DFT Study of the Mechanism of Nucleophilic Displacements on Chloro-substituted Methylphosphonates: P-O *vs.* P-C Bond Cleavage.

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Supporting Infromation

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Table S1: Calculated absolute energies and no. of imaginary frequencies at B3LYP/6-31+G(d)

Compound	**B3LYP/6-31+G(d) (water)**	**ZPVE (water)**	**G (water)**	N_{imag}
OH^-	-75.93487755	5.11101	-75.943010	0
OMe^-	-115.22926539	23.23214	-115.213489	0
MeOH	-115.73596633	31.67146	-115.708310	0
Dimethyl phosphate	-722.78802216	65.33770	-722.718257	0
Dimethyl phosphate anion	-722.34148354	58.88539	-722.281636	0
DMMP (**1**)	-686.84984671	80.76137	-686.756257	0
Methyl methylphosphonate	-647.55658082	61.71999	647.490848	0
Methyl methylphosphonate anion	-647.10462207	55.45365	-647.047847	0
CH_3^-	-39.93952410	18.18292	-39.928647	0
CH_4	-40.52077932	28.19478	-40.493124	0
1-INT1	-762.77112128	88.62670	-762.665559	0
1-INT2	-762.78262101	88.38048	-762.677535	0
1-INT3	-762.78888527	88.38438	-762.683813	0
1-INT4	-762.77158939	88.69360	-762.665606	0
1-TS1	-762.75588350	87.41132	-762.652777	1
1-TS2	-762.76903571	87.43800	-762.666551	1
1-TS3	-762.78454559	87.55746	-762.681427	1
1-TS4	-762.76854374	86.71091	-762.666711	1
1-TS5	-762.71145951	84.87081	-762.613717	1
1-TS6	-762.75792919	88.24757	-762.652986	1
1-TS7	-762.76598219	88.46742	-762.659716	1
1-TS8	-762.73159851	85.75860	-762.632205	1
1-TS9	-762.77576614	88.02086	-762.670839	1
Cl-DMMP (**2**)	-1146.43539061	75.29429	-1146.353580	0

Methyl chloromethylphosphonate	-1107.14151024	56.32295	-1107.086999	0
Methyl chloromethylphosphonate anion	-1106.69545671	49.96710	-1106.615829	0
CH_2Cl^-	-499.56286517	14.05470	-499.564161	0
CH_3Cl	-500.11493601	23.80562	-500.100691	0
2-INT1	-1222.37381760	83.61435	-1222.278301	0
2-INT2	-1222.37789651	83.25335	-1222.283494	0
2-INT3	-1222.38274578	83.26070	-1222.288525	0
2-INT4	-1222.37435772	83.41524	-1222.279168	0
2-TS1	-1222.35217307	82.08258	-1222.259652	1
2-TS2	-1222.36048137	81.82694	-1222.269498	1
2-TS3	-1222.33797337	80.60325	-1222.249604	1
2-TS4	-1222.36195423	81.07169	-1222.271540	1
2-TS5	-1222.37589272	82.20425	-1222.283963	1
2-TS6	-1222.35618841	83.34010	-1222.260920	1
2-TS7	-1222.36053479	83.35631	-1222.264890	1
2-TS8	-1222.34870925	81.94610	-1222.257117	1
2-TS9	-1222.37285113	82.30615	-1222.280402	1
Cl_2-DMMP (**3**)	-1606.01930402	69.30551	-1605.948767	0
Methyl dichloromethylphosphonate	-1566.72515140	50.23190	-1566.645102	0
Methyl dichloromethylphosphonate anion	-1566.72515140	50.23190	-1566.682770	0
$CHCl_2^-$	-959.18154548	9.00197	-959.194425	0
CH_2Cl_2	-959.70540582	18.41345	-959.702911	0
3-INT1	-1681.96811558	75.50447	-1681.884704	0
3-INT2	-1681.96489288	77.00254	-1681.882733	0
3-INT3	-1681.97082701	77.25133	-1681.888240	0
3-INT4	-1681.97051846	77.29166	-1681.887429	0
3-TS1	-1681.94127070	75.86263	-1681.860915	1
3-TS2	-1681.94744353	75.93452	-1681.868080	1

3-TS3	-1681.95120905	75.80655	-1681.872449	1
3-TS4	-1681.94828660	75.24629	-1681.869482	1
3-TS5	-1681.96397047	76.08573	-1681.883889	1
3-TS6	-1681.9496635	77.20100	-1681.865840	1
3-TS7	-1681.94854251	77.46130	-1681.862232	1
3-TS8	-1681.95508476	76.16405	-1681.875658	1
3-TS9	-1681.96302091	76.01315	-1681.882370	1
Cl_3-DMMP (**4**)	-2065.59340195	62.65495	-2065.536073	0
Methyl trichloromethylphosphonate	-2026.30143033	43.82528	-2026.270756	0
Methyl trichloromethylphosphonate anion	-2025.86599379	37.67679	-2025.844100	0
CCl_3^-	-1418.79037222	2.97857	-1418.814436	0
$CHCl_3$	-1419.28974044	12.23275	-1419.298454	0
4-INT1	-2141.55482932	70.85084	-2141.483609	0
4-INT2	-2141.55603742	70.59953	-2141.485773	0
4-TS1	-2141.52062524	69.24139	-2141.452508	1
4-TS2	-2141.52681095	70.9673	-2141.413716	1
4-TS3	-2141.55189909	69.62245	-2141.484582	1
4-TS4	-2141.55519933	69.98826	-2141.486544	1
4-TS5	-2141.5443587	69.12261	-2141.476263	1

* ZPVE in kcal/mol, all other energies are in Hartrees.

Table S2: Calculated absolute energies and no. of imaginary frequencies at MP2/6-31+G(d)//B3LYP/6-31+G(d)

Compound	**MP2/6-31+G(d) (water)**	**ZPVE (water)**	**G (water)**	N_{imag}
OH^-	-75.72765861	5.17210	-75.735694	0
DMMP (**1**)	-685.29606785	82.44342	-685.199178	0
1-TS1	-760.99668262	88.73110	-760.890274	1
1-TS2	-761.01142993	88.77459	-760.905660	1
1-INT1	-760.01422674	90.19378	-760.904138	0
1-TS3	-760.94603380	86.16836	-760.849401	1
2	-1144.31689588	76.83567	-1144.231844	0
2-TS1	-1220.02915780	83.23564	-1219.933650	1
2-TS2	-1220.03689130	83.12574	-1219.942520	1
3[(a)]	-1595.49116362[(a)]	70.09487[(a)]	-1595.419587[(a)]	0
3-TS1[(a)]	-1670.77119866[(a)]	76.01877[(a)]	-1670.688573[(a)]	1
3-TS2[(a)]	-1670.77819169[(a)]	76.11674[(a)]	-1670.694126[(a)]	1
4[(b)]	-2052.43477025[(b)]	63.43035[(b)]	-2052.370060[(b)]	0
4-TS1[(a)]	-2127.72117764[(b)]	69.42526[(b)]	-2127.648999[b)]	1
4-TS2[(a)]	-2127.72946427[(b)]	71.13618[(b)]	-2127.653795[(b)]	1

* ZPVE in kcal/mol, all other energies are in Hartrees. [(a)] Calculated at MP2/6-31G*//B3LYP/6-31+G(d). [(b)] Calculated at MP2/3-21G*//B3LYP/6-31+G(d).

Table S3: Calculated absolute energies and no. of imaginary frequencies at B3LYP/6-31+G(d) for **4** in Et_2O

Compound	**B3LYP/6-31+G(d) (Et_2O)**	**ZPVE (Et_2O)**	**G (Et_2O)**	N_{imag}
OH^-	-75.90297885	5.19608	-75.910971	0
OMe^-	-115.20030774	22.90586	-115.185038	0
MeOH	-115.73205662	31.90295	-115.703996	0
Dimethyl phosphate	-722.77948357	65.89748	-722.708691	0
Dimethyl phosphate anion	-722.31332613	58.85818	-722.253537	0
Cl_3-DMMP (**4**)	-2065.59051179	62.92349	-2065.531934	0
Methyl trichloromethylphosphonate	-2026.29317155	44.46642	-2026.261315	0
Methyl trichloromethylphosphonate anion	-2025.84166701	37.55530	-2025.818779	0
CCl_3^-	-1418.771364	2.98376	-1418.795601	0
$CHCl_3$	-1419.2872371	12.33963	-1419.296361	0
4-INT1	-2141.53274508	70.74508	-2141.462622	0
4-INT2	-2141.52735422	70.84452	-2141.456924	0
4-TS1	-2141.50174858	71.22839	-2141.428469	1
4-TS2	-2141.49311512	69.47817	-2141.424234	1
4-TS3	-2141.52447490	70.02543	-2141.455745	1
4-TS4	-2141.53208654	70.29216	-2141.462930	1
4-TS5	-2141.52284465	69.33417	-2141.454387	1

* ZPVE in kcal/mol, all other energies are in Hartrees.

Table S4. Calculated relative free energies and selected bond lengths and angle for the species involved in the reaction of **4** with OH^- in Et_2O.

	ΔG (kcal/mol)[a]	Bond Length P-apical ligand (Å)	∠ L_{ap}-P-L_{ap} (°)
4-S.M.	0.0		
4-TS1	11.7	2.853 (P-O), 1.926 (P-C)	169.2
4-TS2	9.1	1.693 (P-OH)[b], 1.703 (P-OMe)[b], 1.990 (P-C)[b]	142.5
4-TS3	-8.1	2.410 (P-C), 1.692 (P-OH)	174.8
4-TS4	-12.5	1.676 (P-OMe), 2.388 (P-C)	163.3
4-TS5	-7.1	2.257 (P-OMe), 1.954 (P-C)	162.8
4-INT1	-8.8	1.721 (P-OH), 2.090 (P-C)	172.8
4-INT2	-12.3	1.699 (P-OMe), 2.149 (P-C)	168.3
4-PR1a	-38.5		
4-PR1	-67.1		
4-PR2	-50.2		

[a] All energies are relative to the starting materials which were determined as 0.0 kcal/mol. [b] Square pyramid geometry.

Optimized geometries

OH^-

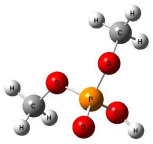
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.108615
2	1	0	0.000000	0.000000	-0.868918

OMe^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.812719
2	6	0	0.000000	0.000000	-0.573265
3	1	0	0.000000	1.024235	-1.020721
4	1	0	0.887013	-0.512117	-1.020721
5	1	0	-0.887013	-0.512117	-1.020721

MeOH

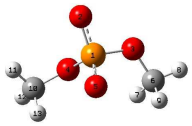
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1	6	0	-0.672416	-0.021457	0.000020
2	1	0	-1.091914	0.988067	-0.001322
3	1	0	-1.025827	-0.550703	0.895482
4	1	0	-1.025307	-0.552700	-0.894479
5	8	0	0.750490	0.125774	0.000032
6	1	0	1.173621	-0.762117	-0.000057



Dimethyl phosphate

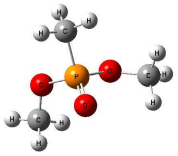
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1	15	0	-0.023176	0.464758	-0.082304
2	8	0	-0.511274	1.691014	-0.774125
3	8	0	1.463429	0.096142	-0.543073
4	8	0	-0.807637	-0.902088	-0.370024
5	8	0	-0.045902	0.523149	1.525357
6	1	0	0.135950	1.438276	1.883102
7	6	0	2.190143	-1.025946	0.019948
8	1	0	1.686886	-1.962039	-0.235513
9	1	0	3.181067	-0.993772	-0.434562
10	1	0	2.269698	-0.916898	1.104988

11	6	0	-2.204861	-1.053831	-0.015856
12	1	0	-2.809640	-0.300637	-0.529298
13	1	0	-2.488842	-2.051940	-0.351329
14	1	0	-2.328100	-0.971445	1.067539



