Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Hydrogen-Bonding Cyclodiphosphazanes: Superior Effect of 3,5-$(CF_3)_2$-Substitution in Anion-Recognition and Counter-Ion Catalysis

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UV/Vis-Spectrometry

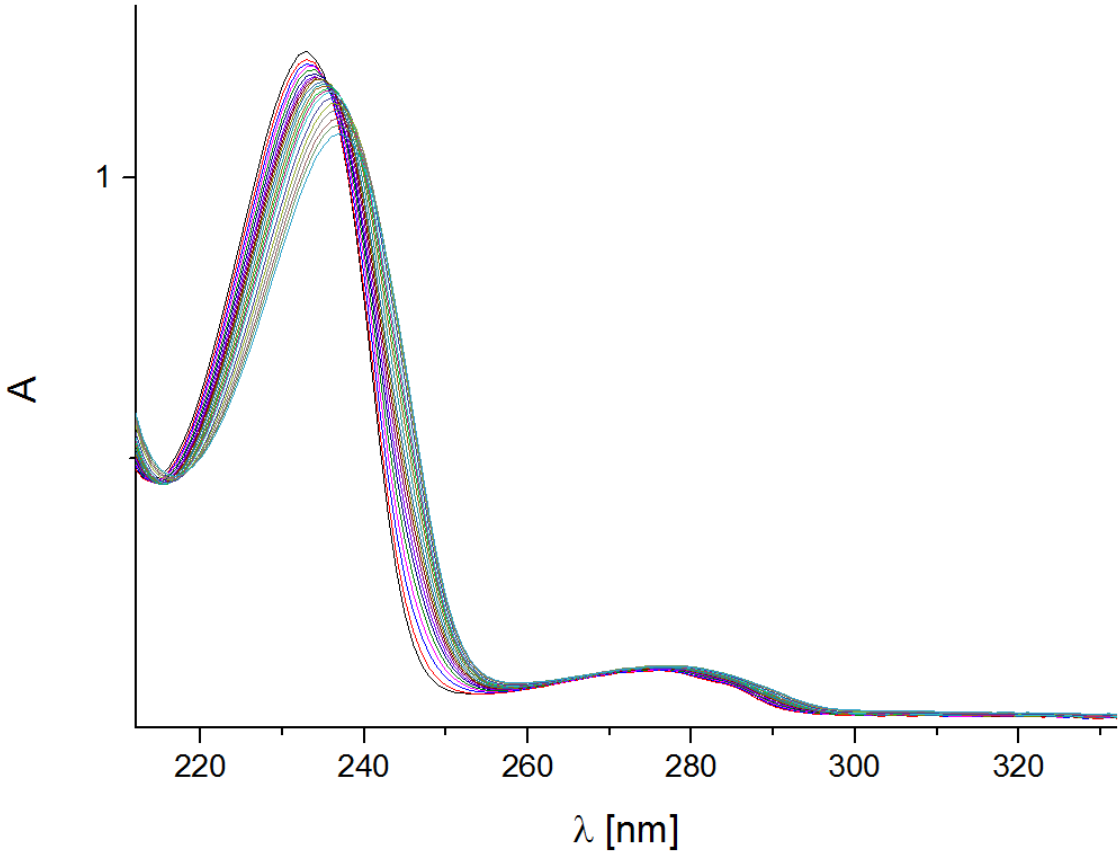
Experimental details

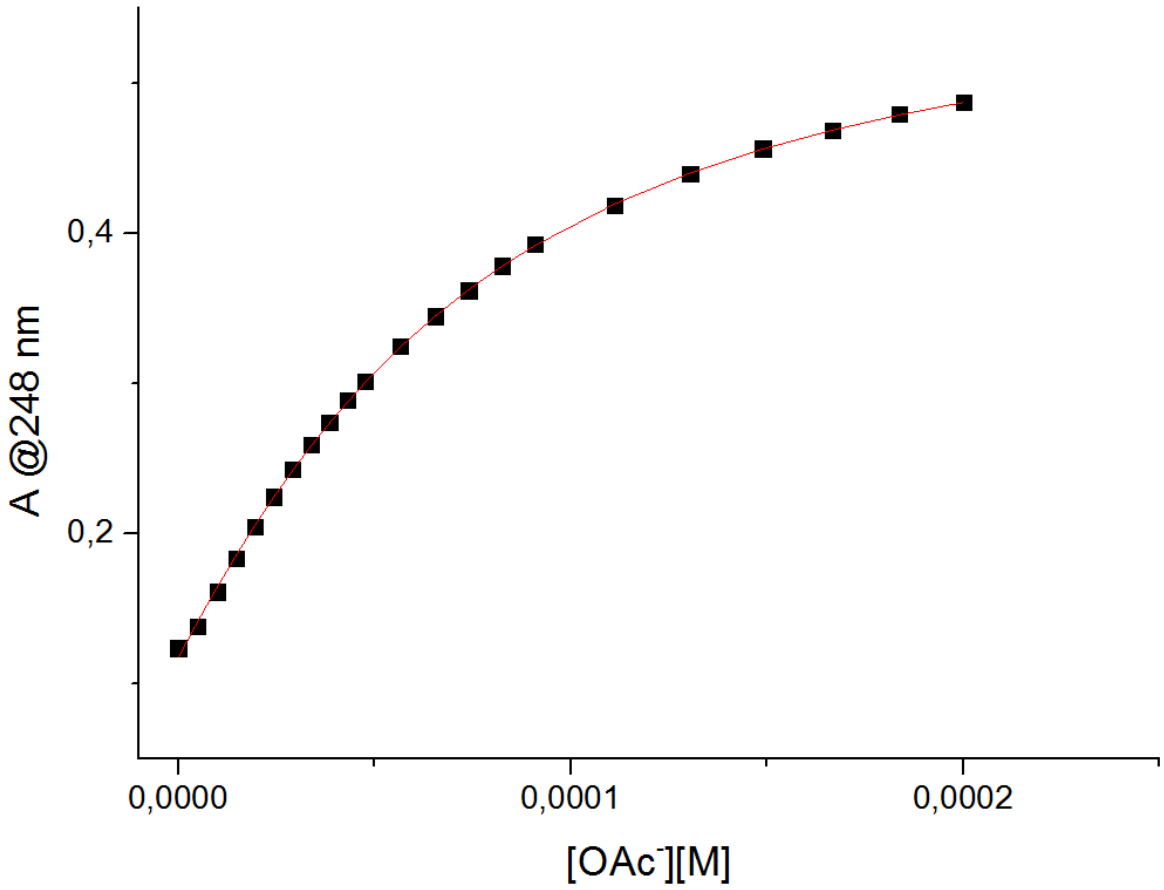
Stock solutions of the employed compounds with a concentration between $1x10^{-2}$ and $1x10^{-4}$ M, depending on the solubility of the molecule, in dry HPLC-grade acetonitrile were prepared. The examined anions Cl^- and OAc^- were employed as the *tert*-butylammonium salt and stock solutions with a concentration of $1x10^{-2}$ M were prepared. The appropriate amount of anion stock solution was added between UV/Vis-measurements. The measurements were recorded on a *Perkin Elmer Lambda35* spectrometer featuring a double-beam and all-reflecting system. A deuterium (UV) and a halogen (Vis) lamp, which automatically change at a wavelength of 326 nm, are used to cover the spectral range.

UV/Vis-Spectra

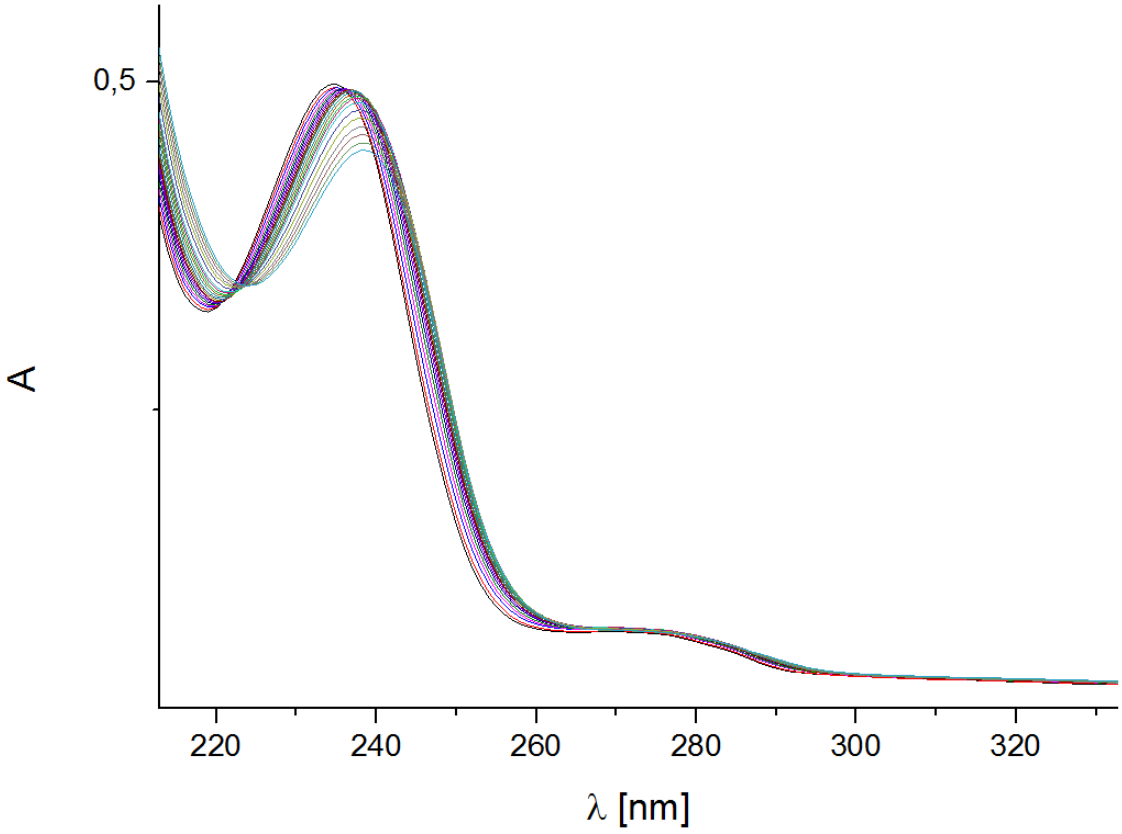
Acetate

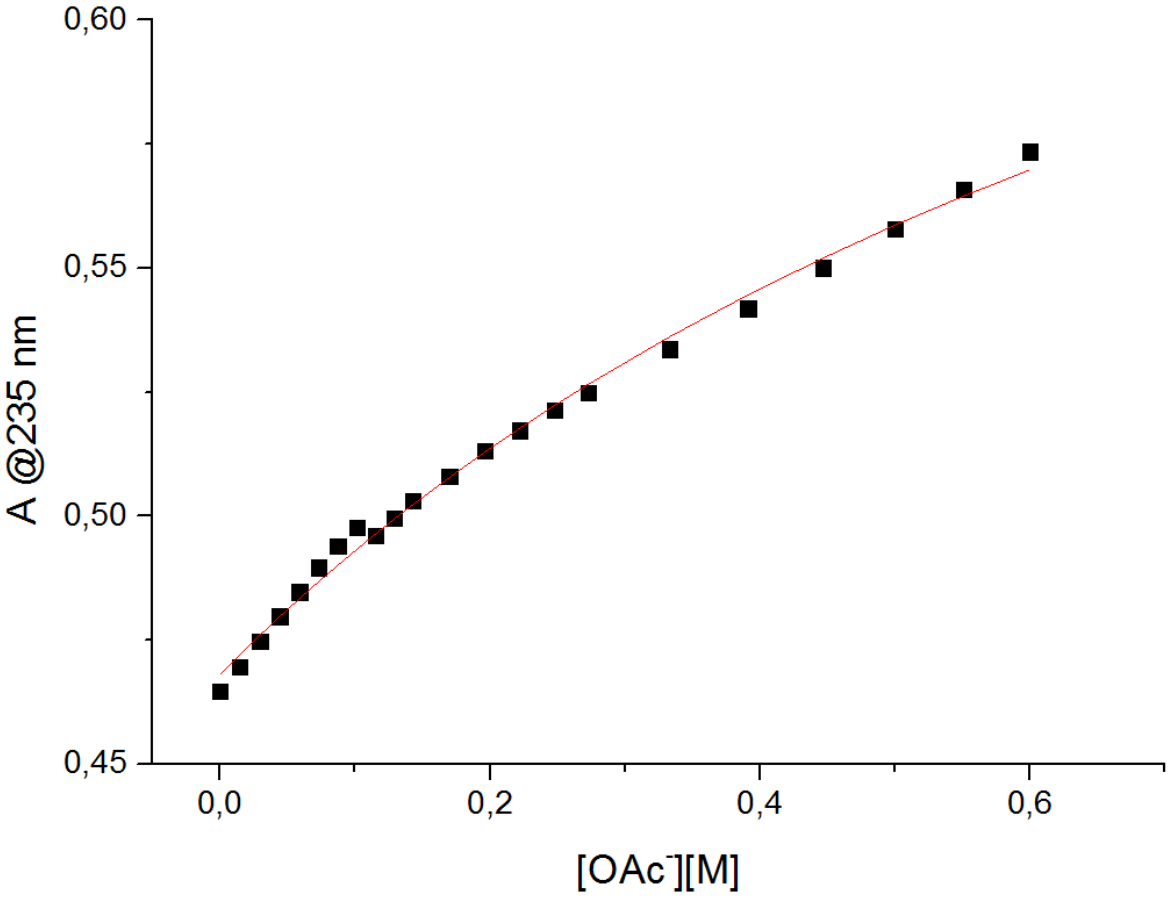
O-cyclodiphosph(V)azane **4**



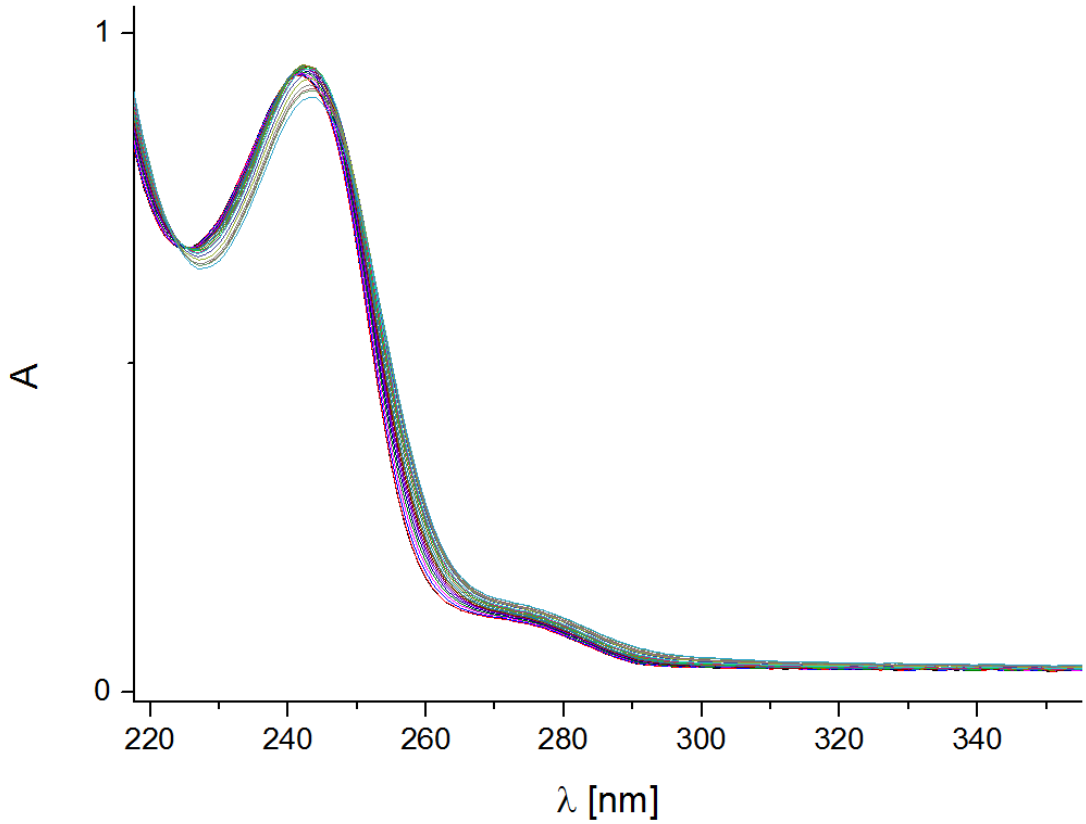

A @248 nm
0,4
0,2
0,0000
0,0001
0,0002
[OAc-][M]

