

Intermolecular Proton Transfer in Cyclic Carbonate Synthesis from Epoxide and Carbon Dioxide Catalyzed by Azaphosphatranes: A DFT Mechanistic Study

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Electronic Supporting Information

Computational Methods

All calculations were carried out with use of Gaussian 09 software package.¹ The B3LYP exchange-correlation functional²⁻⁵ was used in all cases. For the geometry optimization, the polarized split-valence 6-31G(d)^{6, 7} basis set was employed for all atoms. All geometries of minima (intermediates) and transition states were optimized for gas phase molecules. The optimization was conducted with tight convergence criteria and an ultrafine grid. The transition states were confirmed by frequency analysis in which there is only one imaginary frequency for each transition state. To identify the minima connected to the transition states thus identified, the intrinsic reaction coordinate was followed in forward and reverse directions and the two resulting molecular geometries were used as starting points for subsequent geometry optimizations. For all molecular structures (intermediate or transition states), the calculated electronic energy was improved by a single-point calculation in which the 6-31G(d) basis was replaced by the better polarized valence triple- ζ type 6-311++G(2d,p).⁸⁻¹⁰ The above calculations provided the electronic energies ($E_{electron}$) under vacuum. To model the reaction energies more closed resembling experimental conditions, further terms were added, namely zero-point vibrational energy (ZPE), thermal corrections to Gibbs energy ($G_{correct,gas}$), solvation and entropic effects, as well as empirical dispersion corrections ($G_{correct,sol}$). To calculate the zero-point vibrational energies, frequencies analysis was performed based on the optimized molecular geometries using the same basis set which was 6-31G(d), and the calculated harmonic frequencies were scaled by a factor of 0.9614 which was suggested by Scott.¹¹ The $G_{correct,gas}$ were also calculated with the scaled harmonic frequencies. Solvent effect was included by estimating the Gibbs energies of solvation for all intermediates and transition states using a continuum solvation model SMD.¹² This model is an universal solvation model which is applicable for any charged or uncharged solute in any solvent or liquid medium for which a few key descriptors are known (in particular, dielectric constant, refractive index, bulk surface tension, and acidity and basicity parameters).¹² This model is adopted for the object reaction. The Gibbs energy of solvation for an intermediate or transition state was calculated by taking the difference of resulting energies between gas phase and SMD calculation based on the same geometry optimized at gas phase. The Grimme's D3 parametrization¹³ was used to calculate the dispersion correction for all minima and transition states. The calculation for dispersion correction ($E_{dispersion}$) was also performed using 6-31G(d) basis sets based on the geometry optimized at gas phase.

For an intermediate or transition state, the Gibbs energy in gas phase (G_{gas}) was calculated as equation (1):

$$G_{gas} = E_{electron} + E_{dispersion} + ZPE + G_{correct,gas} \quad (1)$$

While the Gibbs energy in solution phase (G_{sol}) was calculated as equation (2):

$$G_{sol} = G_{gas} + G_{correct,sol} \quad (2)$$

Where the empirical dispersion correction has been included in the $G_{correct,sol}$.

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Formation of cyclic carbonate from epoxide and CO₂ without catalysts.

In order to test the role of the catalyst, the objective reaction was investigated using the same method but with the absent catalyst. The first step, namely the epoxide ring opening reaction, is found to be impossible without catalyst as illustrated in **Chart S1**, because the ring opened intermediate **7** does not really exist owing to the high reactivity of oxide anion. Molecular geometric optimizations for **7** always lead to a complex of **1** and chloride anion as illustrated.

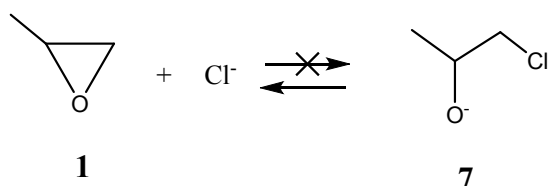


Chart S1 Epoxide ring opening step for cyclic carbonates synthesis.

Thus three elementary reactions in the objective reaction were explored and discussed individually. The model for the second elementary reaction is **8** converting to CO₂ adduct **9**. The species **8** is protonated **7**. The Gibbs free energy profiles of this reaction were depicted in **Fig. S1a**.

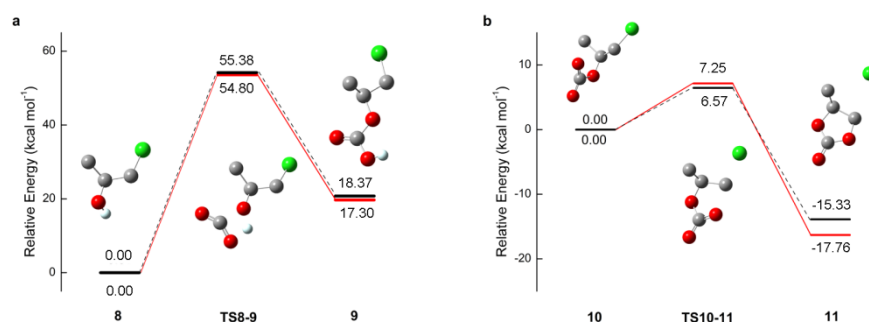


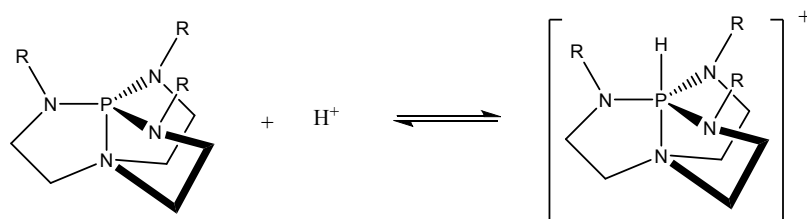
Fig. S1 B3LYP/6-31G(d) optimized structures for cyclic carbonate synthesis from epoxide and carbon dioxide without catalyst. **a**) carbon dioxide addition step. **b**) carbonate ring-closure step. Hydrogens are omitted for clarity except for the one participating the proton transfer. All relative energies were calculated according to the law of Mass Conservation. — $\Delta_r G_{gas}$, — $\Delta_r G_{sol}$. Color code: C, gray; P, orange; Cl, green; O, red; N, navy; H, lightblue.

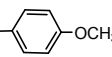
The calculated barriers ($\Delta^\ddagger G_{gas} = 55.38$, $\Delta^\ddagger G_{sol} = 54.80$ kcal mol⁻¹) of this elementary reaction are extremely higher than that of the catalyzed reaction with catalyst **C2a** or **C1a**. The thirdly elementary reaction corresponds to the formation of **2**, whereas we have failed to locate the transition states corresponding to the conversion of **9** to **2**. The conversion of **9** to **2** seems to be impossible without intermolecular proton transfer. The conversion requires a proton leaving process, however, the proton in free stage is dynamically much unfavored. Thus we use **10**, the deprotonated **9**, as the reactant of the thirdly elementary reaction. The Gibbs energy profiles of the thirdly

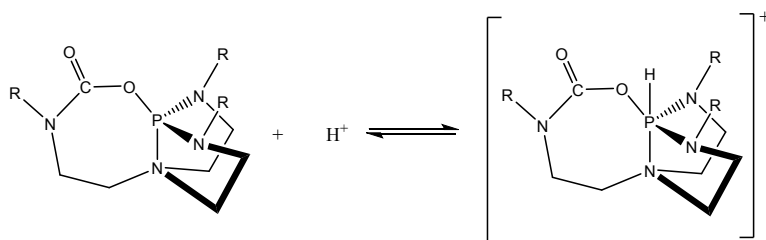
elementary reaction were depicted in **Fig. S1b**. The calculated barrier ($\Delta^\ddagger G_{gas} = 6.57$, $\Delta^\ddagger G_{sol} = 7.25$ kcal mol⁻¹) for the third step is about tenth of the barrier for the second step. The formation of **2** is therefore a fast process compared with the CO₂ addition process. Furthermore, the third step without catalyst is even faster than with catalysts. Thus, the CO₂ addition is generally the rate determining step in which catalyst with high proton affinity will accelerate the reaction rate. The catalytic activity is related to the alkalinity of the catalyst, and a catalyst with strong alkalinity may show high catalytic activity.

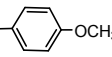
Proton affinity of azaphosphatranes and their CO₂ inserted derivatives

Table S1 The protonation Gibbs free energies of azaphosphatranes



B	A	R=	$\Delta G_{sol}/\text{Hartree}$	${}^a\Delta\Delta G_{sol}/\text{kcal mol}^{-1}$
15	12	-CH ₃	-0.31475199	0.00
17	18	-CH ₂ - 	-0.32049344	-3.60
19	20	-CH ₂ -t-C ₄ H ₉	-0.31753482	-1.75



B	A	R=	$\Delta G_{sol}/\text{Hartree}$	${}^a\Delta\Delta G_{sol}/\text{kcal mol}^{-1}$
16	14	-CH ₃	-0.29293879	13.69
22	21	-CH ₂ - 	-0.29511370	12.32

$${}^a\Delta\Delta G_{sol} = \Delta_{A-B}G_{sol} - \Delta_{12-15}G_{sol}$$

CO₂ insertion into the P–N bond of Catalyst C1a.

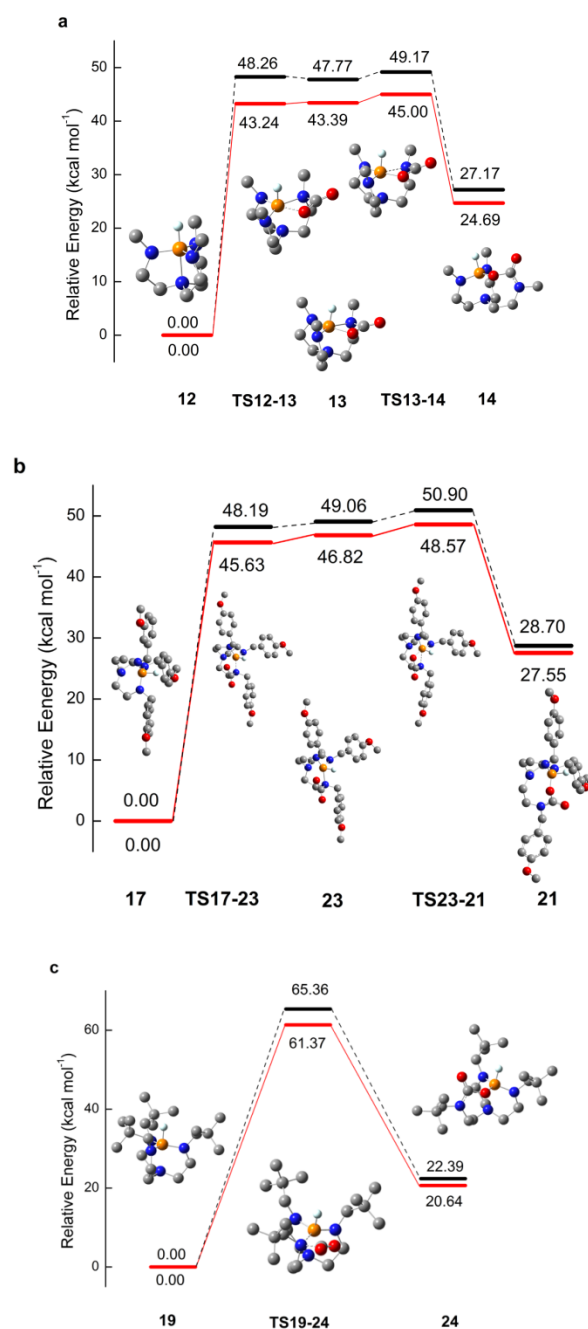


Fig. S2 a) B3LYP/6-31G(d) optimized structures for CO₂ insertion into P–N bond of the acidic form of **C1a**. b) B3LYP/6-31G(d) optimized structures for CO₂ insertion into P–N bond of the acidic form of **C1b**. c) B3LYP/6-31G(d) optimized structures for CO₂ insertion into P–N bond of the acidic form of **C1c**. Hydrogens are omitted for clarity except for the P–H moiety of **C1a**–**C1c**. Each energy reference was calculated as the sum of corresponding azaphosphatrane and CO₂ and defined as zero. Other relative energies were calculated according to the law of Mass Conservation and with respect to corresponding reference. — Δ_rG_{gas}, — Δ_rG_{sol}. Color code: C, gray; P, orange; Cl, green; O, red; N, navy-blue; H, light-blue.

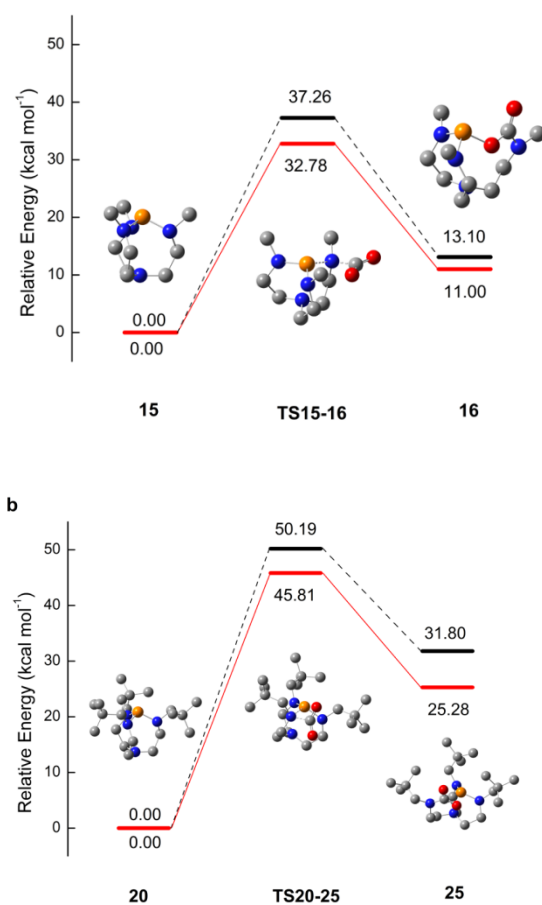


Fig. S3 a) B3LYP/6-31G(d) optimized structures for CO₂ insertion into P–N bond of the basic form of **C1a**. **b)** B3LYP/6-31G(d) optimized structures for CO₂ insertion into P–N bond of the acidic form of **C1c**. Each energy reference was calculated as the sum of corresponding azaphosphatrane and CO₂ and defined as zero. Other relative energies were calculated according the law of Mass Conservation and with respect to corresponding reference. — $\Delta_r G_{gas}$, - - $\Delta_r G_{sol}$. Color code: C, gray; P, orange; Cl, green; O, red; N, navy-blue.

Energies and corrections to Gibbs free energy of all molecular structures

Table S2 Electronic energies ($E_{electron}$), zero-point vibrational energy (ZPE), thermal corrections to Gibbs energy ($G_{correct,gas}$) at 100 °C and 1.0 atm, solvent effect in toluene solution ($G_{correct,sol}$), empirical dispersion corrections ($E_{dispersion}$). All energies are given in Hartree.

Structure	$E_{electron}$	ZPE	$G_{correct,gas}$	$G_{correct,sol}$	$E_{dispersion}$
CO₂	-188.65033425	0.011145	-0.026986	-0.000068	-0.000189
HCl	-460.83557820	0.006436	-0.023322	-0.003875	-0.000003
H+	0.00000000	0.000000	-0.013178	-0.127054	0.000000
C1a	-1376.98465020	0.317106	-0.059999	-0.027459	-0.048884
C1b	-2414.00460490	0.646282	-0.109350	-0.046902	-0.100228
C1c	-1848.87971208	0.644636	-0.088866	-0.034243	-0.108307
C2a	-1565.59230689	0.328412	-0.066668	-0.027856	-0.056847
C2b	-2602.62880400	0.661378	-0.113834	-0.051082	-0.107101
1	-193.17299603	0.082617	-0.034714	-0.004746	-0.004084
2	-381.84539003	0.099451	-0.040469	-0.009078	-0.007947
TS1-3	-1570.11444463	0.398927	-0.078226	-0.045548	-0.055654
3	-1570.18255331	0.398792	-0.079932	-0.016228	-0.056382
TS3-4	-1758.79470910	0.407967	-0.081130	-0.020521	-0.069214
4	-1758.81552002	0.415334	-0.081367	-0.029367	-0.062288
TS4-2	-1758.79356245	0.415350	-0.080351	-0.037940	-0.061607
TS1-5	-1758.73706325	0.412896	-0.083929	-0.049440	-0.063610
5	-1758.83507702	0.414407	-0.083738	-0.018407	-0.062667
TS5-6	-1947.43440884	0.423795	-0.084954	-0.024606	-0.075764
6	-1947.48068836	0.429171	-0.088640	-0.019933	-0.066941
TS6-2	-1947.41681316	0.428574	-0.087826	-0.040025	-0.067850
8	-654.05214866	0.096262	-0.039994	-0.008030	-0.008801
TS8-9	-842.62781804	0.105527	-0.047530	-0.009023	-0.012969
9	-842.69331862	0.111165	-0.047139	-0.009797	-0.012472
10	-842.15447085	0.097952	-0.046419	-0.049058	-0.013018
TS10-11	-842.14603032	0.097761	-0.044777	-0.047962	-0.012441
11	-842.18099642	0.099988	-0.046933	-0.052941	-0.012436
12	-916.55179473	0.316352	-0.056477	-0.052802	-0.040082
TS12-13	-1105.13972880	0.329852	-0.058503	-0.060880	-0.053066
13	-1105.14057077	0.330508	-0.059565	-0.059841	-0.052618
TS13-14	-1105.13986459	0.330093	-0.058853	-0.059511	-0.051383
14	-1105.17566895	0.331008	-0.062044	-0.056824	-0.048364
15	-916.12174905	0.301174	-0.058770	-0.010580	-0.039895
TS15-16	-1104.73168884	0.315968	-0.060021	-0.017788	-0.050487
16	-1104.77053260	0.316190	-0.063704	-0.013987	-0.046688
17	-1953.57900478	0.645590	-0.107160	-0.065856	-0.091467
18	-1953.14014202	0.631133	-0.106058	-0.030167	-0.091940

19	-1388.45173775	0.643823	-0.084473	-0.055926	-0.101548
20	-1388.01821396	0.628632	-0.085793	-0.016108	-0.100612
21	-2142.20529279	0.660832	-0.109652	-0.067929	-0.100507
22	-2141.78933521	0.646171	-0.110928	-0.032697	-0.100414
TS17-23	-2142.16231287	0.659032	-0.106829	-0.070194	-0.107168
23	-2142.16409709	0.659865	-0.107873	-0.069619	-0.105915
TS23-21	-2142.16404679	0.659650	-0.105926	-0.069747	-0.104622
TS19-24	-1577.01006966	0.656562	-0.089090	-0.062362	-0.113541
24	-1577.08556450	0.658010	-0.090789	-0.058787	-0.106276
TS20-25	-1576.60455995	0.642676	-0.089744	-0.023160	-0.110742
25	-1576.63866420	0.643564	-0.092517	-0.026565	-0.104060

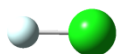
Optimized Cartesian coordinates (Å) from B3LYP/6-31G(d) calculations.