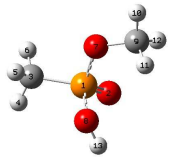
Dimethyl phosphate anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.017534	0.506889	0.062885
2	8	0	-0.388325	1.799684	-0.636113
3	8	0	1.462731	0.096303	-0.518557
4	8	0	-0.878505	-0.753475	-0.573437
5	8	0	-0.056521	0.434090	1.576525
6	6	0	2.132128	-1.068521	-0.009323
7	1	0	1.571542	-1.975457	-0.261843
8	1	0	3.113418	-1.098847	-0.489216
9	1	0	2.254497	-1.001304	1.076867
10	6	0	-2.176343	-1.051407	-0.041351
11	1	0	-2.876591	-0.226490	-0.224374
12	1	0	-2.531009	-1.944446	-0.562196
13	1	0	-2.118596	-1.250038	1.034185



1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.003995	0.371111	0.164938
2	8	0	0.125951	0.238919	1.653715
3	6	0	0.436671	1.988690	-0.510719
4	1	0	1.480576	2.210612	-0.265265
5	1	0	0.309779	1.995146	-1.597098
6	1	0	-0.202898	2.754896	-0.061356
7	8	0	-1.468737	0.143459	-0.450582
8	8	0	0.869615	-0.733200	-0.652390
9	6	0	2.132971	-1.219139	-0.142670
10	1	0	2.016191	-1.588066	0.879442
11	1	0	2.429743	-2.033635	-0.805359
12	1	0	2.888113	-0.426308	-0.172608
13	6	0	-2.224613	-1.048827	-0.126795
14	1	0	-3.187074	-0.937548	-0.627958
15	1	0	-1.707553	-1.936393	-0.503121
16	1	0	-2.371614	-1.123143	0.954418



Methyl methylphosphonate

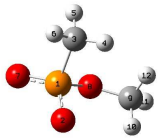
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3	6	0	1.689830	1.113736	-0.127879
4	1	0	2.655551	0.601055	-0.074224
5	1	0	1.589274	1.595662	-1.104793
6	1	0	1.640770	1.871075	0.660615
7	8	0	-0.939030	0.809069	-0.121790
8	8	0	0.395375	-1.057529	-1.196553
9	6	0	-2.258806	0.223347	-0.020515
10	1	0	-2.962842	1.037548	-0.197862
11	1	0	-2.387574	-0.553029	-0.780768
12	1	0	-2.413676	-0.193781	0.978771
13	1	0	0.662230	-1.993465	-0.980820

CH_3^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.128864
2	1	0	0.000000	1.035188	-0.257728
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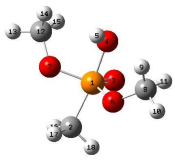
CH_4

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3	1	0	-0.631684	-0.631684	0.631684
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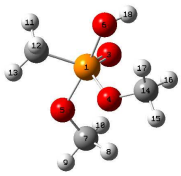
Methyl methylphosphonate anion

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3	6	0	-0.754000	1.651765	-0.047407
4	1	0	0.005128	2.199061	0.521673
5	1	0	-0.734406	1.988684	-1.089114
6	1	0	-1.736025	1.885457	0.378571
7	8	0	-1.457881	-0.882652	-0.866851
8	8	0	1.003840	-0.353678	-0.694360
9	6	0	2.201558	0.070255	-0.031680
10	1	0	2.274842	-0.373698	0.967123
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12	1	0	2.241388	1.164082	0.053039



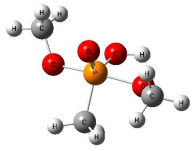
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3	8	0	0.007526	0.443437	1.725790
4	8	0	-0.002358	-1.508938	0.284707
5	1	0	-0.003352	-1.919939	-0.606020
6	8	0	1.527060	0.169260	-0.617080
7	8	0	-1.530956	0.174611	-0.607580
8	6	0	2.523242	-0.802984	-0.300211
9	1	0	2.339541	-1.762674	-0.798564
10	1	0	3.477475	-0.396583	-0.657127
11	1	0	2.589682	-0.978453	0.779564
12	6	0	-2.525944	-0.801363	-0.299313
13	1	0	-3.480789	-0.391638	-0.650814
14	1	0	-2.342626	-1.755551	-0.808309
15	1	0	-2.590974	-0.988468	0.778534
16	1	0	-0.890392	2.560113	0.025283
17	1	0	-0.000965	2.160693	-1.462584
18	1	0	0.894897	2.557919	0.021939



1-INT2

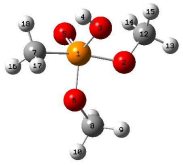
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.089122	-0.398070	0.131690
2	6	0	0.174308	-1.898446	-0.953958
3	8	0	-0.224416	-0.372399	1.643717
4	8	0	0.374908	1.054356	-0.665057
5	8	0	-1.606988	-0.234741	-0.431614
6	8	0	1.861667	-0.664978	0.374013
7	6	0	-2.400977	0.807994	0.099246
8	1	0	-1.973390	1.797726	-0.122343
9	1	0	-3.395281	0.747546	-0.364525
10	1	0	-2.514737	0.715865	1.189159
11	1	0	0.387843	-2.763595	-0.317337
12	1	0	1.013029	-1.786902	-1.647103
13	1	0	-0.753185	-2.060752	-1.503045
14	6	0	1.459377	1.919066	-0.330520
15	1	0	1.266383	2.861263	-0.854985
16	1	0	1.498923	2.118851	0.747854
17	1	0	2.420073	1.504500	-0.649668
18	1	0	2.075885	-0.393032	1.289569



1-INT3

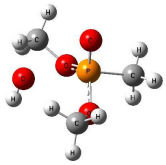
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.043811	0.053532	-0.011846
2	6	0	0.397050	1.845395	0.071192
3	8	0	0.035641	-0.741892	-1.320328
4	8	0	-0.441245	-0.690936	1.432044
5	1	0	0.371801	-1.110696	1.790160
6	8	0	-1.741613	0.562407	-0.112266
7	8	0	1.697872	-0.329666	0.550449
8	6	0	-2.747417	-0.422833	-0.261214
9	1	0	-2.842063	-1.051082	0.636857
10	1	0	-3.702690	0.092549	-0.426921
11	1	0	-2.547416	-1.074867	-1.124048
12	6	0	2.744177	-0.354034	-0.390408
13	1	0	3.679766	-0.594966	0.134404

14	1	0	2.574391	-1.106372	-1.174498
15	1	0	2.887084	0.620704	-0.891325
16	1	0	1.379749	2.016131	-0.373454
17	1	0	0.443401	2.141153	1.124905
18	1	0	-0.354960	2.453994	-0.435009



1-INT4

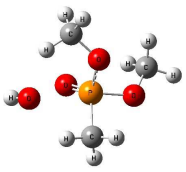
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.327130	-0.286141	0.106833
2	8	0	1.311232	0.240635	-0.306750
3	8	0	-0.027378	-1.494433	-1.090201
4	1	0	-0.798627	-2.080949	-1.213392
5	8	0	-0.071798	-0.640821	1.587730
6	8	0	-0.800925	1.297321	-0.310148
7	6	0	-2.185355	-0.684130	0.038897
8	6	0	0.001592	2.463311	-0.114424
9	1	0	0.768630	2.561633	-0.888715
10	1	0	-0.685707	3.316921	-0.165560
11	1	0	0.492918	2.455081	0.864915
12	6	0	2.411667	-0.550387	0.086453
13	1	0	3.326285	0.002279	-0.169848
14	1	0	2.405437	-0.741941	1.168661
15	1	0	2.432496	-1.518390	-0.437731
16	1	0	-2.710476	-0.068485	0.775817
17	1	0	-2.628080	-0.490311	-0.947071
18	1	0	-2.352408	-1.738107	0.299817



1-TS1

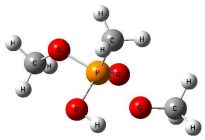
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000019	0.393397	0.173201
2	6	0	0.003544	2.206024	-0.174449
3	8	0	-0.000599	0.277194	1.683680
4	8	0	-0.001925	-1.989494	0.274164
5	1	0	0.001749	-2.296805	-0.654007
6	8	0	1.342447	0.104248	-0.736612
7	8	0	-1.344066	0.109725	-0.735358
8	6	0	2.475534	-0.642271	-0.258902
9	1	0	2.128472	-1.572720	0.193343

10	1	0	3.103006	-0.837871	-1.133421
11	1	0	3.041016	-0.039010	0.462379
12	6	0	-2.476024	-0.640244	-0.259811
13	1	0	-3.104661	-0.831573	-1.134436
14	1	0	-2.127292	-1.572638	0.187103
15	1	0	-3.040675	-0.041042	0.465453
16	1	0	0.895992	2.661876	0.268485
17	1	0	0.003180	2.408683	-1.250800
18	1	0	-0.886254	2.665707	0.269860



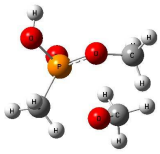
1-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.062407	-0.355567	0.104856
2	6	0	0.344203	-1.879093	-0.808957
3	8	0	-0.025679	-0.231919	1.610036
4	8	0	0.255077	0.988066	-0.765765
5	8	0	-1.681963	-0.441616	-0.330670
6	8	0	2.443316	-0.520354	0.274720
7	6	0	-2.586176	0.555682	0.151610
8	1	0	-2.314430	1.548091	-0.228968
9	1	0	-3.580443	0.288908	-0.218017
10	1	0	-2.599351	0.577382	1.247487
11	1	0	1.412568	-2.068925	-0.751773
12	1	0	0.014391	-1.758269	-1.845719
13	1	0	-0.224329	-2.700620	-0.359887
14	6	0	1.157210	2.022149	-0.343624
15	1	0	0.894745	2.904572	-0.934202
16	1	0	1.024536	2.241325	0.720721
17	1	0	2.185892	1.710119	-0.529604
18	1	0	2.705097	0.045075	1.026374



1-TS3

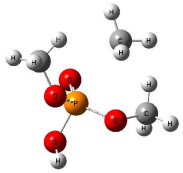
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.208708	0.111737	-0.060607
2	6	0	0.303777	1.862441	0.049712
3	8	0	0.017122	-0.646471	-1.354006
4	8	0	-0.273504	-0.739050	1.341028
5	1	0	0.690054	-0.968505	1.468733
6	8	0	-1.859270	0.495401	-0.037423
7	8	0	1.939981	-0.192449	0.608520
8	6	0	-2.819129	-0.556392	-0.138790
9	1	0	-2.786905	-1.209069	0.742420
10	1	0	-3.805900	-0.086837	-0.201030
11	1	0	-2.650618	-1.158870	-1.040151
12	6	0	2.897847	-0.429259	-0.371539
13	1	0	3.892339	-0.628506	0.073486
14	1	0	2.650503	-1.292741	-1.018980
15	1	0	3.027567	0.441260	-1.050930
16	1	0	1.253338	1.993941	-0.470265
17	1	0	0.441008	2.137435	1.099108
18	1	0	-0.470371	2.495652	-0.394528



1-TS4

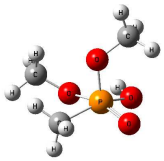
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.732901	-0.145876	0.156409
2	6	0	0.959712	-1.446773	-1.099574
3	8	0	0.267302	-0.398507	1.571136
4	8	0	0.369513	1.303250	-0.510048
5	8	0	-1.604131	-0.776872	-0.530170
6	8	0	2.381734	0.159160	0.260215
7	6	0	-2.632234	-0.603333	0.375777
8	1	0	-3.209899	0.345139	0.232395
9	1	0	-3.394879	-1.416118	0.325647
10	1	0	-2.273637	-0.582446	1.428024
11	1	0	1.366746	-2.329006	-0.593047
12	1	0	1.693058	-1.098102	-1.833109
13	1	0	0.004832	-1.689214	-1.559197
14	6	0	-0.902600	1.960614	-0.380128