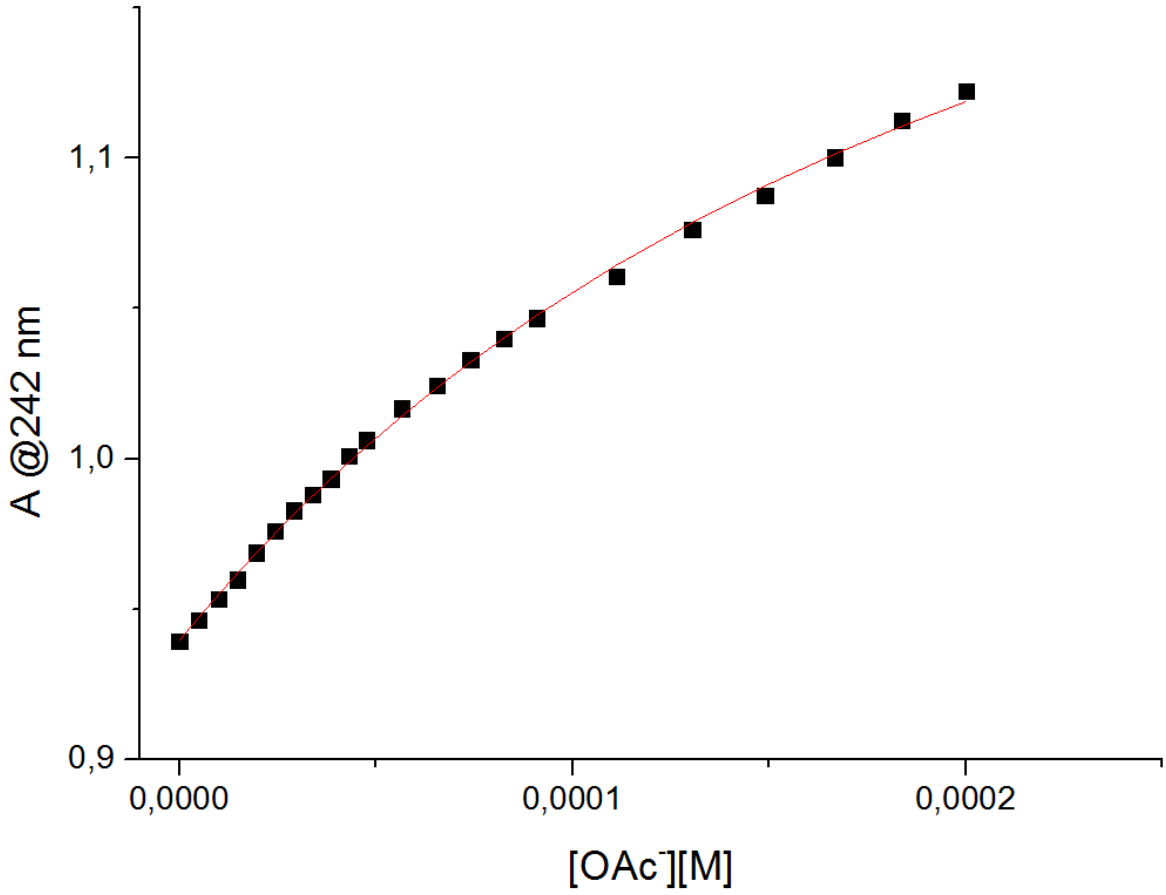
O/S-cyclodiphosph(V)azane **13**



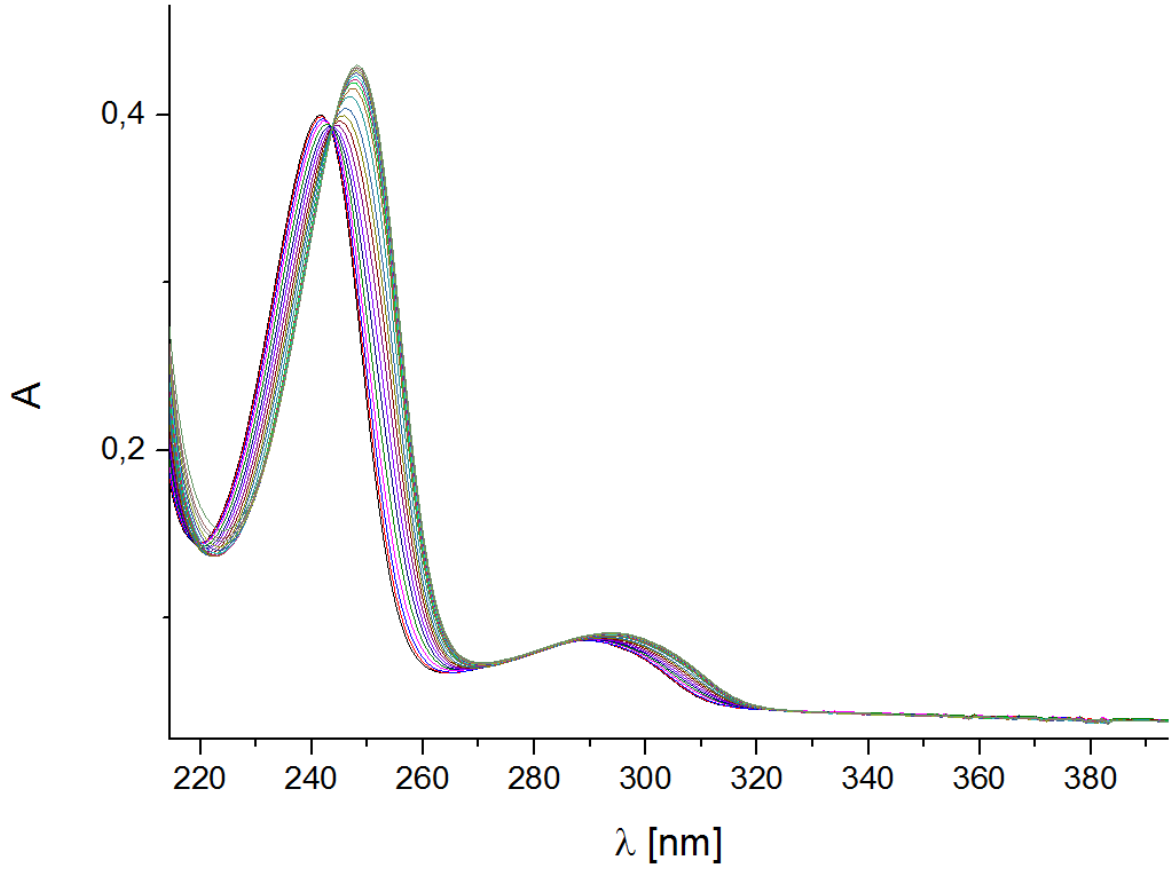


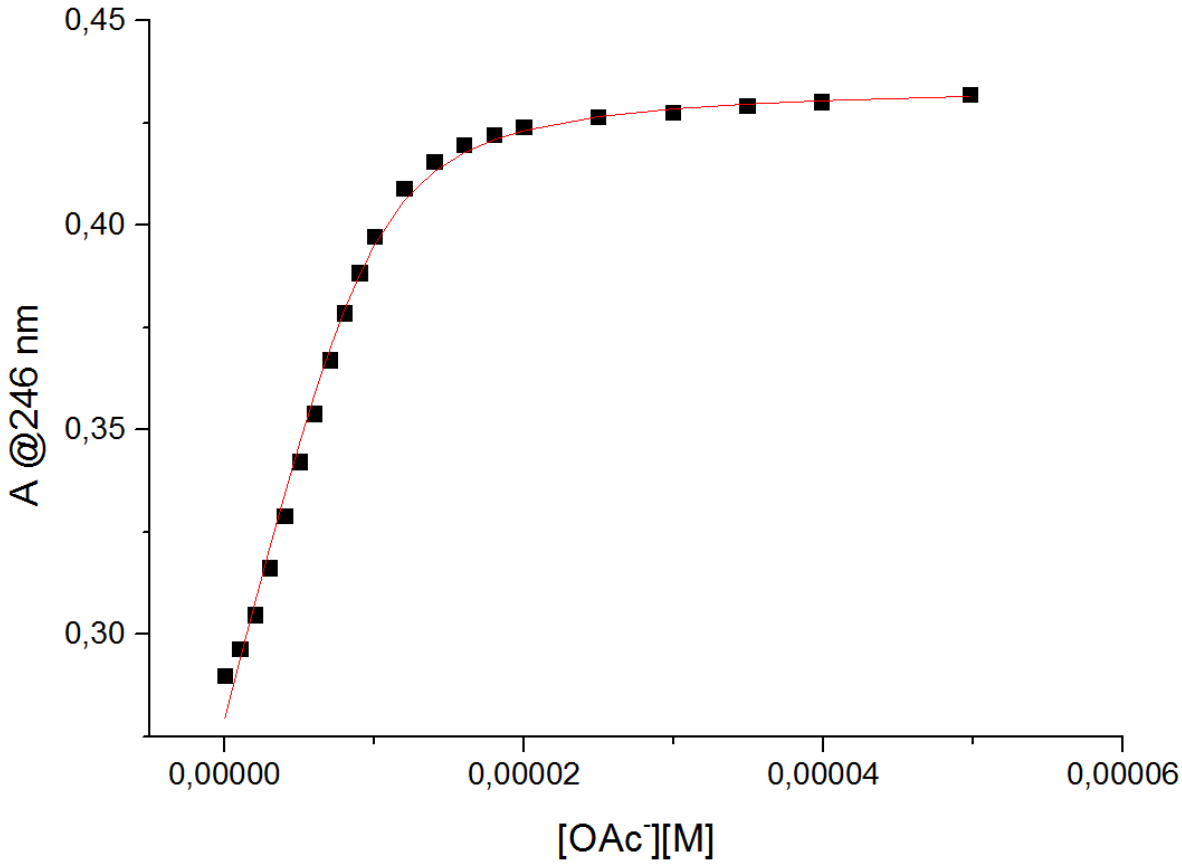
S-cyclodiphosph(V)azane **11**





O-cyclodiphosph(V)azane **5**





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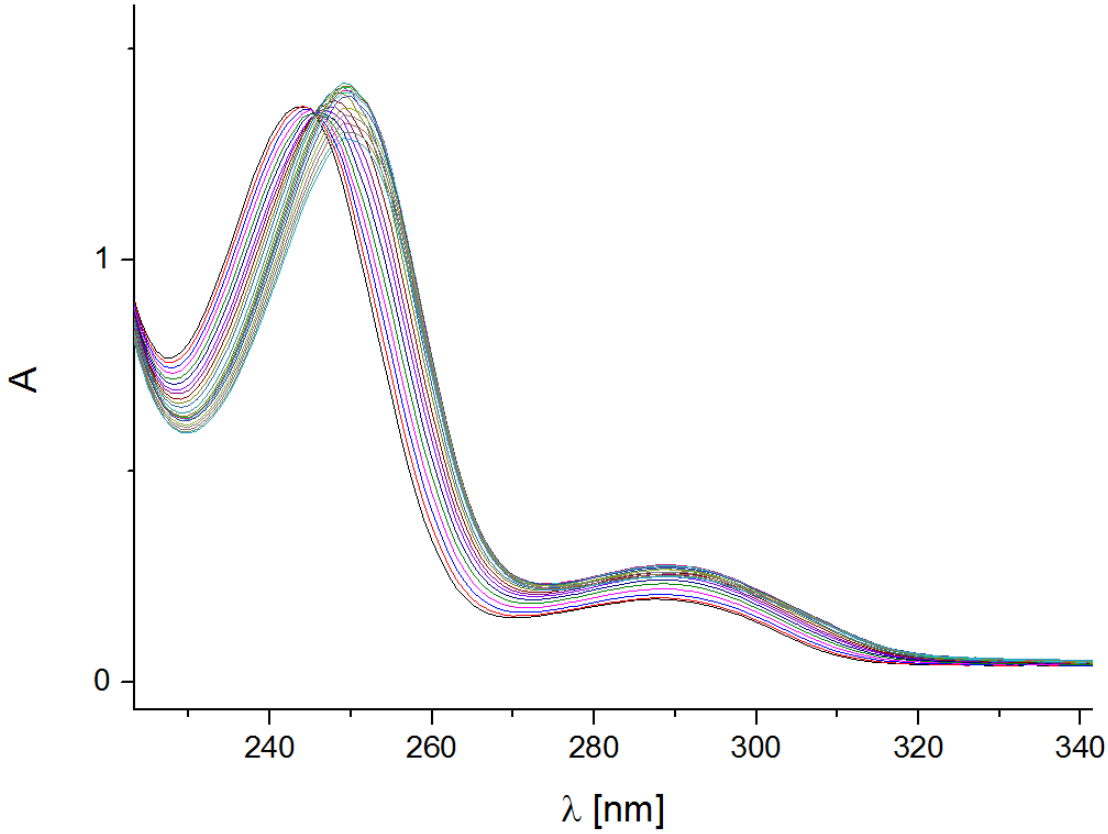
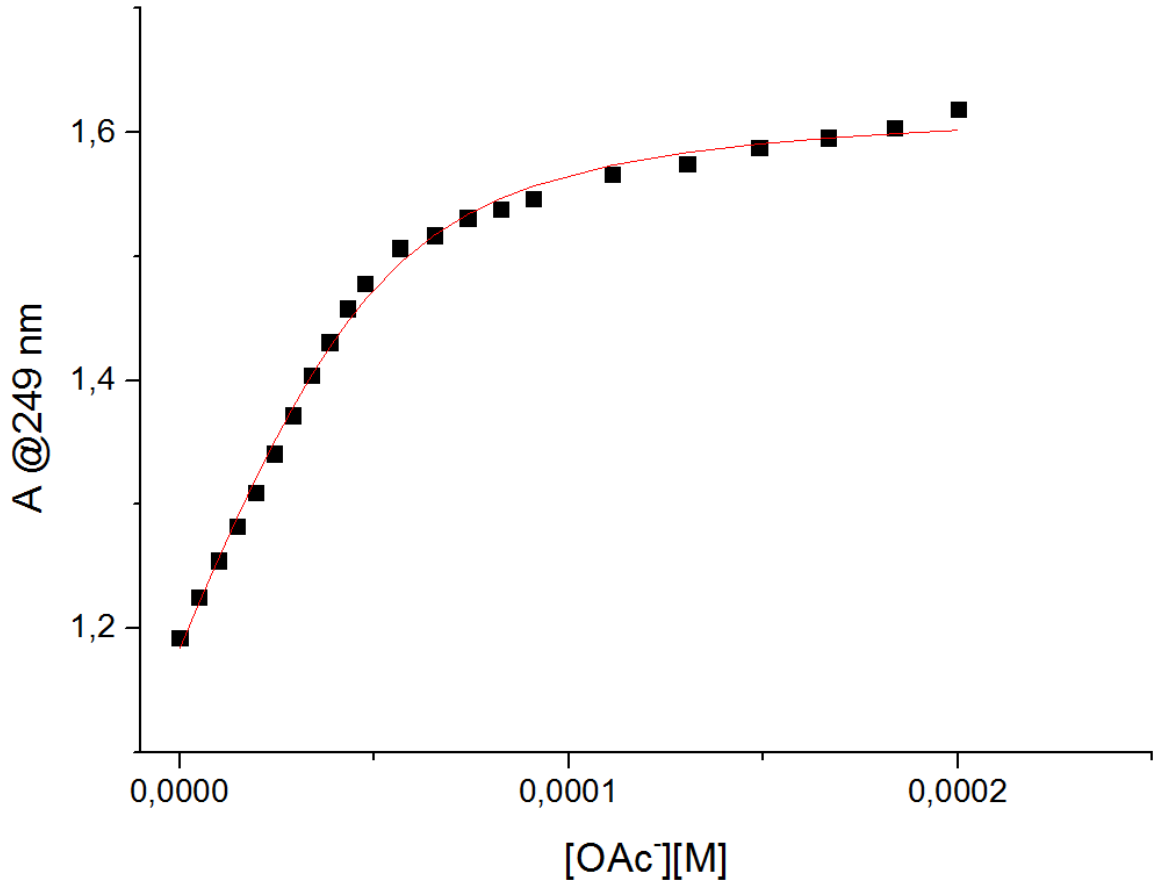
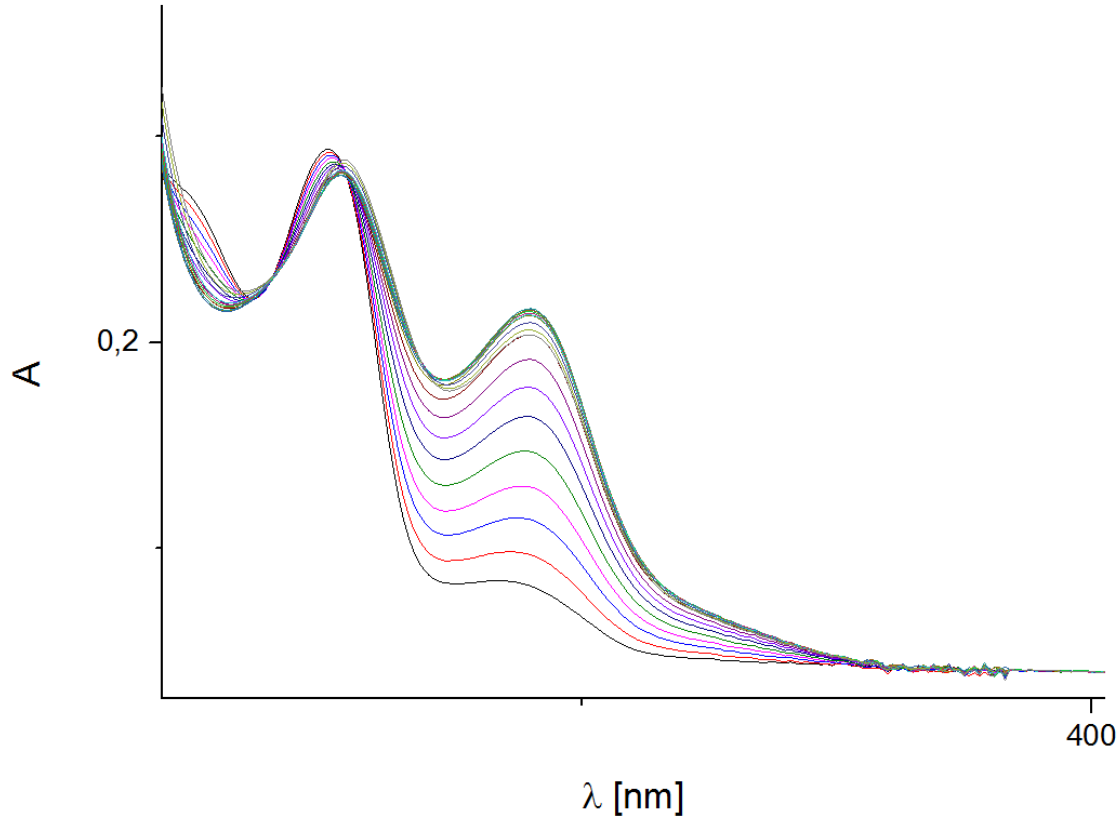
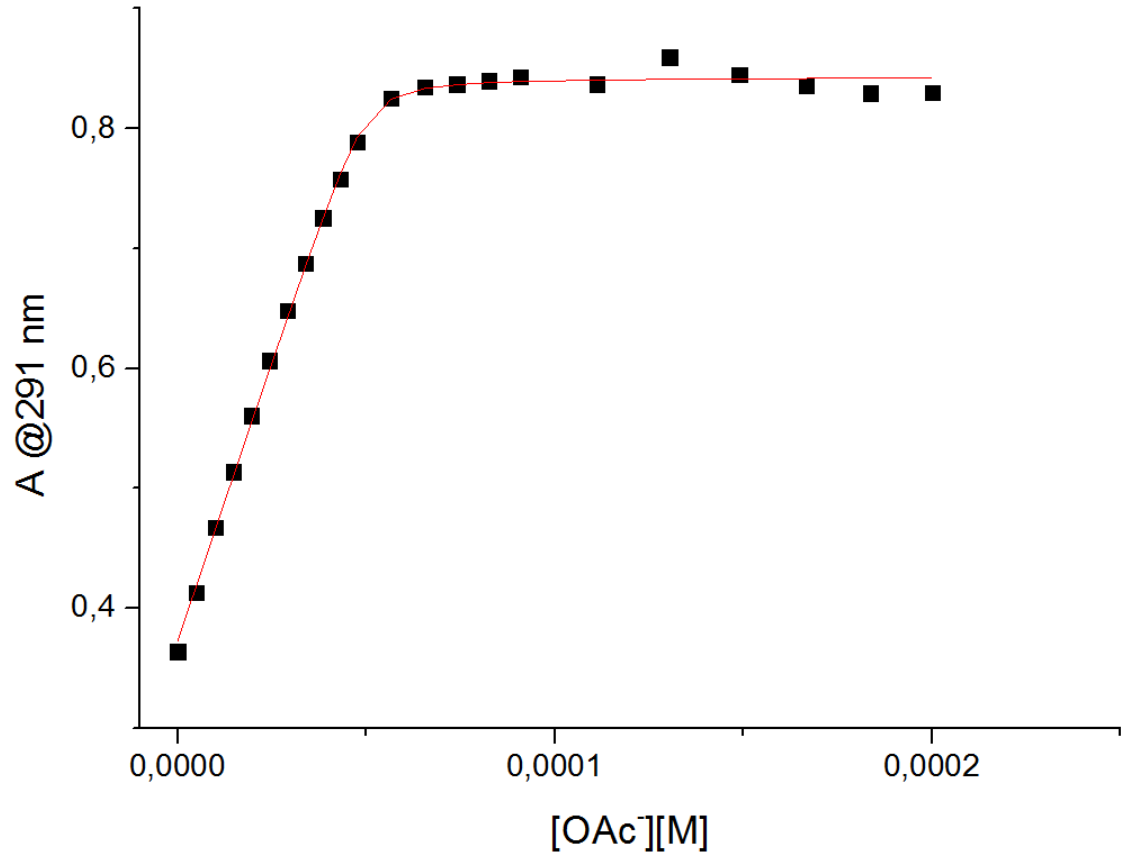