Structure CO₂



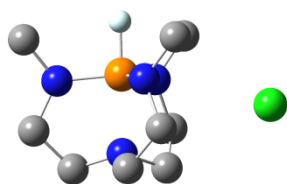
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169160
O	0.000000	0.000000	-1.169160

Structure of HCl



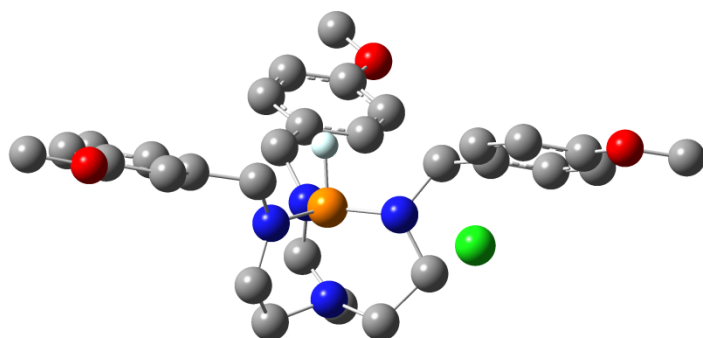
Cl	0.000000	0.000000	0.071641
H	0.000000	0.000000	-1.217896

Structure of C1a



P	0.518881	0.545661	0.491174
N	0.530581	-1.106722	-0.776037
N	-0.093584	1.412993	-0.834206
C	-0.518716	0.678649	-2.028619
C	0.379109	-0.546589	-2.145547
C	1.834118	-1.770552	-0.553602
C	2.856396	-0.663854	-0.313128
N	2.223255	0.333763	0.529179
N	-0.361897	-0.433921	1.534733
C	-0.780994	-1.780968	1.154588
C	-0.639659	-1.923022	-0.357420
C	3.087780	1.456277	0.874922
C	-1.137790	0.145457	2.639116
C	-0.931085	2.598741	-0.581161
H	0.541786	1.657829	1.356642
H	-0.387257	1.315502	-2.912801
H	-1.580538	0.406235	-1.937035
H	-0.035310	-1.306422	-2.816731
H	1.372138	-0.264335	-2.506287
H	1.741142	-2.394509	0.338386
H	2.096442	-2.410356	-1.403924
H	3.741198	-1.076589	0.189052
H	3.206330	-0.229242	-1.266162
H	-1.841657	-1.907124	1.393159
H	-0.195670	-2.531171	1.709324
H	-0.507700	-2.961423	-0.683335
H	-1.544409	-1.489447	-0.799505
H	3.983657	1.086292	1.388887
H	3.408731	2.024489	-0.012420
H	2.573689	2.140596	1.553356
H	-0.737061	1.123792	2.916212
H	-2.186843	0.249977	2.336856
H	-1.058294	-0.506745	3.517449
H	-0.585065	3.122853	0.313809
H	-0.828299	3.285334	-1.430006
H	-1.981520	2.306117	-0.457440
Cl	-3.409538	-0.025540	-0.203863

Structure of C1b

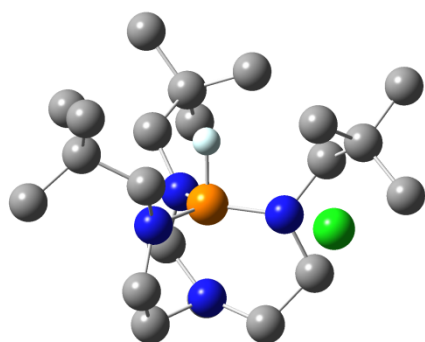


P	-0.367764	-0.084567	0.542573
N	-0.320828	0.000993	2.603739
N	0.367695	-1.599470	0.724552
C	0.710619	-2.115162	2.045651
C	0.778628	-0.925706	2.994829
C	-0.033124	1.423474	2.926334
C	0.906925	1.951155	1.850839
N	0.482711	1.376542	0.564754
N	-2.076710	-0.016325	0.722906
C	-2.667993	0.120348	2.045351
C	-1.663674	-0.434452	3.051069
C	1.458978	1.633061	-0.533284
C	-2.921479	0.464496	-0.373829
C	0.380223	-2.576939	-0.369903
H	-0.430996	-0.162740	-0.863735
H	1.693299	-2.593977	2.014754
H	-0.025162	-2.873284	2.365012
H	0.667643	-1.215989	4.045674
H	1.743430	-0.418432	2.843423
H	-0.983035	1.965170	2.920580
H	0.405939	1.498104	3.926699
H	0.833632	3.042293	1.801675
H	1.950111	1.668931	2.053533
H	-3.605238	-0.444413	2.100149
H	-2.914448	1.173181	2.264286
H	-1.859767	-0.092451	4.073400
H	-1.684214	-1.526415	3.040062
H	2.414259	1.167066	-0.261460
H	1.077016	1.146352	-1.437543
H	-2.330812	0.436842	-1.296206
H	-3.194804	1.518624	-0.209312
H	0.065153	-2.057007	-1.282751

H	-0.383467	-3.349536	-0.180014
C	1.659992	3.109951	-0.791348
C	2.877871	3.714643	-0.472479
C	0.651397	3.904681	-1.359485
C	3.101487	5.073797	-0.716190
H	3.662991	3.113774	-0.018837
C	0.854956	5.255376	-1.605597
H	-0.307104	3.455499	-1.611694
C	2.086870	5.849291	-1.286147
H	4.060423	5.507936	-0.457131
H	0.081512	5.874434	-2.050165
C	-4.186590	-0.358367	-0.562723
C	-5.419239	0.280085	-0.664784
C	-4.125289	-1.757193	-0.669977
C	-6.595061	-0.455400	-0.884151
H	-5.499411	1.360601	-0.581347
C	-5.291250	-2.484627	-0.882103
H	-3.168478	-2.263621	-0.582120
C	-6.532731	-1.848141	-0.992892
H	-5.244967	-3.567227	-0.967639
H	-7.426305	-2.438577	-1.158962
C	1.719198	-3.257131	-0.607818
C	1.738216	-4.563455	-1.100124
C	2.943006	-2.601349	-0.397868
C	2.937433	-5.212825	-1.406497
H	0.801028	-5.095710	-1.256734
C	4.142641	-3.242076	-0.682095
H	2.981880	-1.602032	0.033968
C	4.150200	-4.545971	-1.197385
H	2.911805	-6.226757	-1.789648
H	5.087378	-2.741206	-0.496405
C	3.416716	7.833505	-1.281385
H	3.283941	8.872621	-1.588853
H	3.650684	7.800100	-0.208943
H	4.250444	7.392570	-1.843699
C	-8.963586	-0.399706	-1.195924
H	-9.733497	0.372917	-1.232658
H	-8.950354	-0.944284	-2.149118
H	-9.192358	-1.101244	-0.382791
C	5.448124	-6.400525	-1.960051
H	6.509753	-6.621525	-2.087477
H	5.009253	-7.127623	-1.262888
H	4.942120	-6.487003	-2.931572
O	2.190070	7.182310	-1.569600

O	5.382713	-5.081023	-1.450735
O	-7.739532	0.282038	-0.968036
Cl	3.832372	0.167338	1.802529

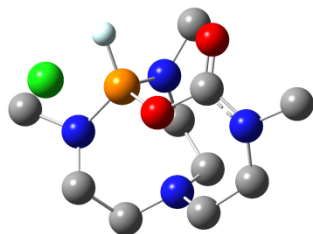
Structure of **C1c**



P	-0.260731	-0.032429	0.377768
N	0.102690	-0.093853	2.419640
N	0.573461	-1.504927	0.318399
C	1.046226	-2.138020	1.546874
C	1.233606	-1.046552	2.586578
C	0.461985	1.294248	2.807931
C	1.211077	1.898807	1.633090
N	0.505793	1.491209	0.404520
N	-1.936779	-0.083948	0.816894
C	-2.293392	0.052054	2.224043
C	-1.159928	-0.556174	3.036966
C	1.162504	1.975427	-0.834431
C	-2.948034	0.420755	-0.128117
C	0.507068	-2.380397	-0.866098
H	-0.535130	-0.000589	-1.002613
H	2.014534	-2.609995	1.379830
H	0.336311	-2.919282	1.871260
H	1.247566	-1.432524	3.612400
H	2.176724	-0.528740	2.357346
H	-0.464426	1.840772	3.006352
H	1.066062	1.281072	3.721321
H	1.199536	2.987156	1.724841
H	2.254442	1.549243	1.593427
H	-3.224301	-0.477526	2.442473
H	-2.456379	1.109278	2.495642
H	-1.197322	-0.272801	4.095008
H	-1.191372	-1.645891	2.965545
H	2.242244	2.005469	-0.640813
H	1.022805	1.227333	-1.619596
H	-2.437235	0.868743	-0.986266
H	-3.492599	1.243228	0.361247
H	-0.265958	-1.989210	-1.535479
H	0.143934	-3.362353	-0.523459

C	0.673634	3.335240	-1.403493
C	-0.808335	3.255412	-1.807366
C	0.863087	4.498529	-0.412075
C	1.531587	3.607729	-2.656686
H	-0.977638	2.464757	-2.550083
H	-1.442840	3.050695	-0.938089
H	-1.143231	4.201217	-2.250441
H	1.897547	4.557318	-0.053312
H	0.625237	5.453305	-0.897095
H	0.200363	4.402385	0.455294
H	1.233176	4.549215	-3.132909
H	2.595366	3.681528	-2.402160
H	1.421331	2.807940	-3.399355
C	-3.980374	-0.602900	-0.679773
C	-3.273089	-1.686373	-1.510667
C	-4.788051	-1.276807	0.444376
C	-4.944646	0.189952	-1.585205
H	-2.718804	-1.248630	-2.350266
H	-2.568468	-2.257202	-0.897329
H	-4.001934	-2.391499	-1.927585
H	-5.284808	-0.537873	1.086096
H	-5.568286	-1.919610	0.019707
H	-4.151615	-1.911027	1.071391
H	-5.690920	-0.476474	-2.032574
H	-5.483139	0.961187	-1.020288
H	-4.409090	0.686398	-2.403762
C	1.791408	-2.596512	-1.718409
C	2.287853	-1.266695	-2.308848
C	2.941827	-3.242875	-0.921919
C	1.369762	-3.548228	-2.858700
H	1.498343	-0.765728	-2.887121
H	2.649411	-0.601354	-1.517809
H	3.126607	-1.448027	-2.991722
H	2.610997	-4.148386	-0.394533
H	3.742437	-3.542885	-1.609213
H	3.380539	-2.535987	-0.208971
H	2.218429	-3.742881	-3.523777
H	1.023235	-4.515576	-2.471671
H	0.562037	-3.120819	-3.467629
Cl	4.005672	0.010704	0.968566

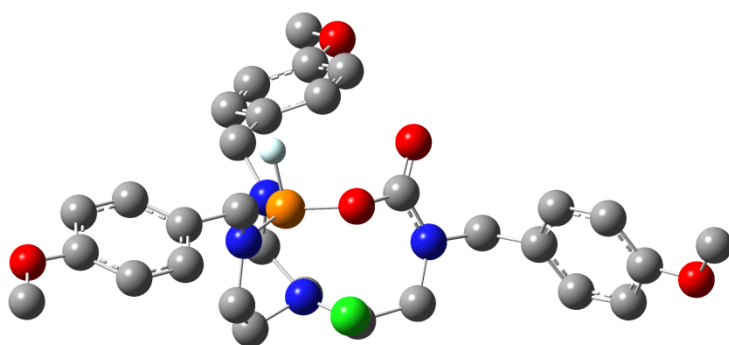
Structure of C2a



P	-0.927621	-0.530257	0.560664
N	0.452859	1.827257	-0.595045
N	-2.040073	0.563776	-0.014346
C	-1.819679	1.210637	-1.318756
C	-0.796935	2.344018	-1.139305
C	0.879726	2.269518	0.716891
C	-0.066379	1.753820	1.825815
N	-0.247148	0.291657	1.862303
N	2.540389	-0.702932	-0.653014
C	2.643186	0.645329	-1.234903
C	1.398314	1.442065	-1.631269
C	0.328360	-0.422367	3.006497
C	3.843803	-1.291892	-0.348375
C	-3.443165	0.290963	0.353128
H	-1.384155	-1.691097	1.170919
H	-2.780914	1.616002	-1.650032
H	-1.509421	0.472558	-2.067929
H	-0.627061	2.855090	-2.100940
H	-1.210783	3.093162	-0.454723
H	1.883980	1.878608	0.906489
H	0.945776	3.370936	0.812136
H	0.328234	2.063827	2.799554
H	-1.047744	2.225024	1.710096
H	3.231137	0.547959	-2.156609
H	3.262941	1.246383	-0.551831
H	1.802354	2.327630	-2.161442
H	0.843251	0.862601	-2.375951
H	1.423800	-0.373677	3.018300
H	-0.058357	0.002234	3.940920
H	0.054965	-1.478895	2.964567
H	3.709733	-2.333764	-0.063039
H	4.479469	-1.232425	-1.237962
H	4.342316	-0.761242	0.475075
H	-3.494942	-0.067522	1.386342
H	-3.993224	1.236334	0.303966

H	-3.879759	-0.463647	-0.308993
O	0.259197	-0.817007	-0.531654
C	1.467999	-1.283012	-0.046528
O	1.524537	-2.160051	0.794751
Cl	-2.248866	-2.308150	-1.186595

Structure of C2b

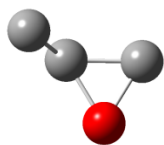


P	0.892438	0.643774	-0.124629
N	0.494873	0.013860	1.883100
N	2.427733	0.055609	0.129546
C	2.810147	-0.531838	1.424240
C	1.864997	0.035206	2.467324
C	-0.374572	1.047563	2.483432
C	0.006412	2.373634	1.832949
N	0.283496	2.119965	0.422316
N	-2.189298	-0.832137	0.532610
C	-1.538854	-1.580550	1.621263
C	-0.044373	-1.389774	1.907854
C	0.397446	3.341328	-0.408498
C	-3.666805	-0.868083	0.545834
C	3.131955	-0.560584	-1.048707
H	1.147868	1.110457	-1.421522
H	3.838552	-0.238987	1.655251
H	2.750462	-1.629119	1.359073
H	1.890747	-0.540441	3.399008
H	2.115941	1.075504	2.695648
H	-1.409478	0.811405	2.238053
H	-0.265433	1.076768	3.574324
H	-0.822448	3.082965	1.914870
H	0.878673	2.835174	2.321962
H	-1.666384	-2.657670	1.454648
H	-2.120927	-1.334824	2.518509
H	0.112206	-1.783042	2.921566
H	0.567793	-2.010217	1.236720
H	1.213043	3.966043	-0.016091
H	0.690031	3.034271	-1.416403
H	-3.994438	-0.124209	-0.181874
H	-3.998326	-0.542167	1.539391
H	2.818704	-0.009748	-1.941633
H	2.791522	-1.599963	-1.125915

