Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*

Supporting Information for

Stepwise Walden Inversion in Nucleophilic Substitution at Phosphorus

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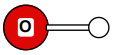
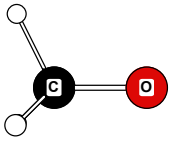
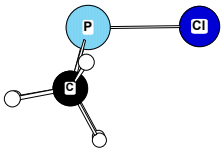
Contents

Table S1. Structures of all species discussed in the main text, including energies *E* of all species relative to ADF's basic atoms, computed at OLYP/TZ2P.[a]

Cl^- (-84.18)	OH^- (-207.45)	CH_3O^- (-580.16)	**1aR** (-1074.02)
			
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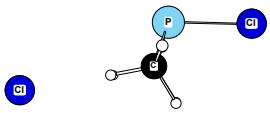	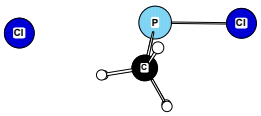	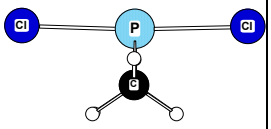	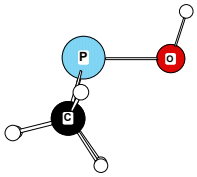
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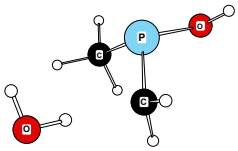	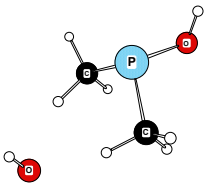	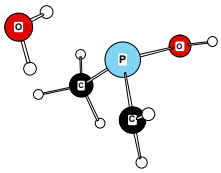	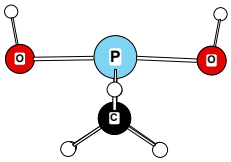
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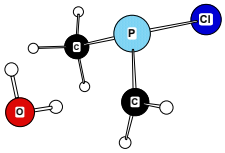	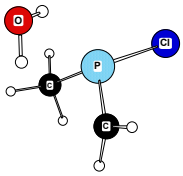	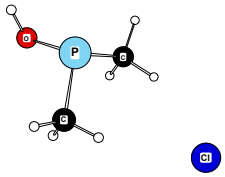	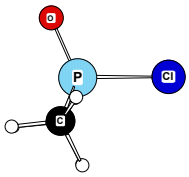
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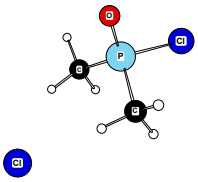	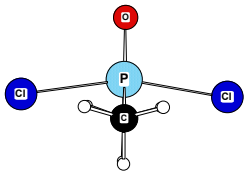	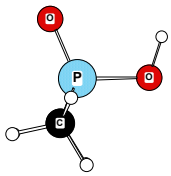	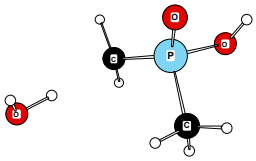
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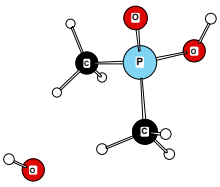
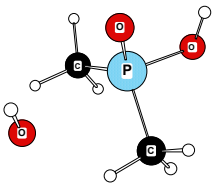
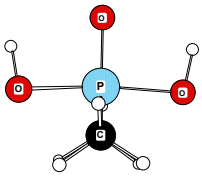
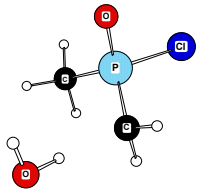
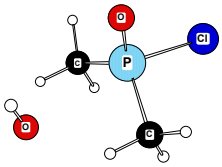
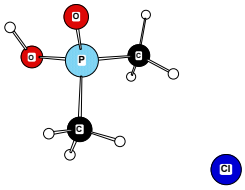
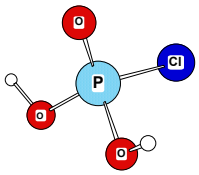
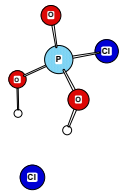
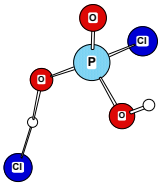
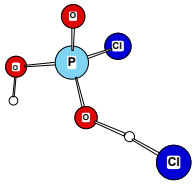
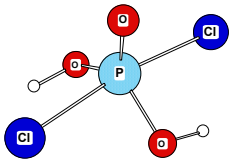
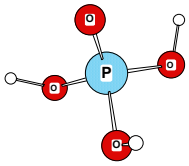
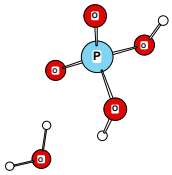
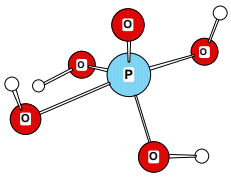
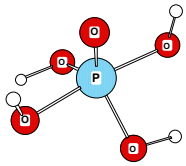
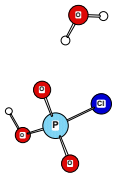
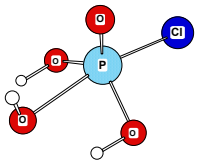
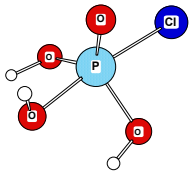
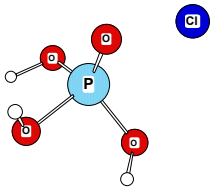
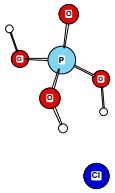
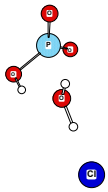
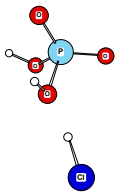
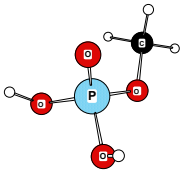
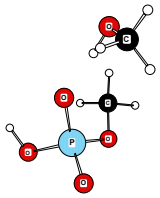
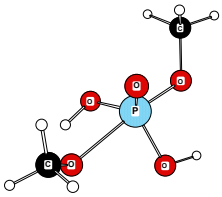
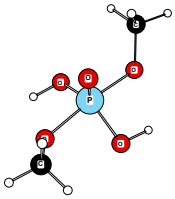
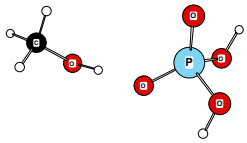
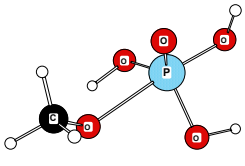
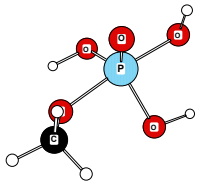
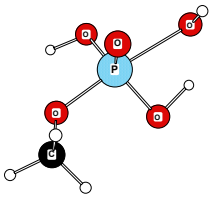
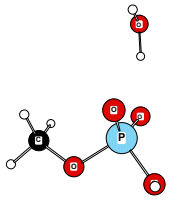
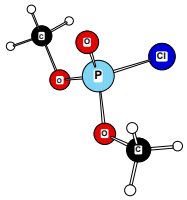
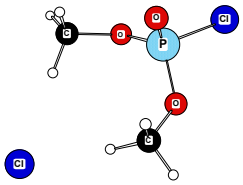
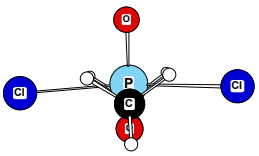
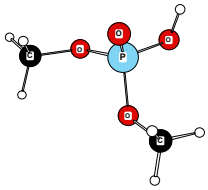
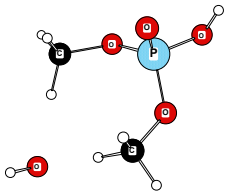
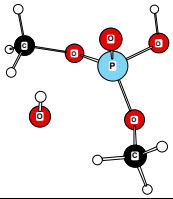
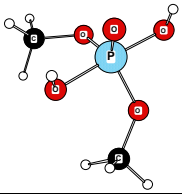
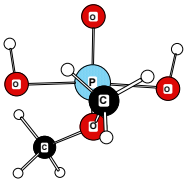
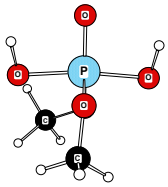
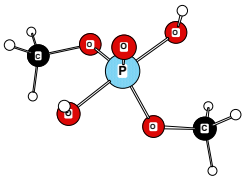
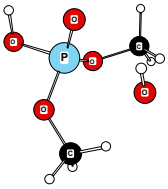
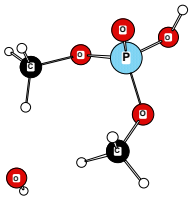
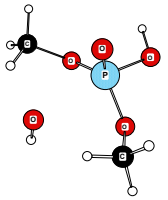
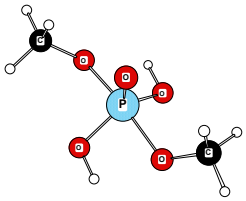
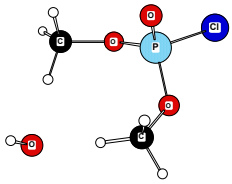
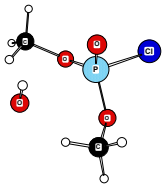
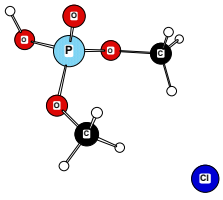
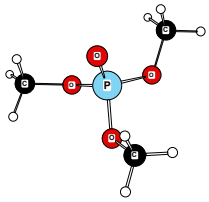
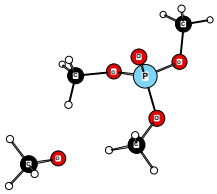
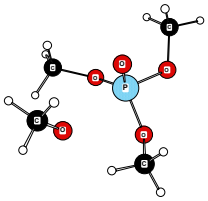
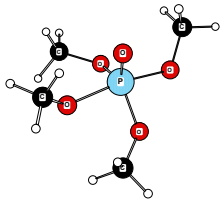
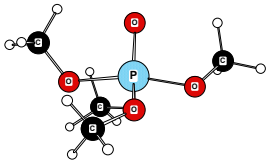
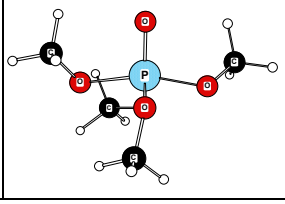
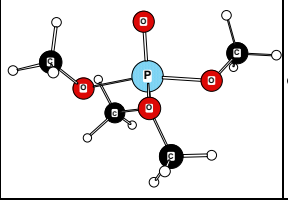
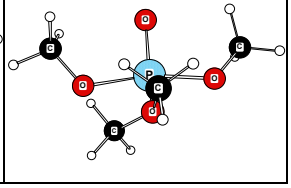
			

2c-preTS(u) (-1491.07) 	**2cPC**(u) (-1539.99) 	**3aR** (-850.22) 	**3aRC** (-976.90) 
3aRC-alt (-968.74) 	**3aRC**-alt2 (-968.67) 	**3aTS** (-946.51) 	**3bR**(u) (-1043.61) 
3bRC(wu) (-1333.33) 	**3b-preTS**(uu) (-1292.74) 	**3bTC**(uu) (-1299.60) 	**3cRC**(w) (-1150.75) 
3c-preTS(u) (-1117.61) 	**3cTC**(u) (-1120.84) 	**3c-postTS**(u) (-1116.56) 	**3cPC**(u) (-1164.08) 
3c-preTS-f (-1125.36) 	**3cPC**-f (-1145.09) 	**3dR**(u) (-1399.27) 	**3dRC**(m) (-2043.16) 
3d-preTS(uu) (-2002.44) 	**3dTC**(uu) (-2007.03) 	**3eRC**(m) (-1689.18) 	**3e-preTS**(uu) (-1648.79) 

3eTC(uu) (-1653.24) 	**3e-postTS**(uu) (-1646.46) 	**3ePC**(uw) (-1687.20) 	**4aR** (-1561.91) 
4aRC (-1660.19) 	**4aTS** (-1643.62) 	**4bR**(u) = **4eR**(u) (-1754.72) 	**4bRC**(uu) (-1988.49) 
4b-preTS(uu) = **4b-postTS**(uu) (-1980.85) 	**4bTC1**(uu) (-1995.61) 	**4bTS12**$_{clock}$(uu) (-1994.09) 	**4bTS12**$_{count}$(uu) (-1992.98) 
4bTC2(uu) (-1996.50) 	**4b-postTS**(uu)-alt (-1981.72) 	**4bRC**(du) = PC(ud) (-1989.02) 	**4b-preTS**(ds) = **4b-postTS**(sd) (-1978.45) 
4bTC1-alt (-2007.03) 	**4cRC**(u) (-1799.73) 	**4c-preTS**(u) (-1796.00) 	**4cPC**(u) (-1850.52) 
4dR(u) (-2109.97) 	**4dRC**(uu) (-2706.33) 	**4d-preTS**(uu) (-2694.68) 	**4dTC1**(uu) (-2701.29) 
4dTS12$_{count,1}$(uu) (-2700.88) 	**4dTC12**$_{count}$(uu) (-2701.71) 	**4dTS12**$_{count,2}$(uu) (-2701.39) 	**4dTS12**$_{clock}$(uu) (-2699.45) 

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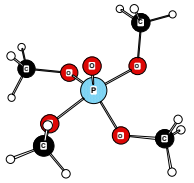
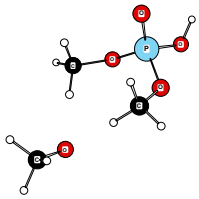
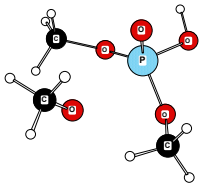
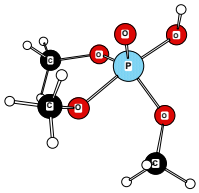
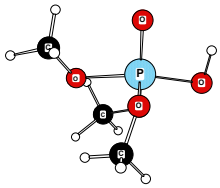
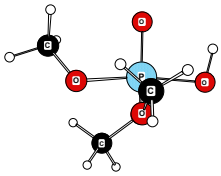
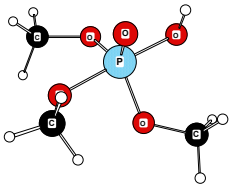
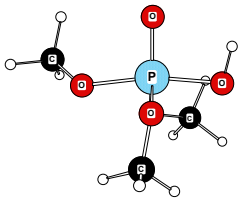
			
4eTS12$_{count}$(uu) (-2346.50)	**4eTS12**$_{clock}$(uu) (-2345.95)	**4eTC2**(uu) (-2349.98)	**4eTS23**$_{count}$(uu) (-2347.29)
			
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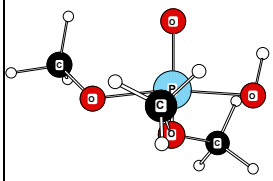
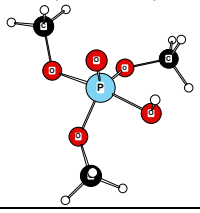
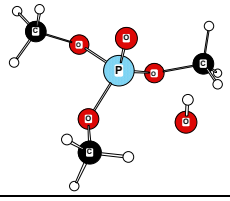
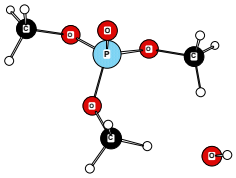
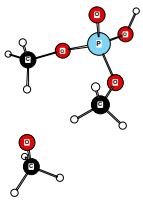
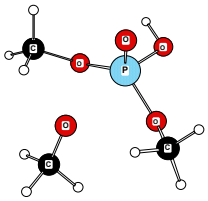
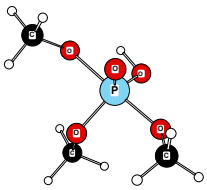
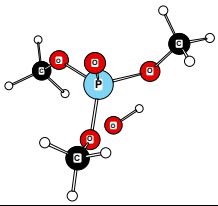
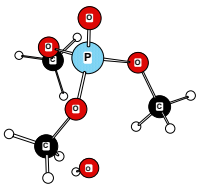
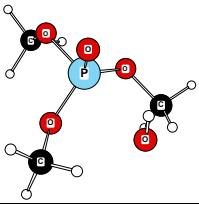
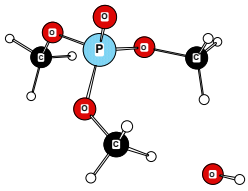
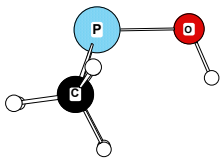
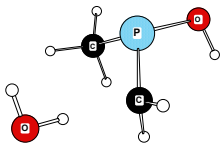
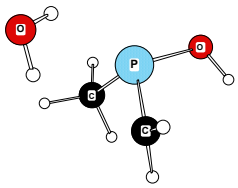
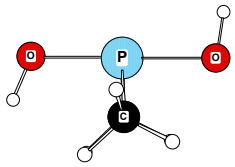
			
4eRC(du) (-2351.66)	**4e-preTS**(ds) (-2338.36)	**4eTC1**-alt (-2354.73)	**4e-postTS**-alt (-2321.64)
			
4ePC-alt (-2344.80)	**4e-postTS**(du)-alt (-2334.88)	**4ePC**(du) (-2343.31)	
			

[a] To enhance numerical precision, energies in the ADF program are computed directly relative to (spherical, average-of-configuration) atoms and not relative to separate electrons and nuclei.

Table S2. Structures of additional species *not* discussed in the main text, including energies *E* of all species relative to ADF's basic atoms, computed at OLYP/TZ2P.[a]

1bR(d) (-1255.10)	**1bRC**(ws)-alt (-1493.25)	**1b-preTS**(ws)-alt (-1490.20)	**1bTC**(du) = **1bTC**(ud) (-1494.24)
			