15	1	0	-1.634188	1.483539	-1.032052
16	1	0	-1.255118	1.916078	0.654062
17	1	0	-0.723607	3.001336	-0.665965
18	1	0	2.568570	0.797646	0.991589



1-TS5

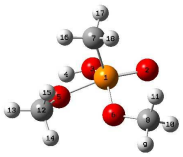
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.068142	-0.519685	0.160430
2	6	0	0.381297	2.490647	0.111872
3	8	0	-0.094559	-0.434391	1.656553
4	8	0	-0.355845	-2.125255	-0.139127
5	1	0	-0.425152	-2.321473	-1.107330
6	8	0	1.302628	-0.407040	-0.693220
7	8	0	-1.253151	0.085866	-0.772189
8	6	0	2.496858	0.210028	-0.168319
9	1	0	2.985339	-0.477295	0.531220
10	1	0	3.146785	0.384566	-1.028828
11	1	0	2.223875	1.149175	0.317391
12	6	0	-2.376926	0.753386	-0.169258
13	1	0	-2.924230	1.223467	-0.989321
14	1	0	-3.023132	0.026771	0.336486
15	1	0	-2.017098	1.510794	0.529319
16	1	0	-0.561608	3.058375	0.229752
17	1	0	0.656386	2.517405	-0.960673
18	1	0	1.161016	3.045679	0.673626



1-TS6

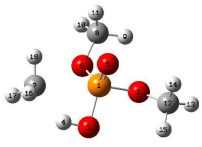
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.229818	0.490210	0.131849
2	8	0	1.386478	1.535290	0.177341
3	8	0	0.658667	-0.119216	1.676598
4	1	0	-0.045326	-0.746500	1.954589
5	8	0	-1.417124	-0.332766	0.734541
6	6	0	-2.341585	-0.942562	-0.138666
7	1	0	-2.845323	-1.760962	0.398781

8	1	0	-3.123878	-0.244658	-0.483445
9	1	0	-1.851709	-1.377354	-1.023130
10	6	0	1.782282	-1.543569	-0.661308
11	1	0	2.663378	-0.920730	-0.465035
12	1	0	1.617386	-2.210729	0.192336
13	1	0	1.954053	-2.141196	-1.561609
14	8	0	0.629217	-0.740099	-0.918320
15	6	0	-0.875584	1.505219	-0.990850
16	1	0	-1.591314	0.904735	-1.554533
17	1	0	-1.433830	2.217399	-0.372395
18	1	0	-0.239277	2.066642	-1.679634



1-TS7

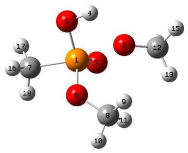
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.116525	-0.513445	-0.043919
2	8	0	-1.505288	-1.218387	-0.152361
3	8	0	0.667354	-1.788574	-0.882255
4	1	0	1.604724	-1.544673	-1.043203
5	8	0	1.499372	0.291685	-0.458100
6	8	0	-0.684118	1.077526	-0.360214
7	6	0	0.269551	-0.644889	1.755334
8	6	0	-2.045557	1.424044	-0.130004
9	1	0	-2.129279	2.496090	-0.347092
10	1	0	-2.725312	0.862088	-0.777863
11	1	0	-2.338235	1.247037	0.913668
12	6	0	1.871976	1.567017	0.023494
13	1	0	2.967250	1.640793	-0.044097
14	1	0	1.424654	2.378497	-0.565913
15	1	0	1.584895	1.721068	1.075061
16	1	0	1.256356	-0.263197	2.027416
17	1	0	0.205853	-1.703581	2.027207
18	1	0	-0.497417	-0.107479	2.324098



1-TS8

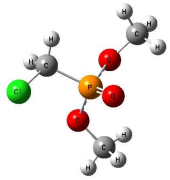
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.072223	-0.220438	0.049400
2	8	0	1.496621	0.197762	-0.394548
3	8	0	-0.192660	-1.444167	-1.023726
4	1	0	-1.184252	-1.594961	-0.819966

5	8	0	-0.001840	-0.417666	1.546742
6	8	0	-0.716177	1.152559	-0.571583
7	6	0	-2.523384	-0.908607	0.159332
8	6	0	-0.332939	2.420510	-0.005349
9	1	0	0.740013	2.595276	-0.128228
10	1	0	-0.900317	3.177429	-0.552145
11	1	0	-0.597005	2.463489	1.057190
12	6	0	2.589327	-0.559580	0.122356
13	1	0	3.505979	-0.086375	-0.243047
14	1	0	2.589343	-0.555917	1.218369
15	1	0	2.558944	-1.598301	-0.234309
16	1	0	-2.768201	-1.829111	0.718848
17	1	0	-3.221750	-0.828513	-0.694421
18	1	0	-2.724976	-0.058297	0.823596



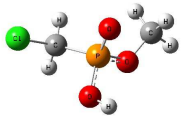
1-TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.597527	-0.201277	0.103673
2	8	0	1.383149	-0.540651	-0.586429
3	8	0	-0.775030	-1.310330	-1.121679
4	1	0	0.159786	-1.550879	-1.346263
5	8	0	-0.218663	-0.603018	1.526189
6	8	0	-0.356485	1.372216	-0.376832
7	6	0	-2.434552	0.052725	0.197390
8	6	0	0.854969	2.096066	-0.130641
9	1	0	1.633418	1.803610	-0.837627
10	1	0	0.600475	3.153809	-0.253094
11	1	0	1.212355	1.926664	0.890629
12	6	0	2.449558	-0.741734	0.292469
13	1	0	2.912890	0.210337	0.624463
14	1	0	2.145671	-1.283185	1.203857
15	1	0	3.247008	-1.328111	-0.199755
16	1	0	-2.846815	0.409758	-0.753166
17	1	0	-2.919848	-0.895904	0.452861
18	1	0	-2.665642	0.784964	0.977713



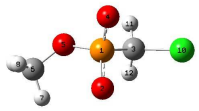
Cl-DMMP (**2**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.312839	-0.028140	0.141052
2	8	0	-0.391589	-0.118133	1.630576
3	6	0	1.142114	-0.823086	-0.631853
4	8	0	-0.235127	1.441527	-0.496785
5	8	0	-1.563813	-0.688714	-0.638550
6	6	0	-2.341766	-1.770233	-0.063761
7	1	0	-2.627072	-1.528815	0.962552
8	1	0	-3.228140	-1.862493	-0.692677
9	1	0	-1.768114	-2.701807	-0.089609
10	6	0	-1.169121	2.477985	-0.097165
11	1	0	-0.848733	3.380831	-0.617988
12	1	0	-2.183063	2.207170	-0.405427
13	1	0	-1.123870	2.630542	0.984390
14	17	0	2.703929	-0.208758	0.040638
15	1	0	1.140081	-0.639729	-1.709473
16	1	0	1.101564	-1.900147	-0.443644



Methyl chloromethylphosphonate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.401756	0.363409	0.103819
2	8	0	-0.491766	0.427964	1.594442
3	6	0	0.870762	-0.773368	-0.559140
4	8	0	-0.041286	1.716697	-0.675889
5	8	0	-1.754846	-0.127699	-0.632232
6	6	0	-2.675772	-1.046352	0.009347
7	1	0	-2.951275	-0.677225	0.999862
8	1	0	-3.552546	-1.084773	-0.638356
9	1	0	-2.227806	-2.042104	0.086669
10	17	0	2.524338	-0.404518	0.074771
11	1	0	0.903287	-0.703266	-1.649583
12	1	0	0.626940	-1.798643	-0.266041
13	1	0	-0.552761	2.514319	-0.352767



Methyl chloromethylphosphonate anion

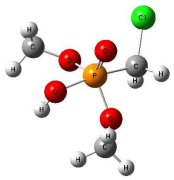
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.388361	0.392015	0.016032
2	8	0	-0.580299	0.522090	1.517789
3	6	0	0.924123	-0.862459	-0.353926
4	8	0	-0.150698	1.640165	-0.815765
5	8	0	-1.639291	-0.469253	-0.652744
6	6	0	-2.847852	-0.725830	0.078265
7	1	0	-2.628650	-1.088114	1.087001
8	1	0	-3.459607	0.181346	0.145632
9	1	0	-3.393866	-1.489347	-0.481837
10	17	0	2.594780	-0.271960	0.086057
11	1	0	0.947018	-1.102247	-1.419420
12	1	0	0.753943	-1.772828	0.224910

CH_2Cl^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.337717	-0.000001	-0.174034
2	17	0	-0.654992	0.000000	0.006021
3	1	0	1.554283	-0.872027	0.470928
4	1	0	1.554272	0.872036	0.470922

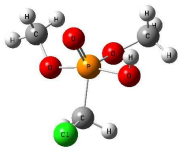
CH_3Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000003	1.148681	0.000000
2	1	0	-1.036725	1.485323	0.000000
3	17	0	0.000003	-0.667535	0.000000
4	1	0	0.518331	1.485348	0.897853
5	1	0	0.518331	1.485348	-0.897853



2-INT1

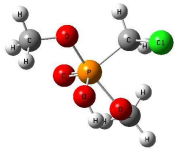
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.372443	-0.006104	0.221850
2	6	0	1.039929	-1.093466	-0.501270
3	8	0	-0.075450	-0.229654	1.712636
4	8	0	-1.794487	0.975700	0.547498
5	1	0	-2.246219	1.281796	-0.266778
6	17	0	2.741255	-0.601362	0.026864
7	8	0	-1.322529	-1.104499	-0.671208
8	8	0	0.326614	1.257808	-0.662778
9	6	0	-2.673461	-1.443406	-0.342974
10	1	0	-3.381235	-0.687917	-0.702571
11	1	0	-2.880275	-2.394640	-0.844920
12	1	0	-2.805954	-1.567251	0.737098
13	6	0	0.125099	2.646417	-0.388285
14	1	0	0.951178	3.174669	-0.876427
15	1	0	-0.823480	3.011009	-0.799307
16	1	0	0.147998	2.852247	0.686725
17	1	0	1.072320	-1.091187	-1.592399
18	1	0	0.928403	-2.116120	-0.139877



2-INT2

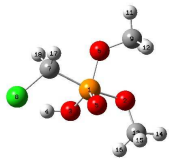
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.235601	-0.064433	0.172639
2	6	0	-1.261509	-0.041066	-0.973756
3	8	0	0.300317	0.282366	1.668651
4	8	0	1.619076	-0.481815	-0.667341
5	8	0	0.488790	1.592132	-0.437400
6	8	0	-0.189975	-1.778582	0.437338
7	6	0	1.579717	2.343092	0.064932
8	1	0	2.542140	1.862008	-0.164807
9	1	0	1.559805	3.328832	-0.418183
10	1	0	1.507594	2.478965	1.152635
11	1	0	-1.265685	0.831322	-1.621322
12	6	0	2.373809	-1.663820	-0.384414

13	1	0	3.318495	-1.549520	-0.926014
14	1	0	2.586672	-1.758650	0.686776
15	1	0	1.853298	-2.563374	-0.723507
16	1	0	-0.063579	-1.970870	1.389801
17	17	0	-2.833792	0.031282	-0.039202
18	1	0	-1.296042	-0.966040	-1.549088



2-INT3

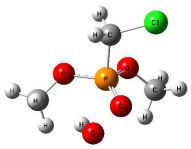
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.367968	0.387819	-0.033293
2	6	0	-0.788911	-0.754753	-0.966945
3	8	0	0.960216	1.573653	-0.798381
4	8	0	0.666666	0.105689	1.577159
5	1	0	0.047582	0.654173	2.111091
6	8	0	1.618844	-0.809297	-0.384963
7	8	0	-1.112753	1.261900	0.607145
8	6	0	2.961905	-0.529579	-0.029074
9	1	0	3.095803	-0.493872	1.061645
10	1	0	3.589195	-1.335056	-0.431423
11	1	0	3.299379	0.425382	-0.456522
12	6	0	-1.754751	2.240294	-0.180693
13	1	0	-2.590632	2.651298	0.401109
14	1	0	-1.072710	3.056368	-0.454533
15	1	0	-2.171856	1.825413	-1.115627
16	1	0	-1.589076	-0.180387	-1.431843
17	17	0	-1.615302	-1.993461	0.093179
18	1	0	-0.240327	-1.323086	-1.715946