O	-0.215516	-0.504739	-0.565187
C	-1.587573	-0.326242	-0.575837
O	-2.150292	0.218447	-1.506626
C	-0.880151	4.154193	-0.462865
C	-2.056749	3.619820	-1.018687
C	-0.908521	5.465295	0.013877
C	-3.214348	4.380563	-1.089614
H	-2.066637	2.599758	-1.394681
C	-2.066702	6.246816	-0.055336
H	-0.008650	5.900294	0.444671
C	-3.228801	5.701485	-0.610343
H	-4.125087	3.976890	-1.520980
H	-2.047856	7.262654	0.322233
C	-4.244820	-2.233109	0.232020
C	-4.080149	-2.801136	-1.036109
C	-4.953330	-2.961382	1.197385
C	-4.594641	-4.061664	-1.338572
H	-3.540902	-2.252152	-1.803736
C	-5.479953	-4.215370	0.910910
H	-5.098858	-2.540392	2.190381
C	-5.298873	-4.777337	-0.360461
H	-4.442077	-4.472569	-2.329722
H	-6.027909	-4.782623	1.656631
C	4.634322	-0.517213	-0.906976
C	5.332558	-1.688807	-0.600077
C	5.362980	0.669240	-1.087246
C	6.725573	-1.689129	-0.479663
H	4.772324	-2.609187	-0.443879
C	6.745971	0.685285	-0.968336
H	4.838583	1.592000	-1.328352
C	7.437198	-0.498872	-0.664599
H	7.235735	-2.616027	-0.243523
H	7.318092	1.596698	-1.113222
O	-4.416004	6.360076	-0.730656
O	-5.843665	-6.012773	-0.545408
O	8.795420	-0.380796	-0.572648
C	-4.488494	7.705273	-0.284001
H	-3.787915	8.349853	-0.830920
H	-5.510432	8.031953	-0.483768
H	-4.286568	7.784715	0.792479
C	-5.651274	-6.653206	-1.798402
H	-6.141966	-7.624491	-1.714888
H	-6.111313	-6.084475	-2.617225
H	-4.585635	-6.801672	-2.014897

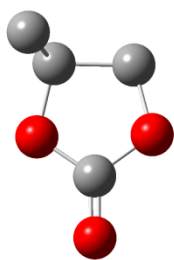
C	9.549940	-1.547395	-0.285678
H	10.594811	-1.231386	-0.267798
H	9.282951	-1.972059	0.691160
H	9.416271	-2.315525	-1.058706
Cl	2.004593	-3.650467	0.321253

Structure of 1



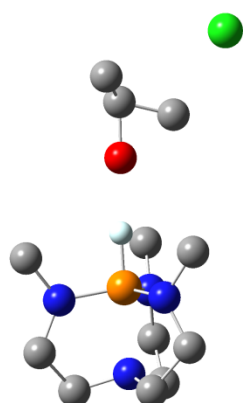
C	1.511499	0.100494	-0.148695
C	0.152115	-0.037588	0.489186
H	2.078324	-0.833080	-0.055847
H	1.416001	0.336765	-1.213308
H	2.089025	0.896380	0.336954
C	-1.045067	0.615258	-0.060247
H	0.155684	-0.255398	1.560129
H	-1.875100	0.879958	0.596012
H	-0.958342	1.222026	-0.962775
O	-0.827110	-0.789454	-0.242829

Structure of 2



O	-0.134411	-0.861459	0.576176
C	1.088708	-0.098745	0.498697
C	0.565077	1.315652	0.179861
C	2.004391	-0.688272	-0.564409
H	1.556671	-0.145655	1.485648
H	1.161254	1.838268	-0.571956
H	0.471622	1.943126	1.072969
H	1.544299	-0.614684	-1.556077
H	2.205342	-1.742381	-0.352623
H	2.958718	-0.149319	-0.583019
C	-1.149978	-0.179679	-0.021273
O	-2.243390	-0.617329	-0.223913
O	-0.740586	1.075902	-0.358787

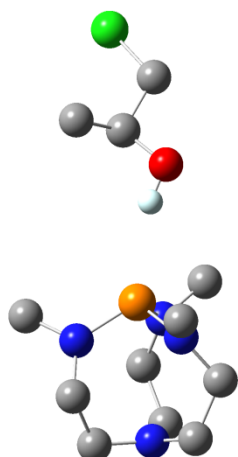
Structure of TS1-3



C	-0.745080	2.727699	-0.746112
N	-1.650869	1.573311	-0.658124
C	-3.059366	1.908727	-0.561199
C	-3.861317	0.612901	-0.657350
N	-3.156496	-0.401063	0.155056
C	-3.263024	-1.777192	-0.375055
C	-2.244002	-1.907687	-1.504066
N	-1.023613	-1.240480	-1.090798
C	0.125269	-1.435208	-1.992188
P	-1.028614	0.106072	-0.060963
N	-1.012837	-0.134491	1.618585
C	0.286881	-0.270660	2.299307
C	-3.417368	-0.296788	1.606614
C	-2.138274	-0.717076	2.326117
H	0.318893	0.431019	-0.200529
H	-2.158561	-0.347844	3.358698
H	-2.052984	-1.815571	2.384838
H	-4.282425	-0.906075	1.896360
H	-3.640651	0.748238	1.834532
H	-3.873687	0.264825	-1.692979
H	-4.898500	0.736459	-0.321950
H	-3.341334	2.577278	-1.384049
H	-3.282152	2.448564	0.375424
H	-2.041073	-2.968400	-1.695726
H	-2.633328	-1.485043	-2.446334
H	-4.286217	-1.994568	-0.705707
H	-3.008137	-2.468458	0.431718
H	-0.956094	3.287104	-1.665197
H	-0.873132	3.404101	0.111435
H	0.295195	2.393586	-0.773377
H	0.984071	-0.852767	-1.645264

H	0.400326	-2.496202	-2.004835
H	-0.124439	-1.126007	-3.017287
H	1.084041	0.160799	1.687500
H	0.247336	0.260097	3.257842
H	0.524701	-1.325859	2.492951
O	2.196576	0.631011	-0.329777
C	3.568329	0.974148	-0.538667
C	3.559630	-0.385979	-0.039866
C	4.133574	2.083239	0.318698
Cl	5.997851	-1.153256	0.115472
H	3.835671	1.085092	-1.596539
H	3.576348	-0.570466	1.021967
H	3.475703	-1.220539	-0.716039
H	3.828180	1.951038	1.362838
H	3.783754	3.065584	-0.024330
H	5.226835	2.052508	0.273257

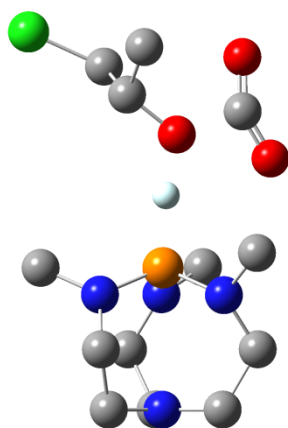
Structure of **3**



C	-0.581743	-0.864358	2.579533
N	-1.342517	-0.885354	1.339614
C	-2.723982	-1.351024	1.394237
C	-3.815556	-0.259708	1.370129
N	-3.805400	0.609906	0.211385
C	-3.261558	1.947481	0.334253
C	-1.785431	2.029065	0.775573
N	-0.812666	1.353739	-0.077293
C	0.029227	2.174357	-0.941345
P	-0.559420	-0.347051	-0.097249
N	-1.610752	-0.901947	-1.342589
C	-1.387740	-2.238435	-1.874659
C	-3.967602	0.033602	-1.108082
C	-2.672858	-0.097610	-1.936580
H	1.768724	-0.582050	-0.757547
H	-2.919650	-0.530082	-2.915777
H	-2.290708	0.912332	-2.131129
H	-4.672309	0.644150	-1.700349
H	-4.436274	-0.950990	-0.990310
H	-3.732368	0.370353	2.264017
H	-4.789721	-0.775324	1.444038
H	-2.843504	-1.951426	2.306732
H	-2.904862	-2.029220	0.551337
H	-1.496559	3.086417	0.845758
H	-1.715069	1.621748	1.792103
H	-3.850235	2.525924	1.068567
H	-3.390566	2.452709	-0.630534
H	-0.881903	-0.054244	3.263164
H	-0.684937	-1.816028	3.119760
H	0.481542	-0.722633	2.352412

H	0.886649	1.585895	-1.287522
H	-0.500501	2.551878	-1.830262
H	0.420099	3.040694	-0.389910
H	-0.416774	-2.611850	-1.528854
H	-2.152955	-2.965273	-1.558791
H	-1.367659	-2.225316	-2.973329
O	2.645346	-0.374384	-1.148685
C	3.595066	-0.308100	-0.089011
C	4.825733	0.321439	-0.743332
C	3.863014	-1.689464	0.508530
Cl	6.128931	0.708677	0.461423
H	3.245072	0.372414	0.703490
H	5.262190	-0.353682	-1.482279
H	4.551658	1.259271	-1.227288
H	4.201907	-2.377308	-0.274599
H	2.942426	-2.096420	0.942465
H	4.622911	-1.646498	1.295350

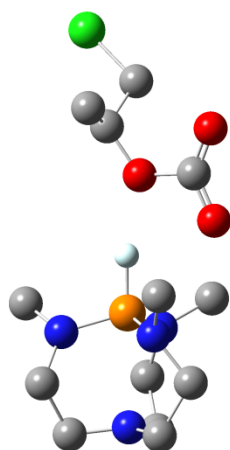
Structure of TS3-4



C	-0.395149	-2.656538	-0.459880
N	-1.173553	-1.468503	-0.803753
C	-2.384554	-1.648095	-1.605583
C	-3.691463	-1.642256	-0.786798
N	-3.832600	-0.455708	0.029430
C	-3.770742	-0.555974	1.470716
C	-2.370917	-0.952924	1.978814
N	-1.294510	-0.069218	1.528368
C	-0.827371	0.954440	2.473113
P	-0.775306	0.004879	-0.076531
N	-1.582785	1.211580	-0.934588
C	-0.787035	2.049163	-1.848987
C	-4.043736	0.829866	-0.600139
C	-2.847690	1.788329	-0.464074
H	0.778509	0.301581	-0.188732
H	-3.041121	2.690014	-1.055518
H	-2.758692	2.116759	0.581328
H	-4.934813	1.332795	-0.186566
H	-4.246140	0.656249	-1.663201
H	-3.722175	-2.516739	-0.126396
H	-4.538296	-1.748920	-1.486831
H	-2.287211	-2.590554	-2.158089
H	-2.431386	-0.844046	-2.348415
H	-2.356456	-0.964472	3.075280
H	-2.157039	-1.977993	1.655172
H	-4.499955	-1.290636	1.854964
H	-4.054077	0.415323	1.892197
H	-0.904112	-3.312547	0.261605
H	-0.181205	-3.240249	-1.363117
H	0.563812	-2.361641	-0.021688

H	-0.039770	1.560376	2.016105
H	-1.640229	1.630366	2.773381
H	-0.425378	0.476755	3.375438
H	0.185104	1.586561	-2.030885
H	-1.308930	2.157255	-2.807755
H	-0.597427	3.037937	-1.417439
O	2.059767	0.723012	-0.405086
C	3.070469	-0.241435	-0.670440
C	3.775020	-0.614362	0.643246
C	4.025497	0.242693	-1.761038
Cl	4.751755	-2.148711	0.474354
H	2.550911	-1.144826	-1.029969
H	4.456776	0.167815	0.971620
H	3.037470	-0.809083	1.424045
H	4.530506	1.156497	-1.438032
H	3.459775	0.461392	-2.672915
H	4.775869	-0.520767	-1.991424
C	2.372435	2.243945	0.400489
O	1.270142	2.707715	0.591781
O	3.553965	2.409464	0.542923

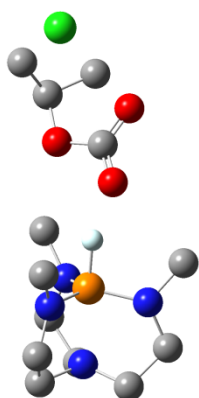
Structure of 4



C	0.156869	1.994074	0.182267
N	-1.218790	1.557190	-0.107061
C	-2.215312	2.581345	0.152297
C	-3.576773	2.073687	-0.311790
N	-3.681498	0.663430	0.100611
C	-4.438194	-0.185710	-0.836143
C	-3.501734	-0.525807	-1.992293
N	-2.194478	-0.844374	-1.448855
C	-1.250597	-1.425163	-2.421789
P	-1.568533	-0.108071	-0.052242
N	-1.956895	-0.787900	1.455744
C	-1.095479	-1.865653	1.976719
C	-4.026639	0.467315	1.519953
C	-3.304756	-0.791216	1.994212
H	-0.259732	-0.607164	-0.150457
H	-3.263570	-0.800389	3.090694
H	-3.852620	-1.701260	1.693119
H	-5.113450	0.401520	1.662256
H	-3.661001	1.332428	2.078674
H	-3.630548	2.111416	-1.402533
H	-4.402998	2.672825	0.093243
H	-1.955884	3.495232	-0.396849
H	-2.236044	2.853843	1.222044
H	-3.892611	-1.393054	-2.538637
H	-3.446604	0.303807	-2.718703
H	-5.356892	0.311501	-1.174795
H	-4.718335	-1.102121	-0.310879
H	0.435774	2.793329	-0.515412
H	0.233997	2.386746	1.207001
H	0.871251	1.172775	0.080384

H	-0.313918	-1.705875	-1.929679
H	-1.701091	-2.328418	-2.850393
H	-1.039734	-0.721045	-3.240087
H	-0.145596	-1.899109	1.434498
H	-0.902456	-1.690678	3.042252
H	-1.588911	-2.842104	1.866540
O	2.514896	-0.336601	0.398980
C	3.844119	0.131836	0.657168
C	4.587704	0.420150	-0.655571
C	4.613012	-0.786812	1.606386
Cl	5.953637	1.615552	-0.381918
H	3.679601	1.096835	1.152492
H	5.024911	-0.473660	-1.089573
H	3.916059	0.891562	-1.374397
H	4.755752	-1.765820	1.144338
H	4.048389	-0.912090	2.536836
H	5.589493	-0.354244	1.849959
C	2.340174	-1.565688	-0.339389
O	1.124480	-1.894948	-0.366971
O	3.336901	-2.096286	-0.829624

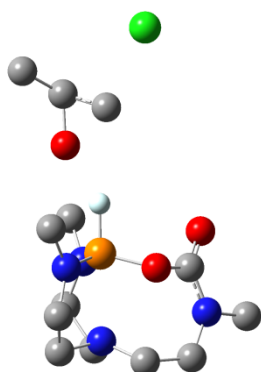
Structure of TS4-2



C	-0.166684	1.977186	-0.326834
N	1.203350	1.559742	0.011913
C	2.200115	2.586301	-0.237591
C	3.546631	2.087357	0.275641
N	3.650074	0.660224	-0.091330
C	4.405828	-0.152025	0.884126
C	3.459572	-0.449558	2.043659
N	2.157443	-0.775166	1.491399
C	1.189548	-1.307733	2.466358
P	1.590143	-0.095425	0.043269
N	1.990140	-0.857727	-1.419126
C	1.145621	-1.962582	-1.906072
C	4.033816	0.426965	-1.499083
C	3.341513	-0.856835	-1.948513
H	0.287402	-0.585680	0.132694
H	3.310885	-0.894037	-3.044535
H	3.900735	-1.749326	-1.618622
H	5.124319	0.375348	-1.607940
H	3.668829	1.269587	-2.091105
H	3.576094	2.157951	1.365419
H	4.388304	2.662270	-0.130106
H	1.922897	3.508116	0.288468
H	2.249767	2.839245	-1.310610
H	3.839858	-1.302359	2.619011
H	3.401965	0.401877	2.743379
H	5.318018	0.365410	1.206654
H	4.693566	-1.085736	0.395133
H	-0.486014	2.773486	0.355457
H	-0.213181	2.360175	-1.356152
H	-0.868924	1.145299	-0.246814
H	0.271088	-1.626553	1.966105

H	1.631617	-2.183010	2.956468
H	0.947647	-0.562796	3.237925
H	0.188729	-1.984071	-1.377655
H	0.962516	-1.832983	-2.979472
H	1.646137	-2.928846	-1.750102
O	-2.470315	-0.501056	-0.630639
C	-3.835103	-0.001376	-0.684008
C	-4.440801	-0.099466	0.706031
C	-4.631374	-0.769939	-1.730094
Cl	-5.923991	1.723441	0.393713
H	-3.742652	1.046797	-0.963646
H	-5.322996	-0.684741	0.898039
H	-4.026045	0.468066	1.522619
H	-4.723778	-1.823197	-1.442310
H	-4.132226	-0.715690	-2.702943
H	-5.629863	-0.332215	-1.814292
C	-2.307942	-1.460903	0.353946
O	-1.209224	-2.035338	0.401942
O	-3.318021	-1.609026	1.112621

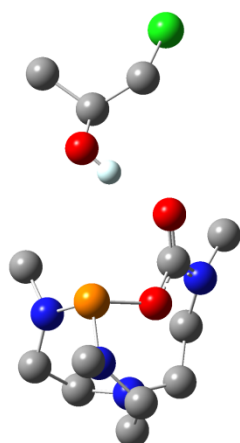
Structure of TS1-5



P	-0.387409	-0.448078	-0.003089
N	-2.780664	-0.980860	-0.176657
N	-0.308215	-1.813591	-0.946209
C	-1.455815	-2.508946	-1.522802
C	-2.657035	-2.386225	-0.590359
C	-3.244064	-0.791052	1.201145
C	-2.063251	-1.061924	2.132909
N	-0.837197	-0.467857	1.600119
N	-2.739568	2.180643	-0.337237
C	-3.758475	1.295254	-0.910225
C	-3.442415	-0.173424	-1.224264
C	0.214811	-0.234236	2.621306
C	-3.263399	3.462567	0.134958
C	1.009139	-2.209828	-1.500637
H	0.963677	-0.135037	0.127916
H	-1.194328	-3.566272	-1.642105
H	-1.682229	-2.122239	-2.527438
H	-3.574391	-2.754676	-1.072967
H	-2.480724	-2.994516	0.300908
H	-3.549949	0.248681	1.322210
H	-4.102300	-1.430768	1.455455
H	-2.265062	-0.614758	3.111987
H	-1.920333	-2.140468	2.301013
H	-4.123130	1.728169	-1.853536
H	-4.611128	1.334571	-0.219711
H	-4.415084	-0.625851	-1.480178
H	-2.817081	-0.228379	-2.115596
H	-0.052762	0.639801	3.224304
H	0.290817	-1.114735	3.270008
H	1.190061	-0.083106	2.149373
H	-2.434083	4.065485	0.500060
H	-3.767369	3.989847	-0.684055