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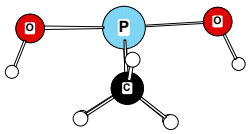	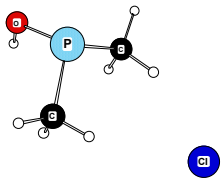	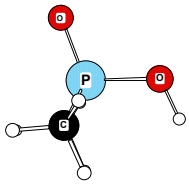	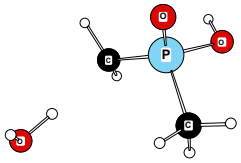
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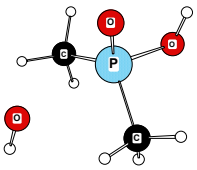	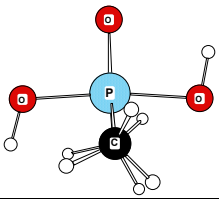	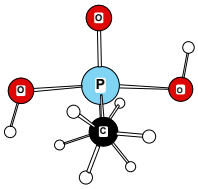	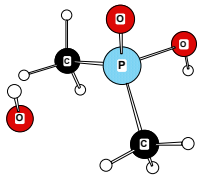
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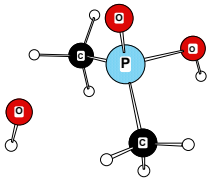	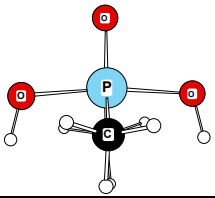	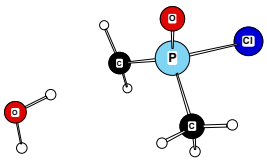	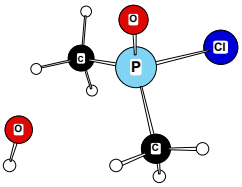
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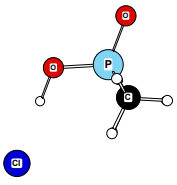	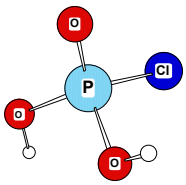	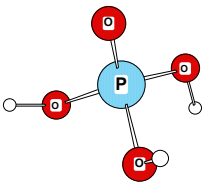	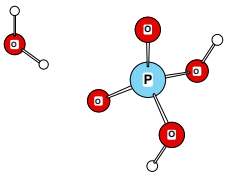
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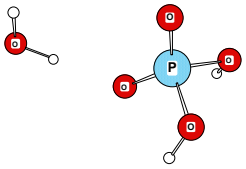
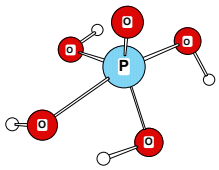
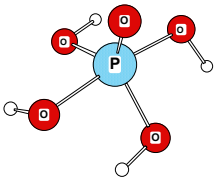
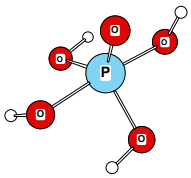
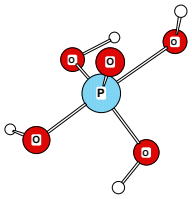
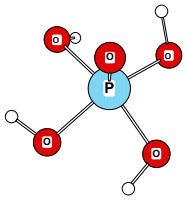
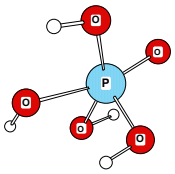
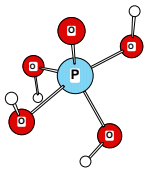
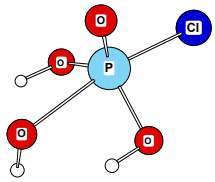
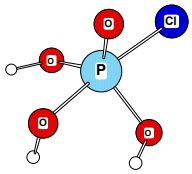
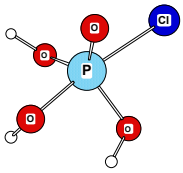
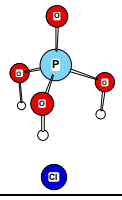
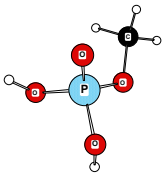
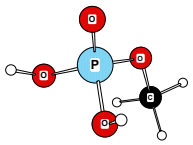
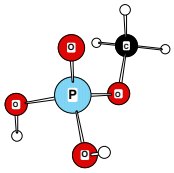
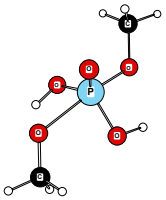
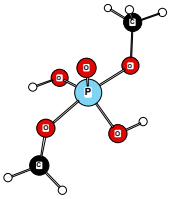
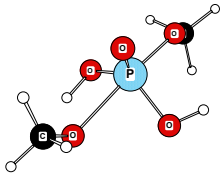
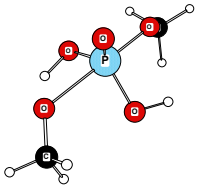
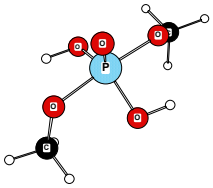
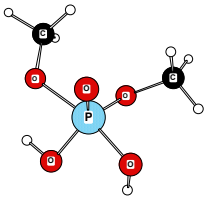
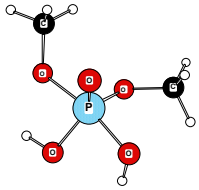
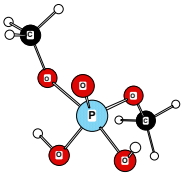
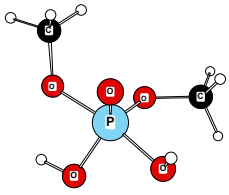
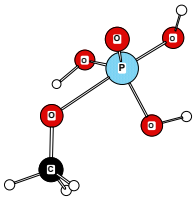
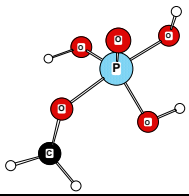
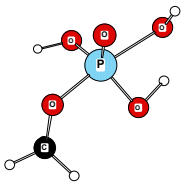
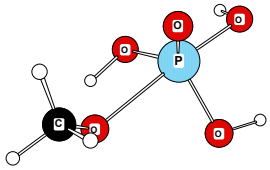
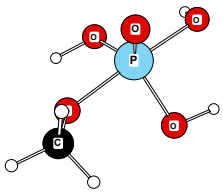
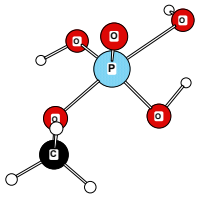
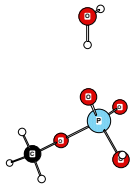
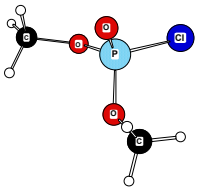
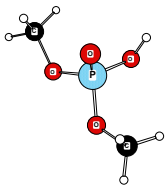
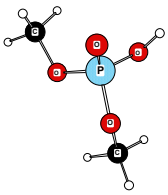
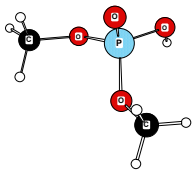
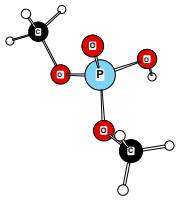
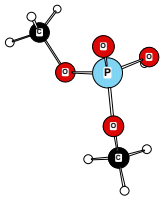
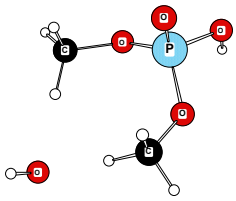
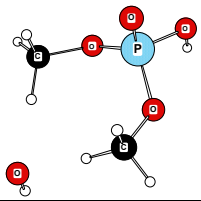
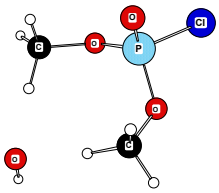
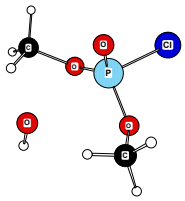
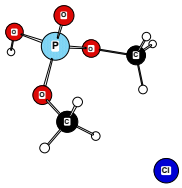
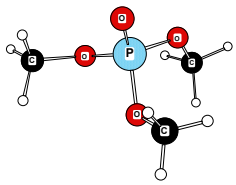
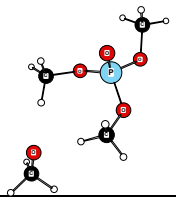
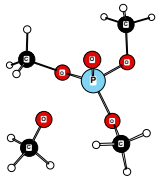
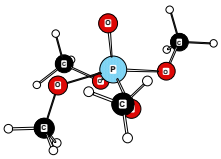
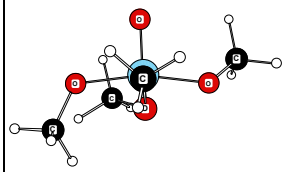
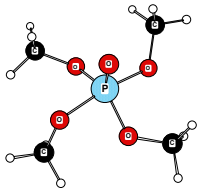
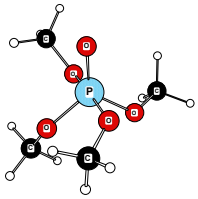
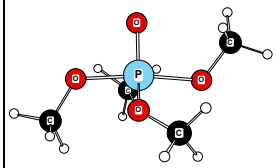
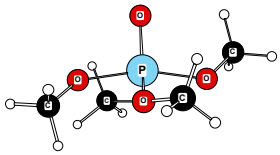
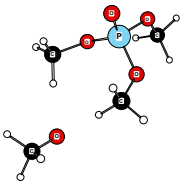
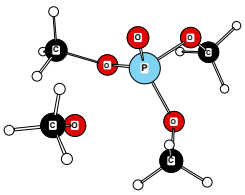
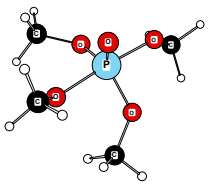
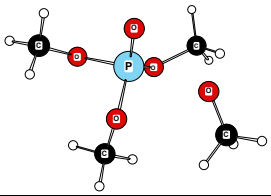
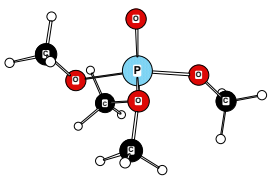
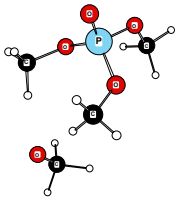
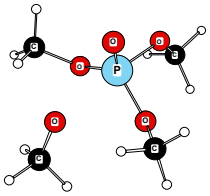
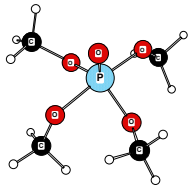
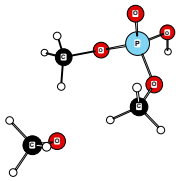
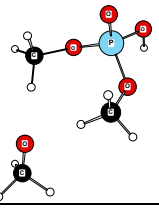
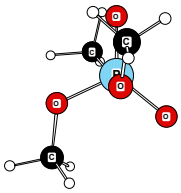
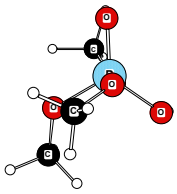
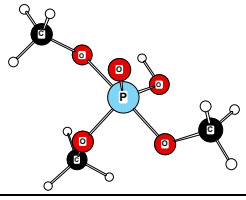
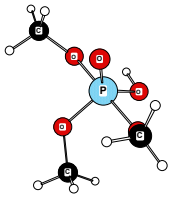
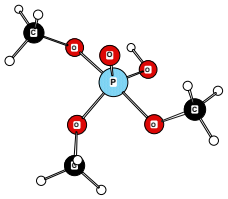
			

3b-postTS(su) (-1291.26) 	**3b-postTS**(su)-f (-1287.42) 	**3bTS**-alt (-1285.46) 	**3bTS**(uu)-rot (-1290.92) 
3c-preTS(d) (-1109.99) 	**3cTC**(d) (-1113.87) 	**3c-postTS**(d) (-1112.79) 	**3cPC**(d)-alt (-1166.57) 
3dR(u)-alt (-1398.38) 	**3dR**(d) (-1398.09) 	**3dR**(u)-alt2 (-1397.74) 	**3d-preTS**(du) (-2000.69) 
3dTC(du) = **3dTC**(ud) (-2003.26) 	**3d-preTS**(ud) (-1999.71) 	**3d-preTS**(dd) (-1998.63) 	**3dTC**(dd) (-1998.63) 
3d-preTS(uu)-f (-1997.49) 	**3dTC**(uu)-f (-2000.32) 	**3d-preTS**(ud)-f (-2000.02) 	**3dTC**(ud)-f (-2002.57) 
3e-preTS(du) (-1647.14) 	**3eTC**(du) (-1649.15) 	**3e-postTS**(du) (-1643.86) 	**3e-preTS**(ud) (-1647.04) 
3eTC(ud) (-1650.29) 	**3e-postTS**(ud) (-1644.48) 	**3ePC**(uw)-alt (-1687.61) 	**4aR**-alt (-1561.41) 

4bR(u)-alt (-1753.90) 	**4bR**(u)-alt2 (-1753.84) 	**4bR**(d) (-1753.58) 	**4bR**(d)-alt (-1752.80) 
4bR(d)-alt2 (-1750.37) 	**4bRC**(ud) (-1989.09) 	**4bRC**(dd) (-1989.34) 	**4cRC**(d) (-1799.92) 
4c-preTS(d) (-1794.08) 	**4cPC**(d) (-1851.01) 	**4dR**(d) (-2108.73) 	**4dRC**(du) (-2706.55) 
4d-preTS(du) (-2693.43) 	**4dTC1**(du) (-2698.27) 	**4dTS12**$_{clock}$(du) (-2698.28) 	**4dTC2**(du) (-2701.06) 
4dTS12$_{count,1}$(du) (-2696.13) 	**4dTS12**$_{count,2}$(du) not found	**4dTS23**$_{clock}$(du) (-2698.17) 	**4dTS23**$_{count}$(du) (-2699.31) 
4dRC(ud) (-2706.51) 	**4d-preTS**(ud) (-2693.12) 	**4dTC1**(ud) (-2699.75) 	**4d-postTS**(ud) (-2689.17) 
4dTS12$_{count}$(ud) (-2695.61) 	**4dTS23**$_{count}$(ud) not found	**4dRC**(dd) (-2706.02) 	**4d-preTS**(dd) (-2691.76) 

4dTC1(dd) (-2695.58)	**4eRC**(ud) (-2352.12)	**4eRC**(dd) (-2352.46)	**4eTS12**$_{\textbf{clock}}$-alt (-2352.84)
			
4eTS12$_{\textbf{count}}$-alt (-2349.06)	**4eTC2**-alt (-2354.25)	**4eTS1**-rot(Nu) (-2353.42)	**4eTC3**-alt (-2356.17)
			

[a] To enhance numerical precision, energies in the ADF program are computed directly relative to (spherical, average-of-configuration) atoms and not relative to separate electrons and nuclei.

Table S3. Cartesian coordinates of all species discussed in the main text, computed at OLYP/TZ2P.

Cl^-

Cl	0.00000	0.00000	0.00000

OH^-

O	0.00000	0.00000	0.00000
H	0.96871	0.00000	0.00000

CH_3O^-

C	0.024843	0.826132	0.000010
H	0.582080	0.347346	0.894958
H	0.582081	0.347342	-0.894940
H	-0.962941	0.222022	0.000013
O	-0.081552	2.137601	-0.000009

$P(CH_3)_2Cl$ (**1aR**)

Cl	-0.057274	-0.157885	-0.556012
P	0.120244	0.178709	1.505526
C	-1.642811	-0.036412	2.024888
C	0.803719	-1.453926	2.045685
H	-1.665414	-0.006716	3.121646
H	-2.080952	-0.976470	1.677484
H	-2.233572	0.804366	1.650299
H	1.831617	-1.551012	1.684827
H	0.210467	-2.304118	1.696985
H	0.826780	-1.450663	3.142831

$Cl^-\cdots P(CH_3)_2Cl$ (**1aRC**)

Cl	4.229423	-0.012908	-0.028683
Cl	-1.902518	0.453392	0.861714
P	0.025200	0.010855	0.023448
C	0.822810	1.666837	0.106347
C	0.850145	-0.790059	1.458991
H	1.891175	1.476914	-0.090269
H	0.711786	2.139327	1.087232
H	0.408704	2.317446	-0.670387
H	0.453398	-1.800638	1.598414
H	0.740054	-0.214822	2.383510
H	1.917080	-0.838317	1.181682

$Cl^-\cdots P(CH_3)_2Cl$ ‡ (**1a-preTS**)

Cl	3.534883	-0.025538	-0.045120
Cl	-2.099845	0.152472	0.274965
P	0.075293	0.024033	0.042449
C	0.457438	1.809131	0.342979
C	0.456811	-0.677737	1.711124
H	1.551848	1.863486	0.376444
H	0.014488	2.182151	1.271902
H	0.088946	2.398478	-0.502810
H	0.087908	-1.707471	1.755956
H	0.013903	-0.092575	2.523299
H	1.551212	-0.678953	1.775070

$ClP(CH_3)_2Cl^-$ (**1aTC**)

P	0.024070	0.026400	0.000120
C	1.898765	0.027309	-0.001524
C	-0.248498	1.881231	0.001789
Cl	-0.019494	-0.024073	2.478980
Cl	-0.019477	-0.023984	-2.478958
H	2.268127	0.515150	0.903225
H	2.267277	0.530962	-0.897966
H	2.245647	-1.011420	-0.011237
H	-1.326711	2.072913	0.012095
H	0.179724	2.317747	-0.903239
H	0.196507	2.319424	0.897920

$P(CH_3)_2OH$ (**1bR**(u))

P	0.147350	0.157042	1.467229
C	-1.615901	-0.032728	1.994495
C	0.794707	-1.469788	2.065690
H	-1.667724	-0.038871	3.089279
H	-2.055323	-0.959144	1.607708
H	-2.198883	0.819346	1.630989
H	1.832371	-1.590753	1.738958
H	0.199003	-2.307406	1.685570
H	0.779049	-1.484101	3.161568
O	-0.030497	-0.218076	-0.168427
H	0.405866	0.470911	-0.682922

$H_2O\cdots PCH_2CH_3OH^-$ (**1bRC**(wu))

O	-3.911733	-0.058958	-0.094653
P	0.061024	0.016708	0.035433
C	-0.107107	1.850182	0.350661
C	-1.102477	-0.246433	-1.223092
H	-1.092914	2.061006	0.774382
H	0.006050	2.410905	-0.587448
H	0.667811	2.184010	1.049820
H	-1.238936	-1.297048	-1.500284
H	-1.162125	0.441231	-2.078273
H	-2.969297	-0.079516	-0.454448
O	1.725576	0.280566	-0.583515
H	2.062547	-0.613396	-0.719672
H	-3.770884	-0.336721	0.819063

$OH^-\cdots P(CH_3)_2OH^-$ (**1bTS**(w))

O	-3.664323	0.320993	-0.389861
P	0.068898	-0.110797	0.120276
C	-0.781077	1.496949	0.365875
C	-0.822503	-0.611159	-1.400848
H	-1.874604	1.262015	0.324135
H	-0.540719	2.190894	-0.450300
H	-0.498676	1.950059	1.323732
H	-0.567254	-1.638838	-1.686276
H	-0.584677	0.067244	-2.230887
H	-1.913755	-0.505252	-1.154077
O	1.589004	0.397143	-0.513658
H	2.256105	-0.052735	0.017164
H	-3.868029	-0.283068	0.337809

$H_2O\cdots PCH_2CH_3OH^-$ ‡ (**1b-preTS**(ws))

O	-3.358454	-0.399749	-0.004764
P	0.141804	0.156806	-0.007473
C	0.372603	1.995781	0.246527
C	-0.109902	0.009615	-1.700233
H	-0.588045	2.504399	0.122173
H	1.090651	2.394420	-0.483104
H	0.756604	2.192062	1.254221
H	-0.504845	-0.943393	-2.057804
H	0.441633	0.598534	-2.443275
H	-2.995857	-0.083308	-0.847962
O	1.855324	-0.110822	0.482442
H	2.029759	-1.009147	0.172704
H	-2.519957	-0.476427	0.488151

$HOP(CH_3)_2OH^-$ (**1bTC**(uu))

O	-1.923153	0.000708	-0.000023
P	0.009174	0.000150	-0.000201
C	-0.019563	1.860894	0.217539
C	-0.021669	-0.079362	-1.871885
H	-0.940156	2.276024	-0.206108
H	0.866952	2.308326	-0.244303
H	-0.000790	2.093743	1.289203
H	-0.011230	-1.131020	-2.183223
H	0.867978	0.407839	-2.284778
H	-0.939345	0.380424	-2.253778
O	1.939078	0.069184	-0.065856
H	2.135543	-0.620991	0.575955
H	-2.072861	-0.695544	0.647803

$H_2O…PCH_2CH_3Cl^-$ (**1cRC**)

O	-4.046253	-0.047061	0.009699
CL	2.347346	0.812062	0.038310
P	-0.042020	0.027412	-0.000538
C	-0.057075	0.000733	1.871610
C	-1.179004	1.251491	-0.328914
H	-0.981199	-0.482153	2.211430
H	-0.007938	1.013327	2.285890
H	0.804610	-0.566067	2.232805
H	-1.384545	1.462001	-1.380282
H	-1.382868	2.085319	0.348909
H	-3.131036	0.322839	-0.056734
H	-3.896908	-0.982717	-0.172017

$H_2O…PCH_2CH_3Cl^{-\ddagger}$ (**1c-preTS**)

O	-3.381294	-0.115346	-0.579713
CL	2.553836	-0.864839	-0.012864
P	0.169706	0.097010	0.262490
C	0.383401	-0.019390	2.118020
C	-0.003063	1.766388	0.038453
H	-0.581757	0.171344	2.602558
H	1.119128	0.708078	2.476264
H	0.732853	-1.021175	2.378017
H	-0.209675	2.125139	-0.971123
H	0.370218	2.524563	0.731809
H	-3.133781	0.778440	-0.304508
H	-2.509180	-0.544743	-0.553655

$HOP(CH_3)_2…Cl^-$ (**1cPC**(u))

O	-1.751318	0.032330	0.053439
CL	3.855990	1.643092	1.585236
P	-0.039708	-0.018547	-0.025302
C	0.358711	-0.192687	1.762669
C	0.325401	1.775240	-0.215873
H	-0.261878	0.477355	2.369895
H	1.416149	0.078333	1.900498
H	0.195302	-1.227797	2.083025
H	0.137478	2.087667	-1.249186
H	1.384903	1.931846	0.034246
H	-0.292153	2.375670	0.463009
H	-2.066178	-0.613649	-0.588096

$PO(CH_3)_2Cl$ (**2aR**)

O	-0.100071	0.000015	-0.618642
P	-0.134248	0.000025	0.863201
Cl	1.745221	-0.000010	1.736980
C	-0.910263	-1.462288	1.615460
C	-0.910284	1.462246	1.615438
H	-0.374881	-2.354514	1.280563
H	-1.945857	-1.515324	1.262152
H	-0.892288	-1.411353	2.707235
H	-0.374850	2.354344	1.280278
H	-0.892122	1.411442	2.707207
H	-1.945894	1.515245	1.262199

$Cl^-…PO(CH_3)_2Cl$ (**2aRC**)

Cl	-4.236203	-0.028055	-0.002738
O	0.472873	1.426928	0.021993
P	0.015627	0.013255	0.001334
Cl	1.701614	-1.288510	-0.018309
C	-0.915960	-0.504057	-1.456623
C	-0.915520	-0.546495	1.443907
H	-0.453757	-0.068136	-2.346871
H	-1.949730	-0.141669	-1.311856
H	-0.938911	-1.593916	-1.535836
H	-0.456057	-0.132351	2.345880
H	-0.934034	-1.638150	1.494263
H	-1.950436	-0.184082	1.307571

$ClP(CH_3)_2Cl^{-\ddagger}$ (**2aTS**)

P	-0.003145	-0.000013	-0.000119
Cl	2.500042	0.002896	0.000191
Cl	-2.393211	0.746393	-0.000108
O	-0.226114	-1.467984	-0.000159
C	0.134651	0.902043	-1.593552
C	0.131226	0.902531	1.593361
H	-0.803948	0.772951	-2.132563
H	0.986644	0.491450	-2.135569
H	0.302469	1.963906	-1.396141
H	-0.801515	0.754770	2.137873
H	0.275330	1.967885	1.396037
H	0.994155	0.508095	2.129883

