,1.2674823883\H,-5.7802696382,1.0796560028,0.0522268331\H,-5.6046296977,2.5920559654,-0.8423548911\H,-5.6629552713,1.0532791702,-1.7147645017\H,3.6841415373,0.2216697137,-1.7336741857\H,3.3837435685,-1.5195905463,-1.5349952296\H,5.829836957,-0.967859618,-1.2595442596\H,5.4306799787,0.1322066191,0.0794293358\H,5.1549445319,-1.6149574345,0.252670714\H,1.9543646127,-2.2577409069,2.1903920491\H,0.4862294954,-2.8316208276,1.3591748089\H,0.534495351,-1.2793065972,4.0230976039\H,0.2391951107,-3.0247093603,3.8554713988\H,-1.2094236398,2.1151250303,1.4309669555\H,-0.9299255006,-1.8577378403,3.1965219041\H,1.0289786857,1.4742065564,-1.3599271258\H,

0.9390692685,1.7989329904,0.372379009\\Version=Al64T-G03RevC.02\\State=1-A\\HF=-1035.8525355\\RMSD=5.946e-09\\RMSF=1.496e-06\\Dipole=0.3838529,0.3986048,0.4837785\\PG=C01 [X(C12H19O3P1)]\\@

Diethyl benzylphosphonate Ring 'up':

I\\N\\GINC-SC31\\FOpt\\RB3LYP\\6-31+G(d)\\C12H19O3P1\\CJJ506\\05-Apr-2005\\0\\#
B3LYP/6-31+G* OPT\\debpu\\0,1\\C,-1.2335268385,-0.0543689454,-1.02427
089\\C,-1.9462059334,-1.2284655694,-0.755561804\\C,-3.1735250662,-1.1898
52511,-0.0873573312\\C,-3.7312745421,0.0235472449,0.3322735807\\C,-3.015
7680677,1.1999942106,0.0577181524\\C,-1.7909579351,1.1640472686,-0.6071
780352\\C,0.0860650068,-0.1016268888,-1.7610287232\\C,-5.0604138791,0.07
46165763,1.0512551552\\C,2.4767211613,1.9227550217,0.8515263677\\C,2.118
6182643,3.3487853808,1.2279082965\\C,1.993096942,-2.3766722275,0.453636
0847\\C,2.0995747475,-2.8938371431,1.8772177078\\P,1.613353103,-0.015975
4436,-0.7525317003\\O,1.4398886932,1.4160873684,-0.0284900532\\O,1.43425
46732,-1.0399179156,0.4986941445\\O,2.8680542817,-0.231763119,-1.529366
7053\\H,-1.5442292619,-2.1877607162,-1.0760271708\\H,-3.7055491211,-2.11
95188453,0.1044670742\\H,-3.4254265068,2.1600510643,0.3669749157\\H,-4.9
596988714,0.5259587991,2.0466892576\\H,-5.7926686919,0.6758056373,0.497
1065507\\H,-5.4827092446,-0.9274357651,1.181302215\\H,3.4370730334,1.875
2718232,0.3268814396\\H,2.5230780657,1.2777385846,1.7362515167\\H,2.8824
055075,3.7559328984,1.9013877476\\H,2.0676999612,3.9856199766,0.3382804
429\\H,1.1510069021,3.3855562559,1.7397076354\\H,2.9688820282,-2.3390295
397,-0.0399981462\\H,1.3249567699,-3.0117334675,-0.1425365488\\H,2.77702
69391,-2.2683821855,2.4685655105\\H,1.1189098145,-2.9005426318,2.364852
4123\\H,2.4917942148,-3.9180925762,1.8705926921\\H,-1.2569015836,2.09086
77935,-0.8005337622\\H,0.1725914983,0.7203954069,-2.4820812655\\H,0.1794
576594,-1.0298560334,-2.337437469\\Version=Al64T-G03RevC.02\\State=1-A\\
HF=-1035.8517583\\RMSD=9.166e-09\\RMSF=1.439e-06\\Dipole=-0.7396463,-0.11
03206,0.8986261\\PG=C01 [X(C12H19O3P1)]\\@

Diethyl benzylphosphonate Transition State:

I\\N\\GINC-SC104\\FTS\\RB3LYP\\6-31+G(d)\\C12H19O3P1\\CJJ506\\05-Apr-2005\\0\\#
B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\\DEBPTS\\0,1\\C,-1.251783994
9,-0.9057093407,0.5579014719\\C,-2.1357055692,-0.2724135929,1.438797803
9\\C,-3.4422912708,0.0322807887,1.0476783948\\C,-3.9109382782,-0.2899146
496,-0.2320969572\\C,-3.022132328,-0.9289532093,-1.1108215623\\C,-1.7178
616459,-1.2334834357,-0.7233389141\\C,0.1600277555,-1.2422712891,0.9839
965151\\C,-5.3281431451,0.0245928803,-0.6552680234\\C,3.67264766,-1.3020
895568,-0.084064288\\C,4.5871588696,-1.3672458744,-1.2945477852\\C,1.360
4519782,2.3650341469,-0.5919215939\\C,0.3329245437,3.2742566262,-1.2405
806438\\P,1.4667736984,0.0252994638,0.6596894248\\O,2.4570372315,-0.6152
868352,-0.4706436952\\O,0.6898313269,1.1372215159,-0.2062668676\\O,2.188
8840405,0.4950150984,1.8778949003\\H,-1.8019488882,-0.0103524395,2.4408
061866\\H,-4.1077215325,0.5248345689,1.7538793693\\H,-3.3567202779,-1.19
54378996,-2.1119176736\\H,-5.3491308044,0.6042064584,-1.5866912036\\H,-5
.9053715403,-0.892415293,-0.8324953832\\H,-5.8539243028,0.6040427779,0.
1109847192\\H,3.4088469245,-2.311145671,0.2605045404\\H,4.1371044332,-0.
7626014466,0.7468473494\\H,5.5061717456,-1.907178762,-1.0361433673\\H,4.
1010040421,-1.8892610773,-2.1258608797\\H,4.8601695486,-0.3607773483,-1
.629525276\\H,2.1674199806,2.113603504,-1.2897780582\\H,1.7960835822,2.8
233891627,0.3022755052\\H,-0.1043954869,2.7995309365,-2.1252443565\\H,0.
8120735054,4.2112698888,-1.5493898989\\H,-1.0511121417,-1.7268876998,-1
.4277291701\\H,-0.4741759447,3.5111884171,-0.5395435732\\H,0.2053845444,
-1.4111280218,2.0652289647\\H,0.4964888965,-2.1644712076,0.4961696268\\
Version=Al64T-G03RevC.02\\State=1-A\\HF=-1035.847882\\RMSD=7.279e-09\\RMSF

=1.075e-06Dipole=-0.2225049,-0.2781184,-0.9514573\PG=C01 [X(C12H19O3P1)]\@

MCS ring 'up':

I\INGINC-SC30\FOpt\RB3LYP\6-31+G(d)\C7H7Cl3N1O3P1S1\CJJ506\22-Apr-2005
\#\ B3LYP/6-31+G* OPT\mcs-up\0,1\O,-2.0601304646,1.5063399423,0.22
00917763\p,-2.3579274879,-0.0393348728,-0.1065334997\S,-3.9773476398,-
0.5249508575,-1.0326643199\O,-2.1064893523,-0.6881451947,1.3446710146\
O,-1.0194544328,-0.3770272807,-1.0052326888\C,-2.9811817581,2.28914580
87,1.0098992496\C,0.2736178808,-0.1612161612,-0.6113995103\C,-2.273803
813,-2.1009865955,1.5944882516\H,-3.9859887579,2.2380397852,0.58024763
01\H,-2.6070710506,3.3128091223,0.9690043631\H,-2.987876341,1.92961118
42,2.0428436898\H,-2.2462302729,-2.2129903425,2.67914362\H,-1.44603137
58,-2.6515902225,1.1400215479\H,-3.2344943051,-2.4434799514,1.19958362
54\C,2.898523717,0.1265681466,0.1130743436\N,0.7730353431,-0.938151558
8,0.3365209018\C,1.0488701377,0.8029951105,-1.2749164206\C,2.381980503
3,0.9380411559,-0.8981131782\C,2.036926757,-0.8095781905,0.7044961818\
Cl,0.3861585012,1.7943758086,-2.5375930097\H,3.016135493,1.6704036507,
-1.38547593\Cl,2.5952504048,-1.8796161918,1.9654674516\Cl,4.5636368124
,0.3013779783,0.586137466\Version=Al64T-G03RevC.02\State=1-A\HF=-2671
.5859725\RMSD=6.940e-09\RMSF=3.208e-06\Dipole=0.4806552,0.634292,0.823
3877\PG=C01 [X(C7H7Cl3N1O3P1S1)]\@

MCS Transition State:

I\INGINC-SC30\FTS\RB3LYP\6-31+G(d)\C7H7Cl3N1O3P1S1\CJJ506\02-May-2005\
0\#\ B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\Reactant\0,1\C,0.2607
402882,0.3318002298,-0.4574047068\C,0.878442615,1.5737263297,-0.237242
985\C,2.2526480021,1.5871655713,-0.0129123962\C,2.9629499907,0.3865955
082,-0.0138275538\C,2.2462756728,-0.7961501157,-0.2554488683\N,0.94366
22796,-0.8006214149,-0.4734623667\O,-1.0713042044,0.2862066801,-0.7561
832148\C,-4.0440136913,-0.6141786199,-1.9019801994\C,-2.2243082919,-2.
2224263104,1.9940285138\p,-2.3171297015,-0.3383675696,0.1213516602\O,-
3.0838183265,-1.2011002504,-0.9983673499\O,-1.556964818,-1.4693801991,
0.9585412665\S,-3.3748679471,0.9643133219,1.0843150793\Cl,-0.023065362
8,3.0590197647,-0.2541588069\H,2.7678774425,2.5249505101,0.163246721\C
1,3.0509517512,-2.3451367115,-0.2944911396\H,-3.5316190537,0.025131672
8,-2.6270683362\H,-4.7873437706,-0.03662292,-1.3455459733\H,-2.9775739
263,-2.8789968089,1.54916798\H,-2.6868187669,-1.5451817733,2.717261618
9\H,-1.4434224866,-2.8160341244,2.4706163447\H,-4.5170831956,-1.453942
0451,-2.4127595759\Cl,4.679494303,0.4053252047,0.2725796627\Version=A
164T-G03RevC.02\State=1-A\HF=-2671.5816626\RMSD=8.121e-09\RMSF=7.298e-
06\Dipole=-0.2245025,-0.2581584,-0.1228447\PG=C01 [X(C7H7Cl3N1O3P1S1)]
\@

MCO ring 'up':

I\INGINC-SC84\FOpt\RB3LYP\6-31+G(d)\C7H7Cl3N1O4P1\CJJ506\25-Apr-2005\
\#\ B3LYP/6-31+G* OPT\mco-up\0,1\O,-2.338277892,1.5520980039,0.23310
41349\p,-2.5739541239,0.0006332719,-0.0756997819\O,-3.8193142742,-0.41
50813812,-0.7500879231\O,-2.2829401558,-0.654825076,1.3567333199\O,-1.
2735904644,-0.3050972958,-1.0227467275\C,-3.3261916213,2.3018351718,0.
9759341708\C,0.0374405203,-0.154941982,-0.6701363415\C,-2.4970017265,-
2.0695669721,1.5748286637\H,-4.3075549764,2.2071581054,0.5028834389\H,
-2.9936379534,3.3400108085,0.945527203\H,-3.3634278056,1.9494246165,2.
010926382\H,-2.4706658478,-2.209422536,2.6562392326\H,-1.687663303,-2.
6354793903,1.1061465637\H,-3.468065254,-2.3721201164,1.1742185968\C,2.
6957341853,0.0068168551,-0.0306862875\N,0.5375118631,-0.9786912815,0.2

372525\C,0.8287653569,0.7966640659,-1.3331108321\C,2.1781645859,0.8678
112729,-0.9995397316\C,1.8172296533,-0.9111203596,0.5642934206\C1,0.16
34409568,1.851707275,-2.5421349369\H,2.8243571,1.5888997131,-1.4878684
192\C1,2.3737310544,-2.0392697491,1.774230505\C1,4.3817411315,0.101158
1431,0.3879712216\Version=Al64T-G03RevC.02\State=1-A\HF=-2348.632589\
RMSD=6.788e-09\RMSF=6.552e-06\Dipole=0.5081652,0.6683177,0.8390189\PG=
C01 [X(C7H7C13N1O4P1)]\@

MCO Transition State:

I\GINC-SC36FTS\RB3LYP\6-31+G(d)\C7H7C13N1O4P1\CJJ506\02-May-2005\0\
\# B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\mcots\0,1\C,0.123351
3766,0.2751801084,-0.4888877272\C,0.8112727827,1.4936447432,-0.3762869
13\C,2.172868242,1.4483836641,-0.0874720365\C,2.8008706948,0.213895797
,0.0776840775\C,2.0180444782,-0.942885955,-0.0659757867\N,0.7278535508
, -0.8919537959,-0.3449847685\O,-1.1965044489,0.2699218644,-0.842469287
4\C,-4.3191069525,-0.6126049304,-1.7388623155\C,-2.6205876476,-1.25892
53891,2.4275167784P,-2.5002787835,-0.0364394565,0.0964800596\O,-3.326
7606237,-1.0785646302,-0.7961427217\O,-1.8578408773,-0.9429586272,1.24
05038207\O,-3.2501627299,1.1688481839,0.5143491998\C1,0.0067056662,3.0
183240062,-0.5925168794\H,2.7414110534,2.3666003995,0.0103435605\C1,2.
7185280017,-2.5321278545,0.1074679376\H,-3.8257201804,-0.1901596464,-2
.6194911271\H,-4.9675438305,0.1338186464,-1.2733742199\H,-3.4179130732
, -1.9655250603,2.1785963051\H,-3.0388431124,-0.3487208707,2.86492453\H
, -1.913954117,-1.7234372476,3.1160423915\H,-4.8935490317,-1.4950995006
, -2.0236450021\C1,4.5015422605,0.159373798,0.4437590297\Version=Al64T
-G03RevC.02\State=1-A\HF=-2348.6287277\RMSD=8.431e-09\RMSF=4.687e-06\
Dipole=-0.2861033,-0.2153083,0.1201229\PG=C01 [X(C7H7C13N1O4P1)]\@

MPS ring 'up':

I\GINC-SC117FOpt\RB3LYP\6-31+G(d)\C8H10N1O5P1S1\CJJ506\16-Apr-2005\
0\# B3LYP/6-31+G* OPT\mps-up\0,1\O,-0.0304286682,1.2445567233,-0.77
6573328P,-1.5899517182,1.0051614272,-1.1949029584\S,-2.2522107014,2.3
706398757,-2.3848720866\O,-2.3830595236,0.8043750214,0.2040152413\O,-1
.5110811897,-0.51849991,-1.7044043961\C,-2.6995397925,-1.2126830421,-2
.1408839907\C,0.74372966,0.3714071654,-0.0221910322\C,-3.0400472223,1.
8992733968,0.8754668318\C,2.4034745063,-1.2498611548,1.4593908532\C,1.
4491222682,-0.6507659386,-0.6623503578\C,0.8696003175,0.5935423886,1.3
508621126\C,1.7075141939,-0.225778075,2.1030426678\C,2.287789002,-1.47
20490087,0.0856210771\H,1.3343385897,-0.7930303099,-1.7309252375\H,0.3
20667065,1.4048007683,1.8167087361\H,1.8279026011,-0.0799053732,3.1697
845451\H,2.8494286982,-2.2735036724,-0.3792361158\N,3.2887351891,-2.11
67644707,2.2510175872\O,3.8917842881,-3.0146883381,1.6602442653\O,3.37
60603538,-1.8971112446,3.4607995586\H,-3.1889381388,-0.6546497788,-2.9
446515384\H,-3.3832047798,-1.349975967,-1.2983817783\H,-2.3575099381,-
2.1806233462,-2.5092509865\H,-3.7594192061,2.3770465323,0.2055538016\H
, -2.3071095854,2.637423436,1.2162226193\H,-3.5487143153,1.45453718,1.7
321509052\Version=Al64T-G03RevC.02\State=1-A\HF=-1481.2776015\RMSD=2.
966e-09\RMSF=8.866e-05\Dipole=-1.7374261,0.2084246,-0.1354528\PG=C01 [
X(C8H10N1O5P1S1)]\@

MPS Transition State:

I\GINC-SC64FTS\RB3LYP\6-31+G(d)\C8H10N1O5P1S1\CJJ506\29-Apr-2005\0\
\# B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\mpsts\0,1\C,-0.41592754
83,-0.4806867342,0.4324785688\C,-1.2515096235,0.0191629516,1.434357970
6\C,-2.6209051888,0.1119241127,1.1997391066\C,-3.1230317003,-0.3002857
474,-0.0357702566\C,-2.2928823256,-0.8056219157,-1.03875145\C,-0.92496