H	-3.984631	3.306372	0.946845
H	1.819407	-1.766462	-0.912022
H	1.094619	-3.299872	-1.436058
H	1.093857	-1.907701	-2.551711
O	-1.002334	0.802879	-0.890633
C	-1.396187	1.973537	-0.234717
O	-0.602961	2.686752	0.331873
C	4.120442	-0.411256	0.900275
C	3.713203	0.470659	-0.171137
O	2.723964	-0.645822	0.654739
H	4.312475	0.073007	1.863860
H	3.775307	0.139031	-1.195169
H	3.341700	1.461234	0.037026
C	5.065559	-1.555385	0.621928
H	4.824563	-2.027487	-0.337119
H	5.011184	-2.316769	1.410093
H	6.085868	-1.163544	0.562310
Cl	5.861015	1.742962	-0.882799

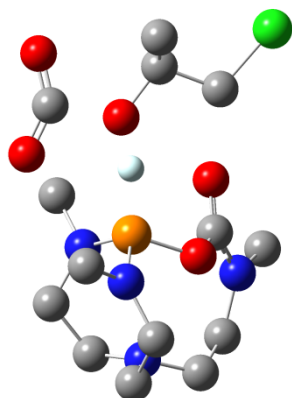
Structure of 5



P	-1.184504	-1.353674	-0.456235
N	-3.101608	1.040544	0.592612
N	-2.796096	-1.504606	-1.044297
C	-3.641701	-0.358044	-1.423555
C	-4.149837	0.483386	-0.240020
C	-2.996248	0.534142	1.940865
C	-2.631671	-0.964006	1.935609
N	-1.395115	-1.297501	1.231716
N	-0.080307	2.307698	-0.385650
C	-1.152037	2.706520	0.549889
C	-2.629916	2.367539	0.256576
C	-0.183638	-1.393474	2.047940
C	1.116463	3.144206	-0.298914
C	-2.981320	-2.668063	-1.922397
H	2.024462	-1.055780	-0.628612
H	-4.520724	-0.766654	-1.938273
H	-3.123084	0.290286	-2.143470
H	-4.791762	1.281047	-0.650598
H	-4.805264	-0.140201	0.380104
H	-2.219522	1.093557	2.472054
H	-3.929044	0.660813	2.528683
H	-2.545101	-1.323679	2.969067
H	-3.446024	-1.527291	1.468300
H	-1.104977	3.800166	0.576434
H	-0.884973	2.374592	1.564949
H	-3.210492	3.149806	0.787916
H	-2.805389	2.527031	-0.811623
H	0.081766	-0.432044	2.514374
H	-0.322426	-2.130554	2.850037
H	0.663770	-1.710103	1.430040

H	1.821996	2.840841	-1.070430
H	0.835006	4.190817	-0.452115
H	1.613247	3.052936	0.678160
H	-2.290100	-3.467088	-1.640593
H	-4.002066	-3.055037	-1.815799
H	-2.812361	-2.432195	-2.985308
O	-1.033387	0.339100	-0.928070
C	0.115155	1.015805	-0.811151
O	1.221944	0.564173	-1.108739
C	3.687102	-0.919025	0.384189
C	4.509765	-0.400030	-0.801605
O	2.608179	-1.678629	-0.147857
H	3.311568	-0.049083	0.944820
H	4.980139	-1.224652	-1.340943
H	3.874115	0.171329	-1.479146
C	4.474828	-1.830097	1.315273
H	4.830816	-2.709401	0.766173
H	3.831289	-2.176946	2.130022
H	5.335752	-1.308391	1.742755
Cl	5.846662	0.732221	-0.287234

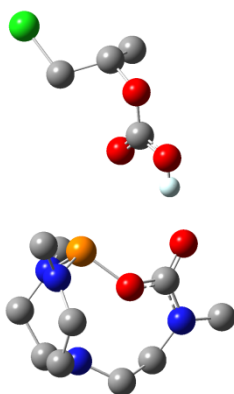
Structure of TS5-6



P	-0.352444	-0.606282	-0.147114
N	-3.353814	-0.458547	-0.410072
N	-0.836767	-1.595358	-1.396123
C	-2.002029	-1.349466	-2.256601
C	-3.329456	-1.435043	-1.489334
C	-3.569525	-0.956884	0.933274
C	-2.331644	-1.733155	1.414726
N	-1.093681	-0.945843	1.316974
N	-2.160057	2.570873	0.256454
C	-3.530094	2.050945	0.084055
C	-3.836234	0.849255	-0.817080
C	-0.285652	-0.838223	2.546563
C	-2.128210	3.792944	1.063621
C	-0.088216	-2.844377	-1.627464
H	1.229232	-0.575189	-0.037645
H	-1.978081	-2.097615	-3.055957
H	-1.908820	-0.367550	-2.733017
H	-4.172453	-1.292153	-2.187656
H	-3.439941	-2.441036	-1.070544
H	-3.726784	-0.108108	1.604713
H	-4.460964	-1.606485	1.023689
H	-2.463585	-2.019111	2.463172
H	-2.230209	-2.668238	0.848372
H	-4.115278	2.879673	-0.333101
H	-3.944715	1.875831	1.088218
H	-4.939605	0.862994	-0.927722
H	-3.426783	1.054508	-1.810989
H	-0.902102	-0.410135	3.345047
H	0.108490	-1.812412	2.850406
H	0.554586	-0.161415	2.381512
H	-2.406021	3.592867	2.107682

H	-1.123309	4.210710	1.046014
H	-2.835843	4.514883	0.643809
H	0.709231	-2.951095	-0.887578
H	-0.755282	-3.711304	-1.537414
H	0.349572	-2.839552	-2.633117
O	-1.006517	0.839807	-0.709535
C	-0.984454	1.883947	0.187530
O	0.028512	2.180909	0.800191
C	3.624665	0.101071	-0.116776
C	3.003498	1.370370	-0.704255
O	2.561174	-0.865419	-0.038943
H	3.981405	0.303969	0.898391
H	2.707171	1.217951	-1.745369
H	2.143651	1.702610	-0.121713
C	4.762498	-0.469806	-0.956772
H	4.405710	-0.713559	-1.964856
H	5.136771	-1.380471	-0.483629
H	5.585217	0.247250	-1.038951
Cl	4.179515	2.760934	-0.705644
C	2.711639	-2.051549	1.079996
O	3.755150	-1.985067	1.683668
O	1.682074	-2.716167	1.021040

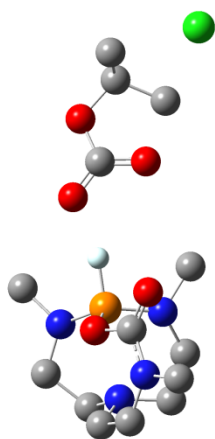
Structure of 6



P	-0.758712	-0.839865	-0.419064
N	-3.864595	-0.737939	0.499600
N	-1.717641	-2.013431	-1.236034
C	-3.110671	-1.779511	-1.660241
C	-4.134836	-1.739883	-0.513332
C	-3.499765	-1.219646	1.811385
C	-2.151603	-1.965649	1.760105
N	-1.037618	-1.188883	1.221717
N	-2.679887	2.439353	0.035112
C	-3.721893	1.793252	0.858577
C	-4.488329	0.558089	0.335260
C	-0.237300	-0.434279	2.188871
C	-2.491913	3.860902	0.324649
C	-0.950322	-2.797438	-2.214899
H	0.964556	1.740598	-1.258775
H	-3.386907	-2.613025	-2.318611
H	-3.188079	-0.861134	-2.258564
H	-5.130321	-1.586524	-0.962879
H	-4.169063	-2.727475	-0.037113
H	-3.418508	-0.368264	2.494541
H	-4.257055	-1.900724	2.251455
H	-1.877826	-2.302538	2.768497
H	-2.262886	-2.861683	1.141254
H	-4.480419	2.569251	1.003666
H	-3.313928	1.586335	1.859465
H	-5.475563	0.598790	0.839913
H	-4.681507	0.708287	-0.731204
H	-0.820229	0.355435	2.687905
H	0.151786	-1.107622	2.963831
H	0.609933	0.042050	1.684656
H	-1.764388	4.273352	-0.372192
H	-3.448145	4.380906	0.208381

H	-2.122903	4.025475	1.347398
H	0.090756	-2.887873	-1.893251
H	-1.367705	-3.808999	-2.287681
H	-0.956928	-2.348387	-3.220735
O	-1.861610	0.500510	-0.773800
C	-1.593694	1.773969	-0.475982
O	-0.515589	2.335106	-0.688991
C	4.987595	0.461044	-0.451325
C	4.669807	-0.838368	0.299004
O	3.868924	0.835658	-1.294848
H	5.762139	0.238218	-1.190208
H	4.044892	-0.666292	1.171717
H	4.186115	-1.550814	-0.371119
C	5.447441	1.613439	0.435246
H	4.681811	1.870286	1.170520
H	5.659395	2.493007	-0.180827
H	6.365194	1.330880	0.959967
Cl	6.203404	-1.628019	0.878277
C	2.680729	1.123759	-0.719243
O	2.433705	1.018396	0.470702
O	1.848983	1.522954	-1.666307

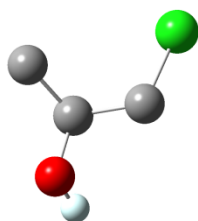
Structure of TS6-2



P	-1.166208	-0.543761	-0.174477
N	-3.570956	-0.771451	0.679600
N	-1.488975	-2.139408	-0.519975
C	-2.793421	-2.796160	-0.423701
C	-3.605763	-2.235100	0.738301
C	-3.467715	-0.106864	1.976723
C	-2.027480	-0.255491	2.465089
N	-1.070524	0.020497	1.388740
N	-3.482710	2.128572	-0.607181
C	-4.666298	1.280937	-0.422282
C	-4.540779	-0.241895	-0.292550
C	0.246953	0.496635	1.880483
C	-3.761591	3.559320	-0.480240
C	-0.523573	-2.884261	-1.365821
H	0.160694	-0.410577	-0.638017
H	-2.622422	-3.866853	-0.263202
H	-3.337162	-2.702131	-1.375672
H	-4.634773	-2.627035	0.715894
H	-3.152107	-2.557448	1.679341
H	-3.678356	0.955080	1.841361
H	-4.175090	-0.499283	2.724515
H	-1.842617	0.462010	3.270862
H	-1.846215	-1.255546	2.887088
H	-5.359439	1.451741	-1.259295
H	-5.178423	1.671691	0.466943
H	-5.558815	-0.588873	-0.042239
H	-4.288685	-0.667490	-1.265092
H	0.111926	1.477524	2.348206
H	0.644593	-0.204253	2.624344
H	0.984261	0.592844	1.080225

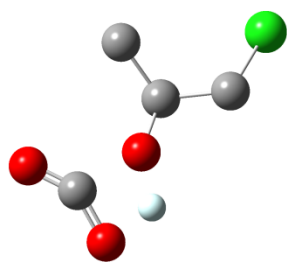
H	-2.845799	4.113553	-0.676243
H	-4.533814	3.858696	-1.199329
H	-4.117294	3.792032	0.531258
H	0.425212	-2.350831	-1.453979
H	-0.340321	-3.862485	-0.907697
H	-0.942372	-3.035529	-2.368849
O	-2.093176	0.397869	-1.168796
C	-2.201778	1.765384	-0.899880
O	-1.244913	2.502234	-0.947749
C	5.165168	-0.163209	-0.727106
C	4.744722	0.358017	0.638858
O	4.026601	-0.841584	-1.336608
H	5.920366	-0.936784	-0.600975
H	4.762862	1.409075	0.868172
H	4.540458	-0.330996	1.441646
C	5.659241	0.934077	-1.659003
H	4.892974	1.708730	-1.779920
H	5.890600	0.516864	-2.643897
H	6.561192	1.383287	-1.235454
Cl	6.977808	0.378356	1.511851
C	2.842066	-0.385391	-0.865642
O	2.930736	0.440873	0.114558
O	1.793577	-0.798905	-1.389150

Structure of **8**



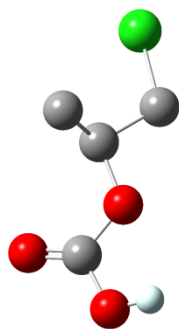
H	-2.005640	-1.628234	-0.447296
C	-0.880251	-0.025699	-0.325621
C	0.308128	-0.692797	0.378774
O	-2.054339	-0.770726	0.003849
H	-0.700172	-0.044173	-1.411255
H	0.214638	-0.603361	1.462942
H	0.373895	-1.750571	0.111226
C	-1.124690	1.405963	0.126909
H	-1.333917	1.429241	1.202394
H	-1.990598	1.818163	-0.399221
H	-0.253158	2.033830	-0.077035
Cl	1.900620	0.046242	-0.091348

Structure of TS8-9



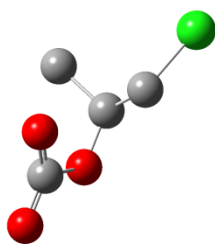
H	-1.468198	-1.412099	0.259856
C	0.261238	0.202914	-0.056615
C	1.423786	-0.625166	0.494766
O	-0.918992	-0.350335	0.584006
H	0.188996	0.042315	-1.140593
H	1.561572	-0.438684	1.561569
H	1.251959	-1.691040	0.332418
C	0.345007	1.688434	0.262165
H	0.412598	1.839260	1.344922
H	-0.544226	2.204997	-0.106612
H	1.228686	2.125319	-0.211358
Cl	2.977453	-0.215530	-0.336669
C	-2.398760	-0.113567	-0.122028
O	-2.823994	0.963871	-0.354559
O	-2.636480	-1.353754	-0.202767

Structure of **9**



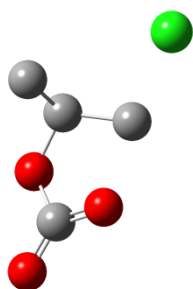
H	-2.833807	-1.362612	0.953714
C	0.250265	0.245641	0.016200
C	1.342998	-0.788832	0.283302
O	-0.970626	-0.441503	0.419357
H	0.180104	0.449026	-1.055023
H	1.458407	-0.977596	1.352720
H	1.113552	-1.724915	-0.227653
C	0.391496	1.542310	0.798975
H	0.395413	1.344499	1.876751
H	-0.440717	2.210567	0.561950
H	1.325081	2.045710	0.532267
Cl	2.945356	-0.223584	-0.337417
C	-2.106640	-0.074566	-0.229434
O	-2.194078	0.743093	-1.106461
O	-3.152521	-0.767973	0.252992

Structure of **10**



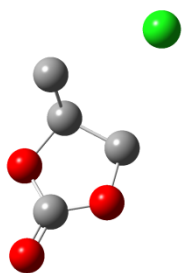
C	0.207618	0.589723	-0.513616
C	0.953367	-0.652762	-0.001955
O	-1.100249	0.241709	-0.920141
H	0.711219	0.901299	-1.441080
H	0.685575	-0.902549	1.019233
H	0.764917	-1.498272	-0.663952
C	0.241653	1.761383	0.474674
H	-0.287621	1.475185	1.386015
H	-0.264152	2.625580	0.028103
H	1.272820	2.047673	0.716751
Cl	2.798594	-0.412882	-0.032382
C	-2.045401	-0.307962	0.088699
O	-1.555138	-0.541001	1.213625
O	-3.169897	-0.447235	-0.391159

Structure of TS10-11



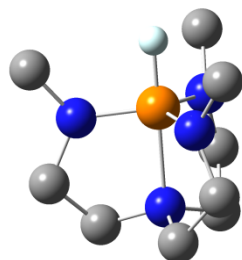
C	0.140641	0.667030	-0.362958
C	0.681780	-0.610559	0.266056
O	-1.181272	0.471892	-0.862622
H	0.743756	0.899373	-1.244051
H	0.877935	-0.673446	1.322289
H	0.577728	-1.538644	-0.272579
C	0.189342	1.840408	0.617153
H	-0.414000	1.606365	1.500671
H	-0.218272	2.739970	0.143260
H	1.221817	2.035978	0.927004
Cl	2.839860	-0.428500	-0.184436
C	-1.978387	-0.357299	-0.028414
O	-1.306232	-0.931964	0.891892
O	-3.170850	-0.417750	-0.303295

Structure of **11**



C	0.048245	0.578663	-0.298558
C	0.061208	-0.828901	0.311659
O	-1.350805	0.722736	-0.713192
H	0.670223	0.620581	-1.190895
H	0.613439	-0.887848	1.247273
H	0.451294	-1.580943	-0.375063
C	0.423120	1.690166	0.664661
H	-0.162581	1.623670	1.590911
H	0.244703	2.671386	0.210394
H	1.488959	1.575565	0.886975
Cl	3.191982	-0.366490	-0.189433
C	-2.110602	-0.217316	-0.112287
O	-1.347412	-1.096932	0.572482
O	-3.314478	-0.266773	-0.177051