$PO(CH_3)_2OH$ (**2bR**(u))

O	0.023208	0.041631	-0.567811
P	-0.094042	0.029276	0.914171
C	-0.892990	-1.444817	1.616015
C	-0.958571	1.460540	1.628381
H	-0.392187	-2.333438	1.220176
H	-1.944753	-1.469336	1.314210
H	-0.826650	-1.448712	2.708385
H	-0.489688	2.374079	1.250274
H	-0.903835	1.452233	2.721393
H	-2.007259	1.448225	1.315206
O	1.347848	0.053182	1.685727
H	2.043205	0.102666	1.013746

$H_2O…POCH_2CH_3OH^-$ (**2bRC**(wu))

O	-3.990194	0.287592	0.157331
O	0.344640	-1.558805	-0.026073
P	0.087764	-0.070226	-0.034217
C	-1.167393	0.588423	0.942841
C	-0.195081	0.557025	-1.748159
H	-1.125371	0.196612	1.966306
H	-3.001997	0.361223	0.390019
H	-1.155499	1.686314	0.938402
H	0.629764	0.238373	-2.395398
H	-0.251004	1.651520	-1.756331
H	-1.136998	0.154714	-2.132246
O	1.599137	0.663436	0.257007
H	2.216078	-0.081373	0.213130
H	-4.073946	-0.651989	-0.045926

$OH^-…PO(CH_3)_2OH^-$ (**2bTS**(w))

O	-3.783782	0.845213	-0.087566
O	0.089099	-1.639727	0.005304
P	-0.174598	-0.161744	0.004009
C	-1.002911	0.491105	1.477647
C	-1.136889	0.495623	-1.364777
H	-0.756291	-0.126847	2.347577
H	-2.093039	0.495149	1.247860
H	-0.685781	1.524470	1.657321
H	-0.989116	-0.129815	-2.252539
H	-0.817437	1.522118	-1.581309
H	-2.229994	0.528832	-1.018713
O	1.288004	0.647573	-0.030393
H	1.949776	-0.058332	-0.056914
H	-4.237823	-0.008266	-0.059386

$OH^-…PO(CH_3)_2OH^{-\ddagger}$ (**2b-preTS**(uu))

O	-2.639032	0.183236	-0.036245
O	-0.046894	-1.561301	0.168183
P	0.070828	-0.078126	-0.039971
C	-0.307787	1.060328	1.335335
C	-0.351192	0.650817	-1.659254

H	0.164767	0.652624	2.237491
H	-1.401149	1.086912	1.411626
H	0.123462	2.047655	1.126851
H	0.051317	-0.017152	-2.430751
H	0.127244	1.633479	-1.758618
H	-1.445694	0.702741	-1.691242
O	1.758434	0.201215	-0.106011
H	2.114138	-0.687668	0.025865
H	-2.850419	-0.750227	0.086915

$HOPO(CH_3)_2OH^-$ (**2bTC**(uu))

O	-1.820378	0.001195	0.002667
O	0.076202	-1.523434	0.206148
P	0.003242	0.000168	-0.000196
C	-0.039355	1.271072	1.362377
C	-0.056945	0.863582	-1.650668
H	0.045846	0.717107	2.305864
H	-0.986711	1.816068	1.365102
H	0.814124	1.950220	1.288376
H	-0.088075	0.074400	-2.412582
H	0.838729	1.468235	-1.813795
H	-0.967362	1.461658	-1.743706
O	1.818816	0.171306	-0.026950
H	2.051632	-0.755779	0.103416
H	-1.963234	-0.944688	0.127569

$H_2O\cdots POCH_2CH_3Cl^-$ (**2cRC**(wu))

O	-4.040043	-0.005543	0.126023
O	0.204185	-1.470724	-0.189897
P	-0.027475	0.002489	-0.038745
CL	2.009043	0.958404	-0.473507
C	-0.077677	0.542653	1.716267
C	-1.298724	0.771734	-0.870578
H	0.834385	0.214263	2.219770
H	-0.952313	0.083773	2.188718
H	-0.159037	1.631104	1.783054
H	-1.377683	0.471091	-1.918365
H	-1.323064	1.856826	-0.737241
H	-3.114095	0.251302	-0.160049
H	-3.981855	-0.968517	0.140779

$OH^-\cdots PO(CH_3)_2Cl^{-\ddagger}$ (**2c-preTS**(u))

O	-2.668682	0.381544	0.094013
O	0.033623	-1.566024	-0.418190
P	0.181790	-0.158933	0.041749
CL	2.359541	0.179920	0.243917
C	-0.297536	0.264134	1.739786
C	-0.174129	1.186840	-1.122323
H	0.088355	-0.513505	2.406035
H	-1.401456	0.288666	1.679610
H	0.124384	1.234520	2.018968
H	0.279662	0.932510	-2.085116
H	0.246697	2.126360	-0.751059
H	-1.279432	1.201732	-1.144341
H	-3.041540	-0.461597	-0.191532

$HOPO(CH_3)_2\cdots Cl^-$ (**2cPC**(u))

O	-1.646447	0.062034	0.020562
O	0.450184	-1.360916	-0.491295
P	0.011317	-0.016093	-0.005288
CL	3.249622	2.962493	1.066805
C	0.484952	0.414318	1.687369
C	0.488885	1.397835	-1.027799
H	0.397705	-0.476058	2.318907
H	-0.169945	1.204360	2.068464
H	1.512447	0.805644	1.688037
H	1.518296	1.693786	-0.779578
H	-0.161098	2.251432	-0.810607
H	0.397325	1.121143	-2.083381
H	-1.941537	-0.805003	-0.291668

$PO(OH)_2Cl$ (**3aR**(u))

P	-0.00387	-0.02584	0.00000
CL	2.03414	0.00322	0.00000
O	-0.38381	-1.00286	-1.20591
O	-0.57838	1.32750	0.00000
O	-0.38381	-1.00286	1.20591
H	-0.49034	-0.49700	-2.02484
H	-0.49034	-0.49700	2.02484

$Cl^-\cdots PO(OH)_2Cl$ (**3aRC**)

P	0.05079	0.64794	0.00000
CL	1.42871	-0.93047	0.00000
O	-0.84153	0.36531	-1.27197
O	0.79552	1.91911	0.00000
O	-0.84153	0.36531	1.27197
H	-1.65171	-0.20126	-1.01432
H	-1.65171	-0.20126	1.01432
CL	-3.07694	-1.13663	0.00000

$Cl^-\cdots PO(OH)_2Cl$ (**3aRC**-alt)

P	0.007601	-0.038247	-0.020055
CL	2.107168	0.253684	-0.037399
O	-0.228158	-1.427116	-0.567373
O	-0.618408	1.164027	-0.625651
O	-0.274256	-0.111870	1.587629
H	0.025231	-2.605031	-0.005778
H	-0.409847	0.797132	1.887559
CL	0.243094	-3.959770	0.527180

$Cl^-\cdots PO(OH)_2Cl$ (**3aRC**-alt2)

P	-0.01845	-0.02047	0.03586
CL	-0.00365	-3.35429	2.25792
O	0.41277	1.54585	0.24122
O	0.48956	-0.50857	-1.26296
O	0.22909	-0.68944	1.37670
H	0.32262	1.74604	1.18267
H	0.09337	-2.00624	1.74025
CL	-2.12903	0.17633	-0.10676

$ClPO(OH)_2Cl^{-\ddagger}$ (**3aTS**)

P	-0.00089	0.14820	0.00007
CL	2.39646	-0.17059	0.01235
O	-0.00331	-0.73603	-1.35546
O	-0.00016	1.62366	0.00000
O	0.00343	-0.73583	1.35553
H	-0.95834	-0.88872	-1.50708
H	0.95888	-0.88814	1.50560
CL	-2.39567	-0.16974	-0.01240

$PO(OH)_2OH$ (**3bR**(u))

P	-0.92339	0.04158	-0.10083
O	0.56183	0.53176	0.25298
O	-1.58120	1.38671	-0.67487
O	-1.58982	-0.05106	1.35484
O	-1.03447	-1.15805	-0.95141
H	-1.54308	1.38736	-1.64218
H	-2.35765	-0.64015	1.33082
H	1.16137	-0.22736	0.29023

$H_2O\cdots POO(OH)OH^-$ (**3bRC**(wu))

P	0.36189	0.13877	0.25635
O	1.46143	-0.33963	-0.90127
O	-0.73095	0.87230	-0.48168
O	1.13599	0.71051	1.40074
O	-0.27075	-1.31374	0.75232
H	-2.03810	0.11855	-1.29824
H	-3.56149	0.03499	-1.19479
H	2.31064	-0.32911	-0.44186
O	-2.82708	-0.36727	-1.67173
H	-1.05213	-1.47483	0.20573

$OH^-\cdots PO(OH)_2OH^{\ddagger}$ (**3b-preTS**(uu))

P	0.05717	-0.00652	0.00775
O	2.26524	0.03815	-0.03779
O	0.27489	-0.97721	-1.30715
O	-0.03749	1.48178	-0.17385
O	0.53837	-0.70930	1.35880
H	-0.62058	-1.28840	-1.50188
H	1.55727	-0.48709	1.09687
O	-1.59826	-0.44658	0.16512
H	-2.03055	0.41607	0.15169
H	2.35172	0.99316	0.06391

$HOPO(OH)_2OH^-$ (**3bTC**(uu))

P	0.00000	-0.05340	0.00000
O	1.78128	-0.21817	-0.01501
O	-0.00250	-0.98883	-1.37620
O	0.00000	1.46951	0.00000
O	0.00250	-0.98883	1.37620
H	-0.95246	-1.08478	-1.54338
H	0.95246	-1.08478	1.54338
O	-1.78128	-0.21817	0.01501
H	-2.02382	0.71477	0.04006
H	2.02382	0.71477	-0.04006

$H_2O\cdots POO(OH)Cl^-$ (**3cRC**(w))

P	-0.35482	1.06378	0.12026
O	-0.87490	2.19685	0.92385
O	-0.53949	1.42942	-1.47631
CL	-1.81124	-0.53354	0.28716
O	0.97579	0.39421	0.29482
H	0.04587	0.82551	-1.95306
H	1.76005	-1.06656	1.32540
O	2.08624	-1.84673	1.82172
H	1.26245	-2.28153	2.07085

$OH^-\cdots PO(OH)_2Cl^{\ddagger}$ (**3c-preTS**(u))

P	-0.00971	0.00242	0.00007
O	-0.11450	1.48512	0.03443
O	0.30912	-0.78953	-1.37698
CL	-2.08911	-0.63792	-0.01466
O	0.30917	-0.85238	1.33903
H	1.29454	-0.65255	-1.35685
H	1.29460	-0.71474	1.32515
O	2.20482	-0.01667	-0.00040
H	2.35256	0.93463	0.02188

$HOPO(OH)_2Cl^-$ (**3cTC**(u))

P	-0.12992	-0.00994	-0.00023
O	-0.27337	1.47966	0.03619
O	-0.08273	-0.88763	-1.39229
CL	-2.39144	-0.46827	-0.01125
O	-0.08260	-0.95439	1.34747
H	0.86439	-0.87402	-1.60741
H	0.86453	-0.95141	1.56293
O	1.70730	-0.04224	-0.00117
H	1.88060	0.90647	0.02234

$HOPO(OH)_2\cdots Cl^{-\ddagger}$ (**3c-postTS**(u))

P	0.50306	-0.18444	-0.00030
O	0.46967	1.29169	-0.00413
O	0.08417	-1.05602	-1.29158
CL	-2.58429	-0.15174	0.00670
O	0.06715	-1.01796	1.30745
H	0.85857	-1.07623	-1.87520
H	0.86882	-1.45951	1.62905
O	2.14652	-0.61317	-0.00528
H	2.59952	0.23199	0.11988

$HOPO(OH)_2\cdots Cl^-$ (**3cPC**(u))

P	-0.00085	-0.28864	-0.01869
O	1.00842	0.99745	0.12546
O	-0.88835	0.04593	-1.28879
O	-0.96517	-0.18175	1.23604
O	0.80095	-1.53241	-0.10288
H	-1.74720	0.50999	-1.01710
H	-1.80734	0.33001	1.00221
H	1.89846	0.62330	0.14033
CL	-3.28932	1.30628	0.02401

$OH^-\cdots PO(OH)_2Cl^{\ddagger}$ (**3c-preTS**-f)

P	-0.40788	1.09533	0.19336
O	-1.84812	0.79767	0.31093
O	0.26547	1.97424	-0.78653
CL	1.72904	-3.73206	-0.58331
O	0.45979	0.66267	1.45226
H	1.71051	-0.58915	-1.10125
H	1.05893	-0.02922	1.02149
O	1.15575	-0.92697	-0.38858
H	1.30032	-1.97764	-0.43110

$HOPO(OH)_2\cdots Cl^-$ (**3cPC**-f)

P	-0.00368	0.00089	-0.00703
O	-0.47841	-1.40260	-0.09151
O	-0.35342	1.13155	-0.93193
CL	3.90838	-1.90940	0.26940
O	-0.21500	0.50479	1.55425
H	1.93650	0.56156	-0.79750
H	-0.24749	1.46933	1.51244
O	1.71810	-0.02641	-0.06336
H	2.80872	-1.09657	0.11662

$PO(OH)_2OCH_3$ (**3dR**(u))

P	-0.92014	0.04431	-0.10474
O	0.54899	0.55296	0.24310
O	-1.56689	1.39131	-0.68953
O	-1.58402	-0.06718	1.35787
O	-1.06513	-1.15336	-0.95462
H	-1.68410	1.30067	-1.64570
H	-2.29639	-0.72189	1.34365
C	1.51219	-0.37057	0.79351
H	1.18585	-0.72611	1.77566
H	1.66217	-1.21823	0.11929
H	2.44124	0.19141	0.89864

CH_3OH…$POO(OH)OCH_3^-$ (**3dRC**(m))

P	0.11195	0.01653	0.02707
O	-0.05091	1.60388	-0.42118
O	-0.87153	-0.03582	1.37790
O	1.51130	-0.21669	0.55619
O	-0.50850	-0.77679	-1.06684
H	-0.26548	-0.23068	2.10339
H	3.22923	-0.06200	0.05947
C	0.54211	2.60873	0.38108
H	1.61327	2.42865	0.53327
H	0.40937	3.56469	-0.14077
H	0.05649	2.68197	1.36687
C	4.47554	-0.82218	-1.23855
H	3.83726	-0.64067	-2.11965
H	5.51908	-0.65463	-1.53884
H	4.37183	-1.88909	-0.97043
O	4.18638	0.04153	-0.16636

CH_3O^-…$PO(OH)_2OCH_3$ ‡ (**3d-preTS**(uu))

P	-0.06864	0.01395	0.05908
O	-1.70276	0.54634	-0.08627
O	0.12090	0.97589	1.37418
O	0.41404	0.69007	-1.31992
O	-0.16630	-1.46432	0.22778
H	-0.77057	1.31200	1.54950
H	1.41450	0.51251	-1.11922
C	-2.52725	-0.11061	-1.02062
H	-2.23216	0.11552	-2.05804
H	-2.50464	-1.20080	-0.88569
H	-3.55720	0.24389	-0.87348
C	2.84646	-1.11603	0.29750
H	2.84387	-1.46514	1.35279
H	2.45703	-1.96461	-0.29965
H	3.91548	-0.99015	0.01818
O	2.14652	0.06345	0.12943

$CH_3OPO(OH)_2OCH_3^-$ (**3dTC**(uu))

P	-0.03741	0.00368	0.11901
O	-1.38603	-1.16154	0.42280
O	-0.88557	0.36111	-1.26248
O	0.95466	-1.32349	0.02052
O	-0.15843	0.82625	1.37143
H	-1.72869	-0.09702	-1.12178
H	1.80742	-0.93589	-0.23089
C	-1.51294	-1.72853	1.69378
H	-0.70547	-2.45040	1.91663
H	-1.50981	-0.96774	2.48921
H	-2.46747	-2.27900	1.73945
C	1.35883	2.26515	-0.65748
H	0.62680	2.68073	-1.37511
H	1.13440	2.68834	0.33333
H	2.35785	2.61399	-0.96864
O	1.35743	0.86790	-0.64348

CH_3OH…$POO(OH)OH^-$ (**3eRC**(m))

P	0.067836	0.171543	-0.292858
O	-0.772289	-0.294367	-1.652648
O	1.487069	-0.289414	-0.510484
O	-0.588836	-0.829244	0.865562
O	-0.341236	1.570354	0.043276
H	2.956009	-0.419495	0.547013
H	-1.193056	-0.258420	1.357006
H	-0.194583	-0.929392	-2.094754
O	3.791127	-0.494724	1.070777
C	4.561146	0.655268	0.826003
H	5.453226	0.610759	1.466289
H	4.906515	0.727430	-0.221879
H	4.024102	1.589937	1.060845

CH_3O^-…$PO(OH)_2OH$ ‡ (**3e-preTS**(uu))

P	0.007408	-0.000718	0.000034
O	-1.636997	0.490640	-0.117815
O	0.288024	0.963408	1.305303
O	0.449306	0.699088	-1.373772
O	-0.120685	-1.480419	0.183258
H	-0.594142	1.293712	1.528054
H	1.456928	0.514677	-1.205767
C	2.909426	-1.212289	0.025059
H	3.990261	-1.068999	-0.194780
H	2.858696	-1.692190	1.024925
H	2.539388	-1.974983	-0.691271
O	2.232028	-0.008992	-0.021118
H	-2.096088	-0.357575	-0.087023

$CH_3OPO(OH)_2OH^-$ (**3eTC**(uu))

P	-2.16422	1.55370	0.81025
O	-2.73328	3.21202	1.17302
O	-0.76100	1.94621	1.62302
O	-2.14571	2.00690	-0.78174
O	-3.32130	0.84388	1.47745
H	-0.99854	2.80031	2.01516
H	-1.76107	1.23342	-1.22255
C	-1.10867	-0.99418	1.07757
H	-0.65080	-1.82211	0.51049
H	-0.43477	-0.76228	1.92291
H	-2.06353	-1.34507	1.49850
O	-1.27995	0.09294	0.21643
H	-3.56093	2.99466	1.61775

$CH_3OPO(OH)_2$…OH^- ‡ (**3e-postTS**(uu))

P	0.056225	-0.006057	-0.010408
O	-2.140984	0.064773	0.090796
O	-0.295145	0.793988	1.334386
O	-0.189856	0.863015	-1.381408
O	0.064899	-1.501366	-0.070214
H	-1.335314	0.601532	1.161709
H	0.698291	1.148636	-1.641253
C	2.582058	-0.180385	0.894225
H	3.612702	0.121061	0.658432
H	2.360165	0.136140	1.926217
H	2.514483	-1.276502	0.848213
O	1.724428	0.433906	-0.038956
H	-2.259957	-0.880169	0.242199

$CH_3OPOO(OH)^-$…H_2O (**3ePC**(uw))

P	0.05538	0.05409	0.01390
O	-3.84680	-0.22695	-0.03815
O	-0.07056	1.38685	0.69464
O	1.25665	0.15770	-1.11842
O	-1.11774	-0.64972	-0.60985
H	-3.78078	0.61286	0.43096
H	1.69542	0.99487	-0.91983
C	0.05112	-1.55979	2.08350
H	0.68366	-2.26905	2.63245
H	-0.28357	-0.77775	2.78250
H	-0.83416	-2.09018	1.70639
O	0.82822	-1.02519	1.02707
H	-2.90071	-0.39773	-0.26941

$PO(OCH_3)_2Cl$ (**4aR**)

P	-0.612139	-0.076381	0.000000
Cl	1.447352	-0.072015	0.000000
O	-1.004263	-1.041664	-1.202544
O	-1.138097	1.299888	0.000000
O	-1.004263	-1.041664	1.202544
C	-0.853677	-0.546957	-2.556017
C	-0.853677	-0.546957	2.556017
H	-1.416420	-1.232062	3.190150
H	0.202381	-0.558804	2.841588
H	-1.254585	0.465643	2.646414
H	-1.416420	-1.232062	-3.190150
H	-1.254585	0.465643	-2.646414
H	0.202381	-0.558804	-2.841588

$Cl^-\cdots PO(OCH_3)_2Cl$ (**4aRC**)

P	0.055003	0.000052	0.002283
Cl	1.661697	-0.211676	1.260580
O	-0.687910	-1.363881	0.325800
O	0.433440	0.234169	-1.404863
O	-0.684884	1.186923	0.750997
C	-1.752576	-1.873250	-0.538073
C	-1.749908	1.949542	0.100511
H	-1.459905	2.188999	-0.925784
H	-2.691898	1.387625	0.123230
H	-1.835861	2.867158	0.686912
H	-2.690692	-1.337129	-0.347680
H	-1.453005	-1.784489	-1.585590
H	-1.852856	-2.926689	-0.267120
Cl	-4.848240	0.007051	-0.034063

$ClPO(OCH_3)_2Cl^{-\ddagger}$ (**4aTS**)