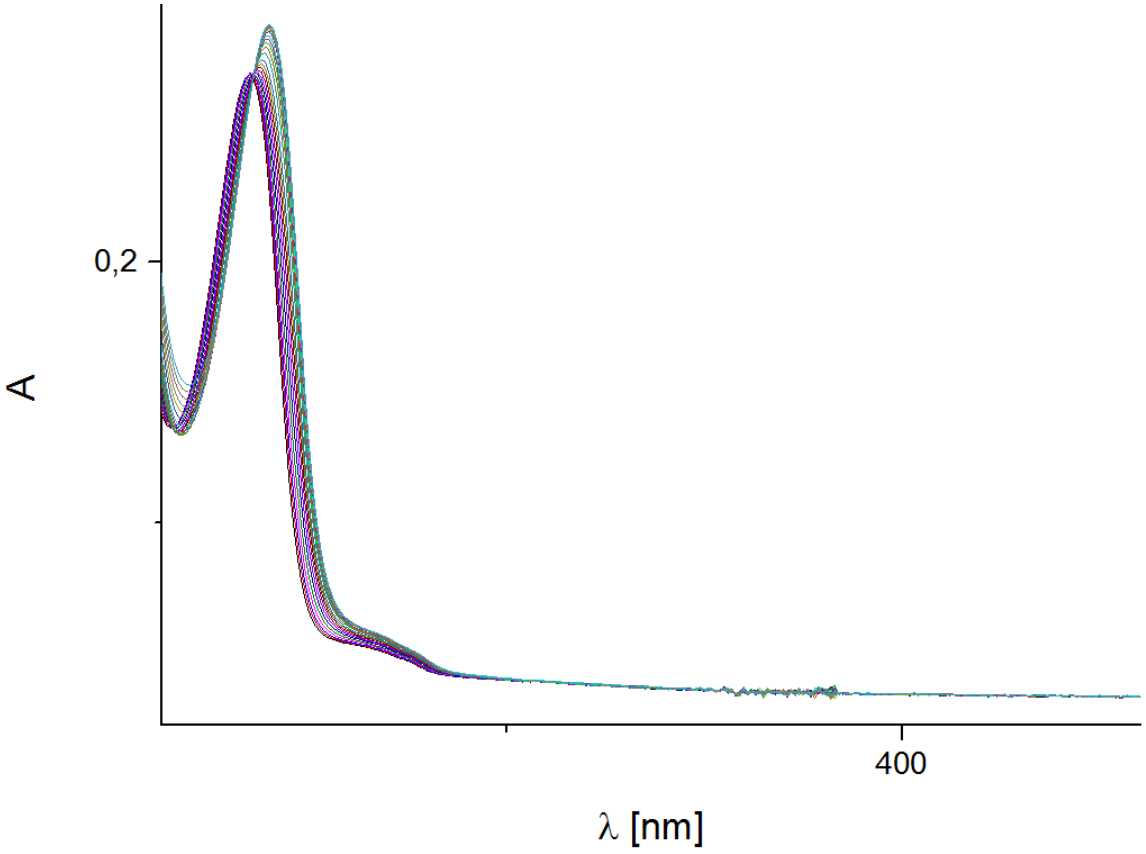


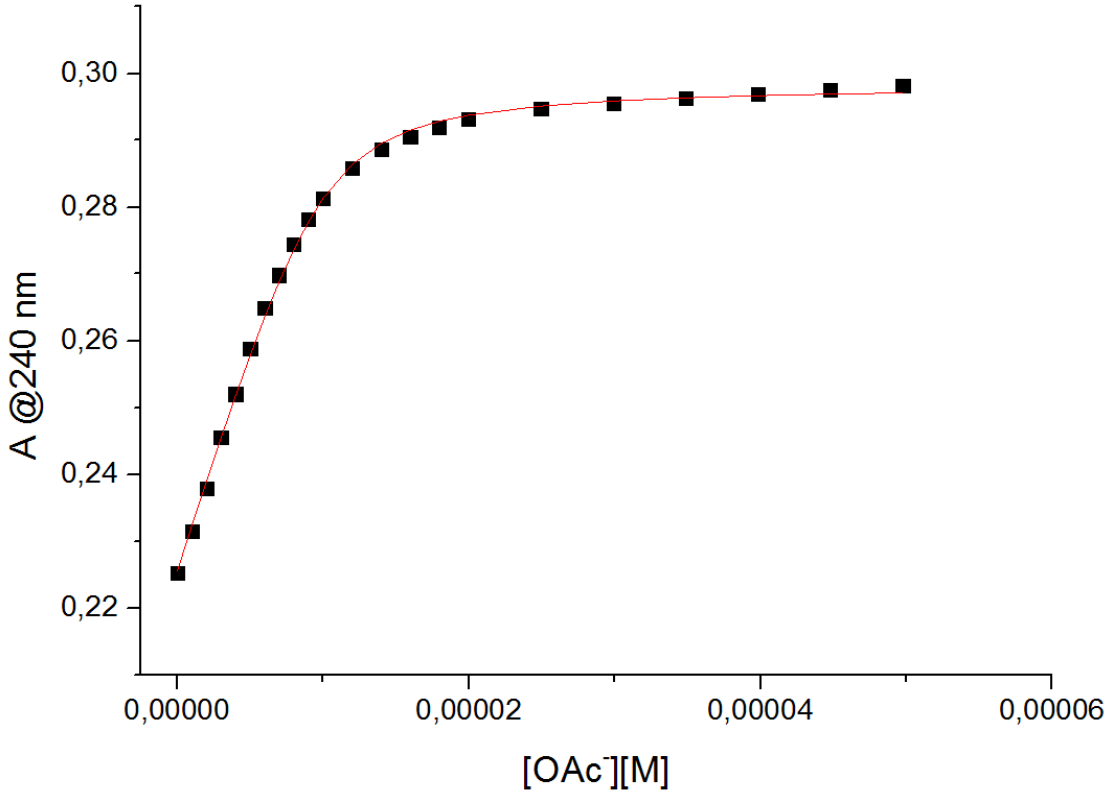
S-cyclodiphosph(V)azane **12**



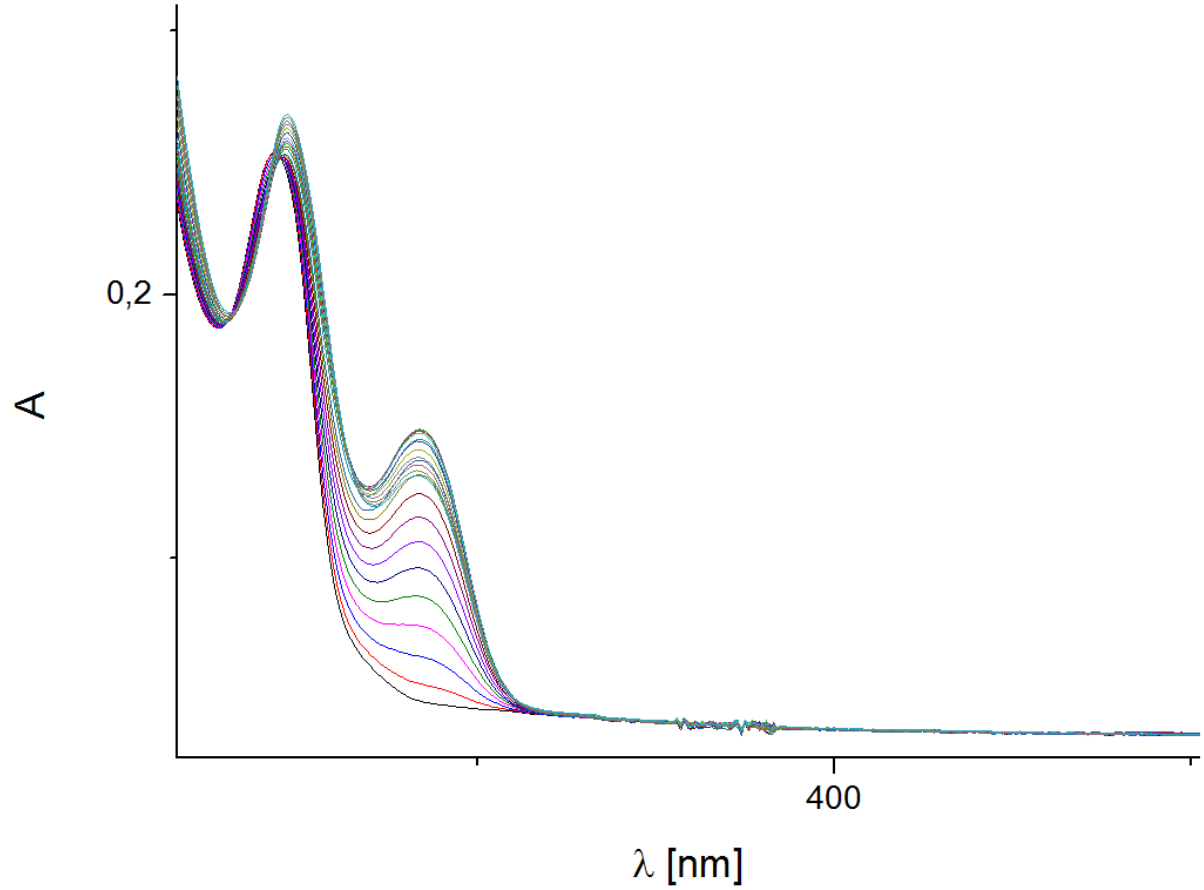


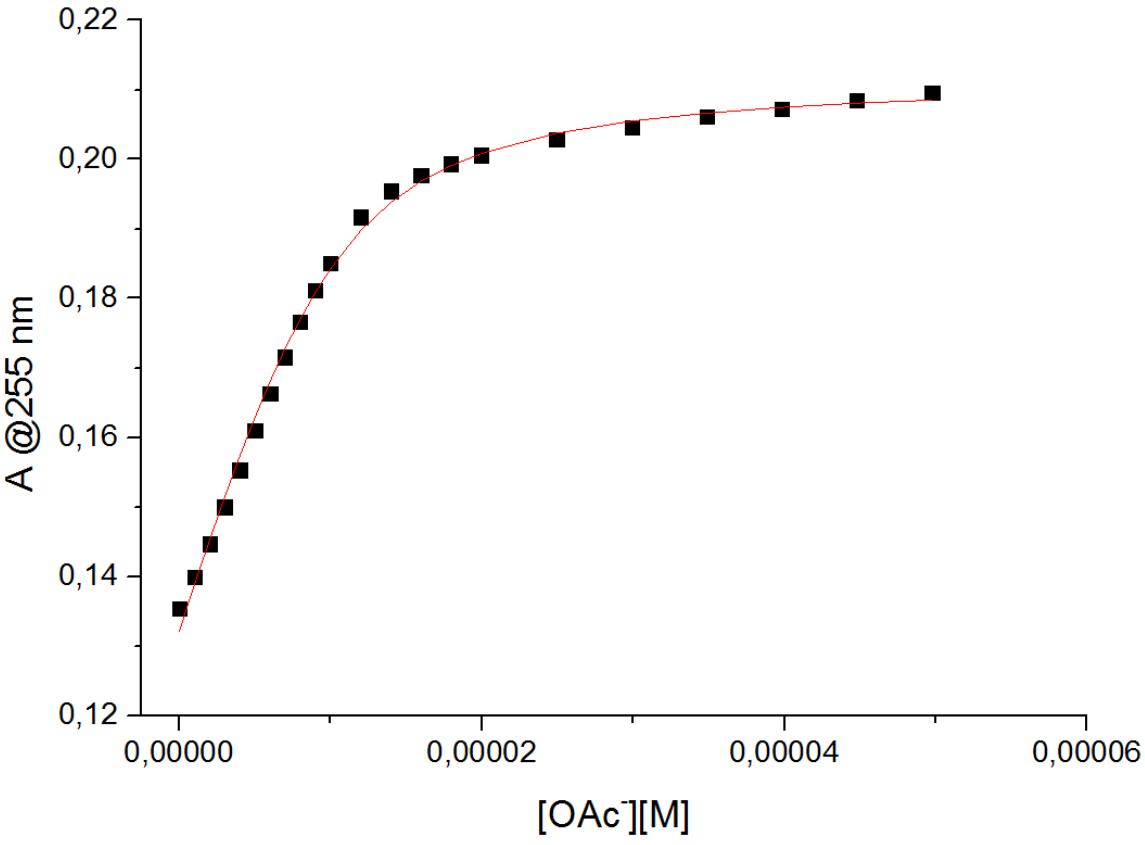
O-Cyclodiphosph(V)azane **15**



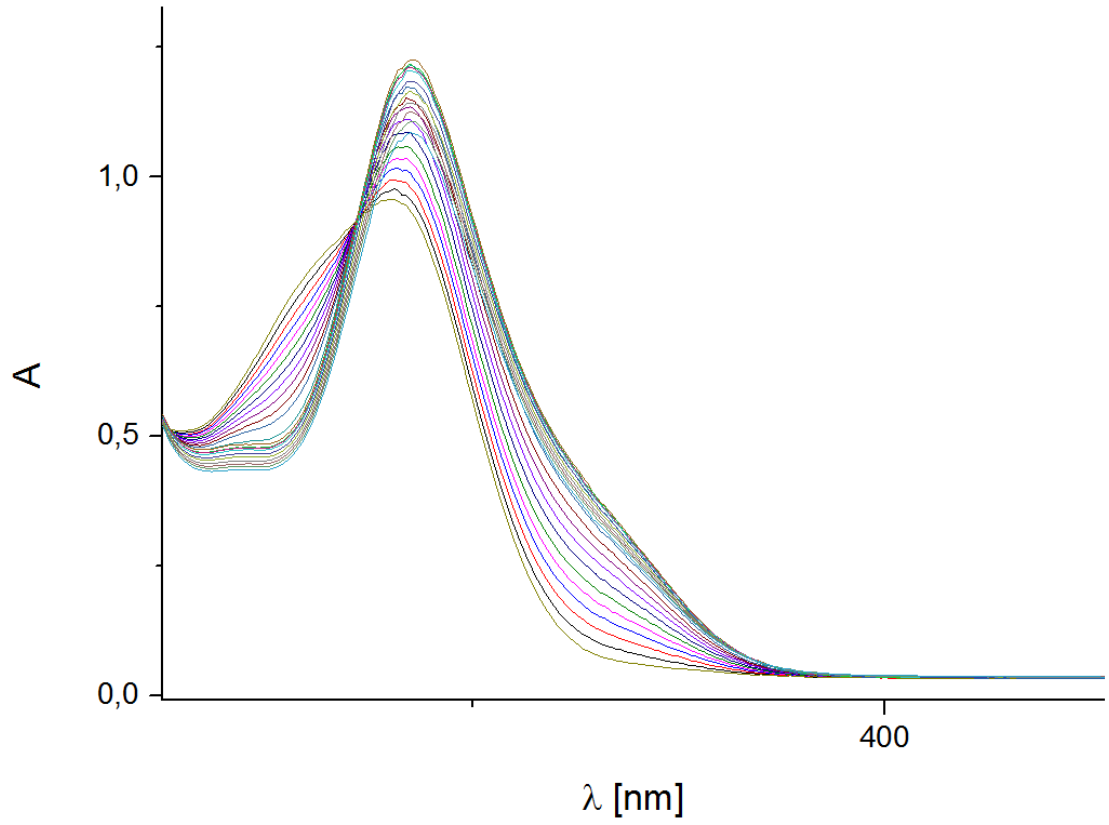