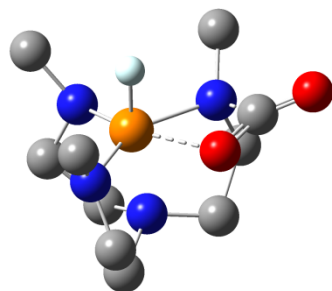
Structure of **12**



P	-0.004189	0.000301	-0.714548
N	0.008569	-0.000768	1.379108
N	-0.849408	-1.462928	-0.564727
C	-1.293865	-1.935495	0.739636
C	-0.315666	-1.396497	1.777374
C	1.382876	0.413656	1.768400
C	2.329877	-0.156555	0.718386
N	1.686759	-0.000421	-0.579355
N	-0.847949	1.464196	-0.563275
C	-1.021750	2.091611	0.739902
C	-1.034127	0.979861	1.783042
C	2.534904	-0.358972	-1.721871
C	-0.972556	2.384376	-1.699469
C	-1.595177	-2.022939	-1.697594
H	-0.012578	0.000810	-2.120668
H	-1.288758	-3.031194	0.761305
H	-2.326917	-1.615651	0.950115
H	-0.718896	-1.421310	2.795031
H	0.609633	-1.976146	1.755537
H	1.422168	1.504936	1.754364
H	1.614808	0.069463	2.781593
H	3.275927	0.396410	0.735038
H	2.572213	-1.212216	0.919963
H	-1.972770	2.635479	0.768473
H	-0.225927	2.827021	0.938930
H	-0.844025	1.346201	2.797190
H	-1.998991	0.468446	1.772960
H	3.431373	0.270227	-1.720668
H	2.845122	-1.411940	-1.681505
H	2.007659	-0.187933	-2.662320
H	-0.865628	1.847523	-2.643961
H	-1.965846	2.845644	-1.686370
H	-0.215798	3.179671	-1.661739
H	-1.191326	-1.657418	-2.643638

H	-1.500102	-3.114028	-1.691537
H	-2.661404	-1.763322	-1.648961

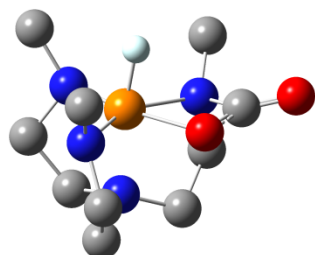
Structure of TS12-13



P	-0.230223	0.044114	-0.614086
N	-0.567948	-0.090145	1.431720
N	-1.339171	1.357033	-0.582932
C	-1.343613	2.118929	0.666245
C	-1.399652	1.106883	1.805373
C	-1.334493	-1.371026	1.621571
C	-2.071686	-1.651556	0.321998
N	-1.105982	-1.424320	-0.750807
N	1.538258	-0.634623	-0.159978
C	1.666165	-1.045526	1.261615
C	0.761685	-0.143579	2.101233
C	-1.621910	-1.788271	-2.081301
C	2.091140	-1.653998	-1.083790
C	-1.328348	2.229369	-1.771767
H	0.169246	0.117906	-1.960624
H	-2.237907	2.749225	0.702201
H	-0.462667	2.770243	0.735522
H	-1.044261	1.518652	2.753678
H	-2.425502	0.760958	1.940528
H	-0.625272	-2.173981	1.822743
H	-1.998596	-1.273888	2.484630
H	-2.411127	-2.692273	0.303359
H	-2.959106	-1.007263	0.214532
H	2.713687	-0.938166	1.559594
H	1.392850	-2.100377	1.347921
H	0.654647	-0.530213	3.119637
H	1.158251	0.871600	2.152220
H	-1.877988	-2.852159	-2.079944
H	-2.518420	-1.213280	-2.354288
H	-0.856709	-1.633686	-2.845302
H	1.949742	-1.324678	-2.115200
H	3.164604	-1.731925	-0.890596
H	1.592106	-2.611584	-0.924441

H	-1.362867	1.631498	-2.684914
H	-2.232522	2.844996	-1.748986
H	-0.447123	2.882709	-1.795759
O	1.313170	1.605677	-0.320632
C	2.274019	0.788184	-0.308550
O	3.472122	0.804560	-0.340243

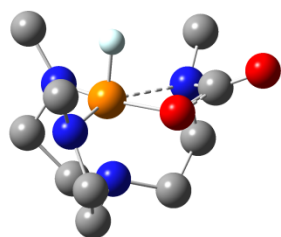
Structure of **13**



P	0.247120	-0.012474	-0.606715
N	0.434221	-0.045948	1.441923
N	1.635519	-1.035284	-0.634564
C	1.662325	-1.983549	0.478295
C	1.376733	-1.187799	1.754798
C	1.038516	1.283973	1.819956
C	1.769484	1.818392	0.599616
N	0.863753	1.604321	-0.521845
N	-1.703907	0.475923	-0.179597
C	-1.904264	0.694089	1.277286
C	-0.923041	-0.194608	2.047000
C	1.342628	2.203936	-1.775990
C	-2.409626	1.475595	-1.012044
C	1.949024	-1.662740	-1.929395
H	-0.075552	0.059832	-1.974489
H	2.660688	-2.427291	0.552711
H	0.939886	-2.799096	0.339748
H	0.943213	-1.807781	2.543015
H	2.301159	-0.748975	2.131400
H	0.230147	1.964918	2.086262
H	1.681443	1.154976	2.693943
H	1.967127	2.888003	0.726954
H	2.735106	1.308803	0.452950
H	-2.936779	0.445482	1.545064
H	-1.744886	1.756000	1.477410
H	-0.889939	0.091858	3.102870
H	-1.211878	-1.244719	1.986920
H	1.428898	3.286673	-1.639465
H	2.324337	1.814139	-2.083920
H	0.626799	2.030813	-2.583480
H	-2.210576	1.269655	-2.065660
H	-3.486495	1.400274	-0.835533
H	-2.042801	2.470802	-0.755191
H	1.955658	-0.912177	-2.723201

H	2.954907	-2.090076	-1.873497
H	1.240612	-2.460342	-2.194756
O	-0.902587	-1.544799	-0.503780
C	-2.067278	-0.958994	-0.492121
O	-3.186411	-1.353640	-0.640615

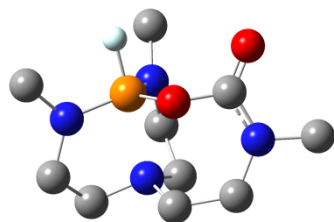
Structure of TS13-14



P	0.321101	-0.060881	-0.630836
N	0.474633	0.084937	1.410414
N	1.762219	-0.986391	-0.584369
C	1.842045	-1.831977	0.606610
C	1.532455	-0.928156	1.801452
C	0.933411	1.488821	1.700753
C	1.627405	2.006641	0.448876
N	0.779395	1.588771	-0.654189
N	-1.867126	0.354298	-0.152167
C	-1.968934	0.571552	1.311122
C	-0.854364	-0.177084	2.049869
C	1.033283	2.249197	-1.938531
C	-2.787742	1.209298	-0.925275
C	2.152101	-1.669548	-1.828879
H	-0.038736	-0.075208	-1.989976
H	2.860987	-2.219606	0.709137
H	1.157480	-2.689527	0.554466
H	1.190427	-1.487386	2.675682
H	2.427352	-0.368661	2.075604
H	0.056061	2.101262	1.906698
H	1.571481	1.488372	2.587811
H	1.691709	3.098941	0.487152
H	2.650089	1.608428	0.358068
H	-2.941978	0.227083	1.684465
H	-1.914006	1.649949	1.479951
H	-0.814865	0.147691	3.094893
H	-1.027042	-1.253477	2.036877
H	0.889405	3.328467	-1.823421
H	2.053455	2.069975	-2.306914
H	0.324996	1.900489	-2.694618
H	-2.653988	1.008335	-1.990098
H	-3.829239	1.002309	-0.656961
H	-2.547391	2.255074	-0.721383
H	2.118538	-0.971079	-2.668596

H	3.185802	-2.013716	-1.728196
H	1.511643	-2.533575	-2.055523
O	-0.739179	-1.531181	-0.386979
C	-1.987545	-1.081671	-0.439752
O	-3.000225	-1.678154	-0.664004

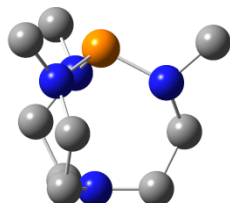
Structure of **14**



P	0.826829	0.678789	-0.431925
N	0.364768	-1.108027	0.753682
N	2.213293	-0.162055	-0.824794
C	2.496623	-1.505976	-0.328881
C	1.714632	-1.695085	0.963471
C	-0.231237	-0.610214	2.016533
C	0.380461	0.761666	2.284628
N	0.507780	1.462103	1.007664
N	-2.469094	-0.399777	-0.430229
C	-2.001311	-1.755055	-0.120166
C	-0.498081	-2.060324	-0.019926
C	0.647237	2.925529	1.120700
C	-3.904630	-0.188691	-0.211098
C	3.103486	0.294610	-1.905542
H	1.156681	1.833619	-1.147225
H	3.569810	-1.599826	-0.129215
H	2.239106	-2.263711	-1.082098
H	1.645718	-2.747779	1.258596
H	2.201477	-1.143483	1.771454
H	-1.304183	-0.496564	1.869252
H	-0.060477	-1.309266	2.843096
H	-0.279143	1.333838	2.944694
H	1.356051	0.691086	2.787041
H	-2.395548	-2.461926	-0.864565
H	-2.481844	-2.025072	0.827630
H	-0.429699	-3.046400	0.458748
H	-0.064077	-2.145285	-1.014816
H	-0.238244	3.333076	1.618020
H	1.539577	3.188665	1.700764
H	0.717237	3.385647	0.134595
H	-4.151974	0.835403	-0.484231
H	-4.488649	-0.881512	-0.827772
H	-4.154279	-0.357234	0.842430
H	2.831061	1.297880	-2.236351

H	4.137301	0.318702	-1.545248
H	3.040203	-0.381471	-2.766151
O	-0.455666	0.188601	-1.339730
C	-1.762694	0.603266	-1.014970
O	-2.140920	1.723363	-1.251837

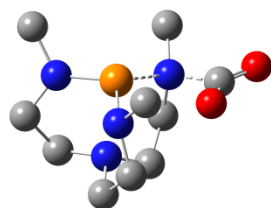
Structure of **15**



P	1.333966	0.007272	-0.008979
N	-2.001051	-0.009801	0.012951
N	0.582345	1.574851	-0.137228
C	-0.565881	1.965873	0.681085
C	-1.913082	1.425212	0.169547
C	-1.912477	-0.590548	-1.308583
C	-0.571568	-0.399870	-2.039891
N	0.587543	-0.897295	-1.298374
N	0.604812	-0.667165	1.423731
C	-0.542826	-1.573273	1.369612
C	-1.894369	-0.862607	1.176109
C	1.520741	-1.692739	-2.096384
C	1.550109	-0.953115	2.503243
C	1.511027	2.665324	-0.435829
H	-0.621505	3.062296	0.690218
H	-0.425359	1.643534	1.723742
H	-2.693507	1.775992	0.868402
H	-2.134896	1.879203	-0.803946
H	-2.119426	-1.663488	-1.213785
H	-2.702130	-0.171252	-1.957537
H	-0.625014	-0.940762	-2.993773
H	-0.446636	0.666088	-2.282548
H	-0.584183	-2.129210	2.315421
H	-0.412413	-2.315186	0.567479
H	-2.673687	-1.644902	1.141767
H	-2.104876	-0.246909	2.059071
H	1.043325	-2.623524	-2.430539
H	1.887601	-1.160196	-2.990406
H	2.390681	-1.964096	-1.491006
H	2.410803	-0.281555	2.431985
H	1.077644	-0.787634	3.480641
H	1.930381	-1.988688	2.481653
H	2.373762	2.279189	-0.986716
H	1.024372	3.422005	-1.065523

H	1.889975	3.170322	0.469075
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Structure of TS15-16



P	0.398250	-0.175487	-1.195159
N	0.621193	0.369005	1.526094
N	1.641874	-1.232992	-0.541960
C	1.532091	-1.807178	0.809746
C	1.517378	-0.728121	1.891276
C	1.276236	1.659224	1.399561
C	2.066315	1.681090	0.074200
N	1.198304	1.334360	-1.039564
N	-1.724515	0.387808	-0.193823
C	-1.761982	0.978459	1.149576
C	-0.722343	0.350590	2.088247
C	0.566576	2.463644	-1.716207
C	-2.655832	1.069810	-1.103497
C	1.851753	-2.325873	-1.515136
H	2.406440	-2.452097	0.970227
H	0.634729	-2.435367	0.879829
H	1.229304	-1.174258	2.854141
H	2.527417	-0.324047	2.021972
H	0.518155	2.448064	1.388092
H	1.954459	1.871424	2.243963
H	2.511557	2.668281	-0.095546
H	2.875660	0.945661	0.117784
H	-2.758908	0.832511	1.592096
H	-1.599611	2.059266	1.053550
H	-0.778144	0.865610	3.063775
H	-0.995681	-0.693852	2.263996
H	-0.041603	3.083227	-1.040264
H	1.335261	3.103583	-2.166615
H	-0.080558	2.095295	-2.517672
H	-2.514376	0.682000	-2.117281
H	-3.693667	0.883752	-0.798640
H	-2.460802	2.147090	-1.104410
H	1.908793	-1.926498	-2.531623
H	2.811780	-2.808337	-1.295522

H	1.055401	-3.083244	-1.476797
O	-1.087321	-1.810238	-0.422839
C	-2.086618	-1.104946	-0.110409
O	-3.222527	-1.387662	0.243208

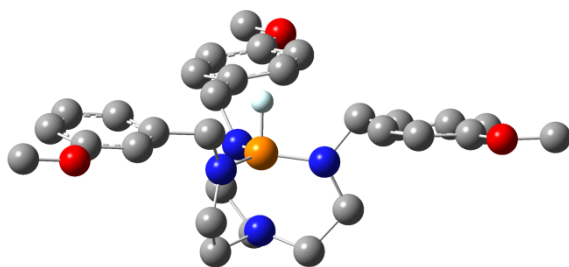
Structure of **16**



P	-0.920267	-1.390645	0.035987
N	-0.311304	1.799710	0.054722
N	-2.130609	-0.485816	-0.795421
C	-1.832133	0.699277	-1.619676
C	-1.457288	1.958912	-0.818170
C	-0.557977	1.842743	1.476270
C	-1.442408	0.658319	1.916548
N	-0.922040	-0.665954	1.587821
N	2.555788	0.040504	-0.579927
C	2.211385	1.344175	0.018749
C	0.988302	2.142866	-0.484198
C	-0.092382	-1.310285	2.601296
C	3.969473	-0.305241	-0.446244
C	-3.200927	-1.321009	-1.353640
H	-2.741784	0.930673	-2.188868
H	-1.043638	0.479318	-2.352350
H	-1.289295	2.774632	-1.541847
H	-2.323132	2.263796	-0.217155
H	0.399506	1.798291	2.005034
H	-1.051172	2.781640	1.804535
H	-1.603102	0.705079	3.002243
H	-2.425132	0.755336	1.443839
H	3.078134	1.982110	-0.185026
H	2.169937	1.246104	1.115396
H	1.237622	3.206207	-0.287190
H	0.942182	2.033441	-1.571881
H	0.860218	-0.785388	2.775374
H	-0.628244	-1.364829	3.558519
H	0.148229	-2.330426	2.283460
H	4.151033	-1.254252	-0.948518
H	4.578580	0.478582	-0.908679
H	4.273925	-0.411165	0.606387
H	-3.340468	-2.214426	-0.738681
H	-4.146350	-0.764383	-1.354912
H	-2.995008	-1.648928	-2.385491
O	0.410639	-0.629933	-0.789369

C	1.686799	-1.037021	-0.599670
O	2.035868	-2.202222	-0.519623

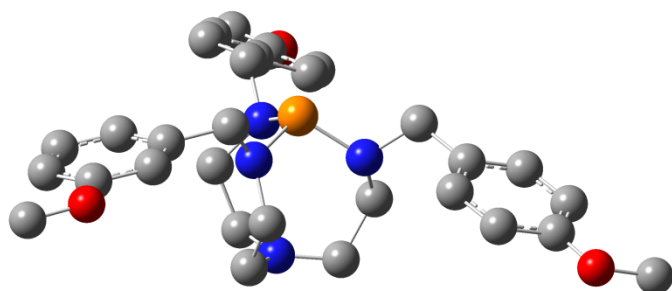
Structure of 17



P	0.098577	-0.107615	0.451551
N	0.099603	-0.143132	2.551343
N	1.603874	-0.878723	0.585247
C	2.081204	-1.351856	1.878030
C	1.506468	-0.425064	2.940914
C	-0.364658	1.205921	2.970295
C	0.163792	2.193958	1.939002
N	0.008987	1.577361	0.627890
N	-1.319652	-1.031755	0.585054
C	-1.949034	-1.237467	1.883633
C	-0.842065	-1.229940	2.929196
C	0.231697	2.490848	-0.517111
C	-2.212574	-1.244976	-0.573231
C	2.261640	-1.504648	-0.585350
H	0.097043	-0.084239	-0.954664
H	3.174616	-1.315461	1.901582
H	1.786878	-2.399574	2.052064
H	1.545907	-0.854307	3.947728
H	2.051459	0.521353	2.943397
H	-1.456721	1.205151	2.959579
H	-0.024867	1.428325	3.987424
H	-0.414840	3.121839	1.979046
H	1.216011	2.458204	2.132972
H	-2.466176	-2.201633	1.893879
H	-2.704633	-0.461575	2.086831
H	-1.217307	-1.074701	3.946313
H	-0.295610	-2.175053	2.899001
H	1.240046	2.924124	-0.444301
H	0.211440	1.890761	-1.432504
H	-1.669926	-0.955168	-1.478568
H	-3.082142	-0.576571	-0.494065
H	1.737048	-1.166034	-1.484527
H	2.130993	-2.595575	-0.534310
C	-0.793169	3.602522	-0.596477
C	-0.409447	4.940447	-0.492623