2-INT4

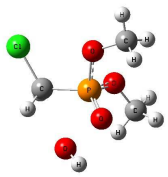
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.226049	-0.020790	0.047127
2	8	0	1.863540	-0.570511	-0.217296
3	8	0	-0.174637	-1.027544	-1.258683
4	1	0	-1.128493	-1.017938	-1.471293
5	8	0	0.046788	-0.510710	1.492558
6	8	0	0.786208	1.534988	-0.293922
7	6	0	-1.477687	0.905477	-0.096817
8	17	0	-2.970823	-0.183128	0.100628
9	6	0	2.093633	2.020448	0.033954

10	1	0	2.845894	1.632985	-0.658233
11	1	0	2.037571	3.111762	-0.046020
12	1	0	2.376119	1.745245	1.055629
13	6	0	2.218626	-1.888515	0.151068
14	1	0	3.295566	-2.001692	-0.029332
15	1	0	2.012566	-2.079089	1.212851
16	1	0	1.683796	-2.639462	-0.449874
17	1	0	-1.560274	1.630286	0.713016
18	1	0	-1.632109	1.408682	-1.054797



2-TS1

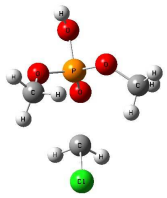
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.225354	-0.132561	0.109627
2	6	0	-1.287985	-1.073796	-0.426287
3	8	0	0.227545	-0.088321	1.613129
4	8	0	2.447075	1.074026	0.380141
5	1	0	2.783959	1.218551	-0.526396
6	17	0	-2.849911	-0.299379	0.117071
7	8	0	-0.084950	1.186296	-0.781899
8	8	0	1.197321	-1.141081	-0.721552
9	6	0	0.029492	2.534249	-0.271685
10	1	0	0.999323	2.636881	0.219045
11	1	0	-0.051683	3.189311	-1.142825
12	1	0	-0.798945	2.733641	0.416613
13	6	0	2.354603	-1.779104	-0.132759
14	1	0	2.881309	-2.259850	-0.960897
15	1	0	2.965825	-1.009263	0.341986
16	1	0	2.030094	-2.540095	0.585939
17	1	0	-1.342503	-1.152397	-1.514013
18	1	0	-1.271798	-2.074368	0.011761



2-TS2

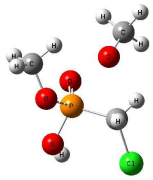
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.298923	0.157188	0.298798
2	6	0	-1.002131	-1.140195	0.100654
3	8	0	1.039029	0.253795	1.603333
4	8	0	1.194275	0.214929	-1.048240

5	8	0	-0.608198	1.492511	0.049489
6	8	0	1.201313	-2.468689	0.447257
7	6	0	0.016661	2.786344	0.140554
8	1	0	0.783785	2.897710	-0.633277
9	1	0	-0.775774	3.520482	-0.020478
10	1	0	0.460948	2.931530	1.130373
11	1	0	-1.117262	-1.667936	1.043518
12	6	0	2.567073	-0.239848	-1.104215
13	1	0	2.882743	-0.087265	-2.138909
14	1	0	3.187319	0.365796	-0.435888
15	1	0	2.597841	-1.293918	-0.818149
16	1	0	1.794017	-2.228189	1.184821
17	17	0	-2.688570	-0.549030	-0.374286
18	1	0	-0.692743	-1.840682	-0.667783



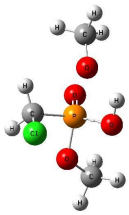
2-TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.320109	-0.027954	0.287314
2	6	0	-1.526945	0.187608	0.808675
3	8	0	1.097048	0.499737	1.670652
4	8	0	2.944331	-0.219720	0.189173
5	1	0	3.234285	-0.644761	-0.658722
6	17	0	-3.386041	0.003429	0.024803
7	8	0	1.052337	0.903954	-1.000610
8	8	0	0.919035	-1.531809	-0.135668
9	6	0	0.259067	2.109816	-0.985659
10	1	0	0.669165	2.823913	-0.264464
11	1	0	0.333621	2.518886	-1.995515
12	1	0	-0.769078	1.851840	-0.727672
13	6	0	-0.232183	-1.932382	-0.910115
14	1	0	-0.559617	-1.125402	-1.564962
15	1	0	0.099318	-2.798138	-1.490816
16	1	0	-1.048546	-2.202708	-0.241398
17	1	0	-1.689097	1.130140	1.364567
18	1	0	-1.610641	-0.600309	1.581825



2-TS4

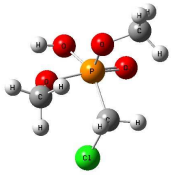
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.020292	-0.611310	0.299532
2	6	0	-0.915889	0.798169	-0.438909
3	8	0	0.565523	-0.378129	1.678979
4	8	0	0.960368	-1.319550	-0.804244
5	8	0	1.500280	1.461371	-0.614922
6	8	0	-1.074729	-1.839408	0.303411
7	6	0	1.889395	2.270454	0.431013
8	1	0	2.550511	1.758269	1.168786
9	1	0	2.447381	3.174702	0.094101
10	1	0	1.033532	2.664591	1.036896
11	1	0	-0.678965	1.721859	0.074651
12	6	0	2.404102	-1.299072	-0.683593
13	1	0	2.727230	-0.256297	-0.643257
14	1	0	2.710548	-1.858326	0.206213
15	1	0	2.776354	-1.802209	-1.579025
16	1	0	-1.770896	-1.722668	0.997787
17	17	0	-2.779603	0.623078	-0.276554
18	1	0	-0.723994	0.885817	-1.504577



2-TS5

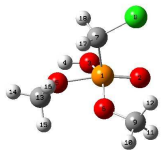
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.323314	-0.437324	-0.127687
2	6	0	0.395930	1.051528	-0.958482
3	8	0	-0.283001	-1.703233	-0.954834
4	8	0	-0.340784	-0.513497	1.498220
5	1	0	0.621867	-0.756046	1.674544
6	8	0	-1.888524	0.163771	-0.260681
7	8	0	1.831220	-0.666565	0.535074
8	6	0	-2.987433	-0.641454	0.174212
9	1	0	-2.961212	-0.790998	1.260148
10	1	0	-3.901890	-0.104024	-0.093388
11	1	0	-2.982995	-1.616705	-0.327829
12	6	0	2.610056	-1.635309	-0.097238

13	1	0	3.602989	-1.723526	0.383136
14	1	0	2.147869	-2.640325	-0.082149
15	1	0	2.794137	-1.392667	-1.164478
16	1	0	1.388718	0.809390	-1.327815
17	17	0	0.573498	2.501790	0.124057
18	1	0	-0.271865	1.351933	-1.769029



2-TS6

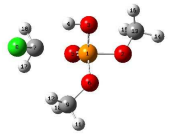
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.457524	-0.188137	0.378558
2	8	0	-0.636801	-1.709386	0.654716
3	8	0	-0.976013	0.194937	1.971067
4	1	0	-0.896594	1.161855	2.121504
5	8	0	0.178034	1.499445	0.518220
6	6	0	0.520145	2.334208	-0.577020
7	1	0	0.413746	3.372885	-0.238152
8	1	0	1.562333	2.190265	-0.897687
9	1	0	-0.149043	2.184819	-1.434137
10	6	0	-2.559439	-0.648837	-1.226949
11	1	0	-2.004472	-1.348007	-1.862540
12	1	0	-3.110226	-1.217581	-0.470908
13	1	0	-3.262647	-0.080138	-1.842574
14	8	0	-1.689601	0.316003	-0.622830
15	6	0	0.939337	-0.526545	-0.906137
16	1	0	1.058189	0.237058	-1.672954
17	1	0	0.756780	-1.494663	-1.369124
18	17	0	2.593505	-0.679140	-0.112973



2-TS7

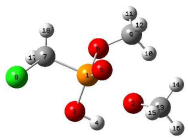
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.287473	-0.090974	0.570474
2	8	0	0.541637	0.740543	1.579511
3	8	0	-0.591484	-1.313947	1.744930
4	1	0	-1.237935	-1.965200	1.396163
5	8	0	-1.646148	-0.981630	-0.244356
6	8	0	-0.952347	1.239139	-0.279593
7	6	0	0.882380	-0.894493	-0.644760
8	17	0	2.606759	-0.275817	-0.635163
9	6	0	-0.410496	2.550901	-0.163862

10	1	0	-1.009764	3.185379	-0.828154
11	1	0	-0.476707	2.928788	0.861110
12	1	0	0.639270	2.589145	-0.479072
13	6	0	-2.277895	-0.624092	-1.463808
14	1	0	-2.858271	-1.499057	-1.786925
15	1	0	-2.954655	0.229292	-1.338168
16	1	0	-1.558913	-0.370962	-2.255387
17	1	0	0.530555	-0.747974	-1.665443
18	1	0	0.946411	-1.962650	-0.432824



2-TS8

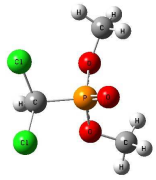
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.820138	0.021401	0.120813
2	8	0	2.356103	0.178661	-0.488850
3	8	0	0.468119	-1.314391	-0.748512
4	1	0	-0.481185	-1.451864	-0.508246
5	8	0	0.941173	-0.010074	1.623234
6	8	0	0.332153	1.373876	-0.629303
7	6	0	-1.639652	-0.465635	0.772814
8	17	0	-3.258512	-0.590322	-0.293518
9	6	0	-0.647517	2.283971	-0.101916
10	1	0	-0.529240	2.403671	0.978759
11	1	0	-0.460110	3.237867	-0.601159
12	1	0	-1.653208	1.927967	-0.331503
13	6	0	3.331199	-0.820801	-0.165191
14	1	0	4.276883	-0.485453	-0.598930
15	1	0	3.444566	-0.920096	0.920608
16	1	0	3.057362	-1.790473	-0.596722
17	1	0	-1.889444	0.362799	1.445148
18	1	0	-1.717559	-1.379745	1.382870



2-TS9

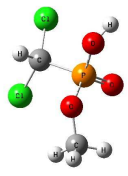
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.011997	0.049450	-0.011692
2	8	0	2.004291	-0.787129	-0.556560
3	8	0	-0.233926	-0.939766	-1.288542
4	1	0	0.686470	-1.340753	-1.379275
5	8	0	0.138189	-0.449983	1.411927
6	8	0	0.679305	1.500698	-0.402958
7	6	0	-1.694829	0.816221	-0.113813

8	17	0	-3.054518	-0.374585	0.184165
9	6	0	1.933803	1.942979	0.145718
10	1	0	2.753447	1.384036	-0.307021
11	1	0	2.002126	3.008029	-0.091138
12	1	0	1.947073	1.806695	1.232251
13	6	0	2.797821	-1.407962	0.409177
14	1	0	3.333285	-0.674819	1.046119
15	1	0	2.215154	-2.050921	1.093459
16	1	0	3.569681	-2.042010	-0.065668
17	1	0	-1.886056	1.253522	-1.096053
18	1	0	-1.797969	1.584418	0.654463