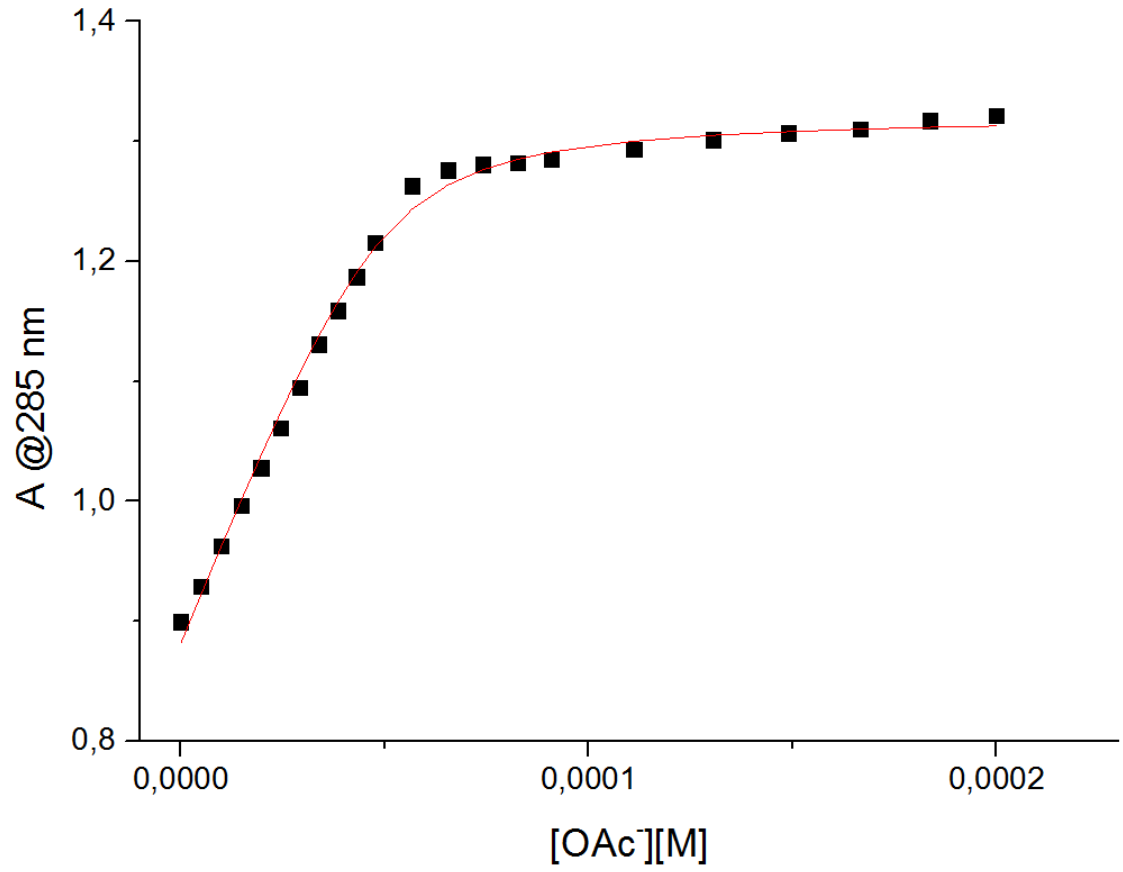
S-Cyclodiphosph(V)azane **16**



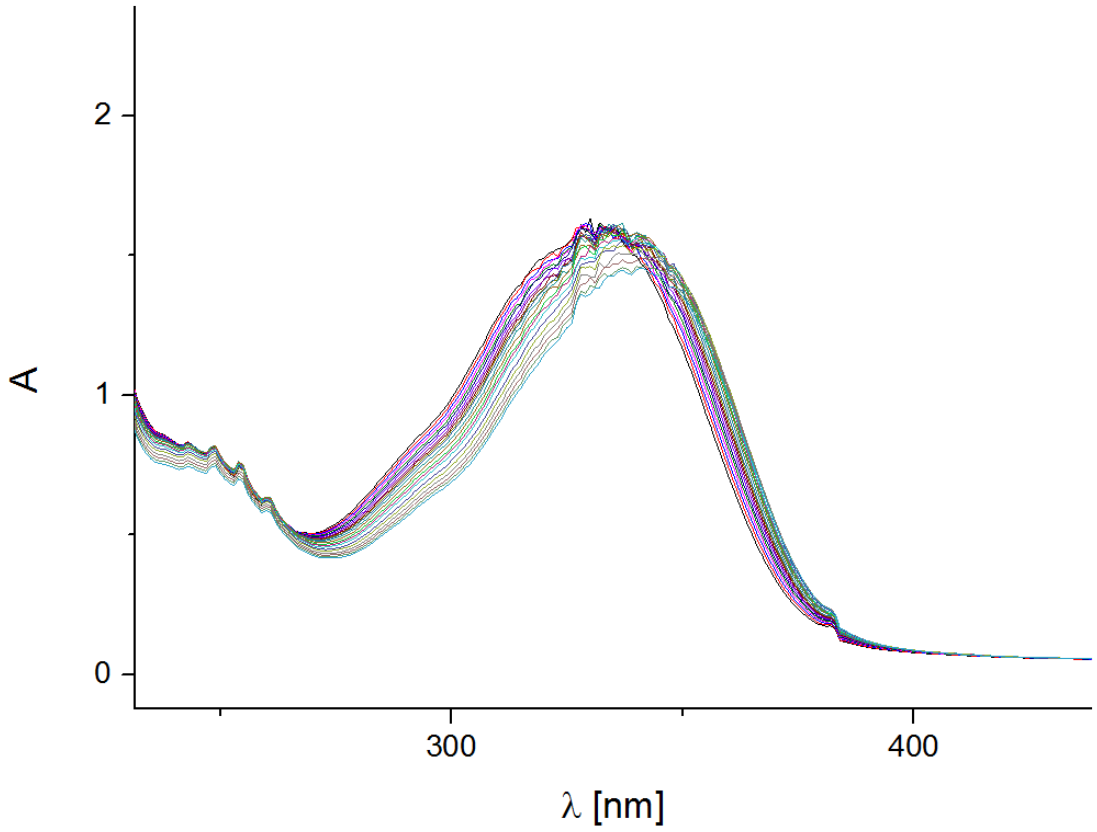


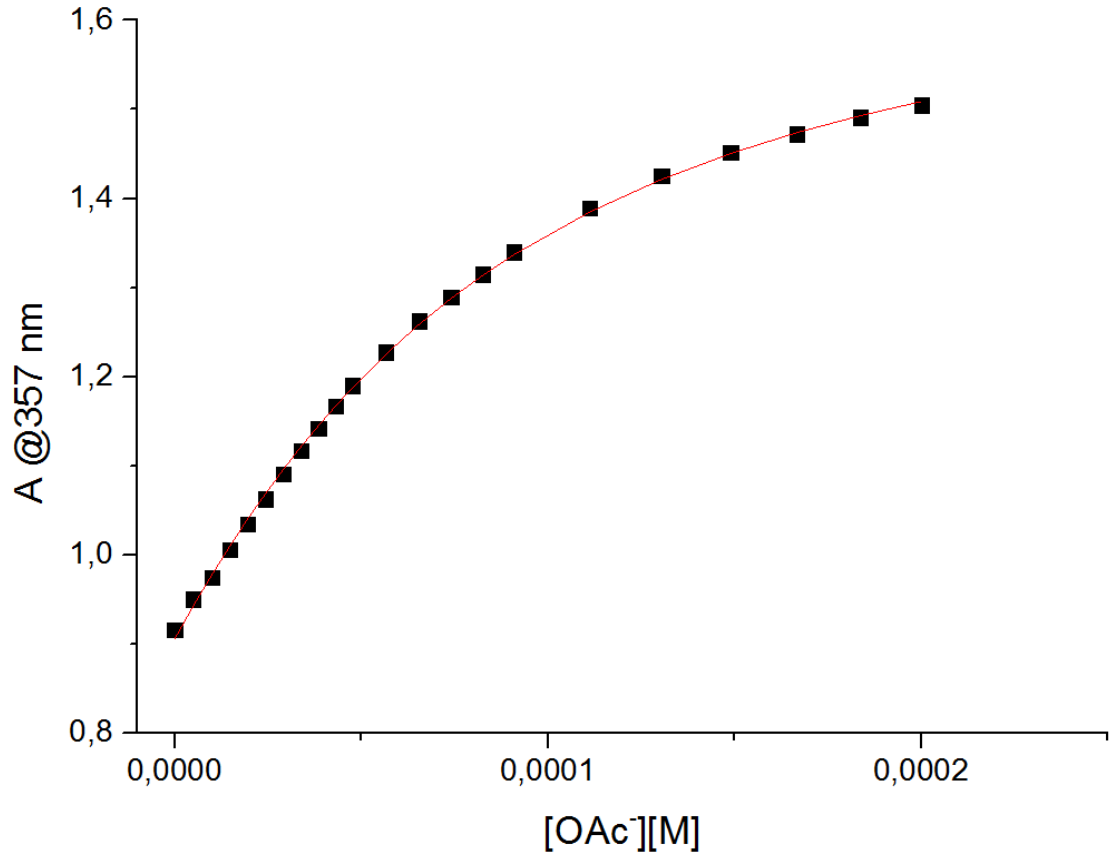
Thiourea **18**



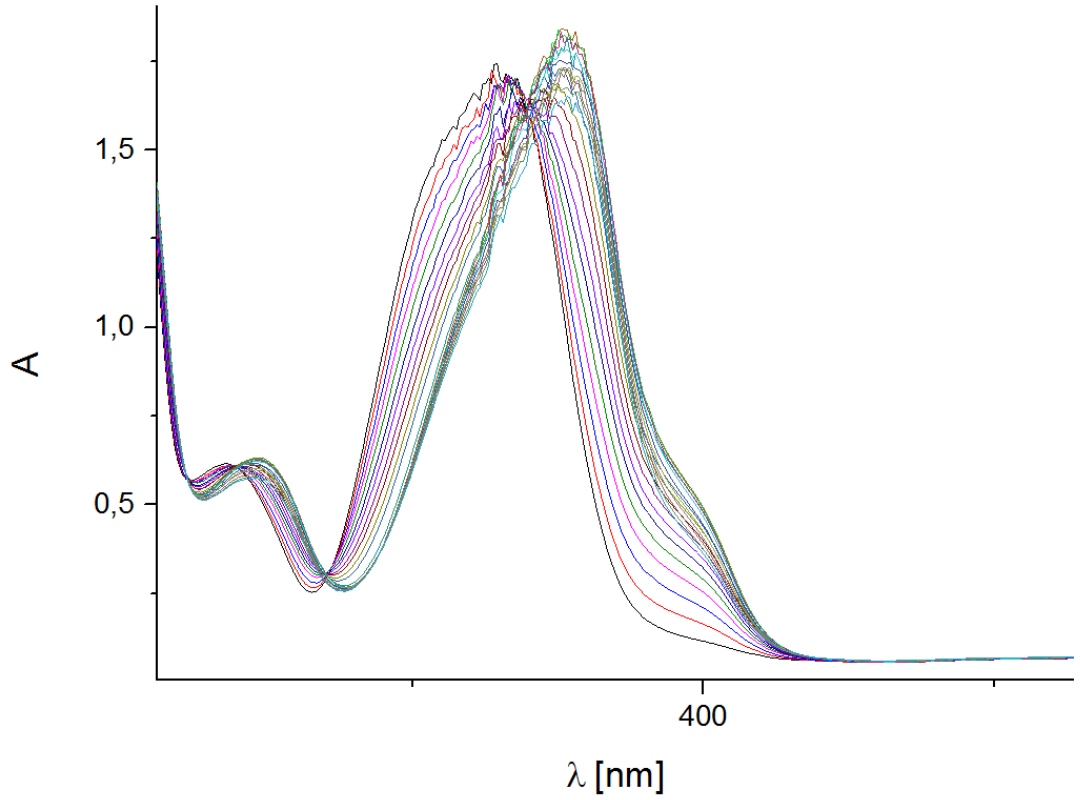