C	-2.154511	3.317982	-0.800991
C	-1.339196	5.979979	-0.592121
H	0.638812	5.189399	-0.340188
C	-3.091893	4.333688	-0.897651
H	-2.481984	2.284218	-0.888955
C	-2.690928	5.678645	-0.795609
H	-1.001187	7.006326	-0.511177
H	-4.143331	4.120565	-1.062160
C	-2.684925	-2.682277	-0.696085
C	-4.046750	-2.967570	-0.660685
C	-1.762654	-3.727392	-0.867200
C	-4.509401	-4.287364	-0.804209
H	-4.784193	-2.179733	-0.533034
C	-2.221281	-5.033064	-1.005188
H	-0.697163	-3.515177	-0.897198
C	-3.588784	-5.327054	-0.976096
H	-1.511733	-5.844083	-1.144942
H	-3.918913	-6.352900	-1.089405
C	3.736053	-1.174422	-0.683317
C	4.702194	-2.179652	-0.619514
C	4.169731	0.150232	-0.865605
C	6.066021	-1.894766	-0.736991
H	4.393999	-3.214529	-0.484949
C	5.516839	0.453592	-0.979580
H	3.438461	0.953774	-0.922202
C	6.480381	-0.570038	-0.917955
H	6.785274	-2.703704	-0.687203
H	5.857496	1.473483	-1.127223
C	-3.347859	7.977451	-0.841639
H	-4.287358	8.516897	-0.966878
H	-2.905900	8.236307	0.128761
H	-2.656131	8.258037	-1.645536
C	-6.400877	-5.746345	-0.916540
H	-7.483221	-5.626758	-0.855410
H	-6.135617	-6.171610	-1.892339
H	-6.063425	-6.420983	-0.119674
C	8.797078	-1.153957	-1.018896
H	9.732959	-0.609263	-1.148452
H	8.816341	-1.688192	-0.060652
H	8.678085	-1.874547	-1.837472
O	-3.684041	6.595417	-0.906629
O	7.769695	-0.168474	-1.043037
O	-5.857826	-4.439931	-0.755712

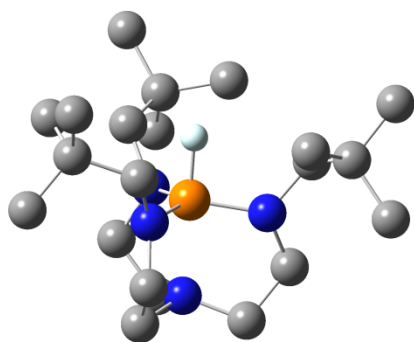
Structures of **18**



P	0.069257	-0.105157	-0.933930
N	0.105955	-0.046127	2.351877
N	1.519459	-0.778552	-0.227920
C	1.505241	-1.622104	0.972412
C	1.304491	-0.849374	2.283715
C	0.200273	1.392118	2.255920
C	0.726570	1.928706	0.917252
N	-0.050104	1.498530	-0.250620
N	-1.238432	-0.998280	-0.192560
C	-1.960660	-0.519875	0.992163
C	-1.189173	-0.684750	2.309043
C	-0.196114	2.552385	-1.273816
C	-2.112675	-1.661907	-1.176197
C	2.500567	-1.219940	-1.238315
H	2.471037	-2.137596	1.033517
H	0.727140	-2.395997	0.888627
H	1.318039	-1.589010	3.104439
H	2.163705	-0.187607	2.441926
H	-0.796828	1.808645	2.438866
H	0.860090	1.787258	3.049173
H	0.692629	3.023747	0.960130
H	1.782544	1.639421	0.803925
H	-2.891002	-1.093963	1.075534
H	-2.240592	0.537460	0.869351
H	-1.835139	-0.297093	3.117160
H	-1.045262	-1.753286	2.505755
H	0.783097	2.987042	-1.539458
H	-0.576175	2.074673	-2.184484
H	-1.543660	-1.767819	-2.107348
H	-2.989026	-1.036766	-1.417832
H	2.275131	-0.686149	-2.169063
H	2.384441	-2.294287	-1.463469
C	-1.129914	3.675687	-0.861827
C	-0.687329	4.996889	-0.799398

C	-2.478043	3.422220	-0.555137
C	-1.542885	6.048094	-0.447325
H	0.351149	5.223019	-1.033251
C	-3.342535	4.448273	-0.203947
H	-2.849292	2.401516	-0.594764
C	-2.879292	5.773213	-0.146781
H	-1.156083	7.060193	-0.409784
H	-4.385159	4.254684	0.029486
C	-2.598317	-3.031825	-0.730719
C	-3.962251	-3.302283	-0.658196
C	-1.684225	-4.050987	-0.413047
C	-4.429439	-4.570680	-0.277413
H	-4.695752	-2.536986	-0.897701
C	-2.146658	-5.306001	-0.036474
H	-0.618327	-3.850805	-0.465834
C	-3.517975	-5.581776	0.037243
H	-1.437756	-6.094256	0.204794
H	-3.853055	-6.568590	0.335463
C	3.942326	-0.960511	-0.841111
C	4.866268	-2.001653	-0.753563
C	4.397907	0.342365	-0.575305
C	6.206489	-1.775380	-0.416481
H	4.542017	-3.020691	-0.955269
C	5.720748	0.588875	-0.239409
H	3.698458	1.172074	-0.634699
C	6.637683	-0.472110	-0.156869
H	6.890376	-2.614613	-0.358457
H	6.075184	1.595167	-0.037374
C	-3.398295	8.064846	0.279923
H	-4.283333	8.631876	0.574882
H	-2.608505	8.211068	1.029126
H	-3.041694	8.430128	-0.692608
C	-6.323939	-5.965993	0.134852
H	-7.409246	-5.855175	0.093880
H	-6.015026	-6.761943	-0.556091
H	-6.026565	-6.242114	1.155521
C	8.885080	-1.154441	0.275289
H	9.820262	-0.662576	0.549749
H	8.622480	-1.889547	1.048025
H	9.016955	-1.673942	-0.683425
O	-3.808413	6.709735	0.210578
O	7.915333	-0.124722	0.182427
O	-5.789146	-4.708921	-0.243480

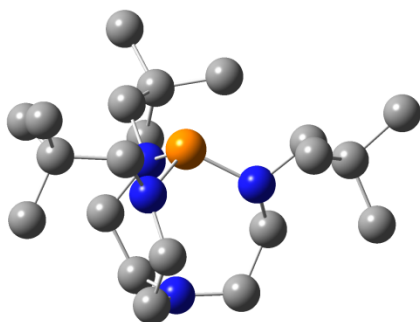
Structure of **19**



P	-0.000864	-0.000384	0.310769
N	-0.000601	-0.001906	2.453101
N	0.877164	1.449363	0.478463
C	1.527399	1.726347	1.758976
C	0.553193	1.317356	2.852094
C	-1.420095	-0.182401	2.851594
C	-2.260912	0.458016	1.758975
N	-1.695355	0.035052	0.478301
N	0.815840	-1.485765	0.476950
C	0.731423	-2.188686	1.756745
C	0.865258	-1.141466	2.850709
C	-2.573778	0.223443	-0.701345
C	1.094278	-2.338400	-0.703746
C	1.478921	2.116222	-0.701282
H	-0.000994	0.000553	-1.095623
H	1.750023	2.790965	1.844530
H	2.482822	1.184686	1.847329
H	1.018343	1.255309	3.841919
H	-0.270401	2.033642	2.897425
H	-1.628575	-1.253864	2.895849
H	-1.599168	0.250425	3.841829
H	-3.294219	0.118311	1.843547
H	-2.269804	1.556164	1.848752
H	1.541981	-2.914013	1.840760
H	-0.215374	-2.745283	1.845302
H	0.579547	-1.514077	3.840404
H	1.897419	-0.786429	2.895676
H	-3.225533	1.082695	-0.492987
H	-1.957029	0.513453	-1.557908
H	0.537021	-1.946796	-1.560668
H	0.674924	-3.332718	-0.498784
H	1.419927	1.437844	-1.558345
H	2.549385	2.249615	-0.494316

C	-3.444935	-0.989230	-1.126430
C	-2.555009	-2.160782	-1.573938
C	-4.374293	-1.459950	0.007140
C	-4.301772	-0.512215	-2.317264
H	-1.904790	-1.873578	-2.410042
H	-1.923840	-2.519867	-0.753146
H	-3.168284	-3.003605	-1.911009
H	-5.021071	-0.649265	0.365558
H	-5.028466	-2.263700	-0.348231
H	-3.808206	-1.858656	0.857379
H	-4.931965	-1.327785	-2.687613
H	-4.963254	0.314405	-2.031280
H	-3.677281	-0.170944	-3.151904
C	2.581025	-2.486449	-1.125744
C	3.153116	-1.128604	-1.565923
C	3.450283	-3.061161	0.007643
C	2.598486	-3.462243	-2.320352
H	2.583308	-0.705623	-2.403007
H	3.144731	-0.405716	-0.742273
H	4.191143	-1.237379	-1.898696
H	3.069939	-4.027549	0.361802
H	4.473959	-3.225620	-0.346315
H	3.511838	-2.374761	0.860510
H	3.620757	-3.599818	-2.688411
H	2.211484	-4.449108	-2.039329
H	1.993386	-3.088006	-3.155124
C	0.865309	3.478194	-1.123891
C	-0.595684	3.295766	-1.567672
C	0.926707	4.517326	0.010489
C	1.704670	3.981671	-2.316279
H	-0.675520	2.590192	-2.404399
H	-1.220175	2.928419	-0.745366
H	-1.018647	4.249266	-1.902358
H	1.953198	4.669804	0.366936
H	0.558862	5.486745	-0.343276
H	0.299568	4.227000	0.861790
H	1.314750	4.936784	-2.683946
H	2.752506	4.138241	-2.033104
H	1.683838	3.271689	-3.152062

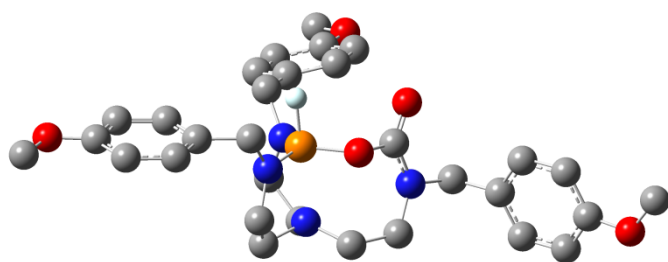
Structure of **20**



P	0.000285	0.000101	-0.551442
N	0.000551	-0.000795	2.771416
N	1.275887	-0.973312	0.150722
C	1.075166	-1.790260	1.354978
C	1.027113	-1.012982	2.677656
C	0.363789	1.394373	2.678299
C	1.012914	1.825500	1.355865
N	0.205452	1.591170	0.151265
N	-1.480350	-0.618032	0.150952
C	-2.086942	-0.036166	1.355723
C	-1.389338	-0.383714	2.678034
C	0.294520	2.660958	-0.864440
C	-2.451585	-1.074879	-0.864907
C	2.157578	-1.585066	-0.865300
H	1.898262	-2.509639	1.422291
H	0.147716	-2.376676	1.266552
H	0.899213	-1.759051	3.482696
H	1.994297	-0.527882	2.853528
H	-0.539897	1.989338	2.854601
H	1.073934	1.656217	3.483396
H	1.223890	2.898065	1.423791
H	1.984703	1.315977	1.267360
H	-3.121513	-0.389182	1.423285
H	-2.130883	1.060274	1.267777
H	-1.971161	0.099946	3.483394
H	-1.452878	-1.463912	2.853657
H	1.252006	3.190482	-0.744607
H	0.325140	2.195336	-1.857781
H	-2.063324	-0.815870	-1.858218
H	-3.388401	-0.509529	-0.745222
H	1.738833	-1.377998	-1.858407
H	2.137086	-2.679112	-0.746167
C	-0.849458	3.713269	-0.885540

C	-2.180274	3.044777	-1.272176
C	-1.000133	4.415561	0.474624
C	-0.480122	4.758832	-1.956756
H	-2.110762	2.565770	-2.256878
H	-2.464903	2.277377	-0.545797
H	-2.989841	3.783966	-1.316183
H	-0.072788	4.922965	0.770329
H	-1.791582	5.174196	0.432475
H	-1.264902	3.702318	1.262322
H	-1.262535	5.522245	-2.043471
H	0.458684	5.270713	-1.709943
H	-0.358473	4.293824	-2.943205
C	-2.792545	-2.591330	-0.885939
C	-1.549283	-3.410996	-1.273171
C	-3.325312	-3.072523	0.474452
C	-3.883467	-2.793066	-1.956619
H	-1.169675	-3.112114	-2.258299
H	-0.741654	-3.274331	-0.547493
H	-1.785756	-4.481474	-1.316579
H	-4.227912	-2.522487	0.770493
H	-3.587333	-4.137079	0.432418
H	-2.574874	-2.945695	1.261880
H	-4.154219	-3.852133	-2.043585
H	-4.795612	-2.235414	-1.709041
H	-3.541932	-2.455074	-2.943147
C	3.641113	-1.121143	-0.886351
C	3.728431	0.365880	-1.271748
C	4.324960	-1.343245	0.473457
C	4.361285	-1.963277	-1.958415
H	3.278812	0.546333	-2.256220
H	3.206794	0.995838	-0.544702
H	4.773589	0.696721	-1.315665
H	4.300076	-2.400235	0.768482
H	5.377881	-1.037846	0.431212
H	3.840332	-0.757502	1.261690
H	5.413778	-1.667919	-2.045063
H	4.334619	-3.032438	-1.712489
H	3.897656	-1.835050	-2.944682

Structures of **21**

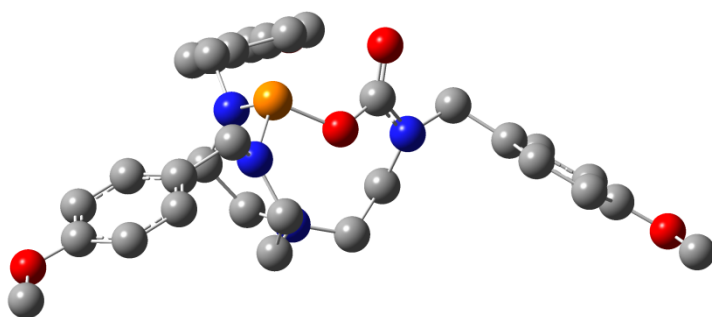


P	0.990945	-0.388654	-0.265634
N	0.460051	-0.836588	1.818131
N	2.183613	-1.528211	-0.022562
C	2.332864	-2.259034	1.233004
C	1.731752	-1.404436	2.338277
C	0.136447	0.474085	2.430675
C	0.978419	1.517641	1.708759
N	0.981794	1.190886	0.283082
N	-2.380384	-0.524917	0.500103
C	-2.071151	-1.392366	1.642525
C	-0.631924	-1.859358	1.896894
C	1.404712	2.313348	-0.612909
C	-3.761913	0.031061	0.502355
C	3.025342	-2.027834	-1.146633
H	1.358589	-0.075308	-1.578022
H	3.397321	-2.424131	1.425124
H	1.852090	-3.245602	1.168856
H	1.560544	-1.972524	3.259491
H	2.405744	-0.575187	2.565937
H	-0.916342	0.687006	2.251203
H	0.319439	0.466685	3.511497
H	0.537874	2.508919	1.843098
H	2.006898	1.560945	2.097462
H	-2.678342	-2.305642	1.583011
H	-2.431187	-0.855272	2.527695
H	-0.633663	-2.277535	2.912809
H	-0.366959	-2.662198	1.210745
H	2.431473	2.599214	-0.347720
H	1.427622	1.928711	-1.635806
H	-3.770295	0.818947	-0.251069
H	-3.918771	0.495474	1.482570
H	2.716793	-1.503042	-2.055391
H	2.789437	-3.088377	-1.301198
O	-0.455312	-1.109691	-0.599503
C	-1.662180	-0.391463	-0.642262

O	-1.965099	0.251543	-1.621893
C	0.497171	3.518001	-0.525370
C	-0.815033	3.475312	-1.031646
C	0.953643	4.712568	0.036704
C	-1.634288	4.591227	-0.968711
H	-1.194533	2.562190	-1.483101
C	0.141108	5.847787	0.103520
H	1.969710	4.773892	0.422003
C	-1.163806	5.789715	-0.400988
H	-2.644324	4.571050	-1.365576
H	0.532964	6.759127	0.539479
C	-4.829179	-1.005373	0.231699
C	-5.048911	-1.478962	-1.067289
C	-5.622234	-1.519574	1.269223
C	-6.022013	-2.442095	-1.333036
H	-4.456661	-1.084771	-1.889342
C	-6.596919	-2.477403	1.022028
H	-5.487623	-1.153393	2.285368
C	-6.803868	-2.948692	-0.284008
H	-6.170625	-2.780359	-2.351843
H	-7.218340	-2.871176	1.819808
C	4.507244	-1.854898	-0.902941
C	5.345957	-2.962914	-0.766997
C	5.083633	-0.574708	-0.828700
C	6.721718	-2.820308	-0.564502
H	4.928070	-3.965536	-0.831375
C	6.444037	-0.412351	-0.624157
H	4.457373	0.308126	-0.942030
C	7.278633	-1.537839	-0.490793
H	7.340541	-3.704728	-0.470044
H	6.896204	0.573012	-0.574441
O	-2.045095	6.819985	-0.393235
O	-7.778370	-3.882200	-0.425333
O	8.592850	-1.271136	-0.296913
C	-1.624903	8.075382	0.130713
H	-0.772426	8.476915	-0.430929
H	-2.479537	8.743646	0.019533
H	-1.359641	7.997146	1.192626
C	-8.064337	-4.380560	-1.727579
H	-8.875361	-5.098238	-1.598222
H	-8.392005	-3.577957	-2.399887
H	-7.194361	-4.889107	-2.162007
C	9.503443	-2.361094	-0.186773
H	10.487825	-1.911456	-0.052809