Cl_2-DMMP (**3**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.635902	-0.041893	0.182045
2	8	0	0.710878	0.019915	1.669980
3	6	0	-1.079566	-0.174081	-0.519079
4	8	0	1.287706	-1.304229	-0.550447
5	8	0	1.292790	1.204567	-0.589339
6	6	0	1.472228	2.511232	0.020408
7	1	0	1.710958	2.407207	1.081003
8	1	0	2.302934	2.975612	-0.512668
9	1	0	0.560049	3.097735	-0.111923
10	6	0	2.653479	-1.716839	-0.271946
11	1	0	2.806337	-2.630109	-0.847303
12	1	0	3.350523	-0.941776	-0.602487
13	1	0	2.775228	-1.917483	0.795568
14	17	0	-1.998768	1.327189	-0.142632
15	17	0	-1.919705	-1.632023	0.110829
16	1	0	-1.038353	-0.264490	-1.610054



Methyl dichloromethylphosphonate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.631367	-0.672825	0.122420
2	8	0	0.729946	-0.716016	1.608692
3	6	0	-0.856212	0.250089	-0.509585

4	8	0	0.550722	-2.066023	-0.665080
5	8	0	1.838767	0.015853	-0.673421
6	6	0	2.753435	0.955848	-0.048231
7	1	0	3.059409	0.591059	0.934664
8	1	0	3.613536	1.013596	-0.716116
9	1	0	2.274309	1.933968	0.037798
10	17	0	-0.802698	1.967722	0.027258
11	17	0	-2.374933	-0.556218	0.021930
12	1	0	-0.858586	0.253596	-1.605218
13	1	0	0.121727	-2.801537	-0.138258



Methyl dichloromethylphosphonate anion

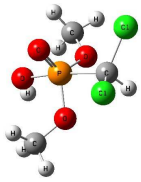
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.636452	-0.811672	0.076498
2	8	0	0.769142	-0.718007	1.579573
3	6	0	-0.829937	0.213405	-0.507495
4	8	0	0.489608	-2.143433	-0.628632
5	8	0	1.865929	-0.020842	-0.678680
6	6	0	2.673555	0.976313	-0.025601
7	1	0	2.760237	0.766093	1.043703
8	1	0	3.660393	0.936807	-0.494213
9	1	0	2.235275	1.968260	-0.173409
10	17	0	-0.747597	1.945734	0.020495
11	17	0	-2.393002	-0.522648	0.044033
12	1	0	-0.871643	0.231405	-1.600031

$CHCl_2^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.026349	0.980913	0.000000
2	17	0	-0.026349	-0.208705	1.539397
3	17	0	-0.026349	-0.208705	-1.539397
4	1	0	1.053951	1.210477	0.000000

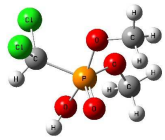
CH_2Cl_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.779093	0.000000
2	1	0	-0.904328	1.385366	0.000000
3	17	0	0.000000	-0.218979	1.494499
4	17	0	0.000000	-0.218979	-1.494499
5	1	0	0.904325	1.385370	0.000000



3-INT1

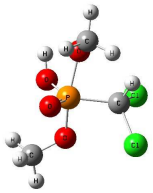
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.693933	-0.000452	0.236235
2	6	0	1.153239	-0.000293	-0.488347
3	8	0	-0.291383	-0.003805	1.711531
4	8	0	-2.402518	-0.001418	0.587209
5	1	0	-2.964637	-0.001440	-0.216745
6	17	0	2.117115	-1.473067	0.020860
7	17	0	2.117364	1.474392	0.012942
8	8	0	-0.830624	-1.381709	-0.710657
9	8	0	-0.828081	1.386299	-0.701372
10	6	0	-1.700068	-2.474100	-0.387321
11	1	0	-2.733414	-2.269093	-0.687025
12	1	0	-1.324536	-3.334890	-0.949004
13	1	0	-1.676079	-2.700399	0.683454
14	6	0	-1.703899	2.473977	-0.379745
15	1	0	-1.326816	3.338697	-0.934313
16	1	0	-2.734045	2.266905	-0.688954
17	1	0	-1.689469	2.695123	0.692240
18	1	0	1.197058	-0.003103	-1.579011



3-INT2

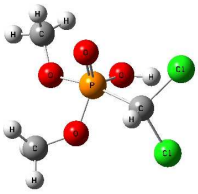
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.612473	0.164945	0.428835
2	6	0	-1.191323	-0.525296	0.375306
3	8	0	0.925619	1.177994	1.535745
4	8	0	1.784544	-0.338116	-0.647549
5	8	0	0.080190	1.230554	-0.834494
6	8	0	0.950560	-1.311081	1.366645
7	6	0	0.924704	2.287398	-1.254296
8	1	0	1.839957	1.909727	-1.730868
9	1	0	0.364973	2.883974	-1.985421
10	1	0	1.205218	2.934321	-0.411373
11	1	0	-1.354174	-1.182415	1.226012
12	6	0	2.963836	-1.059650	-0.274175
13	1	0	3.651286	-0.955377	-1.120669

14	1	0	3.427325	-0.637710	0.623377
15	1	0	2.746690	-2.116448	-0.098889
16	1	0	0.702634	-1.133713	2.300913
17	17	0	-1.480107	-1.572227	-1.085263
18	17	0	-2.512928	0.721282	0.515887



3-INT3

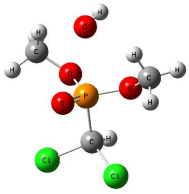
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.803764	0.173502	-0.000805
2	6	0	0.935735	-0.624060	-0.127810
3	8	0	-1.591701	0.379099	-1.290477
4	8	0	-1.445693	0.468348	1.502907
5	1	0	-1.979462	-0.310312	1.782902
6	8	0	0.010585	1.692582	0.127477
7	8	0	-1.357219	-1.546585	0.332622
8	6	0	-0.739872	2.891834	0.031410
9	1	0	-1.435863	3.005204	0.874983
10	1	0	-0.028389	3.726087	0.050010
11	1	0	-1.310262	2.931545	-0.906099
12	6	0	-1.624409	-2.421802	-0.746065
13	1	0	-2.018114	-3.358062	-0.329971
14	1	0	-2.359224	-1.995267	-1.439845
15	1	0	-0.717967	-2.668046	-1.327031
16	1	0	0.856514	-1.666567	-0.418898
17	17	0	1.788011	-0.655239	1.475918
18	17	0	2.017443	0.108740	-1.393531



3-INT4

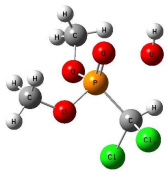
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.627600	-0.185477	-0.116040
2	8	0	-2.290681	-0.138826	0.334227
3	8	0	-0.310138	-0.665250	1.460566
4	1	0	0.633378	-0.840776	1.658938
5	8	0	-0.697671	-1.203847	-1.259946
6	8	0	-0.689208	1.448529	-0.422920

7	6	0	1.322856	0.127876	-0.449935
8	17	0	2.177863	1.368266	0.618682
9	17	0	2.324117	-1.414209	-0.376919
10	6	0	-1.874027	2.231177	-0.624560
11	1	0	-2.446390	2.327895	0.301363
12	1	0	-1.521439	3.215189	-0.950620
13	1	0	-2.514628	1.794908	-1.396748
14	6	0	-2.991422	-1.352132	0.539880
15	1	0	-4.033681	-1.092539	0.761720
16	1	0	-2.963074	-1.987757	-0.354886
17	1	0	-2.582136	-1.918433	1.388848
18	1	0	1.465440	0.498312	-1.465733



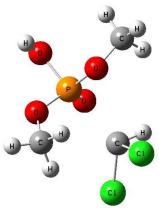
3-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.489508	0.000400	0.092572
2	6	0	1.309576	-0.000560	-0.484895
3	8	0	-0.491640	-0.000397	1.588649
4	8	0	-3.114365	-0.000178	0.454520
5	1	0	-3.500471	0.000027	-0.443457
6	17	0	2.180833	-1.482303	0.083822
7	17	0	2.184171	1.481179	0.078471
8	8	0	-0.884361	-1.299215	-0.774194
9	8	0	-0.884826	1.301338	-0.771833
10	6	0	-1.590405	-2.436439	-0.217327
11	1	0	-2.475983	-2.062217	0.301292
12	1	0	-1.857016	-3.062004	-1.072125
13	1	0	-0.922538	-2.988722	0.451559
14	6	0	-1.590682	2.437275	-0.211925
15	1	0	-1.858183	3.064487	-1.065252
16	1	0	-2.475768	2.061648	0.306504
17	1	0	-0.922393	2.988355	0.457508
18	1	0	1.380509	-0.002489	-1.575860



3-TS2

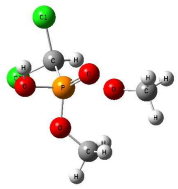
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.583854	0.153151	-0.328023
2	6	0	1.111720	-0.581030	0.019218
3	8	0	-1.080042	0.302458	-1.738611
4	8	0	-1.631299	-0.248873	0.832484
5	8	0	-0.180884	1.636458	0.260008
6	8	0	-0.628636	-2.352517	-0.864965
7	6	0	-1.140907	2.701876	0.193742
8	1	0	-2.037258	2.452631	0.773004
9	1	0	-0.659075	3.580183	0.629819
10	1	0	-1.417266	2.911258	-0.845111
11	1	0	1.068108	-1.637944	-0.227269
12	6	0	-2.793371	-1.082598	0.618512
13	1	0	-3.275783	-1.160736	1.595582
14	1	0	-3.471215	-0.598601	-0.091839
15	1	0	-2.463701	-2.052288	0.241695
16	1	0	-1.138059	-2.335844	-1.697599
17	17	0	2.350135	0.170011	-1.069580
18	17	0	1.606000	-0.427988	1.754398



3-TS3

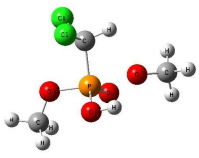
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.321205	-0.386430	-0.154843
2	6	0	1.189247	0.247162	-0.417908
3	8	0	-1.024070	-0.818360	-1.563398
4	8	0	-2.942244	-0.709976	-0.051776
5	1	0	-3.299558	-0.540467	0.855915
6	17	0	2.219636	1.488313	0.637557
7	17	0	2.440228	-1.096914	-0.962755
8	8	0	-1.313671	1.187732	0.264200
9	8	0	-0.935128	-1.215448	1.172858
10	6	0	-1.924941	2.148319	-0.620465
11	1	0	-2.990525	1.932410	-0.751127
12	1	0	-1.799640	3.120926	-0.140627

13	1	0	-1.422376	2.149098	-1.592970
14	6	0	0.253807	-1.142510	1.983298
15	1	0	0.464180	-0.111391	2.268369
16	1	0	0.021408	-1.742251	2.867439
17	1	0	1.107232	-1.560411	1.450722
18	1	0	1.131886	0.825352	-1.351346



3-TS4

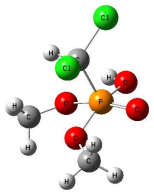
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.300917	-0.262271	0.746246
2	6	0	-0.959975	0.330046	-0.513656
3	8	0	0.894787	0.751154	1.680068
4	8	0	1.143027	-1.498101	0.154538
5	8	0	1.469728	1.061298	-1.113728
6	8	0	-0.697970	-1.245956	1.627181
7	6	0	2.559390	1.830965	-0.743863
8	1	0	3.530646	1.280085	-0.795196
9	1	0	2.690675	2.723232	-1.395620
10	1	0	2.480192	2.209045	0.296330
11	1	0	-0.457854	0.967310	-1.237554
12	6	0	2.506660	-1.449921	-0.319757
13	1	0	2.562926	-0.775462	-1.173532
14	1	0	3.167627	-1.106516	0.481567
15	1	0	2.750331	-2.481502	-0.584191
16	1	0	-1.068117	-0.761673	2.407065
17	17	0	-1.738619	-1.037402	-1.409722
18	17	0	-2.219217	1.335394	0.320700



3-TS5

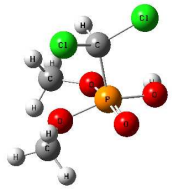
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.455328	0.622597	-0.041121
2	6	0	0.569978	-0.950970	-0.181070
3	8	0	-1.103255	1.074112	-1.325251
4	8	0	-1.159503	0.916702	1.392674
5	1	0	-1.907808	0.239472	1.373585
6	8	0	0.867009	1.589492	0.235699