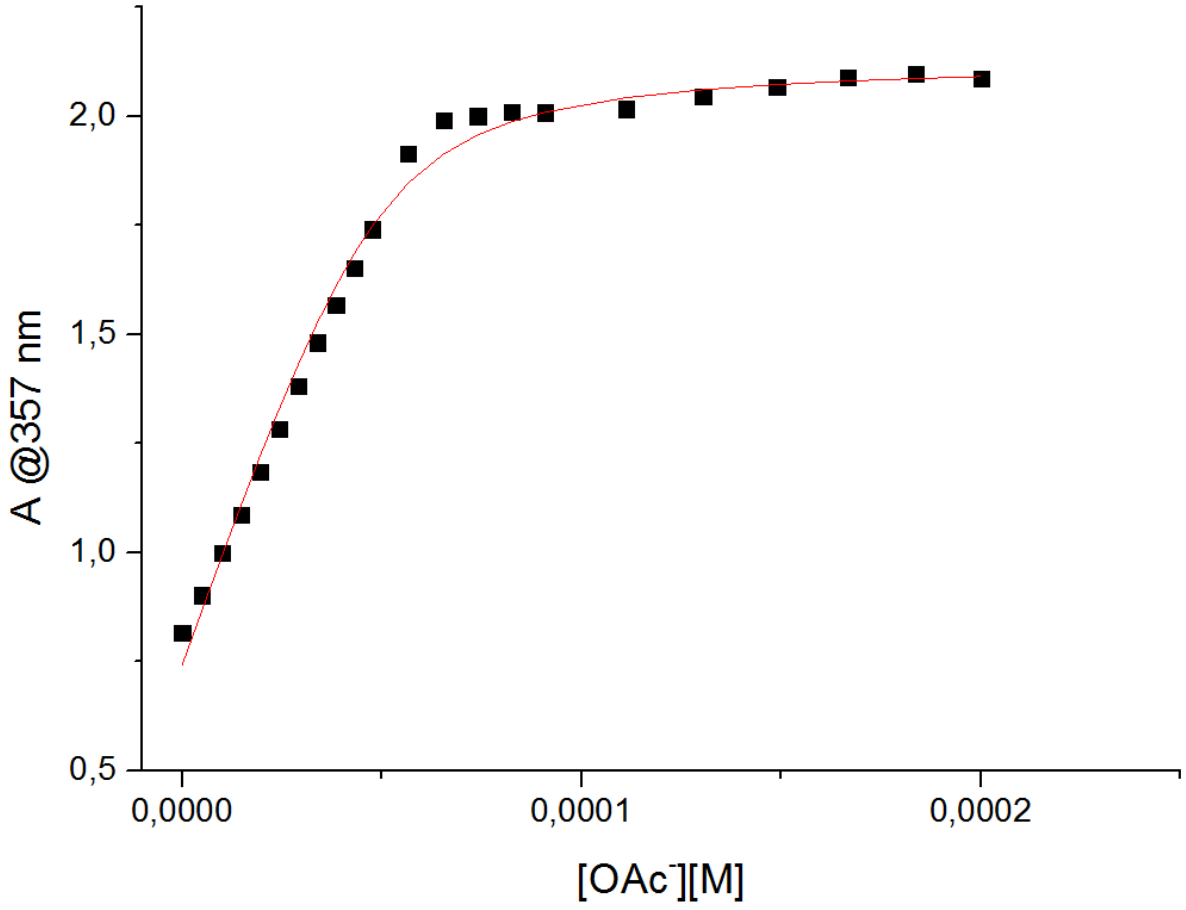
Squaramide **19**





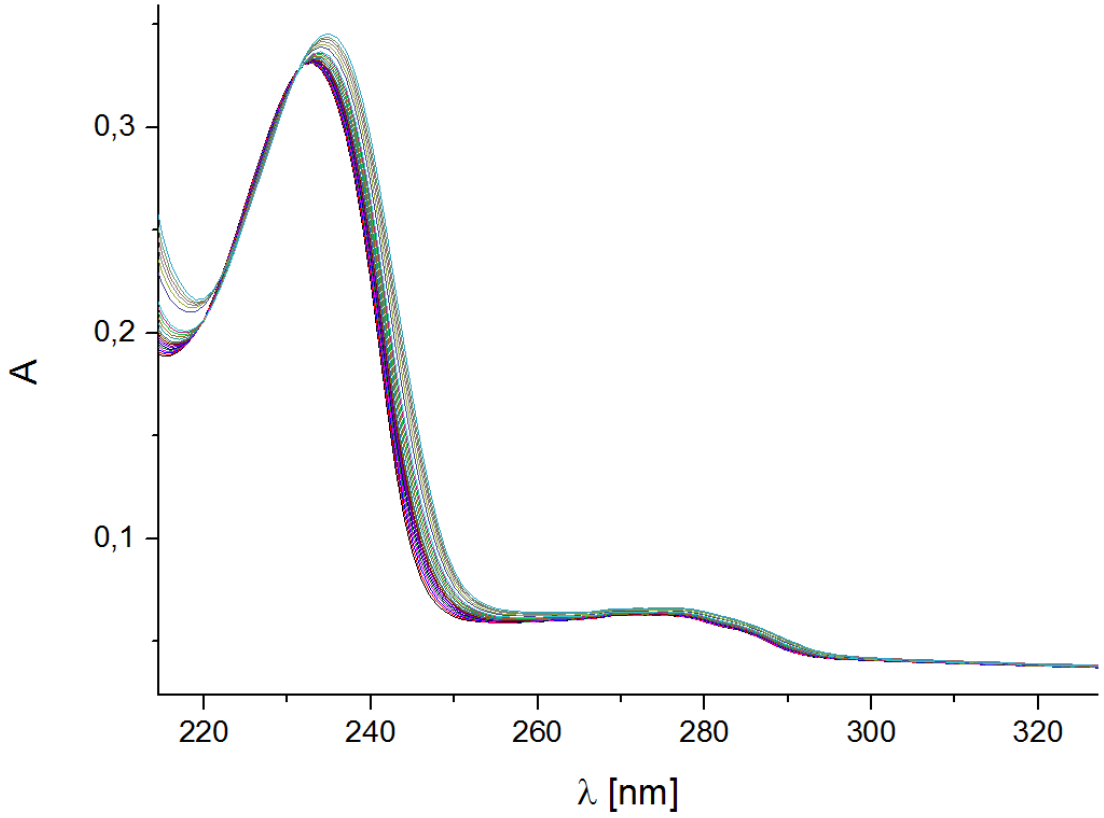
Squaramide **20**

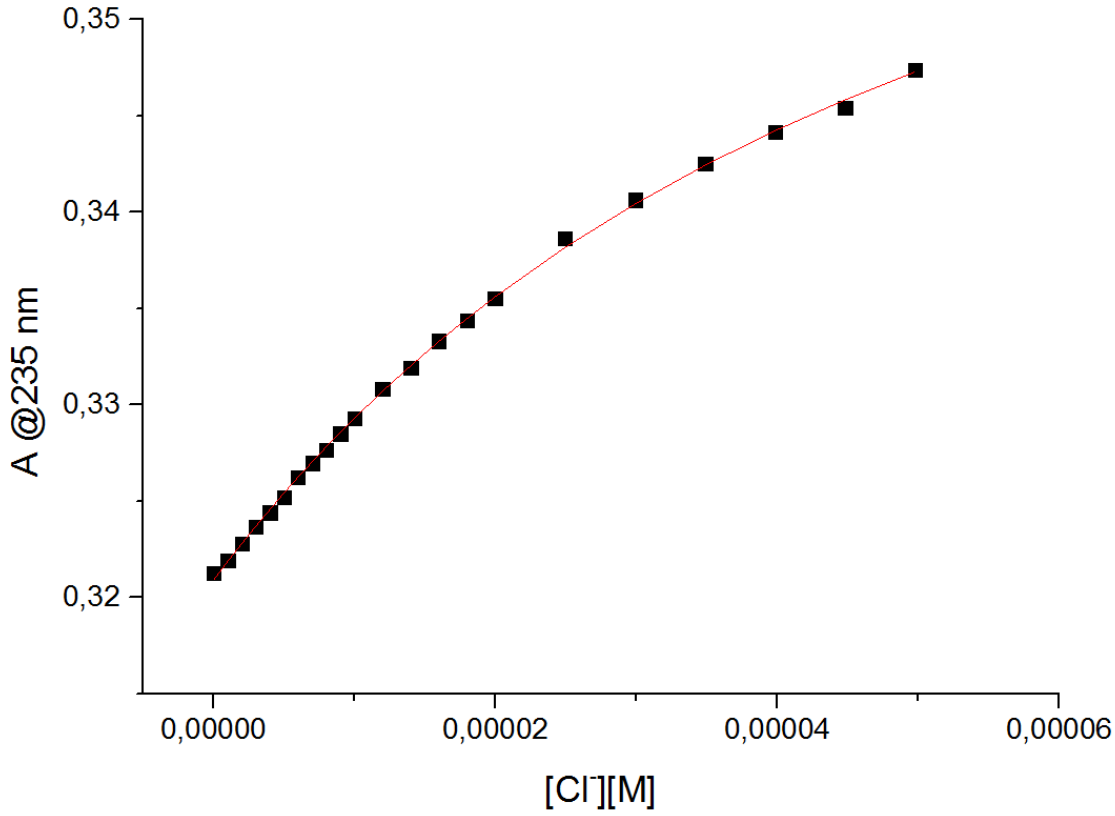




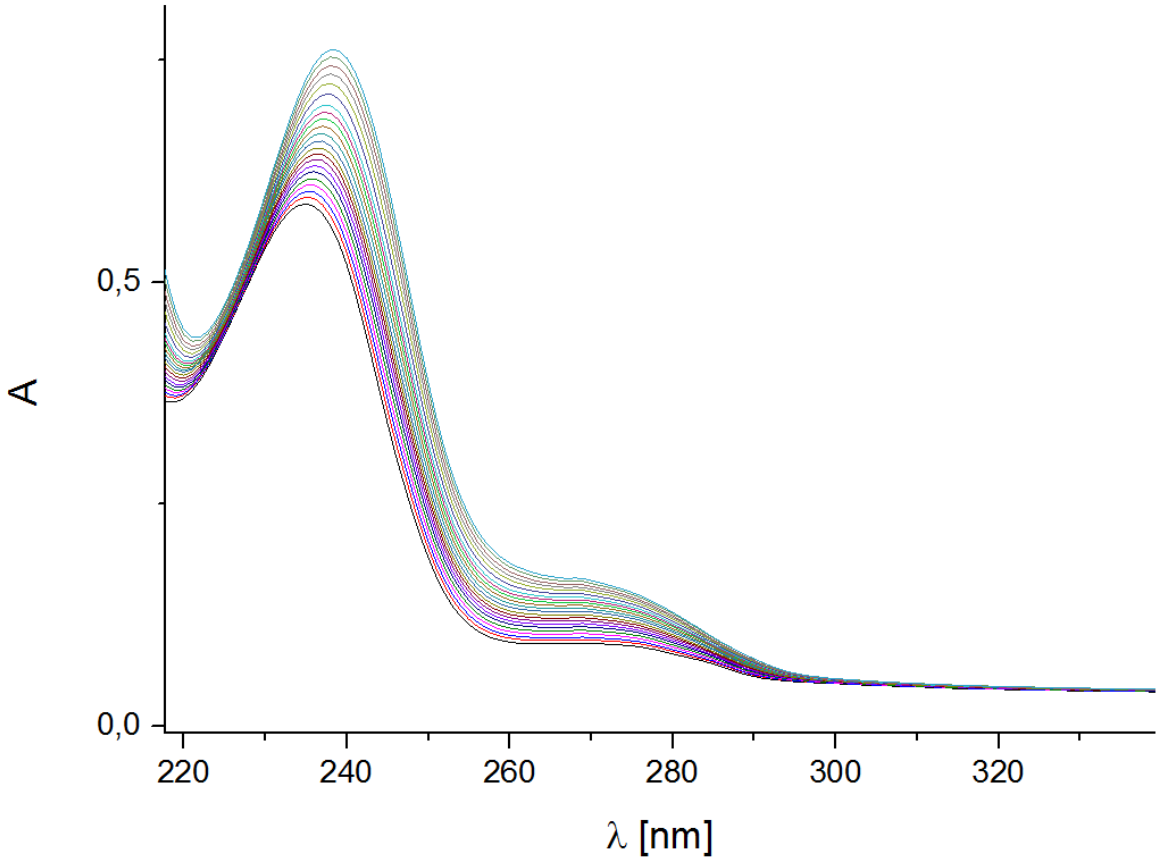
Chloride

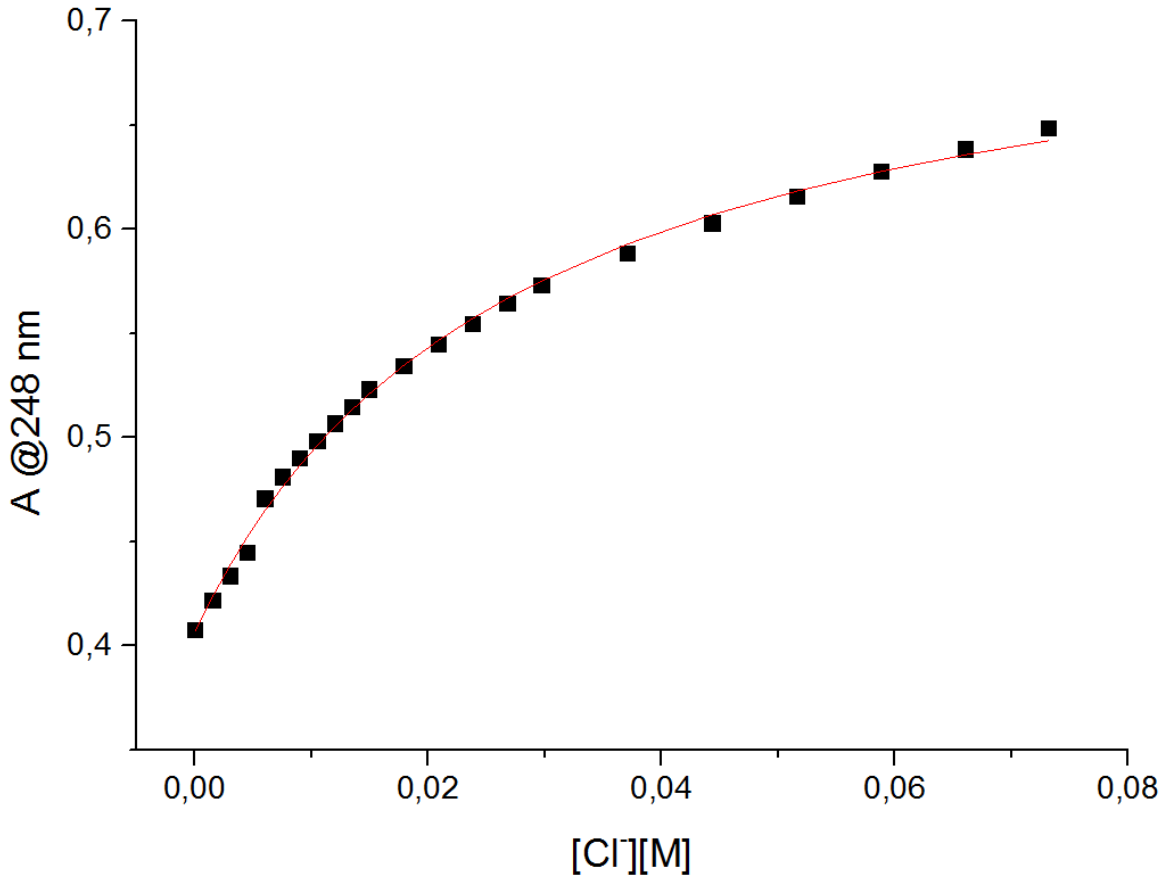