H	9.269382	-2.990912	0.680580
H	9.502835	-2.974152	-1.096322

Structure of **22**

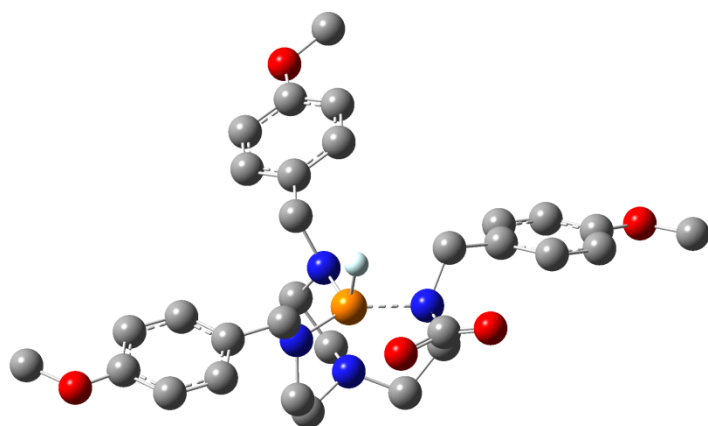


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N	-0.513303	-0.416007	-1.522619
N	-2.505654	-0.823390	0.730985
C	-2.123452	-1.855036	-0.250593
C	-1.656221	-1.303106	-1.607289
C	-0.720008	0.965239	-1.885234
C	-1.703820	1.650385	-0.921404
N	-1.317467	1.605969	0.491930
N	2.190847	-0.607190	0.547708
C	1.968723	-0.355060	-0.892424
C	0.797137	-1.022844	-1.639845
C	-1.041222	2.901459	1.139908
C	3.587948	-0.411159	0.962273
C	-3.654042	-1.208472	1.573911
H	-3.013459	-2.468543	-0.433783
H	-1.350834	-2.515507	0.166577
H	-1.440554	-2.164514	-2.263005
H	-2.492316	-0.769702	-2.074771
H	0.236038	1.493858	-1.843260
H	-1.108896	1.091258	-2.917790
H	-1.812150	2.700407	-1.216613
H	-2.691585	1.184900	-1.029862
H	2.874360	-0.729396	-1.378906
H	1.957926	0.731230	-1.062239
H	1.124180	-1.073824	-2.699270
H	0.721421	-2.057726	-1.292250
H	-1.890744	3.579106	0.967244
H	-0.994472	2.719087	2.219752
H	3.582946	-0.385701	2.053944
H	3.945188	0.573452	0.623338
H	-3.686607	-0.518280	2.425797
H	-3.506230	-2.214628	1.999162
O	-0.001342	-0.696834	1.066010

C	1.233369	-0.388342	1.518483
O	1.471158	-0.023205	2.660997
C	0.235019	3.585916	0.682187
C	1.491130	3.170103	1.159268
C	0.199020	4.650009	-0.220162
C	2.658940	3.788820	0.733806
H	1.553349	2.357091	1.878722
C	1.365913	5.284027	-0.663125
H	-0.760768	5.009136	-0.586984
C	2.605480	4.848890	-0.186019
H	3.629199	3.479946	1.111383
H	1.292193	6.107878	-1.364024
C	4.517465	-1.493175	0.447868
C	4.224195	-2.846942	0.637940
C	5.718961	-1.166397	-0.196237
C	5.093753	-3.850902	0.207935
H	3.294085	-3.125369	1.126579
C	6.600735	-2.151525	-0.627370
H	5.970903	-0.120729	-0.360570
C	6.293148	-3.503600	-0.427312
H	4.830625	-4.889431	0.374493
H	7.530982	-1.898140	-1.126373
C	-4.981980	-1.171508	0.840499
C	-5.791679	-2.303232	0.750887
C	-5.445806	0.016096	0.249111
C	-7.030749	-2.274844	0.099166
H	-5.457791	-3.235905	1.201251
C	-6.669530	0.065899	-0.401425
H	-4.832356	0.911796	0.305349
C	-7.473388	-1.083577	-0.481595
H	-7.628273	-3.178123	0.051093
H	-7.032547	0.983048	-0.855342
O	3.810544	5.386361	-0.541080
O	7.217584	-4.398707	-0.887499
O	-8.658437	-0.930869	-1.144073
C	3.816183	6.473702	-1.450784
H	3.268479	7.337953	-1.051656
H	4.864709	6.744462	-1.588636
H	3.384478	6.192485	-2.420874
C	6.961124	-5.781097	-0.704323
H	7.816823	-6.304373	-1.135291
H	6.877041	-6.039957	0.359641
H	6.045847	-6.095846	-1.223555
C	-9.516228	-2.055069	-1.247811

H	-10.393514	-1.713281	-1.800280
H	-9.040154	-2.878061	-1.797697
H	-9.829047	-2.417621	-0.259439

Structure of TS17-23

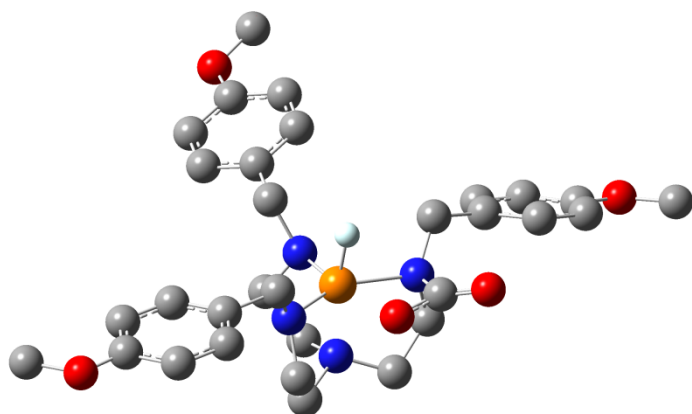


P	0.634785	-0.827823	-0.002108
N	0.515879	-1.263981	2.030303
N	2.333064	-1.012944	0.179610
C	2.734718	-1.946144	1.233045
C	1.912051	-1.602464	2.466447
C	0.027880	0.001695	2.670713
C	0.482734	1.153401	1.790680
N	0.182236	0.773301	0.411731
N	-1.103078	-1.740001	-0.092730
C	-1.634414	-2.098365	1.249192
C	-0.456808	-2.378331	2.180007
C	0.477153	1.854609	-0.576513
C	-2.112574	-1.003309	-0.979391
C	3.113346	-1.192908	-1.080637
H	0.575505	-0.652150	-1.395678
H	3.796312	-1.805249	1.451296
H	2.583917	-2.986077	0.913948
H	1.881046	-2.416705	3.196139
H	2.326740	-0.716595	2.950495
H	-1.060998	-0.024719	2.711535
H	0.410846	0.065309	3.693380
H	-0.063805	2.063667	2.050724
H	1.558137	1.357038	1.925179
H	-2.272894	-2.979243	1.148194
H	-2.262947	-1.281693	1.608463
H	-0.789915	-2.447296	3.220954
H	0.048337	-3.306799	1.909883
O	-1.308388	-3.837136	-1.274923
C	-0.533642	-3.077480	-0.754008
O	0.705702	-3.025571	-0.535361
C	-3.568440	-1.282458	-0.708173

H	-1.908119	0.057340	-0.818025
H	-1.838688	-1.268231	-2.002589
C	-4.340221	-0.332537	-0.014520
C	-5.690850	-0.540225	0.223824
C	-6.312737	-1.714807	-0.232987
C	-5.556710	-2.668574	-0.932026
C	-4.200114	-2.446489	-1.165298
H	-3.879439	0.593349	0.325367
H	-6.292351	0.193546	0.750428
O	-7.632058	-1.826223	0.045744
H	-6.014595	-3.577881	-1.303092
H	-3.623586	-3.193379	-1.700935
C	-8.337160	-2.978785	-0.410026
H	-9.367439	-2.843167	-0.079826
H	-8.310886	-3.054503	-1.503686
H	-7.929814	-3.896017	0.032380
C	-0.401896	3.072320	-0.401451
H	1.535790	2.144460	-0.492325
H	0.334772	1.437108	-1.577651
C	0.061571	4.202281	0.292296
C	-0.738016	5.324637	0.459471
C	-2.036505	5.350919	-0.075036
C	-2.512539	4.236485	-0.781967
C	-1.693255	3.117830	-0.937396
H	1.072046	4.209428	0.696107
H	-0.378173	6.200845	0.988898
O	-2.737558	6.490500	0.137666
H	-3.502159	4.237979	-1.223587
H	-2.071073	2.274631	-1.511675
C	-4.047707	6.603218	-0.409479
H	-4.403601	7.593092	-0.122129
H	-4.031190	6.525083	-1.503475
H	-4.720232	5.840673	0.003079
C	4.577216	-0.864307	-0.888617
H	2.996469	-2.222854	-1.441743
H	2.680733	-0.526925	-1.833674
C	5.552756	-1.869579	-0.974759
C	6.901476	-1.577166	-0.819984
C	7.312333	-0.258490	-0.569946
C	6.349488	0.758308	-0.478056
C	4.999883	0.445203	-0.638732
H	5.252562	-2.895086	-1.178057
H	7.658674	-2.350917	-0.894010
O	8.649166	-0.073092	-0.435246

H	6.641158	1.785725	-0.293770
H	4.264514	1.244249	-0.571496
C	9.139473	1.243883	-0.210783
H	10.224180	1.149265	-0.148675
H	8.879353	1.914097	-1.039568
H	8.756472	1.659257	0.730080

Structure of **23**

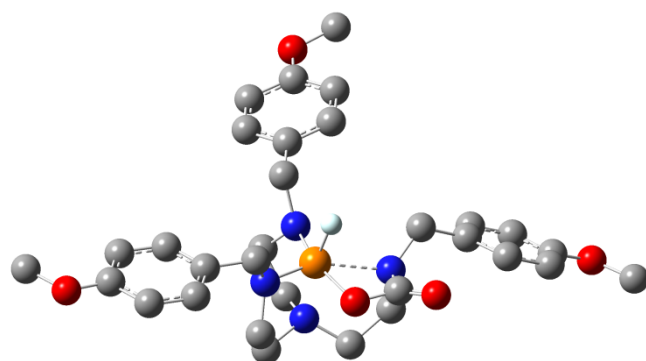


P	0.613335	-0.917259	-0.074391
N	0.486118	-1.329564	1.937130
N	2.320090	-1.104353	0.103408
C	2.667989	-2.140052	1.076810
C	1.847246	-1.855064	2.333122
C	0.192738	-0.012323	2.603226
C	0.714374	1.084257	1.692211
N	0.275056	0.729956	0.348805
N	-1.381862	-1.580421	-0.069270
C	-1.831846	-1.878610	1.316109
C	-0.626800	-2.296106	2.161874
C	0.590773	1.769408	-0.671297
C	-2.390633	-0.802765	-0.891254
C	3.106060	-1.185754	-1.158809
H	0.486380	-0.694001	-1.456988
H	3.731854	-2.066387	1.317614
H	2.477469	-3.150182	0.688475
H	1.722793	-2.738768	2.964302
H	2.334791	-1.075529	2.919877
H	-0.886964	0.087110	2.711723
H	0.642715	-0.001841	3.599370
H	0.286765	2.046509	1.986905
H	1.812381	1.164530	1.753570
H	-2.581168	-2.675128	1.299342
H	-2.319576	-0.982324	1.703242
H	-0.892631	-2.306675	3.224121
H	-0.273645	-3.291010	1.887924
O	-1.522925	-3.680282	-1.228920
C	-0.861365	-2.842892	-0.682291
O	0.424755	-2.772676	-0.450093
C	-3.845368	-1.114100	-0.641885

H	-2.180915	0.242768	-0.648180
H	-2.113432	-0.977449	-1.934340
C	-4.633370	-0.211676	0.094178
C	-5.980320	-0.453101	0.321995
C	-6.581988	-1.615938	-0.187922
C	-5.809652	-2.523882	-0.928866
C	-4.457401	-2.266635	-1.151476
H	-4.188621	0.704550	0.478392
H	-6.593768	0.245235	0.881898
O	-7.899274	-1.763170	0.084869
H	-6.251514	-3.423562	-1.340586
H	-3.871509	-2.979802	-1.722533
C	-8.583935	-2.905774	-0.423297
H	-9.616445	-2.803547	-0.088045
H	-8.556570	-2.931292	-1.519308
H	-8.160617	-3.835051	-0.022843
C	-0.170924	3.059476	-0.460477
H	1.673092	1.974517	-0.666713
H	0.345312	1.357408	-1.655179
C	0.420773	4.145982	0.204489
C	-0.270188	5.333390	0.404265
C	-1.585321	5.471575	-0.068331
C	-2.188670	4.402304	-0.746601
C	-1.477220	3.216592	-0.934547
H	1.446678	4.066540	0.558606
H	0.188924	6.175771	0.911420
O	-2.174485	6.668567	0.171659
H	-3.194216	4.489327	-1.141323
H	-1.951805	2.408237	-1.486747
C	-3.493215	6.893831	-0.315623
H	-3.748776	7.911233	-0.017634
H	-3.534115	6.813187	-1.408890
H	-4.210042	6.193112	0.130849
C	4.585084	-0.964407	-0.928868
H	2.947277	-2.159608	-1.645566
H	2.716812	-0.416648	-1.834617
C	5.508665	-1.994028	-1.164447
C	6.870426	-1.796215	-0.975698
C	7.347218	-0.550583	-0.539292
C	6.436965	0.489260	-0.295732
C	5.073447	0.271637	-0.493403
H	5.157279	-2.963518	-1.510684
H	7.587187	-2.589092	-1.163203
O	8.691944	-0.454594	-0.385250

H	6.779925	1.462755	0.035034
H	4.378996	1.087708	-0.305655
C	9.246890	0.788751	0.027626
H	10.325353	0.632019	0.070704
H	9.023483	1.585690	-0.692689
H	8.882305	1.080638	1.020831

Structure of TS23-21

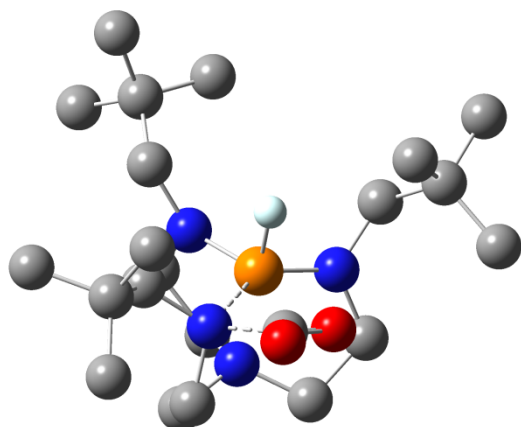


P	0.705094	-0.821362	-0.122177
N	0.516618	-1.240252	1.874806
N	2.393190	-1.069437	0.068774
C	2.688278	-2.114366	1.050317
C	1.868444	-1.778773	2.293714
C	0.221410	0.070670	2.548246
C	0.778457	1.169457	1.659333
N	0.381953	0.815231	0.305501
N	-1.460247	-1.476285	-0.117278
C	-1.831434	-1.800191	1.282160
C	-0.598413	-2.211403	2.090518
C	0.637324	1.869531	-0.713985
C	-2.527640	-0.737058	-0.880860
C	3.202404	-1.156760	-1.178255
H	0.567063	-0.576974	-1.499669
H	3.752127	-2.084815	1.300505
H	2.456577	-3.118468	0.668162
H	1.724095	-2.639443	2.951958
H	2.368502	-0.989276	2.856082
H	-0.859289	0.182187	2.628386
H	0.646572	0.066063	3.555251
H	0.342798	2.131853	1.941113
H	1.873902	1.247126	1.756767
H	-2.571319	-2.607303	1.307098
H	-2.315084	-0.914122	1.698392
H	-0.844118	-2.237526	3.157656
H	-0.243163	-3.200121	1.799354
O	-1.475162	-3.475050	-1.428142
C	-0.890603	-2.660449	-0.769791
O	0.402354	-2.602785	-0.480210
C	-3.959403	-1.130848	-0.603564
H	-2.370918	0.314242	-0.619024