P	0.000000	0.000000	0.000000
Cl	2.459710	-0.254570	-0.000220
O	-0.052600	-0.984150	-1.261390
O	0.073820	1.473030	0.000000
O	-0.052870	-0.984110	1.261370
C	-0.026660	-0.403420	-2.568550
C	-0.015860	-0.403350	2.568260
Cl	-2.472850	0.000000	0.000000
H	-0.038970	-1.243270	3.268230
H	0.907030	0.168320	2.710500
H	-0.890340	0.235560	2.729860
H	-0.046050	-1.243680	-3.268250
H	-0.907210	0.228120	-2.726000
H	0.890720	0.175900	-2.715580

$PO(OCH_3)_2OH$ (**4bR**(u))

P	0.959104	0.572651	0.123175
O	2.226875	0.018521	0.945246
O	1.231772	-0.044145	-1.320859
O	0.757653	2.032740	0.212191
O	-0.239008	-0.348744	0.645970
C	0.377274	0.317371	-2.425678
C	-0.915260	-0.001136	1.872733
H	-1.763758	-0.682287	1.955534
H	-0.249780	-0.141231	2.730838
H	-1.265845	1.033833	1.840550
H	-0.548735	-0.264682	-2.388650
H	0.149641	1.386651	-2.410671
H	0.930679	0.070547	-3.333306
H	2.839942	0.749299	1.107967

$OH^-\cdots PO(OCH_3)_2OH$ (**4bRC**(uu))

P	1.414449	-0.273852	0.187360
O	2.814235	0.254929	-0.445071
O	0.750710	1.121522	0.553974
O	1.614271	-1.231029	1.306987
O	0.731144	-0.852451	-1.124862
C	-0.557797	1.215948	1.207205
C	-0.573458	-1.519513	-1.099437
O	-2.860487	0.527497	-0.735356
H	-0.633000	-2.048804	-2.055656
H	-0.589216	-2.253419	-0.284730
H	-1.410270	-0.786770	-1.001299
H	-0.613833	2.248286	1.566283
H	-1.393453	0.999772	0.498720
H	-0.581768	0.537353	2.068436
H	-3.514571	0.073476	-0.186550
H	3.507855	-0.204390	0.045578

$OH^-\cdots PO(OCH_3)_2OH^{\ddagger}$ (**4b-preTS**(uu) = **4b-postTS**(uu))

P	0.011509	0.002096	0.003543
O	1.652049	0.345250	-0.090384
O	-0.184172	0.866671	1.363602
O	-0.109148	-1.484273	0.038118
O	-0.261089	0.904298	-1.306121
C	-1.221316	0.620133	2.331541
C	-1.161224	0.503524	-2.349917
O	-2.593693	-0.042297	0.000738
H	-1.229762	1.362918	-3.028559
H	-0.745959	-0.353213	-2.900659
H	-2.125709	0.250953	-1.887881
H	-1.281546	1.528610	2.944813
H	-2.155040	0.403399	1.787791
H	-0.933040	-0.225212	2.974631
H	-2.555161	-1.004860	0.043019
H	2.061145	-0.176064	0.611639

$HOPO(OCH_3)_2OH^-$ (**4bTC1**(uu))

P	0.009188	0.000099	0.000153
O	1.723174	0.238314	-0.011769
O	0.020063	1.006801	1.349794
O	0.083744	-1.532215	0.041550
O	0.016769	0.943353	-1.394678
C	-1.106169	1.360040	2.121483
C	-1.115200	1.300452	-2.155946
O	-1.767758	-0.008910	0.000447
H	-0.733587	1.859811	-3.023926
H	-1.679281	0.432378	-2.520493
H	-1.816855	1.944382	-1.609125
H	-0.722487	1.954071	2.965189
H	-1.833771	1.969391	1.569166
H	-1.641394	0.489789	2.522972
H	-1.881762	-0.966805	0.027008
H	2.000118	-0.685256	0.022637

$HOPO(OCH_3)_2OH^{-\ddagger}$ (**4bTS12**$_{clock}$(uu))

P	-0.116000	0.067032	-0.061728
O	1.618910	-0.144248	-0.191336
O	0.211982	1.688542	0.137533
O	-0.257411	-0.978648	1.053229
O	-0.199925	-0.133077	-1.737697
C	-0.760198	2.705220	0.283780
C	-0.246938	-1.449291	-2.224413
O	-1.867683	0.366387	-0.103379
H	-0.238773	-1.397643	-3.322447
H	0.621414	-2.044246	-1.899341
H	-1.165212	-1.976609	-1.913281
H	-0.198132	3.642207	0.411947
H	-1.410077	2.797577	-0.594161
H	-1.402081	2.556957	1.160960
H	-2.119733	-0.191854	0.642259
H	1.770594	-0.688689	0.590838

$HOPO(OCH_3)_2OH^{-\ddagger}$ (**4bTS12**$_{count}$(uu))

P	-0.003824	0.000686	0.000066
O	1.747592	0.004639	-0.014684
O	0.220000	1.672388	-0.002631
O	-0.129097	-1.050286	1.098498
O	-0.039712	-0.625518	-1.566255
C	-0.776823	2.655883	0.173728
C	-0.075304	0.236817	-2.670781
O	-1.752885	0.303991	-0.070635
H	-0.085634	-0.385573	-3.577218
H	-0.980125	0.867048	-2.682467
H	0.807735	0.894797	-2.717676
H	-0.245658	3.619235	0.216174
H	-1.501176	2.690842	-0.649451
H	-1.340966	2.523924	1.104407
H	-2.049235	-0.471372	0.419728
H	1.903950	-0.797228	0.498308

$HOPO(OCH_3)_2OH^-$ (**4bTC2**(uu))

P	-0.189764	0.207733	0.313862
O	0.184449	1.606039	-0.545726
O	-0.219675	0.086766	1.843905
O	-0.525649	-1.035367	-0.770585
C	-0.749650	2.586914	-0.944242
C	0.427391	-1.938967	-1.288968
H	-0.131560	-2.633332	-1.935036
H	1.202089	-1.445649	-1.889545
H	0.933024	-2.519331	-0.506548
H	-0.168108	3.373686	-1.449006
H	-1.502333	2.201758	-1.643722
H	-1.282951	3.035737	-0.096357
O	-1.903116	0.551734	0.193650
O	1.527800	-0.119444	0.207612
H	1.715274	-0.161065	1.153113
H	-2.126984	0.447022	1.126277

$HOPO(OCH_3)_2OH^{-\ddagger}$ (**4b-postTS**(uu)-alt)

P	-0.200273	-0.064480	-0.003787
O	-0.225890	0.746305	-1.406392
O	-0.035310	0.634311	1.307763
O	0.235837	-1.586943	-0.304217
C	0.514016	1.964048	-1.603664
C	1.393404	-2.008368	-1.043237
H	1.598647	-3.036120	-0.718206
H	1.154501	-2.016000	-2.116578
H	2.220212	-1.319826	-0.813183
H	0.554159	2.119971	-2.689047
H	-0.022313	2.806538	-1.142411
H	1.515100	1.831225	-1.164598
O	-1.825179	-0.477695	-0.012217
O	2.379415	0.408204	-0.141584
H	2.276524	0.649306	0.784972
H	-2.160108	-0.006608	0.761336

OH^-…$PO(OCH_3)_2OH$ (**4bRC**(du))

P	0.399139	-0.133663	-0.009664
O	1.816704	0.660646	-0.006291
O	-0.259631	0.495041	1.291881
O	0.569196	-1.609895	-0.021133
O	-0.262523	0.516734	-1.298692
C	-1.564509	0.053556	1.797199
C	-1.573024	0.089811	-1.802005
O	-3.872465	1.014416	0.012198
H	-1.629348	0.510254	-2.811005
H	-1.595385	-1.004054	-1.868380
H	-2.404847	0.479316	-1.165549
H	-1.614548	0.454236	2.814602
H	-2.401929	0.452959	1.174397
H	-1.582692	-1.041471	1.842603
H	-3.851583	1.981030	0.024410
H	2.494473	-0.027729	-0.000080

OH^-…$PO(OCH_3)_2OH^{\ddagger}$ (**4b-preTS**(ds))

P	0.000920	-0.000417	0.000192
O	1.601493	0.509057	-0.056543
O	-0.262358	0.822849	1.392903
O	-0.032296	-1.484561	0.032777
O	-0.289850	0.812307	-1.373383
C	-1.155443	0.296996	2.395167
C	-1.101717	0.212841	-2.397852
O	-2.556858	-0.030031	0.003125
H	-1.310750	1.011595	-3.120156
H	-0.541016	-0.588459	-2.898906
H	-2.022502	-0.163275	-1.934484
H	-1.355098	1.125476	3.086893
H	-2.070376	-0.045557	1.890476
H	-0.661887	-0.518969	2.942882
H	-2.737835	0.919290	-0.038620
H	1.944855	0.409872	0.839520

$HOPO(OCH_3)_2OH^-$ (**4bTC1**-alt)

P	-0.014780	-0.049654	-0.018358
O	0.745988	1.420572	-0.141526
O	-0.054048	0.329609	1.749810
O	0.744275	-1.345843	0.042788
O	-0.251744	0.045933	-1.808883
C	-0.364804	-0.691979	2.651208
C	0.826794	-0.251301	-2.646354
O	-1.672699	0.011572	0.032562
H	0.463446	-0.290408	-3.686951
H	1.619699	0.518312	-2.603270
H	1.288058	-1.219869	-2.399926
H	-0.160680	-0.333440	3.674042
H	-1.431649	-0.980925	2.610330
H	0.234366	-1.597612	2.472301
H	-1.920327	-0.102259	-0.898218
H	0.927096	1.646833	0.784018

OH^-…$PO(OCH_3)_2Cl$ (**4cRC**(u))

P	1.408829	-0.150436	-0.001336
Cl	3.116756	-1.312152	0.002184
O	0.718844	-0.756912	-1.292515
O	1.703127	1.298535	-0.012174
O	0.727565	-0.739950	1.302419
C	-0.434737	-0.083559	-1.916931
C	-0.436766	-0.069435	1.909969
O	-2.787287	-0.215948	-0.004195
H	-0.594251	-0.609067	2.848299
H	-0.170439	0.971024	2.125753
H	-1.333950	-0.133253	1.243299
H	-0.585926	-0.628547	-2.853265
H	-1.337318	-0.138876	-1.257055
H	-0.160295	0.953849	-2.136863
H	-3.168700	0.672455	-0.005331

OH^-…$PO(OCH_3)_2Cl^{-\ddagger}$ (**4c-preTS**(u))

P	-0.026399	-0.000723	0.000595
Cl	2.099956	-0.361185	0.000392
O	-0.270775	-0.896956	-1.297926
O	-0.175244	1.470383	-0.006987
O	-0.267703	-0.883848	1.308226
C	-1.251796	-0.528256	-2.303312
C	-1.255424	-0.512532	2.306329
O	-2.857167	0.022312	-0.000571
H	-1.334669	-1.385660	2.963062
H	-0.885612	0.345393	2.882595
H	-2.194388	-0.283418	1.770222
H	-1.330666	-1.404866	-2.955498
H	-2.192706	-0.293489	-1.773650
H	-0.876801	0.325177	-2.882874
H	-2.831311	0.986672	-0.004121

HOPO(OCH$_3$)$_2$...Cl$^-$ (**4cPC**(u))

P	-0.020721	0.020513	0.002428
Cl	4.084727	-3.155944	0.046330
O	0.362805	-0.866368	-1.263507
O	0.405802	1.440640	-0.036515
O	0.341832	-0.797090	1.319129
C	1.717326	-0.908614	-1.797632
C	1.708500	-0.880735	1.816540
O	-1.625810	-0.179944	0.003798
H	1.618129	-1.183403	2.862413
H	2.290542	-1.626753	1.263568
H	2.190467	0.100182	1.762210
H	1.611255	-1.240905	-2.833325
H	2.161310	0.091278	-1.780225
H	2.339277	-1.619737	-1.241506
H	-2.006927	0.705291	-0.063318

PO(OCH$_3$)$_2$OCH$_3$ (**4dR**(u))

P	-0.323032	-0.255677	-0.008204
O	1.138656	0.283048	0.348912
O	-0.984041	1.012884	-0.720333
O	-1.038829	-0.247636	1.420679
O	-0.382333	-1.525162	-0.758528
C	-0.826627	1.212049	-2.138650
C	2.168322	-0.636472	0.761495
H	2.009706	-0.944555	1.800046
H	2.188029	-1.514913	0.111398
H	3.112029	-0.093139	0.682886
H	-1.623119	1.894083	-2.443216
H	0.146019	1.668245	-2.349605
H	-0.920332	0.265695	-2.677392
C	-2.300405	-0.918846	1.603798
H	-2.438767	-1.019892	2.682075
H	-3.114687	-0.318094	1.185811
H	-2.287177	-1.906217	1.135188

CH$_3$O$^-$...PO(OCH$_3$)$_2$OCH$_3$ (**4dRC**(uu))

P	0.000174	0.004751	0.004344
O	0.734400	0.558793	1.296953
O	0.792346	0.486480	-1.294005
O	-1.236055	1.047661	0.005448
O	-0.382771	-1.427077	0.012032
C	1.900966	-0.287079	-1.849937
C	1.858953	-0.164515	1.889354
H	1.568545	-1.205621	2.064659
H	2.761860	-0.104393	1.251604
H	2.033876	0.330033	2.848676
H	2.067656	0.135351	-2.845351
H	2.807992	-0.180971	-1.222083
H	1.601659	-1.335917	-1.944438
C	-2.293376	0.832901	-0.928457
H	-3.109398	1.501965	-0.639573
H	-1.973476	1.076814	-1.949194
H	-2.645709	-0.204076	-0.899326
O	4.407372	-0.034506	0.035447
C	5.208117	-1.106061	-0.056696
H	6.320174	-0.879714	-0.084777
H	5.058658	-1.753530	-0.982476
H	5.122899	-1.860100	0.791877

CH$_3$O$^-$...PO(OCH$_3$)$_2$OCH$_3$ ‡ (**4d-preTS**(uu))

P	-0.023104	0.005461	0.004479
O	0.283936	0.898396	1.309438
O	0.260873	0.847276	-1.350503
O	-1.637763	0.476356	0.060672
O	-0.007891	-1.480329	0.002482
C	1.229820	0.480047	-2.336942
C	1.051330	0.405458	2.410968
H	0.582626	-0.489274	2.842543
H	2.062370	0.179499	2.060799
H	1.044415	1.207644	3.159260
H	0.953354	1.046818	-3.237190
H	2.232641	0.725050	-1.984044
H	1.182372	-0.591976	-2.556984
C	-2.504647	-0.045774	-0.921812
H	-3.529196	0.226068	-0.635406
H	-2.301562	0.376581	-1.918355
H	-2.435954	-1.140507	-0.987509
O	2.477771	-0.036202	0.036972
C	3.183245	-1.179117	-0.154522
H	4.143357	-1.213575	0.432954
H	3.517358	-1.353710	-1.222073
H	2.640337	-2.115404	0.119232

CH$_3$OPO(OCH$_3$)$_2$OCH$_3^-$ ‡ (**4dTC1**(uu))

P	-0.004401	0.004163	-0.003374
O	0.051588	0.900740	1.402815
O	0.104900	0.952937	-1.381267
O	-1.685078	0.499804	0.040123
O	-0.201284	-1.488330	-0.065538
C	1.137125	0.849836	-2.338170
C	1.056852	0.784376	2.381316
H	1.292785	-0.258656	2.630809
H	1.989080	1.286162	2.093318
H	0.656558	1.266680	3.286230
H	0.756531	1.337338	-3.249026
H	2.056865	1.356355	-2.019884
H	1.385285	-0.190592	-2.584557
C	-2.561897	-0.055923	-0.892733
H	-3.588694	0.216158	-0.596040
H	-2.401945	0.328414	-1.918497
H	-2.493952	-1.154352	-0.930489
O	1.821203	-0.019461	0.027786
C	2.566302	-1.191473	0.067412
H	3.185007	-1.241324	0.989100
H	3.273892	-1.238412	-0.787126
H	1.931773	-2.085566	0.034436

CH$_3$OPO(OCH$_3$)$_2$OCH$_3^-$ ‡ (**4dTS12**$_{count,1}$(uu))

P	0.037369	-0.007088	-0.000696
O	1.538869	-0.133186	0.025474
O	-0.812541	1.429889	0.004946
C	-1.288663	2.141708	-1.110820
O	-0.978470	-1.340869	0.060164
O	-0.236252	0.126152	1.726701
C	-1.009394	-2.362950	-0.912606
H	-0.496355	2.445545	-1.806288
H	-2.044860	1.586339	-1.679622
H	-1.754723	3.053591	-0.706125
H	-1.487738	-3.229294	-0.429689
H	-1.592921	-2.082531	-1.798875
H	-0.006967	-2.662314	-1.244421
C	0.458180	-0.743093	2.569411
H	0.266528	-0.429945	3.609458
H	0.123386	-1.794545	2.475423
H	1.544615	-0.722463	2.394493
O	-0.139051	-0.068274	-1.809906
C	0.944674	0.085840	-2.667763
H	0.993677	1.106042	-3.107748
H	0.847839	-0.618058	-3.517970
H	1.899991	-0.101835	-2.162940

$CH_3OPO(OCH_3)_2OCH_3^-$ (**4dTC12**(uu))

P	0.142222	-0.032966	-0.063945
O	1.618875	-0.270093	0.070729
O	-0.416220	1.537943	-0.272785
C	-1.742424	1.788220	-0.661696
O	-1.028077	-1.232183	0.021172
O	-0.241463	0.243868	1.638973
C	-1.191439	-2.294277	-0.898421
H	-2.018408	1.244721	-1.577417
H	-2.460204	1.527850	0.133151
H	-1.827797	2.866561	-0.860315
H	-1.795393	-3.054759	-0.378777
H	-1.718494	-1.982723	-1.808923
H	-0.237029	-2.744533	-1.195338
C	0.212263	-0.672680	2.589425
H	0.066790	-0.229995	3.589422
H	-0.344985	-1.629520	2.568826
H	1.282336	-0.903036	2.469087
O	0.042314	-0.242107	-1.853421
C	1.037979	0.333357	-2.641488
H	1.039272	1.439437	-2.599032
H	0.857758	0.045663	-3.692650
H	2.045680	-0.004529	-2.354811

$CH_3OPO(OCH_3)_2OCH_3^{-\ddagger}$ (**4dTS12**$_{count,2}$(uu))

P	0.135932	-0.036835	-0.122234
O	1.611094	-0.232027	0.088474
O	-0.457784	1.497774	-0.451301
C	-1.775682	1.895989	-0.169197
O	-1.008761	-1.258302	-0.021255
O	-0.312326	0.301605	1.560482
C	-1.121442	-2.355556	-0.906732
H	-2.520082	1.252023	-0.666157
H	-1.987988	1.903356	0.907873
H	-1.895587	2.915695	-0.564437
H	-1.738409	-3.103825	-0.384813
H	-1.611435	-2.083603	-1.849811
H	-0.150010	-2.804434	-1.145310
C	0.126126	-0.560113	2.564394
H	-0.065614	-0.079439	3.539220
H	-0.407796	-1.530275	2.565081
H	1.205025	-0.768962	2.491689
O	0.120402	-0.327725	-1.890616
C	1.122268	0.234730	-2.679505
H	1.027554	1.333872	-2.776293
H	1.044134	-0.191149	-3.695823
H	2.129478	0.021647	-2.290101

$CH_3OPO(OCH_3)_2OCH_3^{-\ddagger}$ (**4dTS12**$_{clock}$(uu))

P	-0.035046	-0.015878	-0.111576
O	1.456553	0.200678	-0.077134
O	-1.221497	1.152165	-0.260558
C	-0.823116	2.499390	-0.211218
O	-0.816029	-1.479844	0.047606
O	-0.308237	0.148286	1.637504
C	-1.119963	-2.395234	-0.986258
H	-0.295612	2.741822	0.723629
H	-0.175256	2.773548	-1.059894
H	-1.735635	3.109891	-0.264195
H	-1.595319	-3.255197	-0.490860
H	-1.813570	-1.979530	-1.724731
H	-0.230059	-2.756498	-1.516786
C	0.587877	-0.449108	2.525522
H	0.334497	-0.112481	3.545821
H	0.526397	-1.555467	2.522716
H	1.633944	-0.175032	2.318647
O	-0.146902	-0.138043	-1.918561
C	0.996747	-0.403771	-2.670087
H	0.681718	-0.588358	-3.713953
H	1.566231	-1.289509	-2.335347
H	1.715564	0.432997	-2.674257

$CH_3OPO(OCH_3)_2OCH_3^-$ (**4dTC2**(uu))