O-cyclodiphosph(V)azane **4**



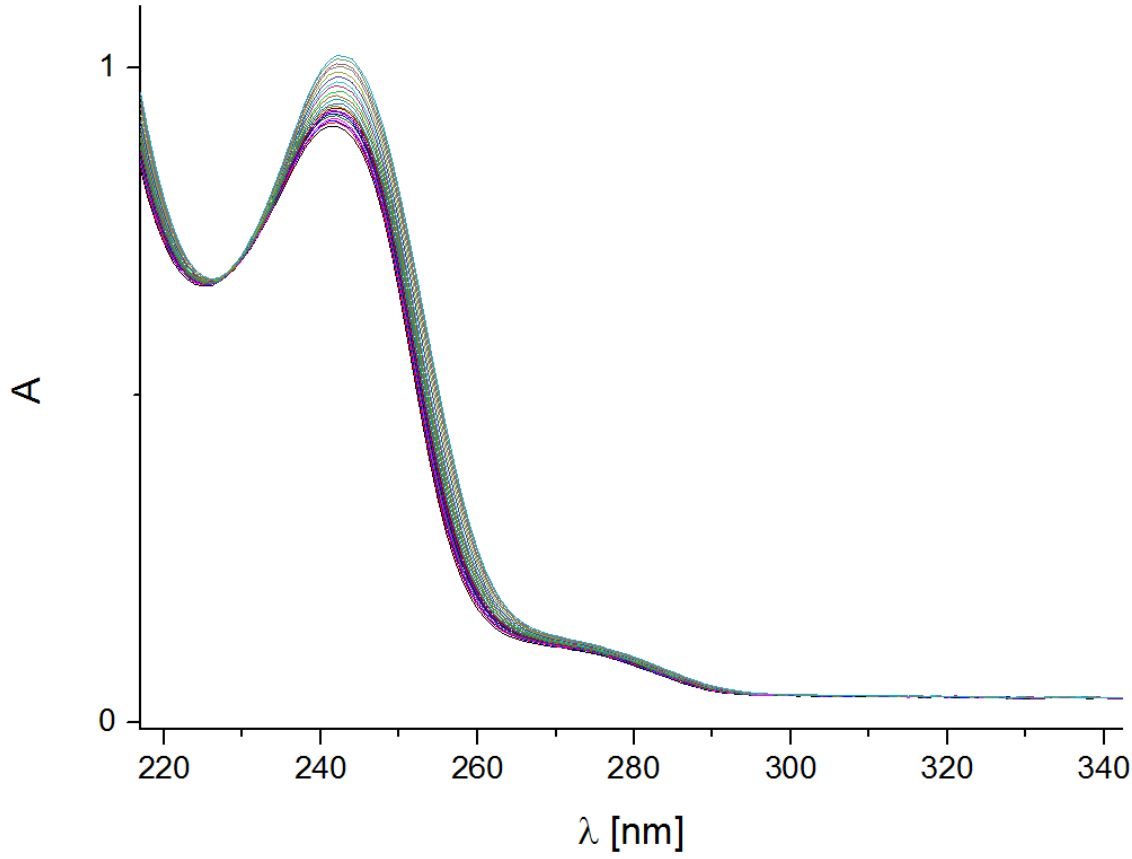


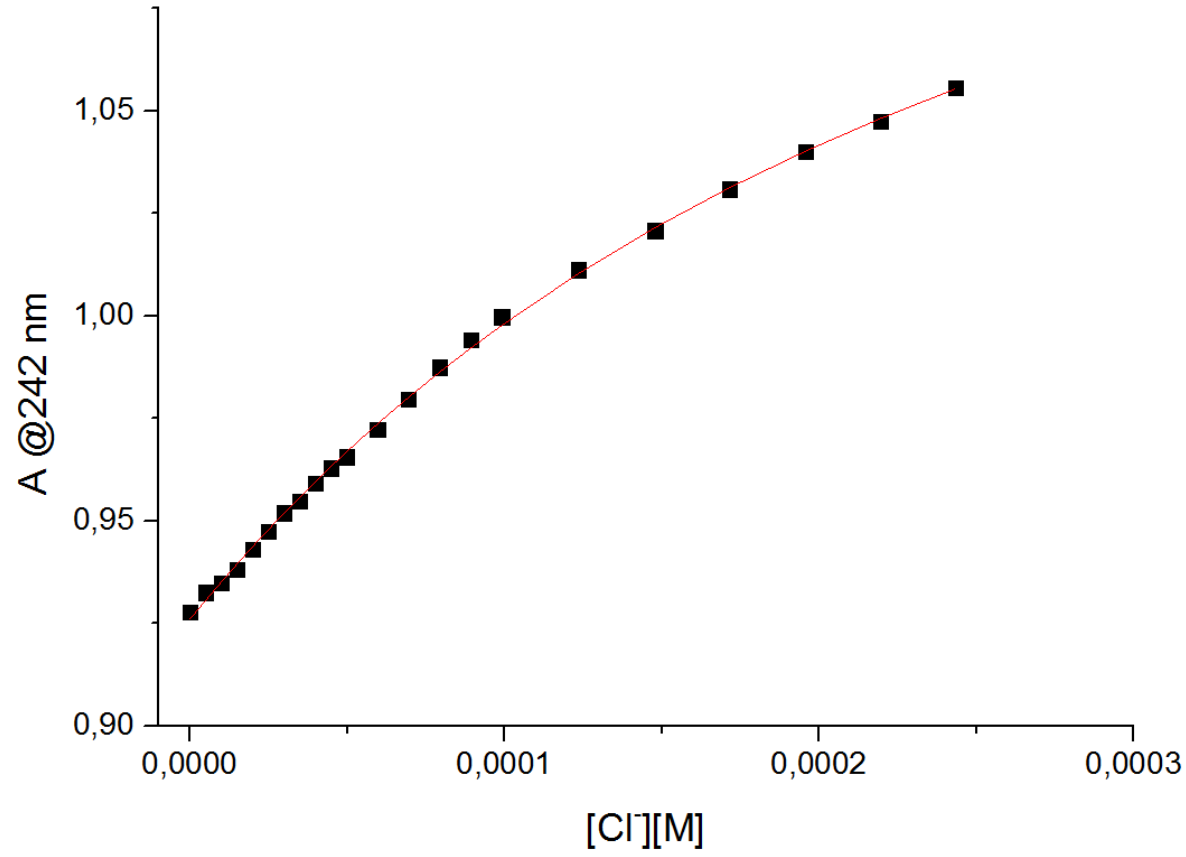
O/S-cyclodiphosph(V)azane **13**



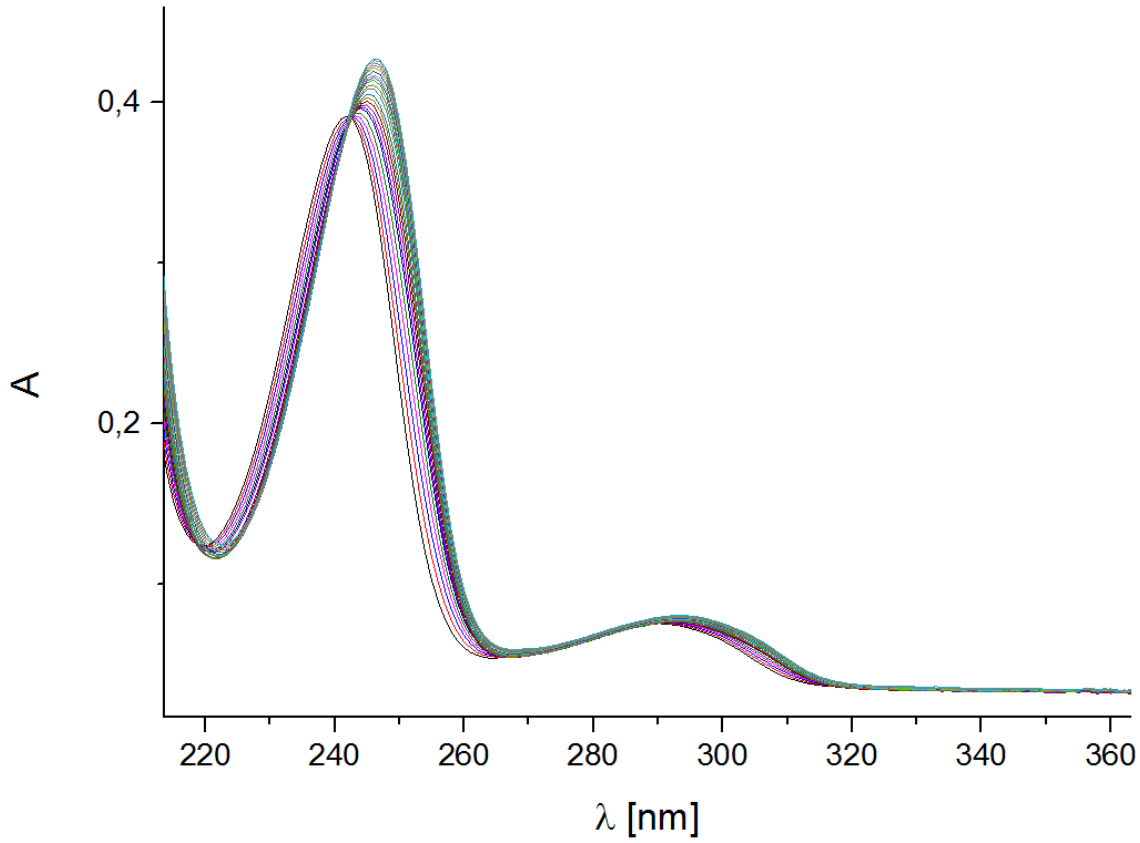


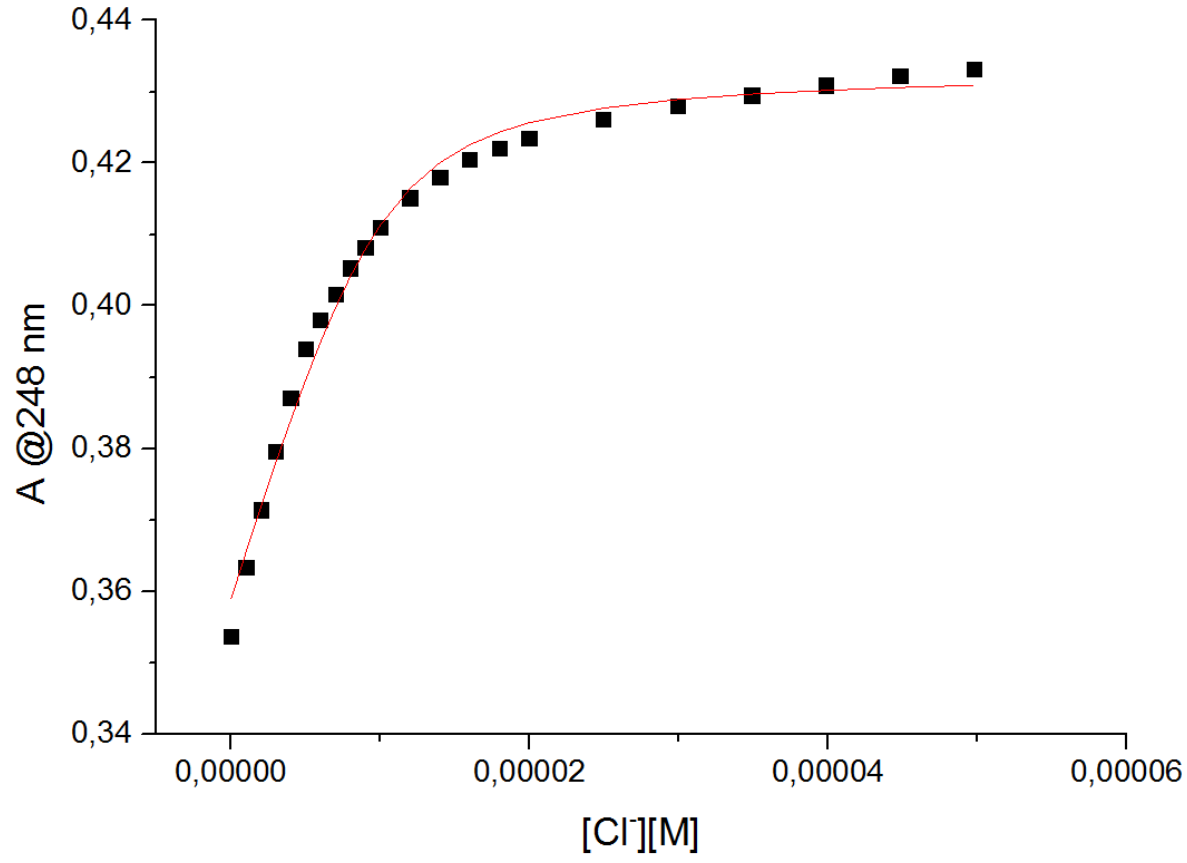
S-cyclodiphosph(V)azane **11**