02698,-0.8982900013,-0.800594812\O,0.9280805623,-0.6298661018,0.728606
6748\C,3.9846178894,-1.7874248173,-0.1111705705\C,2.2059249912,2.04957
64769,-1.7776264935\P,2.2047785514,0.1998734845,0.1354285507\O,3.00511
83428,-0.9154370584,-0.7142102984\O,1.4940870737,1.0329629824,-1.03883
0666\S,3.2239082799,1.1538657976,1.4740149376\H,-0.8216273266,0.325765
759,2.3821297588\H,-3.2958186953,0.4960753408,1.9551973153\H,-2.720620
3739,-1.1207773073,-1.9829712259\H,3.4875544703,-2.5267601033,0.524217
422\H,4.7007233536,-1.2051091195,0.4749387142\H,2.9644645875,1.5848930
68,-2.4142011035\H,2.6690268571,2.7613221992,-1.0888561493\H,-0.254469
329,-1.2881093201,-1.5585850124\H,1.4535842947,2.5477788537,-2.3901616
704\H,4.4864497811,-2.2854484129,-0.9419292959\N,-4.5680216136,-0.2044
764014,-0.2875951845\O,-4.9857405065,-0.5733085753,-1.3874225441\O,-5.
2809560249,0.2396016121,0.6145753206\Version=Al64T-G03RevC.02\State=1
-A\HF=-1481.276179\RMSD=5.386e-09\RMSF=4.356e-06\Dipole=1.9944291,-0.3
485757,-0.7122665\PG=C01 [X(C8H10N1O5P1S1)]\@

MPO ring 'up':

I\GINC-SC88\FOpt\RB3LYP\6-31+G(d)\C8H10N1O6P1\CJJ506\20-Apr-2005\O\
B3LYP/6-31+G* OPT\mpo-up\O,1\O,0.4054467964,-0.808493271,1.2981152
66\P,0.9347747275,-2.2197977269,0.6949307821\O,1.4134243491,-3.1146999
293,1.7669574664\O,1.9699906293,-1.7157254631,-0.4134433534\O,-0.26112
76291,-2.8080240254,-0.2131039695\C,-1.2719765485,-3.6549661621,0.3847
772621\C,-0.0401618664,0.325341521,0.648269099\C,2.8239055696,-2.66421
418,-1.0954266961\C,-0.954129968,2.6895343081,-0.4461190481\C,-0.43472
48805,0.3514023846,-0.6941354519\C,-0.1057989001,1.4762114832,1.442879
9804\C,-0.5647295909,2.668175962,0.8951970001\C,-0.8934943354,1.546433
2458,-1.2432210078\H,-0.3892466979,-0.5434567682,-1.3020336577\H,0.207
8951232,1.4182024806,2.479855938\H,-0.6219754805,3.5728866755,1.488540
8853\H,-1.205285276,1.5975477274,-2.2796227597\N,-1.4385441328,3.94530
44501,-1.0319345546\O,-1.775450573,3.9352739815,-2.2182548095\O,-1.481
9589666,4.9401180524,-0.3047722395\H,-1.9464958394,-3.0548476822,1.003
422196\H,-0.8026231546,-4.43596352,0.9874970969\H,-1.8234811261,-4.092
5520662,-0.4483167347\H,3.3710946424,-3.2703931651,-0.3687571116\H,3.5
176123547,-2.0650123986,-1.6858547003\H,2.2247597431,-3.3016826651,-1.
752464712\Version=Al64T-G03RevC.02\State=1-A\HF=-1158.3256235\RMSD=3.
066e-09\RMSF=6.659e-05\Dipole=0.2408513,-1.9046087,-0.4051738\PG=C01 [
X(C8H10N1O6P1)]\@

MPO Transition State:

I\GINC-SC116\FTS\RB3LYP\6-31+G(d)\C8H10N1O6P1\CJJ506\28-Apr-2005\O\
B3LYP/6-31+G* OPT=(TS,CALCF,NOEIGENTEST)\mpots\O,1\C,0.2020196022
,-0.3260335437,-0.5752468223\C,1.007774237,0.2746887352,-1.5457455153
\C,2.3827160628,0.3531887167,-1.3409295992\C,2.9211491022,-0.175098416
5,-0.1664048976\C,2.1210569516,-0.7816757469,0.8043089556\C,0.74746974
91,-0.8609324279,0.5953840482\O,-1.147473658,-0.4513601974,-0.84850529
28\C,-4.2437248755,-1.6561107262,-0.1819428126\C,-2.4540344009,1.92574
29178,1.9215140348\P,-2.4165542186,0.2617513879,-0.1265205693\O,-3.209
5285341,-0.961055255,0.5521902412\O,-1.7185809092,0.9663239049,1.12694
68666\O,-3.226276293,1.100087213,-1.0375127261\H,0.5502328966,0.670442
8424,-2.4464323803\H,3.0343308416,0.8146003864,-2.0732893304\H,2.57616
7417,-1.1847152388,1.7011289251\H,-3.7905954451,-2.3228051187,-0.92216
34673\H,-4.9072213175,-0.9405478724,-0.6736453535\H,-3.2207857694,1.41
16763464,2.5086843254\H,-2.9091666939,2.681704018,1.2766551633\H,0.100
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