P	0.010271	-0.080050	-0.167686
O	1.485648	-0.067942	0.137153
O	-0.792880	1.327065	-0.619637
C	-0.951852	2.458379	0.211621
O	-0.881855	-1.502506	-0.066421
O	-0.617591	0.225460	1.454876
C	-0.667046	-2.636471	-0.881240
H	-1.789595	2.349677	0.912535
H	-0.048960	2.685432	0.791969
H	-1.159015	3.306775	-0.460092
H	-1.107503	-3.490508	-0.342222
H	-1.153796	-2.547606	-1.861088
H	0.398133	-2.840516	-1.046659
C	-0.101481	-0.496038	2.531224
H	-0.430186	-0.004643	3.463552
H	-0.468301	-1.539249	2.559810
H	0.998717	-0.523956	2.523128
O	0.081807	-0.389897	-1.905480
C	0.973699	0.339956	-2.691133
H	0.635260	1.378327	-2.867297
H	1.048598	-0.154416	-3.675405
H	1.979745	0.382435	-2.246924

$CH_3O^-...PO(OCH_3)_2OH$ (**4eRC**(uu))

P	-0.076243	0.007224	-0.024798
O	0.756934	1.358182	0.064011
O	0.769883	-1.076820	-0.822153
O	-1.138500	0.419367	-1.178086
O	-0.723490	-0.451970	1.230954
C	1.869324	-1.811967	-0.199660
H	-2.012698	0.293314	-0.787198
C	1.849503	1.535341	1.019241
H	1.548558	1.147057	1.998415
H	2.773991	1.046389	0.652628
H	1.987367	2.617799	1.092368
H	1.561998	-2.162424	0.791893
H	2.032820	-2.676874	-0.848697
H	2.783440	-1.189998	-0.144504
O	4.398418	0.042840	-0.036268
C	5.349677	-0.129765	0.892575
H	5.270603	0.543015	1.809596
H	5.409481	-1.170386	1.351137
H	6.412321	0.052439	0.538039

$CH_3O^-...PO(OCH_3)_2OH^{\ddagger}$ (**4e-preTS**(uu))

P	-0.005085	0.001566	0.005029
O	0.322202	0.758611	1.392087
O	0.275719	0.911369	-1.315753
O	-1.599505	0.519790	0.106138
O	-0.013074	-1.480509	-0.114719
C	1.235159	0.556126	-2.320160
H	-2.002785	0.317584	-0.746744
C	1.118912	0.156104	2.417589
H	0.717097	-0.827284	2.694174
H	2.144730	0.055032	2.054594
H	1.045219	0.829435	3.280688
H	1.206937	-0.517725	-2.532135
H	0.931820	1.112944	-3.218194
H	2.239173	0.822412	-1.987869
O	2.506310	-0.027321	0.006474
C	3.227762	-1.149477	-0.238306
H	2.694273	-2.107391	-0.024396
H	3.579231	-1.261302	-1.309116
H	4.181197	-1.206577	0.359373

$CH_3OPO(OCH_3)_2OH^-$ (**4eTC**(uu))

P	0.007341	-0.061367	-0.020162
O	0.121476	0.749056	1.445312
O	0.142765	1.007296	-1.307853
O	-1.656803	0.428519	0.022209
O	-0.261940	-1.548272	-0.172237
C	1.241520	1.094067	-2.187574
H	-2.069885	-0.434557	-0.096124
C	1.233787	0.744405	2.311644
H	1.605995	-0.264972	2.529416
H	2.074299	1.340230	1.933047
H	0.882082	1.189659	3.255277
H	1.561758	0.116733	-2.571652
H	0.898742	1.700297	-3.040398
H	2.114633	1.582401	-1.735790
O	1.821001	-0.182456	-0.019674
C	2.517307	-1.382044	-0.108356
H	1.846646	-2.244774	-0.198999
H	3.198192	-1.379167	-0.985942
H	3.159856	-1.536124	0.784804

$CH_3OPO(OCH_3)_2OH^-$ (**4eTC2**(uu))

P	-0.039768	-0.054724	-0.152667
O	1.431460	-0.006153	0.227386
O	-0.880091	1.284940	-0.743614
C	-1.258812	2.391251	0.049534
O	-1.009719	-1.416067	-0.043549
O	-0.627313	0.279980	1.467826
C	-1.121977	-2.456189	-0.992238
H	0.218070	0.254341	1.931405
H	-2.081159	2.157921	0.736956
H	-0.427623	2.791164	0.645515
H	-1.590727	3.172363	-0.652142
H	-0.150444	-2.881730	-1.272596
H	-1.724470	-3.241443	-0.509744
H	-1.628836	-2.137712	-1.912087
O	0.181005	-0.454268	-1.858848
C	1.127271	0.250500	-2.603839
H	2.116553	0.256513	-2.121811
H	1.220444	-0.237872	-3.589553
H	0.831484	1.301384	-2.782375

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS12**$_{count}$(uu))

P	0.085418	-0.025765	-0.043245
O	1.583055	-0.196594	0.103865
O	-0.529257	1.526926	-0.292721
C	-1.807839	1.722856	-0.839052
O	-1.108785	-1.200043	0.039707
O	-0.236241	0.173268	1.664775
C	-1.413758	-2.176262	-0.935433
H	0.664113	0.091249	2.000059
H	-1.934444	1.212025	-1.804449
H	-2.604651	1.381207	-0.156989
H	-1.936517	2.803595	-0.996106
H	-0.522477	-2.693664	-1.308927
H	-2.064471	-2.910067	-0.434746
H	-1.948413	-1.762949	-1.800245
O	0.039590	-0.285707	-1.828050
C	1.041137	0.289848	-2.609557
H	2.045053	-0.074038	-2.342109
H	0.844858	0.032696	-3.666286
H	1.065829	1.393678	-2.539061

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS23**$_{clock}$(uu))

P	0.027284	-0.078504	0.085498
O	1.671867	-0.392564	0.235748
O	-0.660211	1.277087	0.127789
C	2.494245	0.682065	0.618128
O	-0.753159	-1.548675	-0.056934
O	0.295630	-0.012533	-1.673008
H	-0.164554	0.815075	-1.856757
C	-1.367153	-2.009407	-1.246388
H	-1.942835	-2.902980	-0.962344
H	-2.059282	-1.273590	-1.676715
H	-0.639229	-2.278872	-2.019481
O	-0.014693	-0.388740	1.833447
C	-1.203964	-0.159152	2.529298
H	-1.005118	-0.304397	3.605016
H	-1.590561	0.861695	2.382485
H	-2.009130	-0.865162	2.247367
H	2.458506	1.513306	-0.105934
H	2.226747	1.075922	1.610571
H	3.526616	0.306975	0.656760

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS12**$_{clock}$(uu))

P	-0.014475	0.030405	-0.123089
O	1.471141	0.356057	-0.117583
O	-1.315788	1.077416	-0.313512
C	-1.040896	2.455703	-0.305824
O	-0.711898	-1.470549	0.080054
O	-0.180746	0.201519	1.615981
C	-1.369759	-2.220050	-0.922509
H	0.747804	0.321010	1.849156
H	-0.543679	2.774587	0.623985
H	-0.412313	2.758929	-1.159096
H	-2.002096	2.983366	-0.381472
H	-0.683994	-2.635931	-1.671152
H	-1.858380	-3.055439	-0.398766
H	-2.133248	-1.637556	-1.448984
O	-0.118183	-0.132814	-1.927102
C	1.002145	-0.560357	-2.640134
H	1.817668	0.180905	-2.645253
H	1.446465	-1.501826	-2.265232
H	0.692596	-0.740541	-3.686436

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS23**$_{count}$(uu))

P	-0.037743	0.114062	0.043653
O	1.605789	0.404314	0.206356
O	-1.000713	1.272578	-0.101838
C	2.488014	-0.627364	0.567919
O	-0.448591	-1.519775	0.134280
O	0.222613	-0.079044	-1.701994
H	-0.235550	0.710721	-2.010939
C	-0.963539	-2.277048	-0.944530
H	-1.338945	-3.214346	-0.505397
H	-1.793704	-1.773470	-1.455200
H	-0.202460	-2.514326	-1.697386
O	-0.039488	0.032208	1.818928
C	-1.258258	-0.078710	2.488950
H	-1.070604	0.046860	3.569156
H	-1.980119	0.693121	2.176190
H	-1.739570	-1.066503	2.351551
H	2.208446	-1.100940	1.519310
H	2.551971	-1.410010	-0.207915
H	3.486469	-0.180526	0.678280

$CH_3OPO(OCH_3)_2OH^-$ (**4eTC3**(uu))

P	-0.033976	-0.082631	-0.070350
O	-0.075214	-0.100655	1.613883
O	1.703882	0.319553	-0.017391
O	-0.351204	1.443859	-0.683060
O	0.181579	-1.340559	-0.896436
H	2.033545	-0.434021	-0.520970
C	1.037007	-0.431731	2.419309
H	0.640256	-0.617450	3.429290
H	1.551083	-1.341031	2.078880
H	1.779324	0.374583	2.469412
O	-1.783036	-0.131378	0.025293
C	-2.385641	-1.333117	0.404046
H	-3.475811	-1.215154	0.287156
H	-2.059764	-2.180663	-0.219214
H	-2.192968	-1.598217	1.460865
C	0.561331	2.174180	-1.470211
H	-0.017028	2.989308	-1.931359
H	1.381563	2.606719	-0.883774
H	1.006464	1.572511	-2.274416

$CH_3O^-...PO(OCH_3)_2OH$ (**4eRC**(du))

P	-0.015464	0.012072	0.000488
O	1.039789	1.243070	0.000875
O	-0.858195	0.387939	1.295081
O	0.641412	-1.320481	0.003631
O	-0.855922	0.381741	-1.297011
C	-1.963030	-0.445151	1.768928
C	-1.950889	-0.460338	-1.779771
H	-2.106987	-0.150964	-2.817021
H	-1.641106	-1.511161	-1.763303
H	-2.870740	-0.301029	-1.180717
H	-2.123747	-0.136291	2.805638
H	-2.876420	-0.277790	1.163944
H	-1.662643	-1.498738	1.753029
H	1.916106	0.837000	-0.011859
O	-4.492511	-0.091698	-0.027660
C	-5.051672	1.129641	-0.091046
H	-4.755166	1.756117	-0.991718
H	-4.820508	1.818965	0.781975
H	-6.184753	1.140361	-0.133574

$CH_3OPO(OCH_3)_2...OH^{-\ddagger}$ (**4e-postTS**(uu))

P	-0.014859	0.003613	-0.002736
O	0.219051	1.186563	1.067511
O	0.176888	0.554894	-1.515175
O	-1.665533	0.322585	0.003395
O	0.142796	-1.443722	0.316174
C	1.199913	0.096641	-2.416618
C	1.123707	1.051551	2.174159
H	0.714017	0.350176	2.915662
H	2.089563	0.702442	1.782706
H	1.191354	2.048475	2.627012
H	1.265011	0.854406	-3.208253
H	2.136817	-0.006596	-1.846197
H	0.895486	-0.861372	-2.864643
C	-2.480036	-0.490836	-0.813707
H	-3.525280	-0.245418	-0.585087
H	-2.306970	-0.303799	-1.884808
H	-2.316881	-1.559669	-0.617417
O	2.575326	0.006884	0.007384
H	2.549807	-0.938761	0.194397

$CH_3O^-...PO(OCH_3)_2OH^{\ddagger}$ (**4e-preTS**(ds))

P	0.019102	0.001382	0.000255
O	1.621478	0.512838	-0.059243
O	-0.222246	0.841065	1.395652
O	-0.017556	-1.482104	0.066083
O	-0.239674	0.755432	-1.417433
C	-1.048686	0.278351	2.426927
C	-0.993619	0.091049	-2.438630
H	-1.236132	0.855167	-3.185944
H	-0.381137	-0.690879	-2.908398
H	-1.902322	-0.335989	-2.006163
H	-1.279152	1.096504	3.118947
H	-1.956883	-0.133406	1.975794
H	-0.495594	-0.504492	2.965438
H	1.933421	0.519632	0.853179
O	-2.418127	0.000725	0.002925
C	-3.082617	1.188427	-0.048439
H	-3.024693	1.810112	0.887947
H	-4.182232	1.058695	-0.226483
H	-2.746965	1.889642	-0.857469

$CH_3OPO(OCH_3)_2...OH^-$ (**4ePC**(uu))

P	0.028948	-0.008417	0.003388
O	-0.724579	0.489275	1.318654
O	-0.675760	0.612427	-1.274121
O	-4.323643	0.074088	-0.006155
O	0.338482	-1.458978	-0.034815
C	-1.851645	-0.034696	-1.866884
H	-4.664143	-0.830058	-0.052439
C	-1.873546	-0.237597	1.865940
H	-2.779677	-0.111122	1.225648
H	-1.610738	-1.296335	1.974377
H	-2.033105	0.199298	2.857270
H	-2.748394	0.036464	-1.205126
H	-2.018342	0.503465	-2.804815
H	-1.610188	-1.080804	-2.088074
O	1.325631	0.964841	0.016475
C	2.358129	0.670820	0.955830
H	2.647884	-0.385119	0.911817
H	3.216726	1.293939	0.687817
H	2.043124	0.914328	1.978416

$CH_3OPO(OCH_3)_2OH^-$ (**4eTC1**-alt)

P	-0.029647	-0.002838	-0.013080
O	0.726805	1.463108	0.063633
O	-0.078714	0.294116	1.875205
O	0.561197	-1.377029	0.058555
O	0.009818	0.283858	-1.735895
C	-0.387574	-0.766157	2.722249
C	-0.325117	-0.777249	-2.585072
H	-0.191881	-0.433225	-3.623421
H	0.312545	-1.658286	-2.421551
H	-1.375059	-1.103294	-2.472377
H	-0.299190	-0.430782	3.771906
H	-1.423148	-1.135313	2.586344
H	0.281868	-1.630608	2.581893
H	0.822632	1.574265	1.026664
O	-1.705734	0.016691	0.007975
C	-2.385655	1.250628	0.006790
H	-2.107675	1.875154	-0.855288
H	-2.196687	1.820616	0.929201
H	-3.461117	1.032803	-0.052996

$CH_3OPO(OCH_3)_2...OH^-$ ‡ (**4e-postTS**-alt)

P	0.033482	-0.003501	0.005964
O	2.680620	-0.128118	-0.014257
O	0.551925	-0.862840	1.307313
O	-1.464680	-0.115370	0.010708
O	0.559382	-0.594264	-1.420684
C	-0.442061	-1.472880	2.139307
C	-0.427470	-0.985939	-2.379883
H	0.136052	-1.313988	-3.261436
H	-1.050552	-1.810921	-2.016308
H	-1.091728	-0.158957	-2.656304
H	0.109495	-1.930898	2.969353
H	-1.159912	-0.744360	2.530707
H	-1.003904	-2.247266	1.604635
H	2.755968	-0.474031	0.881940
O	0.295724	1.576234	0.158529
C	1.507115	2.336375	-0.018392
H	1.432134	2.883262	-0.970165
H	2.355024	1.618983	-0.000237
H	1.545403	3.064046	0.804457

$CH_3OPO(OCH_3)_2...OH^-$ ‡ (**4e-postTS**(du))

P	-0.371110	-0.400642	0.034330
O	1.287381	-0.160571	0.051322
O	-2.940717	-0.640303	-0.052579
H	-2.752238	-1.580315	0.036508
O	-0.529366	0.138050	-1.484469
O	-0.730593	0.812838	1.053278
O	-0.449485	-1.832024	0.419634
C	-1.688361	0.755802	-2.065575
C	1.873592	1.089661	-0.236034
H	1.621476	1.443263	-1.245891
H	1.574955	1.863227	0.486677
H	2.962541	0.961464	-0.175510
H	-1.642015	1.842680	-1.898600
H	-1.628885	0.560979	-3.144310
H	-2.583005	0.310088	-1.603790
C	-1.680000	0.662327	2.121523
H	-1.226797	0.099355	2.950344
H	-1.912718	1.678315	2.465696
H	-2.564963	0.148402	1.718479

$CH_3OPO(OCH_3)_2...OH^-$ (**4ePC**-alt)

P	0.041743	-0.000715	0.000046
O	4.264179	0.050381	-0.012756
O	0.662081	-0.399113	1.420863
O	-1.431516	-0.108181	0.000908
O	0.700120	-0.955120	-1.102357
C	1.893236	-1.141342	1.634752
C	1.859919	-0.640873	-1.918953
H	2.054176	-1.551211	-2.494587
H	1.603585	0.168871	-2.612652
H	2.749335	-0.373540	-1.321564
H	2.009248	-1.184669	2.722453
H	1.774612	-2.160200	1.249389
H	2.771065	-0.656070	1.177234
H	4.928374	0.750795	-0.013944
O	0.505585	1.503807	-0.314840
C	1.689386	2.134156	0.231392
H	1.822844	3.052775	-0.349373
H	2.589276	1.500838	0.146965
H	1.507348	2.399287	1.279808

$CH_3OPO(OCH_3)_2...OH^-$ (**4ePC**(du))

P	0.244516	-0.213880	0.016836
O	1.709216	0.458625	0.054409
O	-3.852129	1.508033	-0.423510
H	-4.603513	0.899335	-0.415688
O	-0.302118	0.336993	-1.376068
O	-0.474406	0.573113	1.203105
O	0.317561	-1.684157	0.155758
C	-1.610276	-0.032800	-1.917797
C	1.883176	1.874428	-0.052500
H	1.485459	2.249888	-1.000934
H	1.389971	2.395000	0.774842
H	2.960920	2.059605	-0.009736
H	-1.557229	0.224245	-2.980905
H	-1.749139	-1.116191	-1.821833
H	-2.432681	0.531261	-1.416465
C	-1.850743	0.302741	1.619777
H	-1.994611	-0.780135	1.714842
H	-1.938976	0.759605	2.611054
H	-2.587905	0.752820	0.912707

Table S4. Cartesian coordinates of additional species *not* discussed in the main text, computed at OLYP/TZ2P.

$P(CH_3)_2OH$ (**1bR**(d))

P	0.128365	0.140685	1.448342
C	-1.622394	-0.039624	2.037802
C	0.796184	-1.470947	2.082577
H	-1.641976	0.054661	3.130078
H	-2.068087	-1.004855	1.763963
H	-2.230318	0.768464	1.618687
H	1.808358	-1.621396	1.693844
H	0.172358	-2.330686	1.805063
H	0.857878	-1.425246	3.176411
O	-0.018340	-0.158317	-0.188209
H	-0.498975	-0.975772	-0.388281

$H_2O…PCH_2CH_3OH^-$ (**1bRC**(ws)-alt)

O	-3.948658	0.030264	-0.029657
P	0.029392	-0.012135	0.011812
C	-0.060965	0.997287	1.593242
C	-1.161519	0.801472	-0.957386
H	-0.981467	0.754818	2.136158
H	-0.055251	2.075928	1.377955
H	0.800347	0.764679	2.229901
H	-1.337708	0.366831	-1.946031
H	-1.219866	1.899484	-0.940613
H	-3.014732	0.304846	-0.294490
O	1.667567	0.489168	-0.434348
H	1.544341	1.306851	-0.939667
H	-3.787589	-0.837114	0.362066

$H_2O…PCH_2CH_3OH^{-\ddagger}$ (**1b-preTS**(ws)-alt)

O	-3.350041	-0.272579	-0.312955
P	0.139412	0.119966	0.110603
C	0.397806	1.073239	1.707176
C	-0.095705	1.386462	-1.029236
H	-0.564087	1.450167	2.072925
H	1.077144	1.922643	1.547281
H	0.836874	0.417422	2.467686
H	-0.476656	1.126568	-2.017711
H	0.408940	2.356197	-0.949482
H	-2.997713	0.591995	-0.578694
O	1.810770	-0.500078	0.041780
H	2.203444	0.060312	-0.644237
H	-2.508371	-0.702118	-0.073358

$HOP(CH_3)_2OH^-$ (**1bTC**(du) = **1bTC**(ud))

O	-1.939637	0.004717	0.000552
P	0.017620	-0.000985	-0.000075
C	-0.029921	1.018213	1.580531
C	-0.030286	1.403254	-1.251112
H	-1.008614	1.495960	1.689260
H	0.766211	1.775943	1.595519
H	0.130383	0.351587	2.436387
H	0.124382	0.988717	-2.254518
H	0.768968	2.134869	-1.066610
H	-1.007378	1.895746	-1.224498
O	1.899511	-0.017091	-0.001834
H	2.272128	0.871086	0.119840
H	-2.080393	-0.938838	-0.127792

$HOP(CH_3)_2OH^-$ (**1bTC**(dd))

O	-1.935521	-0.050725	0.000003
P	-0.029920	0.013918	0.000028
C	-0.022252	1.247552	1.432914
C	-0.022917	1.247473	-1.432995
H	-0.967243	1.801762	1.499661
H	0.811040	1.958849	1.346762
H	0.110537	0.693949	2.370082
H	0.103512	0.693204	-2.370633
H	0.813632	1.955233	-1.350186
H	-0.965957	1.805533	-1.495755
O	1.873051	-0.026272	0.000320
H	2.264113	0.861562	0.001112
H	-2.339067	0.831212	-0.001125

$HOP(CH_3)_2…Cl^-$ (**1cPC**(d))