7	8	0	-1.995375	-1.025549	0.296664
8	6	0	0.698846	3.011020	0.272684
9	1	0	0.065288	3.310116	1.116179
10	1	0	1.695667	3.442163	0.398909
11	1	0	0.260173	3.376890	-0.662735
12	6	0	-2.906921	-1.281217	-0.731071
13	1	0	-3.664354	-2.019709	-0.409862
14	1	0	-3.446920	-0.375289	-1.062097
15	1	0	-2.414165	-1.699219	-1.632006
16	1	0	-0.056574	-1.747515	-0.566538
17	17	0	1.184398	-1.516158	1.422030
18	17	0	1.948319	-0.776602	-1.357333



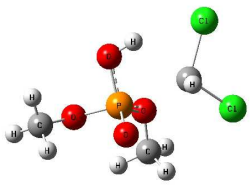
3-TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.694794	-0.161190	-0.482212
2	8	0	-0.261507	0.765847	-1.639997
3	8	0	-1.696946	-1.087572	-1.502169
4	1	0	-2.067389	-1.847119	-0.997876
5	8	0	-0.854502	-1.643756	0.543242
6	6	0	-0.827208	-1.659670	1.965502
7	1	0	-1.656279	-2.290332	2.312585
8	1	0	0.111436	-2.096899	2.338266
9	1	0	-0.960041	-0.660966	2.396416
10	6	0	-2.071478	2.031178	0.206888
11	1	0	-1.207125	2.661163	-0.018214
12	1	0	-2.752169	2.032197	-0.651594
13	1	0	-2.595227	2.416449	1.086400
14	8	0	-1.671955	0.694505	0.539370
15	6	0	1.062179	-0.041406	0.390868
16	1	0	1.118064	-0.451767	1.393666
17	17	0	2.274516	-1.022460	-0.562291
18	17	0	1.686011	1.660244	0.589963



3-TS7

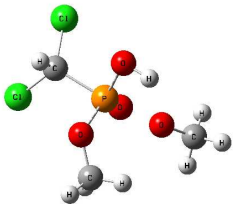
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.502522	-0.448168	-0.535654
2	8	0	0.244947	0.176342	-1.927392
3	8	0	0.060223	-2.007297	-1.088237
4	1	0	0.245403	-2.682806	-0.400149
5	8	0	1.203186	-1.441218	0.781953
6	8	0	1.712581	0.656141	-0.052629
7	6	0	-0.978355	0.072760	0.556674
8	17	0	-2.553857	-0.630298	-0.010097
9	17	0	-1.158191	1.876564	0.675040
10	6	0	2.047153	1.816678	-0.806314
11	1	0	2.844330	2.319143	-0.245123
12	1	0	2.413982	1.555775	-1.804136
13	1	0	1.194274	2.494176	-0.913625
14	6	0	1.890690	-0.957127	1.927948
15	1	0	1.968050	-1.803667	2.622516
16	1	0	2.895464	-0.598337	1.680358
17	1	0	1.350302	-0.141105	2.427788
18	1	0	-0.869233	-0.272778	1.583744



3-TS8

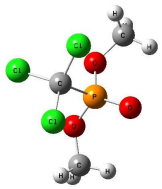
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.004861	-0.159142	0.076044
2	8	0	2.601292	-0.194885	-0.380198
3	8	0	0.662827	-1.617576	-0.555280
4	1	0	-0.292695	-1.804231	-0.468664
5	8	0	1.005826	0.124405	1.555137
6	8	0	0.566674	0.960272	-1.009925
7	6	0	-1.503176	-0.261415	0.526768
8	17	0	-2.690373	-1.485997	-0.427218
9	17	0	-2.320833	1.404652	0.471021
10	6	0	1.038932	2.314259	-0.855408
11	1	0	2.132698	2.345496	-0.874284

12	1	0	0.634975	2.868620	-1.704838
13	1	0	0.661631	2.745195	0.076607
14	6	0	3.557885	-0.866093	0.447491
15	1	0	4.535380	-0.711313	-0.017045
16	1	0	3.560074	-0.448561	1.459619
17	1	0	3.349667	-1.942376	0.496764
18	1	0	-1.718916	-0.581062	1.555545



3-TS9

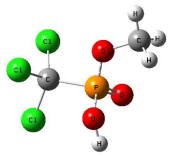
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.394887	-0.156216	-0.078308
2	8	0	2.591871	-0.529541	-0.343678
3	8	0	0.543469	-1.416121	-1.091652
4	1	0	1.562496	-1.504748	-1.052932
5	8	0	0.492184	-0.258059	1.422350
6	8	0	0.698711	1.266730	-0.817585
7	6	0	-1.472364	-0.008789	-0.442470
8	17	0	-2.379875	-1.504166	0.047698
9	17	0	-2.211346	1.429391	0.380031
10	6	0	1.649001	2.208403	-0.283131
11	1	0	2.636876	1.746785	-0.247428
12	1	0	1.639548	3.060096	-0.967447
13	1	0	1.338628	2.534526	0.715005
14	6	0	3.361661	-0.862669	0.775974
15	1	0	3.520897	0.007220	1.440668
16	1	0	2.899477	-1.651982	1.397352
17	1	0	4.359326	-1.226197	0.469420
18	1	0	-1.669457	0.122965	-1.509128



Cl_3-DMMP (**4**)

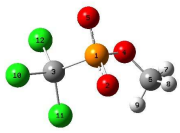
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.972480	0.007009	-0.208102
2	8	0	-1.342529	0.009353	-1.648812
3	6	0	0.908371	-0.006706	0.017002
4	8	0	-1.467270	-1.214253	0.687205

5	8	0	-1.451468	1.235189	0.686677
6	17	0	1.351376	-0.004937	1.756518
7	17	0	1.586727	1.457573	-0.781624
8	17	0	1.562876	-1.486573	-0.772811
9	6	0	-1.841647	-2.509595	0.137191
10	1	0	-0.953978	-3.142951	0.078707
11	1	0	-2.562905	-2.927808	0.840026
12	1	0	-2.295651	-2.388525	-0.848520
13	6	0	-1.795644	2.538872	0.136808
14	1	0	-2.503025	2.975425	0.842558
15	1	0	-0.892927	3.150075	0.073349
16	1	0	-2.257293	2.427847	-0.846559



Methyl trichloromethylphosphonate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.914594	0.546891	-0.144973
2	8	0	-1.169246	1.163379	-1.475874
3	6	0	0.838402	-0.144794	0.005704
4	8	0	-1.742188	-0.754762	0.248839
5	8	0	-1.081603	1.502701	1.127645
6	6	0	-3.180120	-0.833368	0.035114
7	1	0	-3.457228	-1.852580	0.304224
8	1	0	-3.691241	-0.118129	0.685270
9	1	0	-3.413680	-0.639712	-1.014589
10	1	0	-0.954754	2.475336	0.920695
11	17	0	1.980521	1.228887	-0.222787
12	17	0	1.097342	-1.367315	-1.285666
13	17	0	1.112162	-0.890387	1.616054



Methyl trichloromethylphosphonate anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.906667	-0.834449	-0.062171
2	8	0	1.284328	-0.959422	-1.517291
3	6	0	-0.742388	0.150798	0.001155
4	8	0	1.901373	0.194526	0.731336
5	8	0	0.693077	-2.033648	0.826558
6	6	0	2.801833	1.083752	0.041107
7	1	0	3.361429	1.606746	0.820012

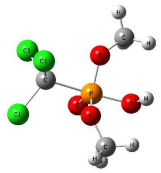
8	1	0	3.489117	0.517444	-0.593779
9	1	0	2.250986	1.807296	-0.565740
10	17	0	-2.050619	-0.847881	-0.755919
11	17	0	-0.619817	1.710650	-0.909573
12	17	0	-1.217119	0.523484	1.706296

CCl_3^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.726880
2	17	0	0.000000	1.739427	-0.085515
3	17	0	-1.506388	-0.869713	-0.085515
4	17	0	1.506388	-0.869713	-0.085515

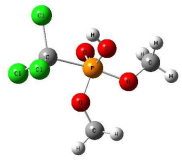
$CHCl_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000003	1.148681	0.000000
2	1	0	-1.036725	1.485323	0.000000
3	17	0	0.000003	-0.667535	0.000000
4	1	0	0.518331	1.485348	0.897853
5	1	0	0.518331	1.485348	-0.897853



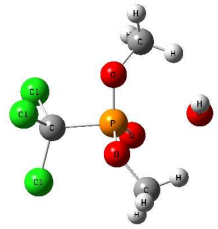
4-INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.013524	0.005373	-0.314930
2	6	0	1.051006	-0.007041	0.010338
3	8	0	-0.818218	0.034391	-1.823694
4	8	0	-2.733559	0.012957	-0.367124
5	1	0	-3.154783	0.011384	0.520981
6	17	0	1.833167	1.494404	-0.691489
7	17	0	1.596471	-0.086213	1.767995
8	17	0	1.833879	-1.437094	-0.829196
9	8	0	-0.929525	1.362463	0.637928
10	8	0	-0.932195	-1.380905	0.590580
11	6	0	-1.794917	2.490331	0.435513
12	1	0	-2.789097	2.313267	0.858059
13	1	0	-1.319470	3.326051	0.956500
14	1	0	-1.892013	2.731240	-0.627972
15	6	0	-1.854530	-2.469904	0.435478
16	1	0	-1.369818	-3.335315	0.896064
17	1	0	-2.801320	-2.267740	0.946886
18	1	0	-2.051805	-2.679703	-0.620328



4-INT2

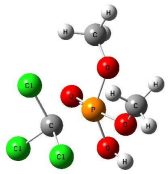
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.951227	-0.184158	-0.058272
2	8	0	-2.630077	-0.070023	0.180341
3	8	0	-0.850324	-1.106876	1.318890
4	1	0	0.028423	-1.478930	1.533374
5	8	0	-0.879583	-0.826088	-1.435483
6	8	0	-0.777365	1.429658	0.199612
7	6	0	1.193067	-0.048521	-0.023944
8	17	0	1.926184	0.669227	1.516431
9	17	0	1.964504	-1.723194	-0.194555
10	17	0	1.817673	0.946699	-1.414271
11	6	0	-1.813936	2.410783	0.033067
12	1	0	-2.572251	2.317243	0.813941
13	1	0	-1.309474	3.378420	0.111030
14	1	0	-2.291404	2.322112	-0.947082
15	6	0	-3.456678	-1.187336	-0.112717
16	1	0	-4.491782	-0.876399	0.066424
17	1	0	-3.347789	-1.499153	-1.158545
18	1	0	-3.225411	-2.040294	0.540323



4-TS1

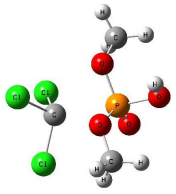
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.722343	-0.000114	-0.216794
2	6	0	-1.186643	0.000228	0.013522
3	8	0	0.959858	0.000702	-1.689200
4	8	0	3.502087	-0.000204	-0.161992
5	1	0	3.738195	0.005000	0.786719
6	17	0	-1.879308	-1.464330	-0.788720
7	17	0	-1.679119	-0.008236	1.751631
8	17	0	-1.876939	1.473165	-0.775294
9	8	0	0.994819	-1.296529	0.676750
10	8	0	0.996341	1.294700	0.678877
11	6	0	1.792854	-2.418187	0.205063

12	1	0	2.757908	-2.022569	-0.122521
13	1	0	1.892791	-3.080084	1.067475
14	1	0	1.258092	-2.931230	-0.599743
15	6	0	1.791985	2.417604	0.206018
16	1	0	1.894728	3.078259	1.069047
17	1	0	2.756186	2.023307	-0.125541
18	1	0	1.254151	2.931637	-0.596112