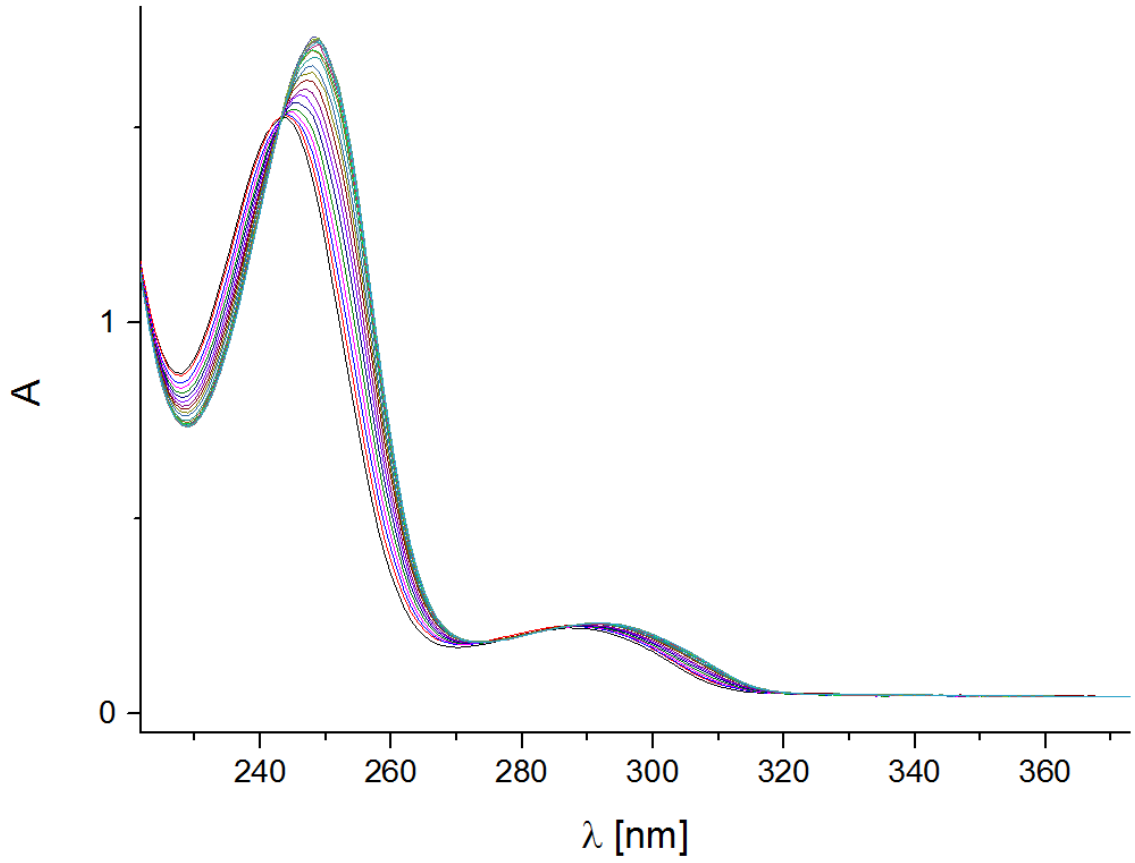


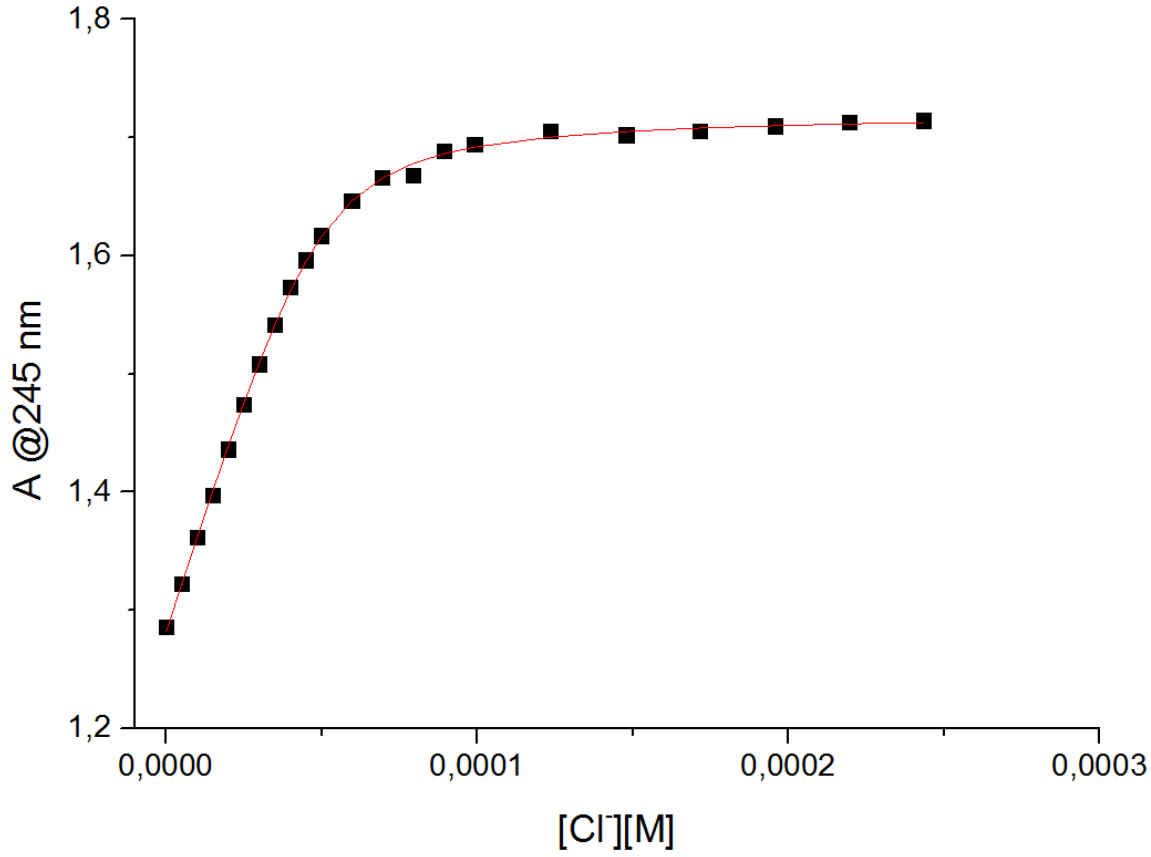
O-cyclodiphosph(V)azane **5**



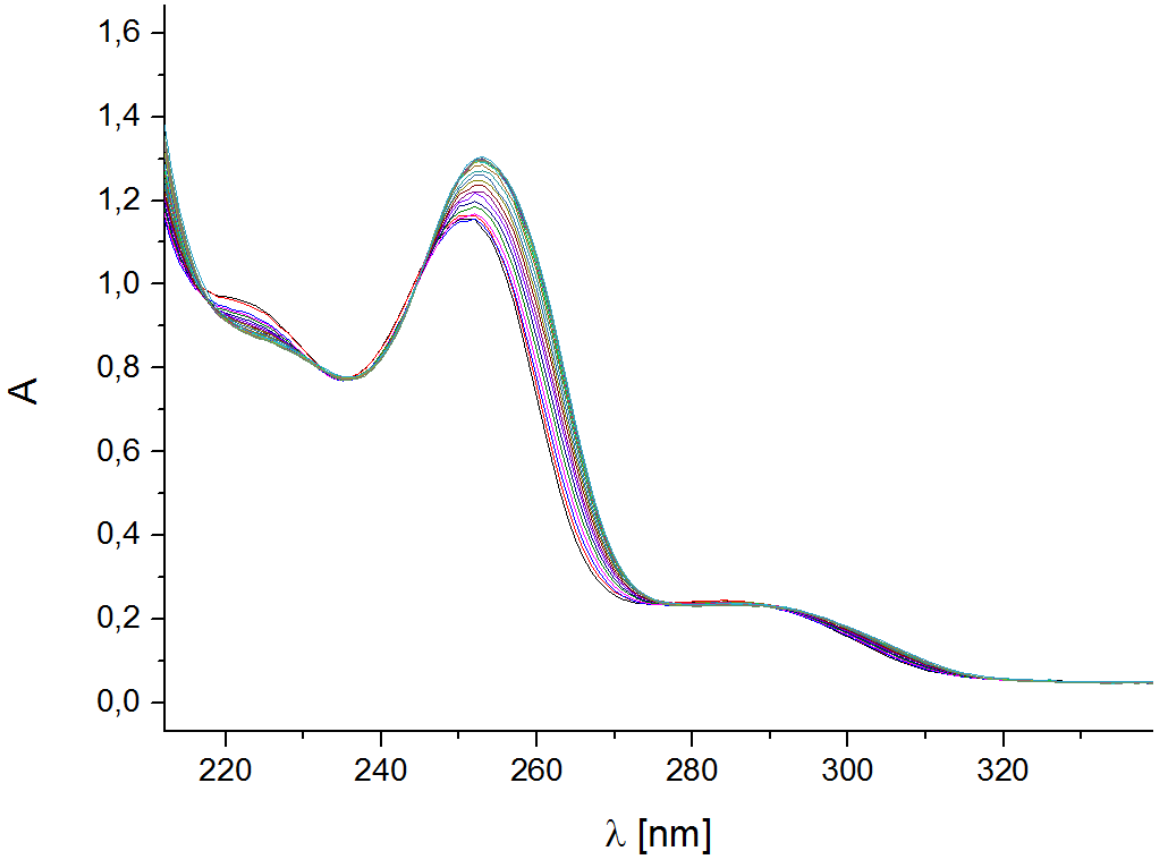


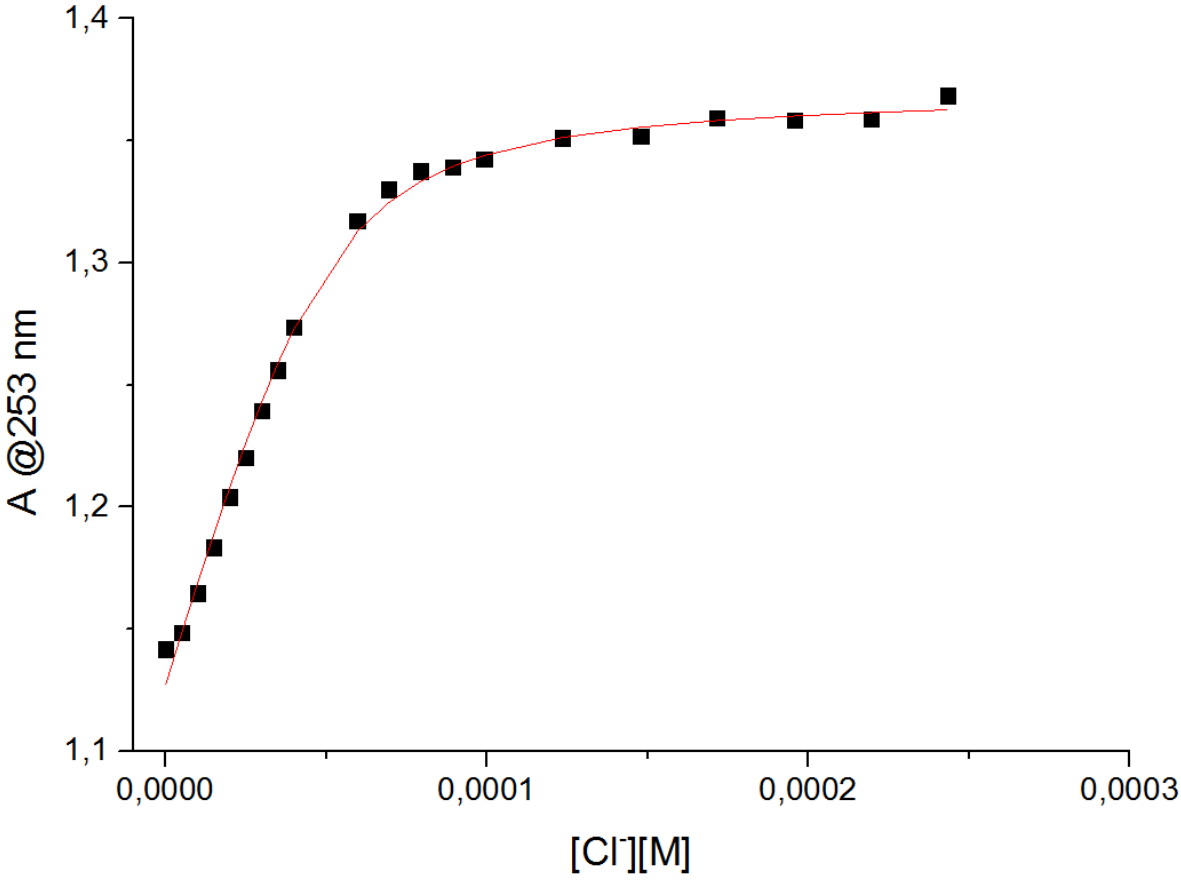
O/S-cyclodiphosph(V)azane **14**