O	-1.746839	0.005946	0.025266
CL	3.847332	2.269261	-0.057125
P	-0.052050	-0.008192	-0.007969
C	0.389172	1.150874	1.358234
C	0.332530	1.108145	-1.427338
H	-0.178744	2.090017	1.297120
H	1.458567	1.394638	1.259218
H	0.201831	0.677389	2.328352
H	0.105537	0.605214	-2.373884
H	1.404495	1.352648	-1.379045
H	-0.232173	2.049500	-1.372200
H	-2.084786	0.914461	0.024840

$PO(CH_3)_2OH$ (**2bR**(d))

O	0.031590	0.033004	-0.543849
P	-0.091300	0.023326	0.930436
C	-0.931605	-1.445319	1.610935
C	-0.967792	1.463333	1.626725
H	-0.392915	-2.339467	1.283385
H	-1.951298	-1.487248	1.214149
H	-0.979425	-1.430421	2.705422
H	-0.451048	2.373921	1.309176
H	-1.015075	1.435447	2.720993
H	-1.988233	1.484922	1.230262
O	1.382635	0.038084	1.630609
H	1.363229	0.031089	2.596842

$H_2O…POCH_2CH_3OH^-$ (**2bRC**(ws))

O	-4.127375	0.006565	0.012782
O	0.498281	-1.418272	0.101996
P	0.002416	-0.001968	-0.002672
C	-1.339860	0.460541	0.983792
C	-0.339650	0.426119	-1.762298
H	-1.387255	-0.099406	1.921533
H	-3.163778	0.140853	0.293392
H	-1.476175	1.540165	1.112417
H	0.583891	0.340485	-2.346200
H	-0.731581	1.444986	-1.851789
H	-1.082317	-0.273664	-2.155729
O	1.274529	1.110218	0.174807
H	1.227521	1.382854	1.101014
H	-4.126500	-0.918081	-0.263368

OH^-…$PO(CH_3)_2OH^{-\ddagger}$ (**2b-preTS**(du))

O	-2.592284	0.729739	0.005130
O	-0.388048	-1.444905	0.002336
P	-0.015989	0.006138	0.000220
C	-0.216847	0.956804	1.549331
C	-0.224001	0.953210	-1.550168
H	0.391625	0.464296	2.319588
H	-1.285075	0.966670	1.779475
H	0.157966	1.977921	1.408116
H	0.389804	0.466281	-2.319813
H	0.140188	1.978227	-1.409494
H	-1.292116	0.953359	-1.781061
O	1.701220	0.021241	-0.002927
H	1.911718	-0.921834	-0.004465
H	-2.656341	1.696214	-0.000488

$HOPO(CH_3)_2OH^-$ (**2bTC**(du))

O	-1.791535	-0.217469	0.025299
O	0.087844	-1.750211	0.052758
P	0.025242	-0.231462	0.037855
C	0.053580	0.808587	1.595065
C	0.051832	0.828285	-1.511268
H	0.693976	0.293371	2.318199
H	-0.941762	0.960693	2.023822
H	0.525632	1.774299	1.379729
H	0.421364	0.178911	-2.313203
H	0.771784	1.644037	-1.395793
H	-0.930294	1.216066	-1.801542
O	1.855093	-0.029951	0.015469
H	2.092961	-0.963150	0.065693
H	-2.086564	0.701812	0.000442

$HOPO(CH_3)_2OH^-$ (**2bTC**(du)-alt)

O	-1.783266	-0.234919	0.005725
O	0.115607	-1.750027	0.021413
P	0.040234	-0.232017	0.033567
C	0.029308	0.825541	1.582842
C	0.005765	0.808492	-1.523707
H	0.515229	0.233969	2.366202
H	-0.973217	1.109671	1.919156
H	0.647911	1.714872	1.421356
H	-0.632495	0.296958	-2.250928
H	1.010267	0.962479	-1.924748
H	-0.448000	1.786811	-1.313223
O	1.864865	-0.013106	0.086541
H	2.113312	-0.945026	0.085064
H	-2.093318	0.678575	0.049494

OH^-…$PO(CH_3)_2OH^{-\ddagger}$ (**2b-preTS**(ud))

O	-2.591328	0.677773	0.000417
O	-0.374659	-1.434877	0.010397
P	-0.010302	0.012255	-0.000007
C	-0.241311	1.018798	1.514512
C	-0.247674	0.997240	-1.527179
H	0.197606	0.462754	2.351967
H	-1.323383	1.160479	1.617247
H	0.275481	1.984345	1.419067
H	0.196802	0.434525	-2.357222
H	0.260907	1.968114	-1.442896
H	-1.330760	1.129780	-1.631574
O	1.701766	-0.037377	-0.002643
H	2.054479	0.862089	-0.006164
H	-2.907924	-0.233607	0.008605

OH^-…$PO(CH_3)_2OH^{-\ddagger}$ (**2b-preTS**(dd))

O	-2.654210	0.025594	-0.003662
O	-0.005049	-1.479019	0.016571
P	-0.025168	0.009148	0.000507
C	-0.475723	0.886282	1.548254
C	-0.475077	0.857270	-1.563813
H	0.284129	0.649741	2.305620
H	-1.479441	0.550032	1.819300
H	-0.489853	1.971844	1.382964
H	0.286462	0.610594	-2.316348
H	-0.494625	1.945413	-1.417076
H	-1.477599	0.512771	-1.829467
O	1.641824	0.427390	-0.003376
H	1.738111	1.388029	-0.038380
H	-2.988533	0.934816	-0.009855

$HOPO(CH_3)_2OH^-$ (**2bTC**(dd))

O	-1.825023	0.223743	-0.029280
O	-0.071872	-1.503685	-0.005590
P	-0.000306	-0.001730	-0.000014
C	0.031110	0.995979	1.597290
C	0.064790	1.005929	-1.590082
H	0.878462	0.673112	2.208591
H	-0.908671	0.872888	2.143084
H	0.163421	2.064319	1.369174
H	-0.811192	0.773808	-2.202209
H	0.987015	0.793780	-2.138493
H	0.040335	2.080439	-1.353990
O	1.837660	0.048894	0.030419
H	2.123911	0.972333	0.023818
H	-2.021875	1.170207	-0.016174

H_2O…$POCH_2CH_3Cl^-$ (**2cRC**(wd))

O	-4.169290	-0.013817	-0.003389
O	0.333361	-1.440497	0.190501
P	-0.007049	0.005346	0.000392
CL	1.946648	1.131632	0.421730
C	-1.336155	0.707825	0.803294
C	-0.074446	0.492715	-1.770629
H	-1.406681	0.413886	1.853826
H	-3.203805	0.126321	0.220512
H	-1.402465	1.791422	0.667077
H	0.867226	0.221290	-2.253318
H	-0.236738	1.569679	-1.870984
H	-0.902836	-0.048165	-2.240187
H	-4.335444	0.691968	-0.639390

OH^-…$PO(CH_3)_2Cl^{-\ddagger}$ (**2c-preTS**(d))

O	-2.700123	0.217034	-0.102990
O	0.102402	-1.547045	0.191284
P	0.162133	-0.083504	-0.052835
CL	2.308062	0.470435	-0.138838
C	-0.293234	1.014770	1.319017
C	-0.278278	0.504664	-1.713759
H	0.311358	0.734967	2.188586
H	-1.374054	0.840535	1.437512
H	-0.092360	2.056117	1.049550
H	0.369177	-0.005465	-2.435299
H	-0.125730	1.586092	-1.781552
H	-1.345222	0.258365	-1.805680
H	-2.996745	1.118922	-0.291400

$HOPO(CH_3)_2\cdots Cl^-$ (**2cPC**(d))

O	-0.836933	1.343906	-0.264758
O	-0.464255	-1.159780	0.233847
P	0.187447	0.158452	-0.032073
CL	0.412392	3.960275	-0.793697
C	1.286275	0.691006	1.333399
C	1.274907	0.124280	-1.505837
H	2.100564	-0.030542	1.463662
H	0.694901	0.724719	2.254337
H	1.691310	1.687352	1.130578
H	2.091102	-0.590985	-1.354403
H	1.677505	1.122221	-1.705783
H	0.677100	-0.200162	-2.363976
H	-0.411080	2.276033	-0.453168

$PO(OH)_2Cl$ (**3aR**-alt)

P	-0.00357	0.00078	-0.01010
CL	2.03930	0.00978	0.02542
O	-0.37147	-0.87166	-1.29012
O	-0.59954	1.33819	0.00412
O	-0.39153	-0.98879	1.19487
H	0.07888	-1.72737	-1.33033
H	-0.48475	-0.49924	2.02608

$PO(OH)_2OH$ (**3bR**(d))

P	0.56973	-0.19461	0.00123
O	1.13810	1.15862	-0.02332
O	1.00671	-1.14544	-1.23215
O	-1.02794	-0.21244	0.01841
O	0.90212	-1.13801	1.25828
H	1.27346	-0.59539	-1.98312
H	-1.40372	-1.10198	-0.03999
H	1.83025	-1.05860	1.52125

$H_2O\cdots POO(OH)OH^-$ (**3bRC**(wu)-alt)

P	-0.049449	0.073085	-0.168048
O	0.589969	1.123980	0.956626
O	0.809722	0.486885	-1.533431
O	-1.466694	0.515348	-0.426868
O	0.360219	-1.307688	0.239464
H	0.212946	1.061870	-2.029247
H	-3.057399	0.056268	0.407279
H	1.190555	0.573507	1.475091
O	-3.890077	-0.242826	0.846057
H	-3.631316	-1.105445	1.189967

$H_2O\cdots POO(OH)OH^-$ (**3bRC**(wd))

P	-0.054949	0.087284	-0.132934
O	0.945729	0.883468	0.937199
O	0.514932	0.636544	-1.599079
O	-1.429115	0.705861	0.042379
O	0.245727	-1.367162	-0.042922
H	-0.122166	1.309773	-1.869685
H	-3.106028	-0.008259	0.399289
H	0.403864	1.602159	1.286805
O	-3.986618	-0.412676	0.587815
H	-3.766462	-1.350270	0.632430

$OH^-\cdots PO(OH)_2OH^{\ddagger}$ (**3b-preTS**(ss))

P	0.029653	0.047962	0.043556
O	-0.261166	1.672270	-0.184095
O	1.696542	0.224159	-0.389828
O	-0.293160	-0.853208	-1.265361
O	0.097760	-0.459803	1.437881
H	1.769359	-0.175145	-1.264858
H	-1.328209	-0.737526	-1.100640
H	0.618738	2.024142	-0.382541
O	-2.131717	-0.058327	-0.064952
H	-2.385526	0.817865	-0.377593

$HOPO(OH)_2OH^-$ (**3bTC**(ss))

P	-0.01647	0.00104	0.00204
O	-0.14312	1.66353	-0.25058
O	1.71824	0.19334	-0.45864
O	-0.13905	-0.97929	-1.36373
O	0.19320	-0.57129	1.36676
H	1.81070	-0.23680	-1.31525
H	-1.10073	-1.08683	-1.43179
H	0.77736	1.89320	-0.45276
O	-1.82220	0.00187	-0.00036
H	-2.08287	0.90526	-0.20758

$HOPO(OH)_2OH^-$ (**3bTC**(su))

P	0.037858	0.000707	-0.002489
O	-0.100425	1.669041	-0.189243
O	1.792619	0.247126	-0.304055
O	0.000134	-0.828671	-1.446098
O	0.203727	-0.712189	1.315972
H	2.141872	-0.202611	0.474141
H	-0.951379	-0.977387	-1.557263
H	0.831354	1.930574	-0.254644
O	-1.757694	-0.015400	-0.027824
H	-2.023598	0.877562	-0.272476

$HOPO(OH)_2\cdots OH^{-\ddagger}$ (**3b-postTS**(su))

P	-0.005658	0.001697	0.001613
O	0.422966	0.863958	1.300886
O	2.166710	0.006789	0.014431
O	0.208666	0.797261	-1.429204
O	-0.076486	-1.489062	-0.032357
H	2.269337	-0.933561	0.201839
H	-0.674508	1.143335	-1.620783
H	1.447935	0.638250	1.097803
O	-1.662027	0.477214	0.113178
H	-1.690343	1.093302	0.854908

$HOPO(OH)_2\cdots OH^{-\ddagger}$ (**3b-postTS**(su)-alt)

P	-0.071367	-0.014568	-0.003668
O	-1.810704	0.470108	-0.031579
O	-0.289235	-0.432615	-1.673185
O	0.981336	-1.346411	-0.027127
O	0.662426	1.289301	0.066549
H	-0.661534	0.378405	-2.042075
H	1.060616	-1.606227	0.897683
H	-2.243899	-0.156878	-0.622452
O	-0.430082	-0.534881	1.625181
H	-1.265628	-0.094841	1.821647

$HOPO(OH)_2OH^{-\ddagger}$ (**3bTS**-alt)

P	0.060906	-0.012151	0.047297
O	-0.233171	1.720498	0.312626
O	-0.059450	-0.115975	-1.605504
O	-0.051328	-1.650384	0.534903
O	1.539128	0.110130	0.376779
H	-1.006580	-0.112278	-1.793012
H	-0.990187	-1.829263	0.670408
H	0.680041	1.987610	0.485584
O	-1.717154	-0.047846	0.318905
H	-1.930996	0.871726	0.518630

$HOPO(OH)_2OH^{-\ddagger}$ (**3bTS**(uu)-rot)

P	0.06266	-0.01013	-0.01326
O	1.79583	0.10011	-0.09077
O	0.10648	1.65733	0.12655
O	0.08218	-0.68927	1.51347
O	-0.09553	-0.99008	-1.16441
H	-0.84333	1.86167	0.09649
H	0.11280	0.03647	2.14713
H	1.98928	-0.61749	-0.70443
O	-1.76625	0.25903	0.12540
H	-2.06527	-0.35636	-0.55373

$OH^-\cdots PO(OH)_2Cl^{\ddagger}$ (**3c-preTS**(d))

P	-0.016939	0.001534	-0.000159
O	-0.086948	1.479841	0.000352
O	0.255887	-0.808684	-1.381943
CL	-2.109146	-0.628540	-0.001253
O	0.254203	-0.809358	1.381744
H	1.220193	-0.602660	-1.455675

H	1.218115	-0.603010	1.457706
O	2.205075	-0.016208	0.000815
H	2.524766	-0.930655	0.001826

$HOPO(OH)_2Cl^-$ (**3cTC**(d))

P	0.48355	0.06072	-0.00495
O	0.52154	1.54544	-0.00681
O	0.34657	-0.83463	-1.38996
CL	-1.86878	-0.13683	0.02337
O	0.37966	-0.83215	1.38456
H	1.23149	-0.76621	-1.78233
H	1.27389	-0.76352	1.75518
O	2.27552	-0.19598	-0.02590
H	2.43752	-1.14989	-0.02734

$HOPO(OH)_2…Cl^{-\ddagger}$ (**3c-postTS**(d))

P	-0.08719	-0.00331	-0.00091
O	-0.01201	1.47706	0.04619
O	-0.35296	-0.91720	-1.33458
CL	-2.59600	0.01965	-0.01823
O	-0.29594	-0.93612	1.35082
H	0.54244	-1.05460	-1.68562
H	0.21063	-0.48492	2.04195
O	1.64357	-0.34232	-0.05849
H	1.76437	-1.24724	0.25753

$HOPO(OH)_2…Cl^-$ (**3cPC**(d))

P	0.04049	-0.08325	0.00456
O	-0.79946	0.18402	1.18359
O	-0.44886	-1.35863	-0.84804
CL	2.01219	-0.70970	-2.76353
O	0.07817	1.14173	-1.03974
H	0.17236	-1.45490	-1.61144
H	0.66211	0.86795	-1.78952
O	1.57933	-0.37918	0.37456
H	2.05699	-0.54442	-0.47547

$PO(OH)_2OCH_3$ (**3dR**(u)-alt)

P	-0.00591	0.01453	0.00303
O	0.29579	1.00759	-1.21182
O	-1.60319	-0.04259	-0.02533
O	0.38028	0.93587	1.27973
O	0.61508	-1.31708	0.00557
H	-2.01839	0.82924	0.02990
H	0.70851	0.36982	1.99299
C	1.66360	1.23781	-1.61756
H	2.22382	1.73672	-0.82055
H	2.14730	0.29333	-1.88021
H	1.61418	1.88748	-2.49243

$PO(OH)_2OCH_3$ (**3dR**(d))

P	-0.00415	0.01323	0.01331
O	1.58292	-0.03704	0.02886
O	-0.40237	1.58350	0.01105
O	-0.35798	-0.40536	1.52575
O	-0.61513	-0.76938	-1.07032
H	-0.70264	1.82829	-0.87580
H	-1.28055	-0.68589	1.59850
C	2.38609	0.69878	0.97261
H	2.19327	1.77211	0.88935
H	2.18609	0.36222	1.99354
H	3.42474	0.48920	0.71326

$PO(OH)_2OCH_3$ (**3dR**(u)-alt2)

P	-0.01793	-0.01282	-0.00442
O	0.31046	-1.00952	-1.21840
O	0.36635	-0.95207	1.24223
O	-1.61931	0.05629	0.09257
O	0.59491	1.32146	-0.05579
H	1.21736	-0.68057	1.61387
H	-2.02977	-0.81371	0.19459
C	0.24692	-0.52463	-2.57735
H	-0.79096	-0.51278	-2.92608
H	0.67687	0.47711	-2.65472
H	0.82743	-1.22541	-3.17993

$CH_3O^-…PO(OH)_2OCH_3^{\ddagger}$ (**3d-preTS**(du))

P	0.02048	-0.11681	-0.03546
O	1.72627	0.16796	0.06922
O	-0.04717	0.94042	-1.29074
O	-0.28414	0.55117	1.40580
O	-0.09310	-1.58168	-0.27552
H	0.88188	1.13844	-1.47972
H	-1.29358	0.57541	1.26145
C	2.48489	-0.66246	0.91533
H	2.29051	-0.45151	1.97987
H	2.27775	-1.72568	0.73200
H	3.54933	-0.46897	0.71910
C	-2.85514	1.00841	-0.78380
H	-2.53563	2.07343	-0.71500
H	-2.80258	0.75025	-1.86245
H	-3.93410	0.99428	-0.51634
O	-2.14058	0.13970	0.01502

$CH_3OPO(OH)_2OCH_3^-$ (**3dTC**(du) = **3dTC**(ud))

P	-0.03082	-0.09362	0.01688
O	1.76898	0.14891	0.02193
O	0.03870	0.88572	-1.31914
O	-0.02473	0.69056	1.49435
O	-0.07488	-1.58874	-0.03799
H	0.99401	0.97910	-1.46059
H	-0.95310	0.62866	1.76297
C	2.56056	-0.68470	0.81679
H	2.44918	-0.46937	1.89561
H	2.32342	-1.74787	0.66216
H	3.61914	-0.51939	0.55518
C	-2.44537	1.33014	-0.32540
H	-2.02360	2.19807	0.21699
H	-2.39737	1.57709	-1.39946
H	-3.51107	1.25913	-0.04697
O	-1.82666	0.11259	-0.01870

$CH_3O^-…PO(OH)_2OCH_3^{\ddagger}$ (**3d-preTS**(ud))

P	-0.03123	0.02059	0.06148
O	2.13210	0.03332	0.14815
O	0.44658	0.81604	-1.26169
O	0.16508	0.89234	1.45435
O	-0.17570	-1.45641	0.15862
H	1.44110	0.64055	-1.08336
H	-0.74235	1.02220	1.76512
C	2.80230	-1.17664	0.18916
H	2.65781	-1.71182	1.14927
H	2.49843	-1.89216	-0.60177
H	3.89623	-1.02022	0.07689
C	-2.06946	1.73676	-0.60168
H	-1.60903	2.57344	-0.04864
H	-1.81066	1.86713	-1.66195
H	-3.16111	1.82461	-0.49779
O	-1.69255	0.47101	-0.11115

CH_3O^-…$PO(OH)_2OCH_3$ ‡ (**3d-preTS**(dd))

P	-0.02670	0.01795	-0.00032
O	-1.71089	0.36488	-0.15373
O	0.16146	0.99622	1.32398
O	0.37215	0.76617	-1.37528
O	-0.08773	-1.45142	0.20218
H	-0.72717	1.04423	1.70375
H	1.37412	0.74918	-1.20708
C	-2.16656	1.60968	-0.63293
H	-1.95106	1.74946	-1.70182
H	-3.25684	1.64490	-0.49109
H	-1.72830	2.46858	-0.09658
C	2.96721	0.41123	1.01206
H	2.86056	1.46205	1.36580
H	2.80172	-0.22632	1.90635
H	4.03775	0.28548	0.73965
O	2.14640	0.07345	-0.04021

$CH_3OPO(OH)_2OCH_3^-$ (**3dTC**(dd))