4-TS2

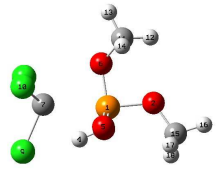
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.815656	-0.142275	0.715066
2	8	0	0.812837	-1.644969	1.075659
3	8	0	0.519840	0.339438	2.312990
4	1	0	0.541336	1.320514	2.387530
5	8	0	1.057852	1.596991	0.506212
6	8	0	2.041332	-0.234039	-0.454626
7	6	0	-0.962312	-0.085304	-0.169793
8	17	0	-2.152403	-1.088657	0.767582
9	17	0	-1.731351	1.551795	-0.355760
10	17	0	-0.821914	-0.808564	-1.834457
11	6	0	2.593302	-1.473651	-0.895903
12	1	0	3.337814	-1.211076	-1.656341
13	1	0	3.078753	-2.010256	-0.075309
14	1	0	1.830781	-2.122337	-1.337075
15	6	0	1.489628	2.259794	-0.675182
16	1	0	1.206331	3.313614	-0.559467
17	1	0	2.576250	2.185806	-0.798136
18	1	0	1.011658	1.865697	-1.579016



4-TS3

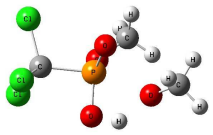
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.292221	0.003561	-0.242558
2	6	0	-1.113209	-0.001399	-0.005148
3	8	0	1.014636	0.015780	-1.721860
4	8	0	2.968145	0.001859	-0.267199
5	1	0	3.358756	0.002747	0.640758

6	17	0	-1.891311	-1.488104	-0.839492
7	17	0	-1.818169	-0.012496	1.737527
8	17	0	-1.901556	1.487446	-0.824997
9	8	0	1.079466	-1.288899	0.727706
10	8	0	1.082649	1.286841	0.741227
11	6	0	1.644042	-2.563179	0.354309
12	1	0	2.731996	-2.498636	0.259897
13	1	0	1.378679	-3.250355	1.160184
14	1	0	1.206067	-2.913918	-0.585535
15	6	0	1.623961	2.568367	0.358001
16	1	0	1.374538	3.249933	1.173678
17	1	0	2.709633	2.514847	0.233694
18	1	0	1.156697	2.918218	-0.567917



4-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.114258	-0.167303	0.006248
2	8	0	-2.762264	-0.082089	0.292415
3	8	0	-0.905642	-1.242563	1.221096
4	1	0	-0.000267	-1.595450	1.334530
5	8	0	-1.004040	-0.555559	-1.447537
6	8	0	-0.854037	1.350688	0.542852
7	6	0	1.253220	-0.088963	-0.020181
8	17	0	2.117012	0.300061	1.601265
9	17	0	2.031680	-1.688121	-0.605372
10	17	0	1.818095	1.199347	-1.203354
11	6	0	-1.590869	2.455449	-0.019159
12	1	0	-2.649329	2.386969	0.243857
13	1	0	-1.148443	3.355181	0.414290
14	1	0	-1.476777	2.481450	-1.107849
15	6	0	-3.612547	-1.121432	-0.192708
16	1	0	-4.639011	-0.825833	0.043599
17	1	0	-3.506460	-1.242680	-1.276347
18	1	0	-3.392193	-2.076106	0.302709



4-TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.672015	-0.152483	-0.040895
2	8	0	-2.826192	-0.414497	0.576659
3	8	0	-0.721408	-1.295185	1.090590
4	1	0	-1.762361	-1.304179	1.184819
5	8	0	-0.965699	-0.391279	-1.495829
6	8	0	-0.820221	1.346481	0.561674
7	6	0	1.276550	-0.071923	-0.022453
8	17	0	1.960000	0.278638	1.621123
9	17	0	1.965723	-1.652989	-0.587729
10	17	0	1.850365	1.221772	-1.154087
11	6	0	-1.796779	2.266177	0.028369
12	1	0	-2.795042	1.842928	0.149581
13	1	0	-1.686628	3.182804	0.611886
14	1	0	-1.586792	2.470119	-1.026216
15	6	0	-3.742144	-0.892806	-0.370396
16	1	0	-3.964320	-0.132507	-1.140521
17	1	0	-3.377932	-1.789027	-0.905371
18	1	0	-4.697805	-1.161907	0.113152

Summary of Natural Population Analysis

1-INT1

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.13457	9.99864	2.83264	0.03416	12.86543
C	2	-0.89237	1.99932	4.88007	0.01298	6.89237
O	3	-1.20345	1.99988	7.19474	0.00883	9.20345
O	4	-1.03823	1.99987	7.02770	0.01066	9.03823
H	5	0.47928	0.00000	0.51980	0.00092	0.52072
O	6	-0.84776	1.99985	6.82945	0.01846	8.84776
O	7	-0.84765	1.99985	6.82930	0.01850	8.84765
C	8	-0.22627	1.99934	4.21436	0.01257	6.22627
H	9	0.16730	0.00000	0.83143	0.00126	0.83270
H	10	0.17780	0.00000	0.82142	0.00078	0.82220
H	11	0.17498	0.00000	0.82367	0.00135	0.82502
C	12	-0.22603	1.99934	4.21411	0.01258	6.22603
H	13	0.17780	0.00000	0.82141	0.00078	0.82220
H	14	0.16716	0.00000	0.83158	0.00126	0.83284
H	15	0.17502	0.00000	0.82364	0.00134	0.82498
H	16	0.20798	0.00000	0.79123	0.00079	0.79202
H	17	0.21193	0.00000	0.78680	0.00127	0.78807
H	18	0.20792	0.00000	0.79129	0.00079	0.79208
* Total *		-1.00000	23.99608	51.86463	0.13929	76.00000

1-INT2

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.36595	9.99870	2.51457	0.12079	12.63405
C	2	-1.05633	1.99941	5.04163	0.01529	7.05633
O	3	-1.24517	1.99987	7.23453	0.01077	9.24517
O	4	-0.87856	1.99980	6.85802	0.02073	8.87856
O	5	-0.90477	1.99984	6.88266	0.02227	8.90477
O	6	-1.14329	1.99989	7.12708	0.01632	9.14329
C	7	-0.31470	1.99952	4.29825	0.01692	6.31470
H	8	0.18930	0.00000	0.80853	0.00217	0.81070
H	9	0.19633	0.00000	0.80276	0.00090	0.80367
H	10	0.19288	0.00000	0.80538	0.00174	0.80712
H	11	0.25661	0.00000	0.74286	0.00053	0.74339
H	12	0.25797	0.00000	0.74117	0.00086	0.74203
H	13	0.25368	0.00000	0.74550	0.00083	0.74632

C	14	-0.31664	1.99950	4.29999	0.01715	6.31664
H	15	0.21324	0.00000	0.78591	0.00085	0.78676
H	16	0.20229	0.00000	0.79618	0.00154	0.79771
H	17	0.21338	0.00000	0.78510	0.00152	0.78662
H	18	0.51785	0.00000	0.48080	0.00136	0.48215

* Total *	-1.00000	23.99654	51.75091	0.25254	76.00000

1-INT3

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.25081	9.99875	2.62844	0.12200	12.74919
C	2	-0.91507	1.99930	4.90132	0.01445	6.91507
O	3	-1.20558	1.99983	7.19687	0.00888	9.20558
O	4	-1.01305	1.99983	7.00183	0.01139	9.01305
H	5	0.51205	0.00000	0.48556	0.00239	0.48795
O	6	-0.88787	1.99983	6.86758	0.02046	8.88787
O	7	-0.92227	1.99984	6.90174	0.02069	8.92227
C	8	-0.19647	1.99936	4.17691	0.02019	6.19647
H	9	0.15245	0.00000	0.84577	0.00178	0.84755
H	10	0.15748	0.00000	0.84169	0.00083	0.84252
H	11	0.15647	0.00000	0.84181	0.00171	0.84353
C	12	-0.18862	1.99938	4.16766	0.02158	6.18862
H	13	0.15522	0.00000	0.84381	0.00098	0.84478
H	14	0.15562	0.00000	0.84264	0.00174	0.84438
H	15	0.13420	0.00000	0.86388	0.00192	0.86580
H	16	0.21259	0.00000	0.78660	0.00081	0.78741
H	17	0.22401	0.00000	0.77516	0.00083	0.77599
H	18	0.21802	0.00000	0.78075	0.00124	0.78198

* Total *	-1.00000	23.99612	51.75001	0.25388	76.00000

1-INT4

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.39032	9.99857	2.48942	0.12169	12.60968
O	2	-0.89198	1.99982	6.86703	0.02513	8.89198
O	3	-1.08455	1.99987	7.06734	0.01734	9.08455
H	4	0.52223	0.00000	0.47698	0.00079	0.47777
O	5	-1.25747	1.99987	7.24662	0.01097	9.25747

O	6	-0.88947	1.99982	6.86751	0.02214	8.88947
C	7	-1.07472	1.99946	5.05895	0.01631	7.07472
C	8	-0.30755	1.99950	4.29223	0.01582	6.30755
H	9	0.20901	0.00000	0.78949	0.00150	0.79099
H	10	0.20497	0.00000	0.79430	0.00073	0.79503
H	11	0.20512	0.00000	0.79326	0.00162	0.79488
C	12	-0.30986	1.99951	4.29351	0.01684	6.30986
H	13	0.19684	0.00000	0.80223	0.00093	0.80316
H	14	0.19631	0.00000	0.80206	0.00163	0.80369
H	15	0.18860	0.00000	0.80954	0.00185	0.81140
H	16	0.24462	0.00000	0.75447	0.00090	0.75538
H	17	0.23119	0.00000	0.76778	0.00103	0.76881
H	18	0.22638	0.00000	0.77309	0.00052	0.77362

* Total *	-1.00000	23.99643	51.74584	0.25773	76.00000

2-INT1

Natural Population

		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
P	1	2.41936	9.99851	2.45675	0.12538	12.58064
C	2	-0.77980	1.99926	4.75704	0.02350	6.77980
O	3	-1.24077	1.99987	7.22900	0.01189	9.24077
O	4	-1.10613	1.99988	7.08821	0.01804	9.10613
H	5	0.51473	0.00000	0.48432	0.00096	0.48527
Cl	6	-0.17940	9.99975	7.16114	0.01851	17.17940
O	7	-0.88632	1.99981	6.86646	0.02005	8.88632
O	8	-0.88800	1.99981	6.86714	0.02105	8.88800
C	9	-0.31439	1.99951	4.29933	0.01555	6.31439
H	10	0.20476	0.00000	0.79414	0.00110	0.79524
H	11	0.21651	0.00000	0.78282	0.00067	0.78349
H	12	0.21159	0.00000	0.78718	0.00123	0.78841
C	13	-0.31430	1.99951	4.29913	0.01567	6.31430
H	14	0.21645	0.00000	0.78283	0.00071	0.78355
H	15	0.20335	0.00000	0.79554	0.00110	0.79665
H	16	0.21236	0.00000	0.78647	0.00117	0.78764
H	17	0.25419	0.00000	0.74429	0.00153	0.74581
H	18	0.25581	0.00000	0.74314	0.00105	0.74419

* Total *	-1.00000	33.99591	57.72493	0.27915	92.00000

2-INT2

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.38051	9.99863	2.49576	0.12511	12.61949
C	2	-0.78945	1.99921	4.76712	0.02313	6.78945
O	3	-1.22666	1.99987	7.21573	0.01107	9.22666
O	4	-0.87526	1.99980	6.85488	0.02057	8.87526
O	5	-0.90018	1.99983	6.87848	0.02186	8.90018
O	6	-1.13670	1.99989	7.12005	0.01676	9.13670
C	7	-0.31628	1.99952	4.30015	0.01662	6.31628
H	8	0.19202	0.00000	0.80594	0.00204	0.80798
H	9	0.20064	0.00000	0.79850	0.00086	0.79936
H	10	0.19758	0.00000	0.80073	0.00170	0.80242
H	11	0.27528	0.00000	0.72345	0.00128	0.72472
C	12	-0.31750	1.99950	4.30100	0.01700	6.31750
H	13	0.21589	0.00000	0.78330	0.00081	0.78411
H	14	0.20662	0.00000	0.79195	0.00143	0.79338
H	15	0.21639	0.00000	0.78222	0.00139	0.78361
H	16	0.52728	0.00000	0.47126	0.00146	0.47272
Cl	17	-0.12493	9.99975	7.10809	0.01709	17.12493
H	18	0.27476	0.00000	0.72398	0.00127	0.72524
* Total *		-1.00000	33.99599	57.72257	0.28143	92.00000