H	-2.274738	-0.864280	-1.937162
C	-4.780333	-0.284900	0.161931
C	-6.105521	-0.606328	0.418691
C	-6.651085	-1.796303	-0.090697
C	-5.845591	-2.649970	-0.859890
C	-4.516062	-2.311855	-1.111286
H	-4.379943	0.650701	0.548367
H	-6.744267	0.048959	1.001935
O	-7.951565	-2.022958	0.211460
H	-6.244501	-3.569522	-1.271739
H	-3.903575	-2.982313	-1.706006
C	-8.580219	-3.197121	-0.295604
H	-9.609010	-3.159363	0.063904
H	-8.576946	-3.208895	-1.392282
H	-8.094843	-4.105103	0.083001
C	-0.180740	3.123161	-0.497467
H	1.709071	2.122764	-0.717029
H	0.405339	1.445920	-1.696315
C	0.360518	4.229169	0.178432
C	-0.382139	5.384109	0.382885
C	-1.699403	5.469063	-0.096611
C	-2.252254	4.380131	-0.786686
C	-1.489602	3.227398	-0.978686
H	1.387449	4.191913	0.536680
H	0.037504	6.241828	0.898435
O	-2.340828	6.637545	0.148673
H	-3.258107	4.427214	-1.187350
H	-1.924470	2.403184	-1.539834
C	-3.664999	6.810238	-0.345645
H	-3.965584	7.813382	-0.041463
H	-3.695406	6.736681	-1.439724
H	-4.353934	6.075988	0.090688
C	4.681218	-0.977338	-0.916009
H	3.027391	-2.119916	-1.680246
H	2.845207	-0.369772	-1.851497
C	5.582319	-2.027782	-1.146699
C	6.944560	-1.868046	-0.927939
C	7.444343	-0.640876	-0.465601
C	6.556519	0.419368	-0.226686
C	5.192218	0.240062	-0.454641
H	5.213127	-2.983219	-1.512937
H	7.644287	-2.676916	-1.111369
O	8.787474	-0.582117	-0.283187
H	6.917850	1.379284	0.123598

H	4.515198	1.071496	-0.270484
C	9.366268	0.640958	0.156946
H	10.439112	0.455127	0.219718
H	9.178665	1.452375	-0.557362
H	8.989143	0.929922	1.146296

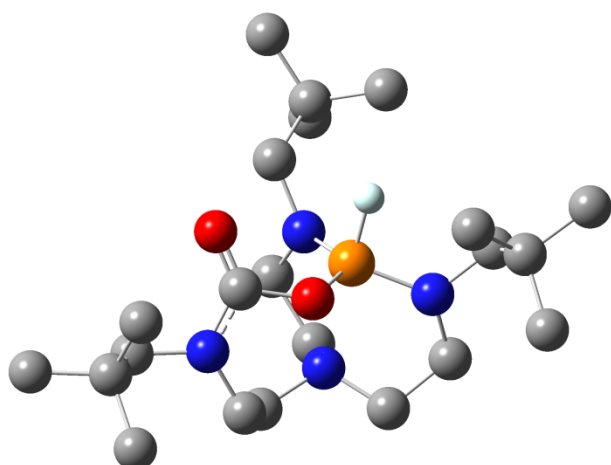
Structure of TS19-24



P	-0.335091	-0.227575	0.365333
N	-0.096073	-0.570386	2.345727
N	-0.229030	1.442596	0.719118
C	-0.237077	1.853675	2.118540
C	-0.685204	0.659770	2.960196
C	-0.908468	-1.792606	2.600907
C	-2.188642	-1.656518	1.759736
N	-1.912267	-0.769313	0.636645
N	1.606611	-0.910151	0.234652
C	2.084284	-1.403691	1.560883
C	1.342485	-0.687025	2.683969
C	-3.014978	-0.469057	-0.300854
C	2.520074	0.125272	-0.371512
C	0.154329	2.455046	-0.287307
H	-0.325625	-0.072966	-1.028678
H	-0.945088	2.667938	2.284104
H	0.752278	2.227754	2.427163
H	-0.363093	0.738671	4.003090
H	-1.769465	0.559679	2.934483
H	-0.324629	-2.650965	2.270743
H	-1.117302	-1.884418	3.671071
H	-2.500446	-2.651633	1.432008
H	-3.009221	-1.236704	2.359684
H	3.155162	-1.233520	1.661762
H	1.920114	-2.480857	1.619309
H	1.457667	-1.222962	3.631333
H	1.735295	0.322664	2.818285
H	-3.905743	-0.359480	0.333910
H	-2.828256	0.524976	-0.721012
H	2.715637	0.829181	0.445941
H	1.921379	0.654918	-1.114526

H	0.183546	1.937588	-1.250734
H	1.179438	2.798291	-0.079957
C	-3.361662	-1.437567	-1.468743
C	-2.284605	-1.404274	-2.569602
C	-3.552928	-2.888665	-0.991623
C	-4.690952	-0.914254	-2.055140
H	-2.114756	-0.382500	-2.934555
H	-1.337235	-1.821485	-2.217129
H	-2.603415	-2.005415	-3.428379
H	-4.294742	-2.957781	-0.185687
H	-3.915886	-3.509533	-1.818332
H	-2.608702	-3.324546	-0.649491
H	-4.989484	-1.518166	-2.918363
H	-5.503401	-0.961292	-1.319765
H	-4.603111	0.125607	-2.394351
C	3.882282	-0.220583	-1.070169
C	4.728139	-1.283383	-0.346969
C	3.663770	-0.628583	-2.542408
C	4.655741	1.120420	-1.059665
H	4.996588	-0.976748	0.672825
H	4.225311	-2.253186	-0.318264
H	5.670928	-1.419303	-0.887671
H	3.100811	0.143372	-3.082933
H	4.633220	-0.732086	-3.041872
H	3.134286	-1.576767	-2.631865
H	5.594924	1.012132	-1.611328
H	4.084444	1.923750	-1.541511
H	4.902974	1.440787	-0.039864
C	-0.743368	3.717483	-0.486289
C	-2.228675	3.343595	-0.598449
C	-0.541954	4.780596	0.616220
C	-0.270584	4.339123	-1.821073
H	-2.406309	2.661470	-1.438730
H	-2.600916	2.863723	0.313818
H	-2.834744	4.239359	-0.772471
H	0.522099	4.972125	0.800800
H	-0.993603	5.728159	0.303629
H	-1.010732	4.513254	1.568198
H	-0.828191	5.257209	-2.032442
H	0.794208	4.600745	-1.788661
H	-0.426049	3.654031	-2.663067
C	1.181520	-2.259266	-0.556800
O	-0.014425	-2.423368	-0.209872
O	2.001969	-2.851348	-1.204702

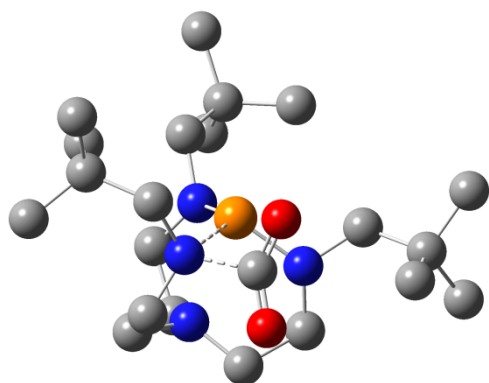
Structure of 24



P	-0.887783	-0.038446	0.069603
N	0.027989	-0.243353	2.173220
N	-0.976566	1.571286	0.516822
C	-0.548780	2.064620	1.830281
C	-0.619175	0.917120	2.827143
C	-0.507892	-1.549246	2.604664
C	-1.891975	-1.727054	2.001060
N	-1.879419	-1.261682	0.611439
N	2.666421	-0.078603	0.154574
C	2.430453	-0.872233	1.367075
C	1.514749	-0.178916	2.390295
C	-3.053533	-1.681335	-0.209775
C	3.941397	0.642679	-0.036619
C	-1.125916	2.612966	-0.546608
H	-1.475525	0.123230	-1.183548
H	-1.209551	2.872789	2.149047
H	0.466478	2.482215	1.766393
H	-0.136474	1.168696	3.779368
H	-1.663688	0.671517	3.033589
H	0.160708	-2.322577	2.218106
H	-0.532639	-1.630976	3.699668
H	-2.160834	-2.784781	2.023933
H	-2.659316	-1.189024	2.576884
H	3.400056	-1.002244	1.851000
H	2.071760	-1.871008	1.106411
H	1.708509	-0.605215	3.384970
H	1.800727	0.874797	2.435572
H	-3.877790	-1.840673	0.495955
H	-3.359386	-0.847234	-0.848239
H	4.306858	0.926141	0.957956
H	3.704194	1.561786	-0.577994

H	-0.796536	2.186582	-1.497986
H	-0.394138	3.394162	-0.307000
C	-2.872176	-2.943403	-1.092464
C	-1.844621	-2.687625	-2.210289
C	-2.432833	-4.162272	-0.261238
C	-4.251791	-3.226578	-1.722952
H	-2.141002	-1.841987	-2.843364
H	-0.844650	-2.485049	-1.811824
H	-1.765047	-3.566954	-2.858594
H	-3.146983	-4.386982	0.541149
H	-2.371261	-5.051200	-0.898276
H	-1.440792	-4.014223	0.181709
H	-4.196915	-4.098650	-2.382929
H	-5.010095	-3.435735	-0.958709
H	-4.602081	-2.378804	-2.324158
C	5.049881	-0.129091	-0.798277
C	5.463488	-1.405024	-0.041599
C	4.575120	-0.498630	-2.215504
C	6.258259	0.824370	-0.889862
H	5.803766	-1.181075	0.978005
H	4.642142	-2.129231	0.017085
H	6.291961	-1.901116	-0.558737
H	4.263222	0.386904	-2.779133
H	5.384942	-0.986038	-2.769546
H	3.730350	-1.196377	-2.190044
H	7.085492	0.341712	-1.420959
H	6.004438	1.741723	-1.434046
H	6.624399	1.109842	0.104214
C	-2.525678	3.253861	-0.728944
C	-3.558046	2.209384	-1.187962
C	-3.030426	3.932646	0.557871
C	-2.358402	4.321977	-1.830974
H	-3.249691	1.718328	-2.119448
H	-3.719915	1.440175	-0.423193
H	-4.526097	2.686567	-1.375062
H	-2.313186	4.671877	0.935654
H	-3.969398	4.461890	0.362205
H	-3.234225	3.203832	1.351467
H	-3.315900	4.812771	-2.034896
H	-1.643991	5.098520	-1.532740
H	-2.003695	3.880367	-2.769765
C	1.645348	0.168962	-0.696435
O	0.556456	-0.675922	-0.382132
O	1.595278	0.959774	-1.610353

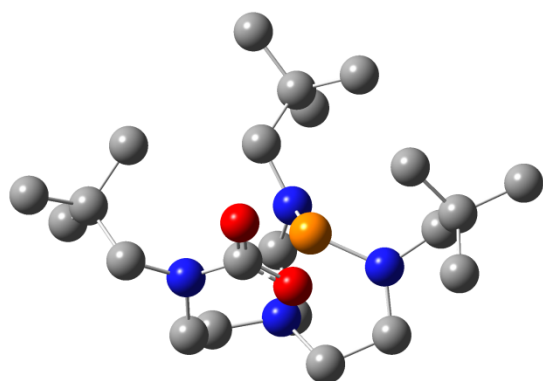
Structure of TS20-25



P	-0.026084	0.156940	-0.109863
N	0.313101	-0.433137	2.245802
N	-1.618418	-0.303835	0.393906
C	-2.053556	-0.514633	1.764418
C	-0.918109	-1.171595	2.542301
C	1.552407	-1.203780	2.335768
C	1.602377	-2.273224	1.239349
N	1.165368	-1.757148	-0.057691
N	0.511800	1.676528	0.627956
C	1.043891	1.865145	1.972013
C	0.388721	0.867551	2.914315
C	2.170944	-1.799422	-1.154879
C	0.999953	2.658930	-0.353629
C	-2.648343	0.115287	-0.583704
H	-2.908488	-1.193136	1.782866
H	-2.384365	0.428598	2.235873
H	-1.129578	-1.193021	3.622310
H	-0.808133	-2.193820	2.179636
H	2.384532	-0.500672	2.223666
H	1.652770	-1.677863	3.325482
H	2.612988	-2.681811	1.192279
H	0.934717	-3.099061	1.497240
H	0.846334	2.877224	2.337596
H	2.142516	1.747229	1.968708
H	0.934249	0.800329	3.867452
H	-0.627535	1.199907	3.138128
H	2.358396	-2.863111	-1.366619
H	1.641980	-1.412114	-2.027844
H	1.046949	2.159945	-1.328869
H	2.031228	2.944247	-0.091992
H	-2.119984	0.217294	-1.537042
H	-3.014894	1.122153	-0.319550

C	3.568976	-1.109135	-1.095882
C	3.471636	0.408567	-0.896420
C	4.532749	-1.695502	-0.042398
C	4.190453	-1.376203	-2.487969
H	2.871440	0.871254	-1.686108
H	3.017073	0.662528	0.065988
H	4.468977	0.865421	-0.923095
H	4.565928	-2.791007	-0.087384
H	5.550352	-1.329025	-0.226278
H	4.271680	-1.401912	0.979676
H	5.180293	-0.910519	-2.562944
H	4.311494	-2.450473	-2.672488
H	3.563989	-0.968158	-3.289541
C	0.163511	3.957561	-0.557468
C	-1.239588	3.616717	-1.083710
C	0.031820	4.786133	0.733458
C	0.915383	4.795685	-1.612009
H	-1.188551	3.045372	-2.018328
H	-1.796961	3.019708	-0.355472
H	-1.812760	4.531087	-1.279975
H	1.012196	5.015513	1.170421
H	-0.465694	5.740956	0.523678
H	-0.570584	4.266163	1.486452
H	0.372786	5.723238	-1.828909
H	1.919482	5.070572	-1.264837
H	1.025257	4.246094	-2.554946
C	-3.904088	-0.780487	-0.839847
C	-3.559539	-2.275591	-0.909195
C	-5.025333	-0.528786	0.193760
C	-4.446906	-0.327167	-2.215349
H	-2.795881	-2.472656	-1.666296
H	-3.167588	-2.658454	0.037385
H	-4.458328	-2.853465	-1.160300
H	-5.258449	0.540762	0.276230
H	-5.942607	-1.042912	-0.117798
H	-4.781327	-0.895450	1.195307
H	-5.381807	-0.848805	-2.451265
H	-4.655185	0.750957	-2.231525
H	-3.729038	-0.546462	-3.013937
C	-0.183365	-2.769765	-0.670421
O	-0.601414	-3.500655	0.209965
O	-0.380530	-2.495761	-1.837454

Structure of **25**



P	-0.652185	-0.035549	0.276496
N	-0.088853	-0.459612	2.137172
N	-2.131962	-0.796291	0.723464
C	-2.198340	-1.640567	1.907998
C	-0.781550	-1.739993	2.486351
C	1.408778	-0.487595	2.325133
C	2.243277	-1.553789	1.597698
N	2.405072	-1.411721	0.160604
N	-0.706855	1.650148	0.803758
C	-0.579453	1.972265	2.214353
C	-0.667167	0.651822	2.975767
C	3.765488	-1.390401	-0.388411
C	-0.179271	2.630073	-0.150153
C	-3.270191	-0.822568	-0.202877
H	-2.542847	-2.650368	1.664010
H	-2.911679	-1.231760	2.646689
H	-0.776880	-1.868862	3.574805
H	-0.236921	-2.537574	1.991702
H	1.766123	0.505972	2.042747
H	1.568184	-0.612386	3.404915
H	3.233050	-1.458353	2.060578
H	1.872480	-2.552562	1.861376
H	-1.362633	2.643292	2.591578
H	0.382057	2.479723	2.399146
H	-0.139100	0.687370	3.933621
H	-1.709846	0.402903	3.168594
H	4.464529	-1.784245	0.364794
H	3.767962	-2.076206	-1.239881
H	0.184866	2.072854	-1.023960
H	0.697807	3.128416	0.296590
H	-3.380168	0.177734	-0.641523
H	-4.167294	-0.975723	0.414883

C	4.293004	-0.014414	-0.875238
C	3.375065	0.548645	-1.973925
C	4.384802	0.989031	0.287541
C	5.703570	-0.246911	-1.450892
H	3.290256	-0.148755	-2.812760
H	2.362947	0.711543	-1.589613
H	3.761272	1.505776	-2.348433
H	5.022045	0.611042	1.098673
H	4.810414	1.942346	-0.049968
H	3.392838	1.202911	0.702263
H	6.135194	0.690717	-1.821900
H	6.386511	-0.649953	-0.691312
H	5.676249	-0.956044	-2.286872
C	-1.153785	3.725452	-0.666052
C	-2.333733	3.083274	-1.413619
C	-1.689004	4.595596	0.486033
C	-0.351798	4.613786	-1.638039
H	-1.986289	2.466025	-2.251312
H	-2.921281	2.445729	-0.744742
H	-3.002415	3.852281	-1.819224
H	-0.871730	5.022107	1.082098
H	-2.281811	5.431060	0.094156
H	-2.338892	4.020994	1.154900
H	-0.986186	5.404674	-2.055076
H	0.494447	5.097095	-1.133407
H	0.047399	4.029475	-2.475965
C	-3.287506	-1.859049	-1.367263
C	-2.236479	-1.514680	-2.441346
C	-3.028315	-3.291062	-0.865750
C	-4.695267	-1.774184	-1.992501
H	-2.347868	-0.479369	-2.790635
H	-1.215179	-1.658301	-2.077059
H	-2.364737	-2.169120	-3.312735
H	-3.752959	-3.591387	-0.096170
H	-3.123105	-4.002115	-1.695674
H	-2.011766	-3.381497	-0.470200
H	-4.777602	-2.454817	-2.847593
H	-5.475990	-2.049180	-1.271004
H	-4.914637	-0.761025	-2.354230
C	1.381161	-2.013642	-0.651928
O	0.275448	-2.199379	-0.010026
O	1.612606	-2.249797	-1.838295