P	-0.16115	0.18144	0.72082
O	-1.87790	-0.43126	0.80026
O	-0.50122	0.65039	-0.84410
O	0.32253	-1.39886	0.95342
O	-0.28755	1.13080	1.86212
H	-1.46714	0.57764	-0.86097
H	1.28464	-1.30153	1.00885
C	-2.27621	-1.65278	0.24581
H	-1.96353	-2.52092	0.85118
H	-3.37853	-1.66919	0.18568
H	-1.89359	-1.83002	-0.77842
C	2.18176	0.27720	-0.87490
H	1.98664	-0.74801	-1.24733
H	1.86285	0.96684	-1.67477
H	3.27550	0.37755	-0.76457
O	1.58305	0.55921	0.35820

CH_3O^-…$PO(OH)_2OCH_3$ ‡ (**3d-preTS**(uu)-f)

P	-0.00194	0.00844	0.00269
O	-0.07987	1.20451	1.16890
O	1.68026	0.26383	-0.31611
O	-0.32310	0.61726	-1.50303
O	0.09559	-1.40940	0.46380
H	1.74144	1.06985	-0.85382
H	-1.30058	0.66391	-1.45396
C	0.76178	1.03240	2.29658
H	0.44280	1.76147	3.05329
H	0.66696	0.02042	2.71358
H	1.81952	1.20024	2.05085
C	-2.75296	0.27021	1.10877
H	-2.33693	-0.17117	2.03290
H	-2.92098	1.34890	1.32411
H	-3.75520	-0.18358	0.97015
O	-1.97256	0.04834	-0.01015

$CH_3OPO(OH)_2OCH_3^-$ (**3dTC**(uu)-f)

P	0.00912	0.00221	0.00056
O	-0.13567	1.19257	1.18481
O	1.69067	0.35808	-0.28508
O	-0.25551	0.58699	-1.54863
O	0.20723	-1.41712	0.44672
H	1.71602	1.08323	-0.92028
H	-1.22402	0.56194	-1.62349
C	0.91946	1.40716	2.10202
H	0.47993	1.90889	2.97694
H	1.38204	0.46827	2.43193
H	1.71292	2.04648	1.68954
C	-2.51671	-0.57846	1.06744
H	-2.14496	-1.58912	1.29600
H	-2.44681	0.02217	1.99478
H	-3.58640	-0.65331	0.80546
O	-1.83298	0.00415	0.00144

CH_3O^-…$PO(OH)_2OCH_3$ ‡ (**3d-preTS**(ud)-f)

P	0.05071	0.01410	-0.02113
O	-0.13374	0.95731	1.32567
O	1.69240	0.44606	-0.27919
O	-0.32017	0.76608	-1.42163
O	0.18984	-1.44635	0.28104
H	2.15287	-0.30526	0.11172
H	-1.29753	0.59014	-1.41082
C	-0.21725	2.36032	1.19467
H	-0.19793	2.78163	2.20837
H	0.63009	2.77267	0.62818
H	-1.15419	2.66483	0.70686
C	-2.72775	-1.13586	0.39969
H	-2.56500	-1.31499	1.48247
H	-3.82058	-0.99126	0.26666
H	-2.46416	-2.08527	-0.10757
O	-2.03781	-0.03597	-0.07430

$CH_3OPO(OH)_2OCH_3^-$ (**3dTC**(ud)-f)

P	0.715130	-0.425330	-0.495089
O	0.358280	0.798303	0.596994
O	2.340885	0.161529	-0.735133
O	0.431489	0.037411	-2.061828
O	1.105572	-1.803614	-0.001000
H	2.832397	-0.630544	-0.489233
H	-0.517098	-0.139170	-2.169274
C	1.344548	1.384693	1.422013
H	0.804467	1.964908	2.185068
H	1.965274	0.636193	1.933921
H	2.012596	2.055279	0.867481
C	-1.707402	-1.350686	0.563259
H	-1.682072	-0.746642	1.490343
H	-2.769065	-1.523325	0.314965
H	-1.242220	-2.323673	0.787579
O	-1.097338	-0.706793	-0.512208

CH_3O^-…$PO(OH)_2OH$ ‡ (**3e-preTS**(du))

P	0.045698	-0.001921	-0.003570
O	1.723434	-0.376650	-0.146249
O	-0.127909	-0.979483	1.313046
O	-0.346525	-0.756437	-1.370089
O	0.081136	1.482810	0.163266
H	0.783316	-1.226053	1.526237
H	-1.354422	-0.696625	-1.200458
C	-2.946776	-0.687985	0.886174
H	-2.766592	-1.783767	0.974255
H	-2.833567	-0.283282	1.914063
H	-4.022571	-0.574006	0.628542
O	-2.148192	-0.045974	-0.036479
H	2.116747	0.504167	-0.127615

$CH_3OPO(OH)_2OH^-$ (**3eTC**(du))

P	0.57278	0.38238	0.10431
O	2.24488	0.53207	-0.53692
O	1.08544	-1.04874	0.78435
O	0.08405	0.24048	-1.48408
O	0.54214	1.70781	0.81712
H	2.03560	-1.01488	0.59390
H	-0.87971	0.19773	-1.39974
C	-1.58369	-1.39162	0.57103
H	-1.35938	-1.93109	-0.36947
H	-1.18224	-2.01189	1.39024
H	-2.68224	-1.36926	0.67783
O	-1.10979	-0.07538	0.60093
H	2.44428	1.42652	-0.23752

$CH_3OPO(OH)_2\cdots OH^-$ ‡ (**3e-postTS**(du))

P	-0.042319	0.004443	0.000935
O	2.128791	0.025500	-0.052158
O	0.345127	0.877496	-1.292670
O	0.209676	0.810372	1.425116
O	-0.108944	-1.485958	0.028484
H	1.369898	0.665260	-1.125919
H	-0.679397	0.894099	1.797755
C	-2.179903	1.647523	-0.464526
H	-1.700005	2.483234	0.072339
H	-2.011117	1.812107	-1.538059
H	-3.261562	1.697957	-0.270216
O	-1.726689	0.381718	-0.041864
H	2.234080	-0.913562	-0.243497

$CH_3O^-\cdots PO(OH)_2OH$ ‡ (**3e-preTS**(ud))

P	0.03898	-0.00733	0.02646
O	1.67209	-0.52496	-0.19556
O	-0.14735	-0.91299	1.39383
O	-0.45153	-0.75875	-1.32819
O	0.16909	1.46686	0.17647
H	0.73845	-1.27555	1.53710
H	-1.44986	-0.58707	-1.12750
C	-2.82040	1.16904	0.19161
H	-3.91533	1.00402	0.10122
H	-2.65888	1.68353	1.16002
H	-2.54325	1.90621	-0.58968
O	-2.13805	-0.03226	0.10965
H	1.64881	-1.12880	-0.94718

$CH_3OPO(OH)_2OH^-$ (**3eTC**(ud))

P	0.66582	0.62459	0.08054
O	2.42181	0.50795	-0.25522
O	0.84819	-0.64187	1.15563
O	0.44907	0.16644	-1.51581
O	0.66720	2.03944	0.57519
H	1.81285	-0.72561	1.19389
H	-0.51409	0.06416	-1.57829
C	-1.83122	0.75441	1.29128
H	-2.90899	0.61071	1.10440
H	-1.57929	0.19515	2.21147
H	-1.64916	1.82123	1.48990
O	-1.12040	0.29879	0.17792
H	2.50376	0.01092	-1.07682

$CH_3OPO(OH)_2\cdots OH^-$ ‡ (**3e-postTS**(ud))

P	-0.053808	-0.002279	0.004790
O	2.141264	0.047330	-0.081904
O	0.307843	0.782710	-1.349604
O	0.203746	0.890061	1.374059
O	-0.111477	-1.488292	0.084569
H	1.341311	0.659606	-1.150826
H	-0.682821	1.186197	1.629844
C	-2.602740	-0.145228	-0.847683
H	-3.622202	0.186299	-0.603080
H	-2.401390	0.118103	-1.899101
H	-2.552205	-1.238716	-0.752182
O	-1.711779	0.495488	0.033950
H	2.378288	0.732259	0.554246

$CH_3OPOO(OH)^-\cdots H_2O$ (**3ePC**(uw)-alt)

P	-0.02741	-0.02829	0.00574
O	3.98508	0.11107	-0.02521
O	1.24403	0.78680	0.09996
O	-1.06755	0.66130	1.11953
O	-0.07998	-1.51007	0.12654
H	3.03175	0.36715	0.01293
H	-0.53217	1.34095	1.54757
C	-0.81835	1.67495	-1.86353
H	-1.39272	2.32992	-1.18962
H	0.19792	2.07870	-1.95543
H	-1.30114	1.68524	-2.84888
O	-0.80955	0.33429	-1.41106
H	3.92903	-0.85134	-0.01241

$PO(OCH_3)_2Cl$ (**4aR**-alt)

P	-0.120698	-0.029580	-0.051908
Cl	1.900851	-0.004697	0.162085
O	-0.254108	-0.971930	-1.328377
O	-0.725649	1.314074	-0.105823
O	-0.638291	-0.987119	1.123953
C	-1.510269	-0.949614	-2.054934
C	-0.824051	-0.428212	2.447695
H	-1.443066	0.471116	2.402578
H	-1.321486	-1.201784	3.033965
H	0.144645	-0.190882	2.898628
H	-2.289702	-1.453799	-1.476091
H	-1.809999	0.078322	-2.270767
H	-1.326093	-1.492422	-2.982186

$PO(OCH_3)_2OH$ (**4bR**(u)-alt)

P	-0.017545	-0.006686	-0.001334
O	1.605202	0.019400	-0.045723
O	-0.439094	1.529264	0.007546
O	-0.526645	-0.876334	1.078535
O	-0.449808	-0.334492	-1.498906
C	-0.376469	2.250212	1.254858
C	-0.405009	-1.706088	-1.941813
H	-0.778632	-1.704843	-2.966497
H	0.622112	-2.085934	-1.930454
H	-1.039661	-2.335785	-1.312488
H	-0.761237	3.249166	1.045972
H	-0.993593	1.762398	2.014211
H	0.657165	2.325882	1.608906
H	1.935242	-0.551932	0.661535

$PO(OCH_3)_2OH$ (**4bR**(u)-alt2)

P	-1.132547	-0.537648	0.252463
O	-1.193561	0.444593	1.543927
O	0.048417	0.121032	-0.602051
O	-2.435904	-0.745561	-0.395974
O	-0.454919	-1.884841	0.752535
C	-0.184742	1.344946	-1.328297
C	0.780266	-1.922190	1.491451
H	1.616217	-1.617937	0.855720
H	0.727016	-1.275437	2.371897
H	0.913605	-2.958700	1.805579
H	0.742761	1.564718	-1.859708
H	-1.002217	1.217175	-2.042987
H	-0.414808	2.164603	-0.640250
H	-2.111063	0.500853	1.845463

$PO(OCH_3)_2OH$ (**4bR**(d))

P	0.023635	-0.007204	0.000846
O	1.625159	0.050674	-0.072305
O	-0.317632	-0.963428	-1.234561
O	-0.577159	1.333797	0.036583
O	-0.340315	-0.969938	1.239777
C	-1.691312	-1.126540	-1.648469
C	-0.486211	-0.412595	2.562936
H	-0.954184	-1.188698	3.171630
H	0.492793	-0.159484	2.983479
H	-1.117549	0.478837	2.539865
H	-2.250297	-1.702512	-0.904197
H	-2.164065	-0.152485	-1.799932
H	-1.661680	-1.675685	-2.590887
H	2.028831	-0.825964	-0.136977

$PO(OCH_3)_2OH$ (**4bR**(d)-alt)

P	0.029733	0.007462	0.000051
O	1.647050	-0.046456	-0.000726
O	-0.375590	0.984933	1.201339
O	-0.519535	-1.355891	0.000364
O	-0.376225	0.984830	-1.201219
C	-0.438669	0.451930	2.540933
C	-0.441907	0.451752	-2.540634
H	-0.908955	1.225630	-3.151804
H	0.562589	0.239638	-2.922065
H	-1.044605	-0.459475	-2.565279
H	-0.913472	1.221872	3.151065
H	-1.033256	-0.464610	2.565113
H	0.567225	0.249039	2.923641
H	2.036987	0.839088	-0.002200

$PO(OCH_3)_2OH$ (**4bR**(d)-alt2)

P	-0.043964	0.016444	-0.006530
O	-1.656073	-0.074506	0.105913
O	0.214241	1.012084	-1.247399
O	0.573860	-1.311094	-0.054218
O	0.457078	0.887654	1.229019
C	0.320915	0.488592	-2.588594
C	-0.000012	2.215057	1.523490
H	0.294097	2.912561	0.733470
H	-1.086923	2.238382	1.660456
H	0.480037	2.501973	2.460700
H	0.782042	1.275473	-3.188588
H	0.943603	-0.408630	-2.604105
H	-0.671149	0.256076	-2.991109
H	-2.102079	0.706884	-0.244709

OH^-…$PO(OCH_3)_2OH$ (**4bRC**(ud))

P	1.807695	-0.291020	-0.002008
O	3.012362	0.791402	0.003244
O	1.004917	0.172360	1.296946
O	2.319792	-1.677314	-0.011824
O	0.999073	0.184249	-1.292646
C	-0.149145	-0.573520	1.810092
C	-0.145788	-0.567193	-1.817481
H	-0.307060	-0.163154	-2.822035
H	0.127251	-1.625899	-1.897739
H	-1.056024	-0.429041	-1.185975
H	-0.315355	-0.171445	2.814607
H	-1.055231	-0.429096	1.173362
H	0.117281	-1.634073	1.889265
H	2.649741	1.686704	0.038543
O	-2.634565	-0.229735	-0.001173
H	-3.033145	-1.110971	-0.000858

OH^-…$PO(OCH_3)_2OH$ (**4bRC**(dd))

P	1.753122	-0.294207	-0.001854
O	2.965436	0.780004	0.010944
O	0.954434	0.163196	1.301771
O	2.258664	-1.682338	-0.024057
O	0.943965	0.195536	-1.286303
C	-0.204912	-0.583215	1.807066
C	-0.202062	-0.553889	-1.816700
H	-0.357250	-0.147105	-2.821180
H	0.068616	-1.612591	-1.896755
H	-1.112619	-0.408720	-1.186847
H	-0.365299	-0.192801	2.817169
H	-1.109477	-0.419102	1.172996
H	0.054259	-1.645959	1.870761
H	2.611167	1.677731	0.063564
O	-2.680245	-0.297723	-0.002305
H	-2.974017	0.623383	-0.003420

OH^-…$PO(OCH_3)_2Cl$ (**4cRC**(d))

P	0.015451	-0.001145	-0.000388
Cl	1.696514	-1.201851	-0.002132
O	-0.685653	-0.581847	-1.297561
O	0.343221	1.440262	-0.000514
O	-0.682870	-0.582435	1.298064
C	-1.830480	0.120995	-1.909397
C	-1.830540	0.117788	1.907544
O	-4.177998	0.024899	-0.001761
H	-1.990579	-0.410299	2.852155
H	-1.543534	1.154655	2.111017
H	-2.731776	0.054730	1.245475
H	-1.987995	-0.404742	-2.855787
H	-2.733462	0.057146	-1.249731
H	-1.541916	1.158056	-2.109603
H	-4.486710	-0.891418	-0.002477

OH^-…$PO(OCH_3)_2Cl^{-\ddagger}$ (**4c-preTS**(d))

P	0.032685	-0.003586	0.000217
Cl	2.155568	-0.428988	-0.000455
O	-0.242190	-0.877122	-1.309956
O	-0.078995	1.467197	0.001163
O	-0.241567	-0.878863	1.309350
C	-1.110645	-0.337194	-2.343219
C	-1.110839	-0.341320	2.343192
O	-2.768662	0.003513	0.000324
H	-1.277924	-1.174326	3.034150
H	-0.596046	0.473054	2.867814
H	-2.040588	-0.010885	1.850686
H	-1.277642	-1.168723	-3.035972
H	-2.040511	-0.007391	-1.850558
H	-0.595297	0.478080	-2.865885
H	-2.981215	-0.940000	-0.000678

$HOPO(OCH_3)_2...Cl^-$ (**4cPC**(d))

P	-0.004454	0.001385	-0.000205
Cl	3.756097	-3.547593	-0.017154
O	0.295952	-0.879530	-1.300376
O	0.540509	1.372565	0.009079
O	0.304143	-0.899521	1.283744
C	1.644912	-1.032851	-1.830602
C	1.653009	-1.045670	1.816329
O	-1.616616	-0.019227	0.003181
H	1.524492	-1.364351	2.853815
H	2.215617	-1.805676	1.261307
H	2.169893	-0.081666	1.793153
H	1.516570	-1.333897	-2.873332
H	2.172930	-0.075432	-1.791096
H	2.197863	-1.806666	-1.285178
H	-1.946917	-0.927784	-0.008762

$PO(OCH_3)_2OCH_3$ (**4dR**(d))

P	0.018565	0.017873	0.007612
O	1.611129	-0.020139	0.033704
O	-0.405806	1.572511	-0.002434
O	-0.352182	-0.399158	1.505206
O	-0.541147	-0.789076	-1.085917
C	-0.581694	2.257546	-1.257273
C	2.424826	0.653080	1.006882
H	2.154410	1.710243	1.085775
H	2.329099	0.172266	1.984437
H	3.454346	0.564097	0.653789
H	-0.984780	3.242179	-1.011694
H	0.375628	2.374858	-1.776261
H	-1.279156	1.713875	-1.899066
C	-1.708350	-0.724678	1.863164
H	-1.653502	-1.266953	2.809299
H	-2.294299	0.190171	1.997590
H	-2.170027	-1.357645	1.100895

$CH_3O^-...PO(OCH_3)_2OCH_3$ (**4dRC**(du))

P	-0.053310	-0.013196	-0.010851
O	0.666857	0.563812	1.278973
O	0.743842	0.455419	-1.311589
O	-1.298190	1.018188	-0.032741
O	-0.424501	-1.448225	0.012861
C	1.880023	-0.303006	-1.831720
C	1.822261	-0.119164	1.863056
H	1.578629	-1.175043	2.020575
H	2.724041	-0.009316	1.228080
H	1.972560	0.366010	2.831208
H	2.036615	0.080977	-2.844248
H	2.781103	-0.142060	-1.208845
H	1.618434	-1.365116	-1.882501
C	-2.349792	0.779348	-0.967024
H	-3.182244	1.427397	-0.677005
H	-2.035044	1.033907	-1.986771
H	-2.676031	-0.266137	-0.940402
O	4.369521	0.037549	0.058499
C	5.090823	1.169952	0.074182
H	6.216263	1.026118	0.105212
H	4.945101	1.856790	-0.820219
H	4.897314	1.861274	0.956404

$CH_3O^-...PO(OCH_3)_2OCH_3$ ‡ (**4d-preTS**(du))

P	-0.018024	-0.001166	-0.003164
O	0.214773	0.907708	1.319623
O	0.189243	0.825113	-1.393504
O	-1.666910	0.373752	0.066445
O	0.081119	-1.483119	0.006958
C	1.022513	0.296177	-2.432326
C	0.895467	0.338088	2.440175
H	0.224597	-0.337924	2.989643
H	1.788505	-0.193070	2.100007
H	1.171276	1.174672	3.092144
H	1.290369	1.140238	-3.078148
H	1.912941	-0.160438	-1.989612
H	0.458375	-0.440346	-3.022780
C	-2.509548	-0.196058	-0.908389
H	-3.546673	0.005228	-0.607801
H	-2.350517	0.245258	-1.905029
H	-2.371642	-1.284064	-0.984261
O	2.387096	0.009454	0.018171
C	3.086969	1.176151	0.024378
H	4.168845	1.026467	0.280569
H	3.110052	1.727562	-0.957691
H	2.728183	1.947498	0.756131

$CH_3OPO(OCH_3)_2OCH_3^-$ ‡ (**4dTC1**(du))

P	-0.000920	-0.001075	0.000414
O	1.690666	0.007054	0.005884
O	-0.779046	1.279003	0.007330
C	2.335847	1.105719	0.610407
O	-0.869661	-1.457833	-0.021809
O	0.249779	-0.281972	-1.708165
C	-1.991097	-1.609478	0.828592
H	2.352226	1.975330	-0.066853
H	1.860121	1.412271	1.549232
H	3.374417	0.808070	0.815544
H	-1.733889	-2.062333	1.795919
H	-2.492748	-0.654282	1.019857
H	-2.691598	-2.280089	0.306814
C	-0.858509	-0.310258	-2.561570
H	-0.484523	-0.248320	-3.596763
H	-1.447197	-1.240602	-2.475036
H	-1.538122	0.540091	-2.392563
O	0.070213	-0.150915	1.817642
C	0.796048	-1.174480	2.424949
H	0.430005	-1.304522	3.459679
H	0.699757	-2.152052	1.919403
H	1.881580	-0.965850	2.491972

$CH_3OPO(OCH_3)_2OCH_3^-$ ‡ (**4dTS12**$_{clock}$(du))