2-INT3

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.38564	9.99862	2.49152	0.12422	12.61436
C	2	-0.79778	1.99918	4.77588	0.02272	6.79778
O	3	-1.21793	1.99987	7.19674	0.02132	9.21793
O	4	-1.06488	1.99985	7.04854	0.01649	9.06488
H	5	0.55190	0.00000	0.44622	0.00188	0.44810
O	6	-0.90495	1.99983	6.88350	0.02162	8.90495
O	7	-0.92393	1.99984	6.90403	0.02006	8.92393
C	8	-0.31732	1.99952	4.30165	0.01616	6.31732
H	9	0.19457	0.00000	0.80375	0.00168	0.80543
H	10	0.20413	0.00000	0.79508	0.00079	0.79587
H	11	0.19755	0.00000	0.80081	0.00165	0.80245
C	12	-0.31153	1.99952	4.29267	0.01934	6.31153
H	13	0.20315	0.00000	0.79572	0.00114	0.79685
H	14	0.20060	0.00000	0.79743	0.00197	0.79940
H	15	0.17478	0.00000	0.82336	0.00187	0.82522

H	16	0.26616	0.00000	0.73293	0.00091	0.73384
Cl	17	-0.11732	9.99974	7.10052	0.01706	17.11732
H	18	0.27716	0.00000	0.72139	0.00145	0.72284

* Total *	-1.00000	33.99597	57.71171	0.29231	92.00000

2-INT4

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.42434	9.99850	2.45195	0.12521	12.57566
O	2	-0.89231	1.99982	6.86781	0.02468	8.89231
O	3	-1.07454	1.99986	7.05708	0.01761	9.07454
H	4	0.52523	0.00000	0.47298	0.00179	0.47477
O	5	-1.23936	1.99987	7.22801	0.01147	9.23936
O	6	-0.88352	1.99980	6.86285	0.02087	8.88352
C	7	-0.79999	1.99930	4.77697	0.02371	6.79999
Cl	8	-0.18366	9.99977	7.16746	0.01643	17.18366
C	9	-0.30883	1.99950	4.29389	0.01544	6.30883
H	10	0.21541	0.00000	0.78318	0.00142	0.78459
H	11	0.21161	0.00000	0.78775	0.00064	0.78839
H	12	0.20916	0.00000	0.78930	0.00154	0.79084
C	13	-0.31250	1.99951	4.29644	0.01655	6.31250
H	14	0.20192	0.00000	0.79724	0.00084	0.79808
H	15	0.19992	0.00000	0.79856	0.00152	0.80008
H	16	0.19188	0.00000	0.80641	0.00171	0.80812
H	17	0.26214	0.00000	0.73662	0.00124	0.73786
H	18	0.25309	0.00000	0.74549	0.00142	0.74691

* Total *	-1.00000	33.99592	57.71999	0.28408	92.00000

3-INT1

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.46187	9.99844	2.41691	0.12279	12.53813
C	2	-0.60348	1.99928	4.57175	0.03244	6.60348
O	3	-1.22714	1.99987	7.20528	0.02199	9.22714
O	4	-1.10642	1.99987	7.08874	0.01780	9.10642
H	5	0.51922	0.00000	0.47979	0.00098	0.48078
Cl	6	-0.10763	9.99967	7.08878	0.01918	17.10763
Cl	7	-0.10754	9.99967	7.08865	0.01923	17.10754

O	8	-0.88362	1.99980	6.86391	0.01991	8.88362
O	9	-0.88365	1.99980	6.86393	0.01991	8.88365
C	10	-0.31536	1.99950	4.30054	0.01532	6.31536
H	11	0.20848	0.00000	0.79044	0.00108	0.79152
H	12	0.22138	0.00000	0.77799	0.00063	0.77862
H	13	0.21474	0.00000	0.78410	0.00116	0.78526
C	14	-0.31526	1.99950	4.30046	0.01530	6.31526
H	15	0.22136	0.00000	0.77801	0.00063	0.77864
H	16	0.20846	0.00000	0.79046	0.00108	0.79154
H	17	0.21482	0.00000	0.78403	0.00115	0.78518
H	18	0.27980	0.00000	0.71824	0.00196	0.72020

* Total *	-1.00000	43.99541	63.69202	0.31257	108.00000

3-INT2

Natural Population

		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
P	1	2.42767	9.99843	2.45180	0.12211	12.57233
C	2	-0.62642	1.99917	4.59526	0.03198	6.62642
O	3	-1.23251	1.99987	7.21078	0.02186	9.23251
O	4	-0.87118	1.99980	6.84996	0.02142	8.87118
O	5	-0.89345	1.99982	6.87028	0.02336	8.89345
O	6	-1.11592	1.99988	7.09870	0.01734	9.11592
C	7	-0.31474	1.99951	4.29886	0.01636	6.31474
H	8	0.19765	0.00000	0.80024	0.00210	0.80235
H	9	0.20598	0.00000	0.79332	0.00070	0.79402
H	10	0.19895	0.00000	0.79941	0.00164	0.80105
H	11	0.29995	0.00000	0.69841	0.00164	0.70005
C	12	-0.31178	1.99950	4.29693	0.01536	6.31178
H	13	0.21367	0.00000	0.78569	0.00065	0.78633
H	14	0.20984	0.00000	0.78888	0.00128	0.79016
H	15	0.21566	0.00000	0.78316	0.00118	0.78434
H	16	0.53080	0.00000	0.46802	0.00118	0.46920
Cl	17	-0.06440	9.99967	7.04505	0.01969	17.06440
Cl	18	-0.06977	9.99967	7.05051	0.01959	17.06977

* Total *	-1.00000	43.99531	63.68527	0.31942	108.00000

3-INT3

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.41007	9.99849	2.46443	0.12701	12.58993
C	2	-0.62772	1.99914	4.59682	0.03177	6.62772
O	3	-1.20973	1.99987	7.18784	0.02202	9.20973
O	4	-1.06045	1.99985	7.04401	0.01659	9.06045
H	5	0.55264	0.00000	0.44499	0.00237	0.44736
O	6	-0.89843	1.99982	6.87619	0.02243	8.89843
O	7	-0.91075	1.99984	6.89032	0.02059	8.91075
C	8	-0.31562	1.99951	4.30022	0.01589	6.31562
H	9	0.19668	0.00000	0.80176	0.00156	0.80332
H	10	0.20842	0.00000	0.79091	0.00067	0.79158
H	11	0.20225	0.00000	0.79619	0.00156	0.79775
C	12	-0.31563	1.99952	4.29892	0.01719	6.31563
H	13	0.20771	0.00000	0.79142	0.00087	0.79229
H	14	0.20653	0.00000	0.79187	0.00160	0.79347
H	15	0.17647	0.00000	0.82179	0.00174	0.82353
H	16	0.29160	0.00000	0.70661	0.00179	0.70840
Cl	17	-0.05366	9.99967	7.03456	0.01943	17.05366
Cl	18	-0.06036	9.99966	7.04131	0.01939	17.06036
* Total *		-1.00000	43.99536	63.68016	0.32448	108.00000

3-INT4

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.47053	9.99838	2.40890	0.12219	12.52947
O	2	-0.89140	1.99981	6.86713	0.02446	8.89140
O	3	-1.07011	1.99985	7.05294	0.01733	9.07011
H	4	0.53605	0.00000	0.46209	0.00186	0.46395
O	5	-1.21991	1.99987	7.19854	0.02150	9.21991
O	6	-0.88102	1.99979	6.86008	0.02114	8.88102
C	7	-0.62395	1.99931	4.59252	0.03212	6.62395
Cl	8	-0.12444	9.99969	7.10563	0.01912	17.12444
Cl	9	-0.11145	9.99968	7.09404	0.01773	17.11145
C	10	-0.30794	1.99949	4.29328	0.01516	6.30794
H	11	0.21731	0.00000	0.78136	0.00133	0.78269
H	12	0.21536	0.00000	0.78408	0.00057	0.78464
H	13	0.21338	0.00000	0.78517	0.00145	0.78662
C	14	-0.31382	1.99951	4.29836	0.01596	6.31382
H	15	0.20688	0.00000	0.79238	0.00074	0.79312

H	16	0.20278	0.00000	0.79577	0.00145	0.79722
H	17	0.19627	0.00000	0.80217	0.00157	0.80373
H	18	0.28549	0.00000	0.71267	0.00185	0.71451

* Total *	-1.00000	43.99538	63.68710	0.31751	108.00000

4-INT1

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.50567	9.99837	2.37086	0.12510	12.49433
C	2	-0.46403	1.99956	4.41956	0.04491	6.46403
O	3	-1.20019	1.99986	7.17785	0.02247	9.20019
O	4	-1.10464	1.99986	7.08714	0.01763	9.10464
H	5	0.52932	0.00000	0.46973	0.00094	0.47068
Cl	6	-0.05970	9.99957	7.03982	0.02032	17.05970
Cl	7	-0.06971	9.99958	7.04986	0.02027	17.06971
Cl	8	-0.06039	9.99957	7.04061	0.02021	17.06039
O	9	-0.87650	1.99980	6.85639	0.02031	8.87650
O	10	-0.87567	1.99980	6.85544	0.02043	8.87567
C	11	-0.31682	1.99949	4.30223	0.01509	6.31682
H	12	0.21230	0.00000	0.78666	0.00105	0.78770
H	13	0.22553	0.00000	0.77392	0.00055	0.77447
H	14	0.21636	0.00000	0.78244	0.00120	0.78364
C	15	-0.31625	1.99949	4.30172	0.01504	6.31625
H	16	0.22563	0.00000	0.77383	0.00055	0.77437
H	17	0.21183	0.00000	0.78716	0.00101	0.78817
H	18	0.21727	0.00000	0.78159	0.00114	0.78273

* Total *	-1.00000	53.99496	69.65681	0.34823	124.00000

4-INT2

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.51584	9.99844	2.36258	0.12314	12.48416
O	2	-0.89237	1.99980	6.86849	0.02407	8.89237
O	3	-1.05744	1.99984	7.04053	0.01707	9.05744
H	4	0.54045	0.00000	0.45769	0.00186	0.45955
O	5	-1.19586	1.99986	7.17363	0.02236	9.19586
O	6	-0.87623	1.99979	6.85474	0.02171	8.87623
C	7	-0.48377	1.99962	4.43995	0.04420	6.48377

Cl	8	-0.08112	9.99960	7.06153	0.01999	17.08112
Cl	9	-0.08008	9.99960	7.06140	0.01907	17.08008
Cl	10	-0.04128	9.99955	7.02013	0.02161	17.04128
C	11	-0.30954	1.99949	4.29518	0.01487	6.30954
H	12	0.22058	0.00000	0.77811	0.00130	0.77942
H	13	0.22073	0.00000	0.77876	0.00051	0.77927
H	14	0.21569	0.00000	0.78295	0.00136	0.78431
C	15	-0.31701	1.99950	4.30191	0.01559	6.31701
H	16	0.21288	0.00000	0.78650	0.00063	0.78712
H	17	0.20800	0.00000	0.79067	0.00132	0.79200
H	18	0.20052	0.00000	0.79805	0.00143	0.79948

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* Total *	-1.00000	53.99510	69.65281	0.35209	124.00000