P	-0.012604	-0.023834	0.050263
O	1.673616	-0.113375	0.138859
O	-0.783640	1.261876	0.044380
C	2.356342	1.114465	0.227797
O	-0.823555	-1.497026	-0.036617
O	0.282507	-0.221241	-1.678625
C	-1.958700	-1.714269	0.784661
H	2.322335	1.672708	-0.721896
H	1.954793	1.762841	1.020547
H	3.406948	0.887791	0.461103
H	-1.702619	-2.161400	1.754134
H	-2.513632	-0.788056	0.970865
H	-2.608545	-2.413698	0.237267
C	-0.792632	-0.117638	-2.565494
H	-0.386104	-0.105961	-3.590539
H	-1.490230	-0.972725	-2.497209
H	-1.374279	0.805644	-2.414720
O	-0.021515	-0.153517	1.861070
C	0.733151	-1.111697	2.535725
H	0.325730	-1.228659	3.556729
H	0.718394	-2.111813	2.064395
H	1.799219	-0.834389	2.639617

$CH_3OPO(OCH_3)_2OCH_3^-$ (**4dTC2**(du))

P	-0.017921	-0.049900	0.138164
O	1.625157	-0.099762	0.588838
O	-0.674630	1.296606	0.080307
C	2.543596	0.776281	-0.033465
O	-0.850381	-1.459939	-0.246538
C	1.035015	-1.209501	-2.173862
H	1.738018	-1.764933	-1.527685
H	0.273775	-1.933842	-2.515582
O	0.473962	-0.086976	-1.564690
H	1.601297	-0.878415	-3.063054
H	3.352572	0.953100	0.692872
H	2.987715	0.355435	-0.946769
H	2.085948	1.739256	-0.289833
C	-1.889940	-2.036855	0.515477
H	-2.590270	-1.288075	0.904499
H	-2.436260	-2.705091	-0.169273
H	-1.515600	-2.626628	1.362051
O	-0.323086	-0.496996	1.817562
C	-0.062449	0.423585	2.833316
H	-0.538827	0.055287	3.758489
H	1.017722	0.536275	3.037982
H	-0.471348	1.419898	2.606268

$CH_3OPO(OCH_3)_2OCH_3^-$ ‡ (**4dTS12**$_{count,1}$(du))

P	-0.033488	0.112469	0.060356
O	1.383420	1.164881	-0.080360
O	-1.029790	1.235268	0.063526
C	2.466396	1.258612	0.779678
O	-1.261064	-1.230060	0.116603
O	0.553595	-0.620612	-1.320261
C	-2.472109	-1.001059	0.765071
H	2.194865	1.566875	1.807894
H	3.059354	0.327451	0.872841
H	3.144795	2.032999	0.378654
H	-3.063494	-1.934733	0.730705
H	-2.360929	-0.724429	1.831782
H	-3.061708	-0.197063	0.297616
C	-0.279248	-1.204879	-2.303749
H	0.295898	-1.192026	-3.242485
H	-0.546104	-2.241863	-2.061805
H	-1.207363	-0.641788	-2.455433
O	0.659476	-0.518647	1.453224
C	0.691544	-1.880719	1.806916
H	1.447644	-1.975895	2.602200
H	-0.268996	-2.250174	2.187107
H	0.991556	-2.522738	0.968302

$CH_3OPO(OCH_3)_2OCH_3^-$ ‡ (**4dTS12**$_{count,2}$(du))

Not found

$CH_3OPO(OCH_3)_2OCH_3^-$ ‡ (**4dTS23**$_{clock}$(du))

P	0.074650	-0.000838	0.119096
O	1.661410	-0.519584	0.314895
O	-0.367217	1.434008	0.134802
C	2.663538	0.469142	0.275044
O	-0.853789	-1.359453	-0.157946
C	0.702397	-1.067003	-2.410179
H	1.544268	-1.630340	-1.970333
H	-0.115333	-1.789553	-2.591422
O	0.301741	0.028749	-1.647105
H	1.036276	-0.696118	-3.395835
H	3.631528	-0.047828	0.205797
H	2.558544	1.134221	-0.593734
H	2.664215	1.087996	1.187106
C	-1.389371	-2.247657	0.801694
H	-2.135253	-1.776712	1.453106
H	-1.888283	-3.041153	0.224188
H	-0.618452	-2.698627	1.435458
O	-0.072149	-0.264582	1.902003
C	-0.944834	0.537746	2.636481
H	-1.028983	0.108027	3.651645
H	-0.593689	1.578574	2.732376
H	-1.966020	0.599206	2.218448

$CH_3OPO(OCH_3)_2OCH_3^-$ ‡ (**4dTS23**$_{count}$(du))

P	-0.022156	0.055089	-0.022576
O	1.474704	-0.052632	0.030921
O	-0.727482	1.586050	-0.126825
C	-0.602959	2.572559	0.876896
O	-1.017822	-1.290780	0.019507
C	-1.033247	-2.307492	-0.959528
O	-0.265349	0.015590	-1.772969
H	-1.657714	-2.045927	-1.823125
H	-0.028267	-2.551068	-1.324675
H	-1.454940	-3.200409	-0.470524
H	-1.287095	2.409628	1.719661
H	0.416863	2.638506	1.276661
H	-0.854667	3.531621	0.397308
C	0.553646	0.793107	-2.592808
H	0.411322	0.459388	-3.635454
H	0.299614	1.868605	-2.551112
H	1.618247	0.687070	-2.335334
O	-0.277199	0.130408	1.744950
C	-1.057534	-0.681907	2.551558
H	-0.968091	-0.311362	3.589993
H	-2.135470	-0.676565	2.297397
H	-0.738499	-1.741221	2.556475

$CH_3O^-...PO(OCH_3)_2OCH_3$ (**4dRC**(ud))

P	0.053569	-0.001795	-0.001076
O	1.158607	1.163768	-0.085423
O	-0.793265	0.285511	-1.321636
O	-0.793314	0.475018	1.263714
O	0.674122	-1.338777	0.096796
C	-1.884392	-0.579192	-1.760653
C	0.807041	2.546656	-0.177599
H	0.222512	2.744963	-1.081720
H	0.235798	2.866903	0.699667
H	1.748535	3.102613	-0.222682
H	-2.034472	-0.333192	-2.816123
H	-1.576445	-1.626943	-1.678140
H	-2.803777	-0.375209	-1.177243
C	-1.885023	-0.312647	1.827924
H	-1.577595	-1.360920	1.905859
H	-2.035791	0.090807	2.833781
H	-2.804405	-0.199161	1.220351
O	-4.424224	0.012666	0.000233
C	-5.280711	-1.016582	0.068403
H	-6.379779	-0.735282	0.055305
H	-5.203425	-1.778219	-0.775487
H	-5.196030	-1.666919	1.000096

$CH_3O^-...PO(OCH_3)_2OCH_3$ ‡ (**4d-preTS**(ud))

P	0.414664	-0.172341	0.220792
O	2.079880	0.032240	0.185296
O	0.203712	0.490730	-1.240779
O	0.178056	0.946704	1.368680
O	0.275578	-1.624219	0.474178
C	-0.793232	0.084523	-2.180282
C	2.708602	1.279112	-0.003699
H	2.472665	1.720063	-0.983594
H	2.437145	2.004683	0.777053
H	3.793032	1.109215	0.045427
H	-0.394688	0.367028	-3.165806
H	-0.950669	-0.997525	-2.151268
H	-1.740444	0.580972	-1.965835
C	-0.662635	0.730442	2.505502
H	-0.276675	-0.095982	3.118279
H	-0.619286	1.658635	3.089800
H	-1.675368	0.513425	2.153576
O	-2.069283	0.017599	0.201578
C	-2.890792	-1.060402	0.169612
H	-3.800967	-0.951737	0.825244
H	-3.324624	-1.288093	-0.851500
H	-2.416148	-2.018453	0.489686

$CH_3OPO(OCH_3)_2OCH_3^{-\ddagger}$ (**4dTC1**(ud))

P	0.031284	-0.076485	0.018330
O	1.771991	0.077379	-0.067379
O	0.035315	0.528289	-1.547570
O	0.057032	1.166457	1.143401
O	0.078419	-1.532481	0.378631
C	-1.074136	0.889619	-2.337748
C	2.476314	1.245547	-0.356941
H	2.255035	1.650506	-1.360444
H	2.301704	2.053408	0.375993
H	3.552417	1.002370	-0.329165
H	-0.658730	1.220695	-3.302657
H	-1.760685	0.055454	-2.527681
H	-1.654012	1.713289	-1.903451
C	-0.890500	1.308775	2.178368
H	-1.153223	0.348989	2.641307
H	-0.418513	1.942297	2.945458
H	-1.816882	1.789344	1.838478
O	-1.779821	0.072026	0.030742
C	-2.573666	-1.071858	0.048331
H	-3.626852	-0.756267	-0.073338
H	-2.343548	-1.788481	-0.758983
H	-2.497021	-1.642337	0.989882

$CH_3OPO(OCH_3)_2...OCH_3^{-\ddagger}$ (**4d-postTS**(ud))

P	-0.177359	-0.077846	0.062930
O	0.112602	0.550132	-1.408395
O	0.120389	-1.510815	0.265789
C	-0.312708	1.860991	-1.750833
O	-0.124730	1.053786	1.209812
C	3.010423	1.209080	-0.333006
H	2.802449	1.443832	-1.416306
H	2.847416	2.203249	0.194537
O	2.332108	0.157999	0.170682
H	4.128056	1.074956	-0.297706
H	0.035087	2.042000	-2.773748
H	-1.406292	1.958475	-1.715468
H	0.132871	2.612586	-1.090492
C	0.748501	0.934838	2.346189
H	1.723367	0.571180	1.991972
H	0.820357	1.939651	2.777915
H	0.300354	0.257258	3.086317
O	-1.868032	0.052653	0.004456
C	-2.556108	-0.897782	-0.781824
H	-3.627245	-0.664112	-0.716552
H	-2.261562	-0.863355	-1.842621
H	-2.389440	-1.920872	-0.420046

$CH_3OPO(OCH_3)_2OCH_3^{-\ddagger}$ (**4dTS12**$_{count}$(ud))

P	-0.018810	0.063998	0.042087
O	1.592426	0.455755	0.353769
O	-0.947153	1.222329	-0.141906
C	2.514325	-0.516833	0.766867
O	-0.401780	-1.560178	-0.061879
C	0.553392	-1.184299	-2.480994
H	1.322832	-1.905881	-2.140853
H	-0.384176	-1.760336	-2.601903
O	0.421485	-0.058270	-1.682698
H	0.858106	-0.846450	-3.488214
H	3.416498	0.008232	1.113812
H	2.133855	-1.130522	1.596834
H	2.811961	-1.187002	-0.056868
C	-1.254890	-2.277907	0.807205
H	-2.159612	-1.715130	1.063213
H	-1.546060	-3.189385	0.261491
H	-0.755875	-2.563273	1.741191
O	-0.247542	-0.150430	1.821265
C	-0.332375	0.987044	2.623673
H	-0.547434	0.665386	3.658605
H	0.607299	1.570799	2.649001
H	-1.130804	1.670721	2.297443

$CH_3OPO(OCH_3)_2OCH_3^{-\ddagger}$ (**4dTS23**$_{count}$(ud))

Not found

$CH_3O^-...PO(OCH_3)_2OCH_3$ (**4dRC**(dd))

P	1.035451	-0.635594	2.080866
O	-0.501788	-1.009053	1.882216
O	1.444970	0.490830	1.028457
O	1.747385	-1.923272	1.436093
O	1.466266	-0.402738	3.475471
C	0.988104	1.872107	1.103064
C	-1.596043	-0.121723	2.254374
H	-1.364666	0.380163	3.200730
H	-1.788565	0.602302	1.439011
H	-2.459470	-0.776335	2.407096
H	1.719839	2.448778	0.528995
H	-0.021189	1.962834	0.656106
H	1.007878	2.216526	2.143328
C	1.497069	-2.314385	0.079803
H	0.429517	-2.481475	-0.091840
H	1.857393	-1.552730	-0.618664
H	2.045838	-3.247522	-0.077928
O	-1.897922	1.886400	-0.144629
C	-1.936697	1.273303	-1.338119
H	-2.233762	0.174770	-1.316334
H	-0.954246	1.255385	-1.912495
H	-2.662070	1.718151	-2.087976

$CH_3O^-...PO(OCH_3)_2OCH_3^{\ddagger}$ (**4d-preTS**(dd))

P	0.020977	0.050409	0.004422
O	-1.663824	-0.098844	-0.009110
O	0.205341	-0.726824	-1.414460
O	0.205949	-0.977543	1.253770
O	0.195667	1.512936	0.141701
C	0.952538	-0.100587	-2.461608
C	-2.327911	-1.335151	-0.123895
H	-2.092643	-1.850304	-1.067658
H	-2.091476	-2.015817	0.708090
H	-3.408088	-1.132618	-0.104288
H	1.139701	-0.874913	-3.214485
H	0.362873	0.707650	-2.917444
H	1.891299	0.288112	-2.056342
C	0.950978	-0.556796	2.400338
H	0.359496	0.150985	2.998637
H	1.139030	-1.457875	2.995464
H	1.889500	-0.097766	2.076354
O	2.426395	-0.090778	-0.008455
C	3.046883	-1.295631	-0.120520
H	2.827277	-1.865083	-1.065657
H	4.165028	-1.206656	-0.104024
H	2.814697	-2.035311	0.694662

$CH_3OPO(OCH_3)_2OCH_3^{-\ddagger}$ (**4dTC1**(dd))

P	-0.039925	0.044427	0.004117
O	-1.787675	-0.139159	-0.008557
O	-0.053192	-0.695929	-1.518397
O	-0.045873	-0.965370	1.362932
O	-0.017927	1.529440	0.143004
C	0.590154	-0.032589	-2.587351
C	-2.450533	-1.362701	-0.120725
H	-2.229059	-1.890460	-1.065921
H	-2.226268	-2.054785	0.710959
H	-3.535496	-1.164225	-0.100691
H	0.636202	-0.738382	-3.429192
H	0.016625	0.852545	-2.904443
H	1.604611	0.291458	-2.329369
C	0.604608	-0.513046	2.532898
H	0.036927	0.301241	3.009908
H	0.649596	-1.362038	3.230131
H	1.619945	-0.151793	2.334714
O	1.784858	-0.121427	-0.015975
C	2.405218	-1.363571	-0.133866
H	2.170419	-1.890327	-1.078309
H	3.499364	-1.213443	-0.108816
H	2.153745	-2.065563	0.683568

$CH_3O^-...PO(OCH_3)_2OH$ (**4eRC**(ud))

P	-0.069475	-0.000836	-0.001029
O	0.728765	0.379688	1.328653
O	0.733782	0.586055	-1.250148
O	-1.292081	1.054390	0.080122
O	-0.548903	-1.393125	-0.112419
C	1.875440	-0.116794	-1.836854
H	-0.951755	1.956754	0.145283
C	1.862040	-0.413068	1.806999
H	1.590850	-1.473842	1.797710
H	2.769353	-0.221396	1.200568
H	2.014983	-0.089502	2.840595
H	1.607292	-1.165210	-2.003746
H	2.039559	0.371102	-2.801880
H	2.775403	-0.025871	-1.197081
O	4.408370	0.078205	0.022711
C	5.199450	-1.002568	-0.057724
H	5.074511	-1.767737	0.776719
H	5.075431	-1.635242	-0.996726
H	6.313866	-0.790686	-0.041284

$CH_3O^-...PO(OCH_3)_2OH$ (**4eRC**(dd))

P	0.051198	-0.005197	0.000866
O	1.282520	1.042636	-0.027194
O	-0.744649	0.520677	1.281947
O	0.519858	-1.405133	0.037065
O	-0.747636	0.452003	-1.304105
C	-1.901249	-0.195691	1.823174
C	-1.896473	-0.299816	-1.813484
H	-2.053220	0.079696	-2.827241
H	-1.640333	-1.363312	-1.862420
H	-2.798015	-0.133626	-1.191622
H	-2.058883	0.234840	2.816193
H	-2.799083	-0.054507	1.190638
H	-1.654158	-1.257514	1.926082
H	0.949264	1.949785	-0.046321
O	-4.432857	0.008046	-0.007830
C	-5.178548	1.122230	-0.077637
H	-5.017163	1.874363	0.760532
H	-6.300733	0.955538	-0.057464
H	-5.031342	1.752913	-1.013089

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS12**$_{clock}$**-alt**)

P	-0.016107	0.028191	-0.098841
O	1.480016	0.021915	-0.157153
O	-0.342598	1.739062	-0.253597
C	0.715571	2.650128	-0.292500
O	-1.000895	0.091187	1.229065
O	-0.194025	-1.849891	0.277403
C	0.662392	-2.749383	-0.347395
H	0.281764	3.658071	-0.402879
H	1.327571	2.645003	0.625918
H	1.406459	2.479294	-1.134126
H	0.461923	-3.768710	0.031498
H	0.524954	-2.781994	-1.446903
H	1.725600	-2.520641	-0.165728
H	-1.012089	-0.842998	1.507726
O	-0.799501	-0.251201	-1.545127
C	-2.172075	-0.567568	-1.576688
H	-2.795975	0.266510	-1.219061
H	-2.399473	-1.461152	-0.978787
H	-2.435291	-0.770543	-2.624096

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS12**$_{count}$**-alt**)

P	0.103789	0.014551	0.025832
O	1.573622	-0.230846	0.139526
O	0.144578	1.759589	0.104071
C	-0.269840	2.632135	-0.894395
O	-0.996151	0.086248	1.255047
O	-0.391134	-1.867263	0.153595
C	0.483009	-2.825819	-0.345383
H	-0.079389	3.659351	-0.540654
H	0.274835	2.505003	-1.847388
H	-1.349859	2.568570	-1.130546
H	0.080163	-3.834815	-0.134877
H	0.618576	-2.760099	-1.444653
H	1.490710	-2.759763	0.096323
H	-1.127198	-0.863765	1.439246
O	-0.553917	0.026590	-1.506797
C	-1.845671	-0.458724	-1.801663
H	-2.612913	-0.028093	-1.141254
H	-1.901928	-1.550124	-1.719760
H	-2.071768	-0.154780	-2.833754

$CH_3OPO(OCH_3)_2OH^-$ (**4eTC2**-alt)

P	0.027572	0.024117	-0.201517
O	1.520146	-0.045087	-0.306747
O	-0.240044	1.714898	-0.545275
C	0.494028	2.655631	0.189533
O	-0.848429	0.239020	1.190792
O	-0.212578	-1.805970	0.321036
C	0.605772	-2.776430	-0.247782
H	0.306787	3.651063	-0.243992
H	0.197252	2.695354	1.253571
H	1.576181	2.457900	0.149703
H	0.391908	-3.754178	0.221962
H	0.435970	-2.898086	-1.336347
H	1.678004	-2.558374	-0.114874
H	-0.831437	-0.657021	1.573280
O	-0.842971	-0.312576	-1.576164
C	-2.223323	-0.590408	-1.504961
H	-2.798415	0.275906	-1.143482
H	-2.432317	-1.451432	-0.855446
H	-2.558517	-0.826937	-2.524053

$CH_3OPO(OCH_3)_2OH^{-\ddagger}$ (**4eTS1**-rot(Nu))

P	-0.037552	0.016950	-0.081244
O	1.455208	0.123546	0.060539
O	-0.925890	1.421912	-0.302301
C	-1.966936	1.846285	0.549575
O	-0.466424	-0.089172	1.621145
C	0.432350	0.403013	2.572189
O	-0.965608	-1.346579	-0.226085
O	-0.042718	-0.099467	-1.937622
C	0.865532	0.644596	-2.687952
H	-0.050276	0.320909	3.561039
H	1.376054	-0.161892	2.595362
H	0.706038	1.462180	2.419813
H	0.839081	0.291363	-3.734251
H	0.622175	1.725735	-2.704398
H	1.896964	0.545584	-2.315924
H	-0.946781	-1.491387	-1.187399
H	-1.607410	2.222993	1.516895
H	-2.696459	1.051154	0.750060
H	-2.480449	2.667253	0.026935

$CH_3OPO(OCH_3)_2OH^{-}$ (**4eTC3**-alt)

O	-0.761617	-0.406395	-1.222854
P	-0.015041	-0.046107	0.033868
O	1.557349	0.332072	-0.659972
C	2.106749	-0.561606	-1.584145
O	0.790163	-1.142484	0.991826
O	-1.366963	-0.382035	1.227888
C	-2.661467	0.036361	0.922932
H	2.978359	-0.078280	-2.057154
H	2.462614	-1.495822	-1.111452
H	1.389423	-0.836034	-2.372220
H	-3.352988	-0.377700	1.676775
H	-2.768956	1.137582	0.949386
H	-2.987426	-0.305510	-0.071943
H	0.083757	-1.483974	1.563745
O	-0.075552	1.511228	0.630999
C	0.445973	2.619745	-0.077877
H	0.224826	2.571170	-1.151323
H	1.532588	2.715289	0.043114
H	-0.041389	3.512658	0.341809