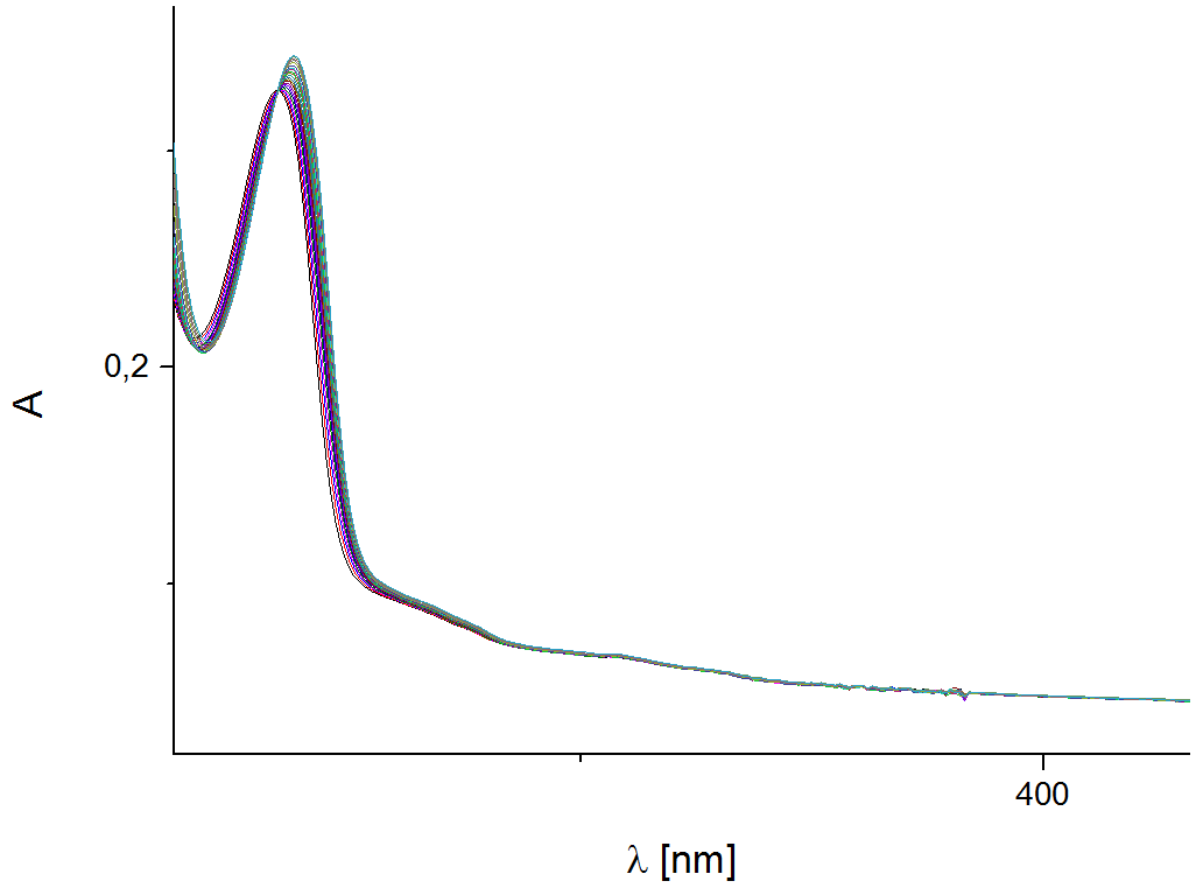


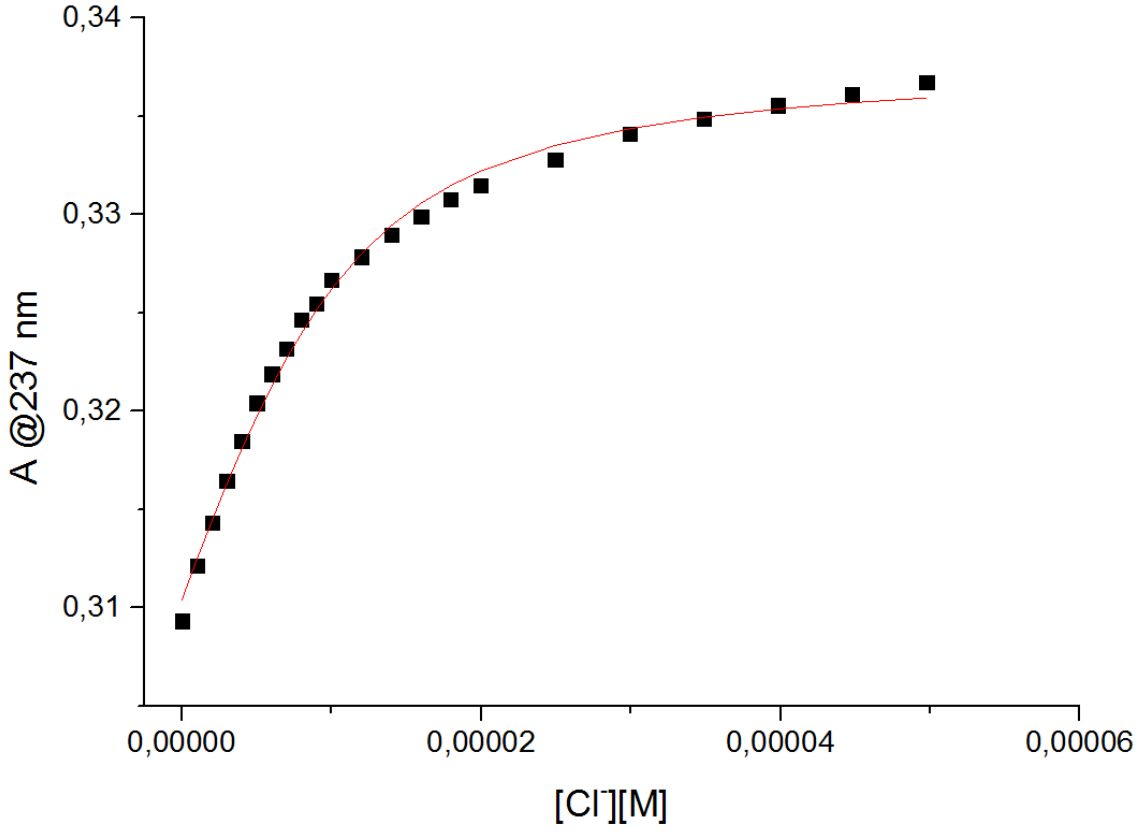
S-cyclodiphosph(V)azane **12**



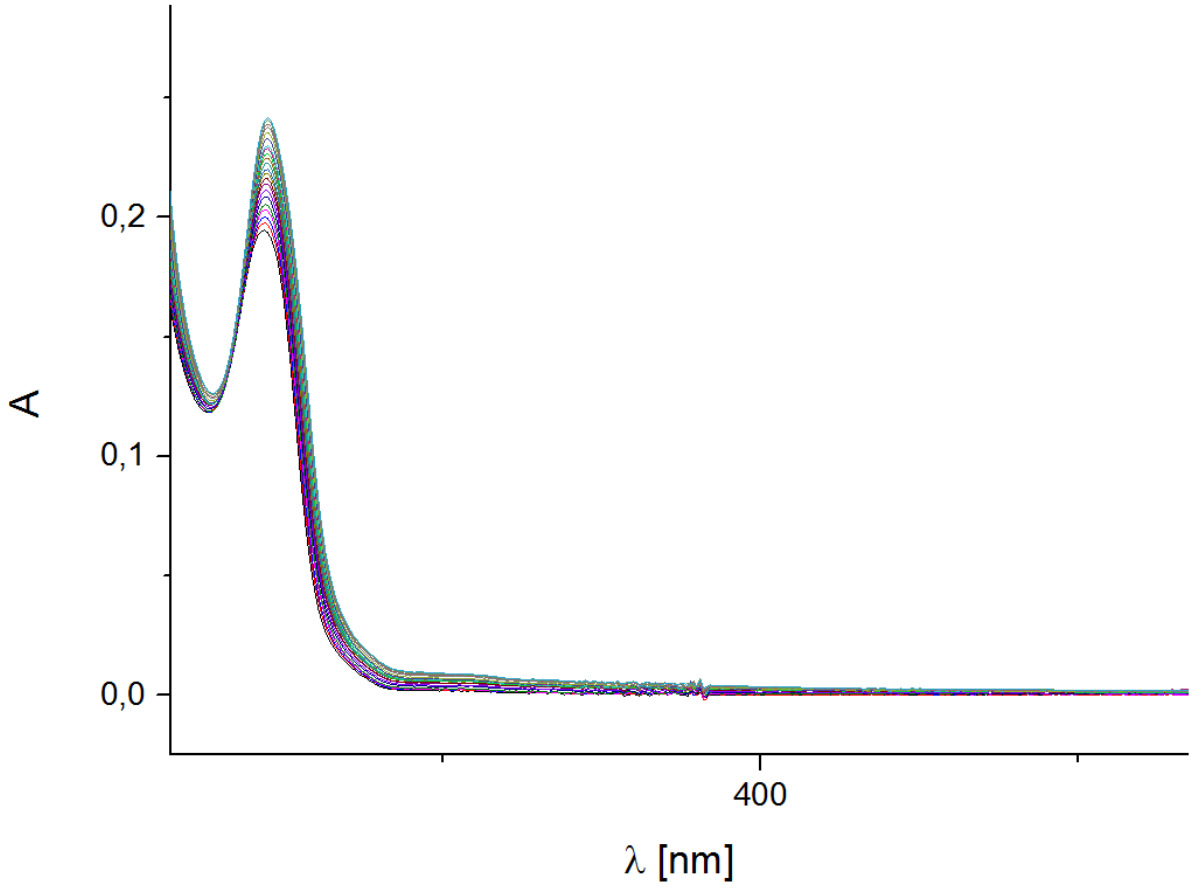


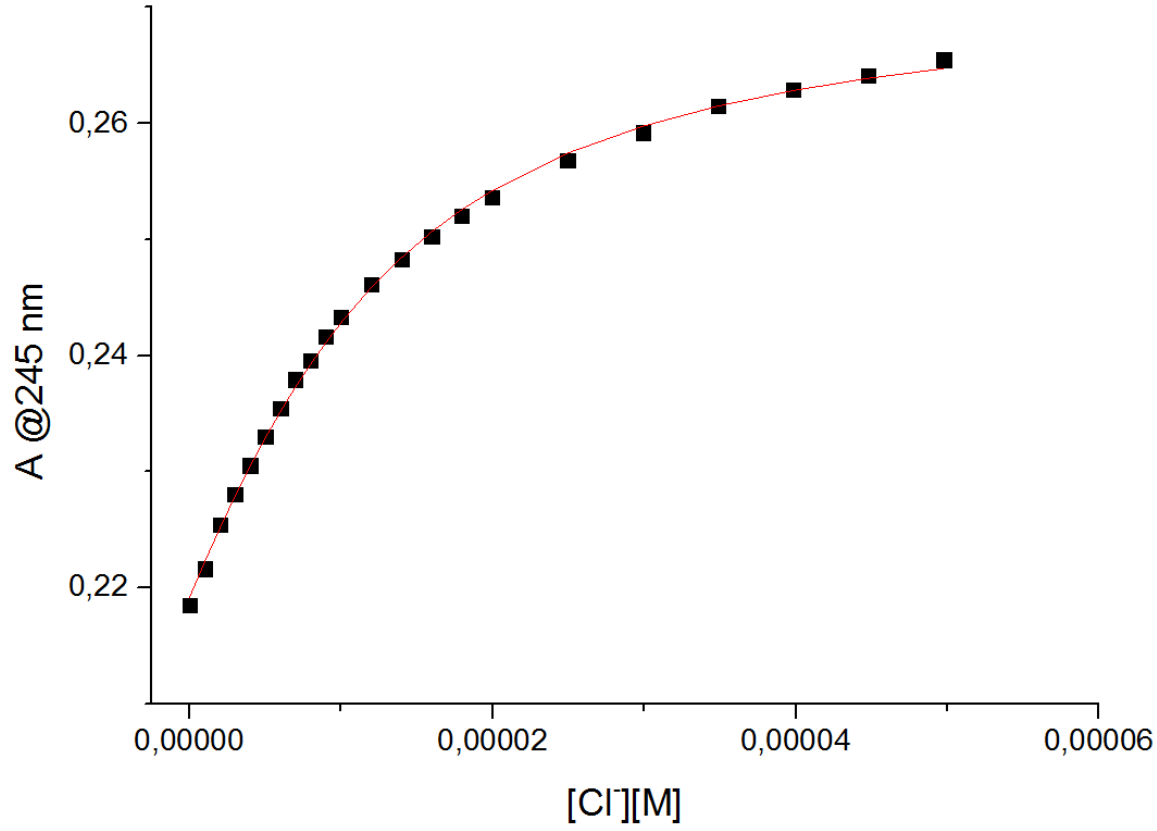
O-Cyclodiphosph(V)azane **15**



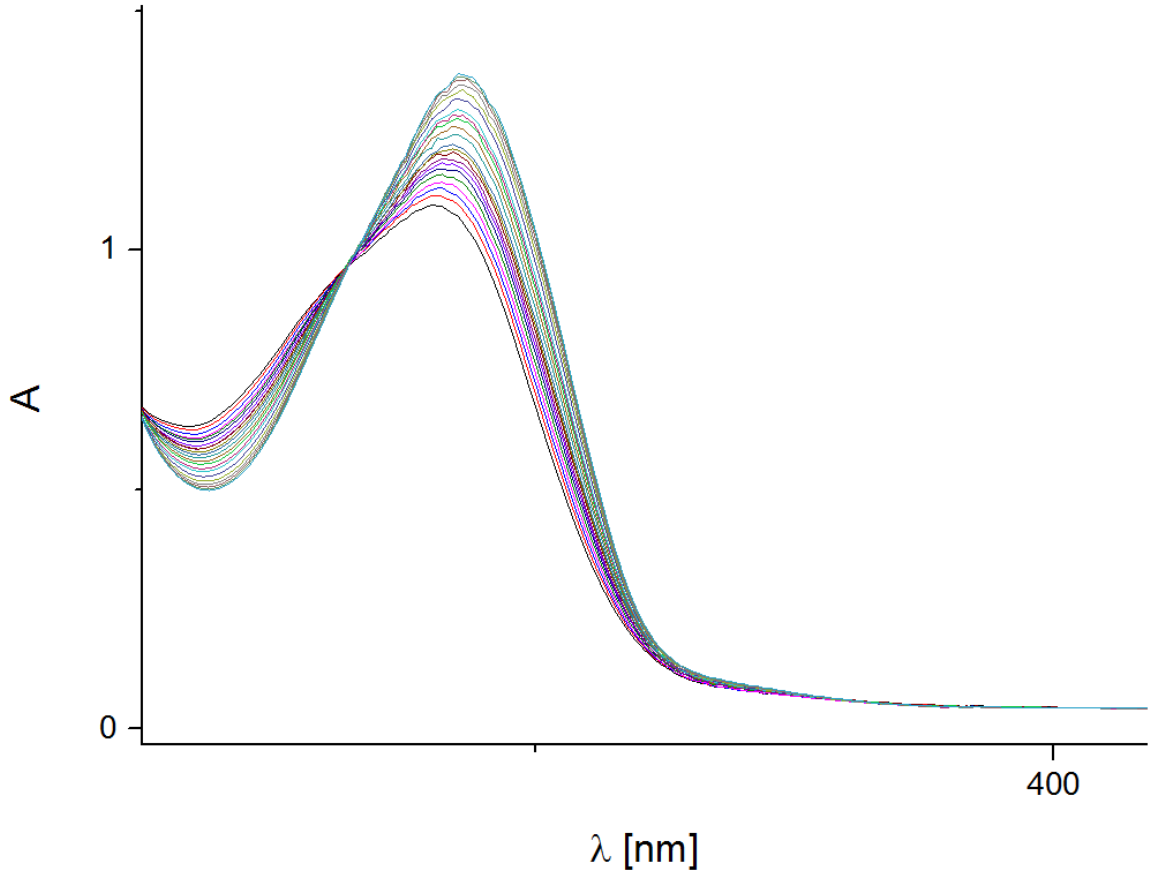


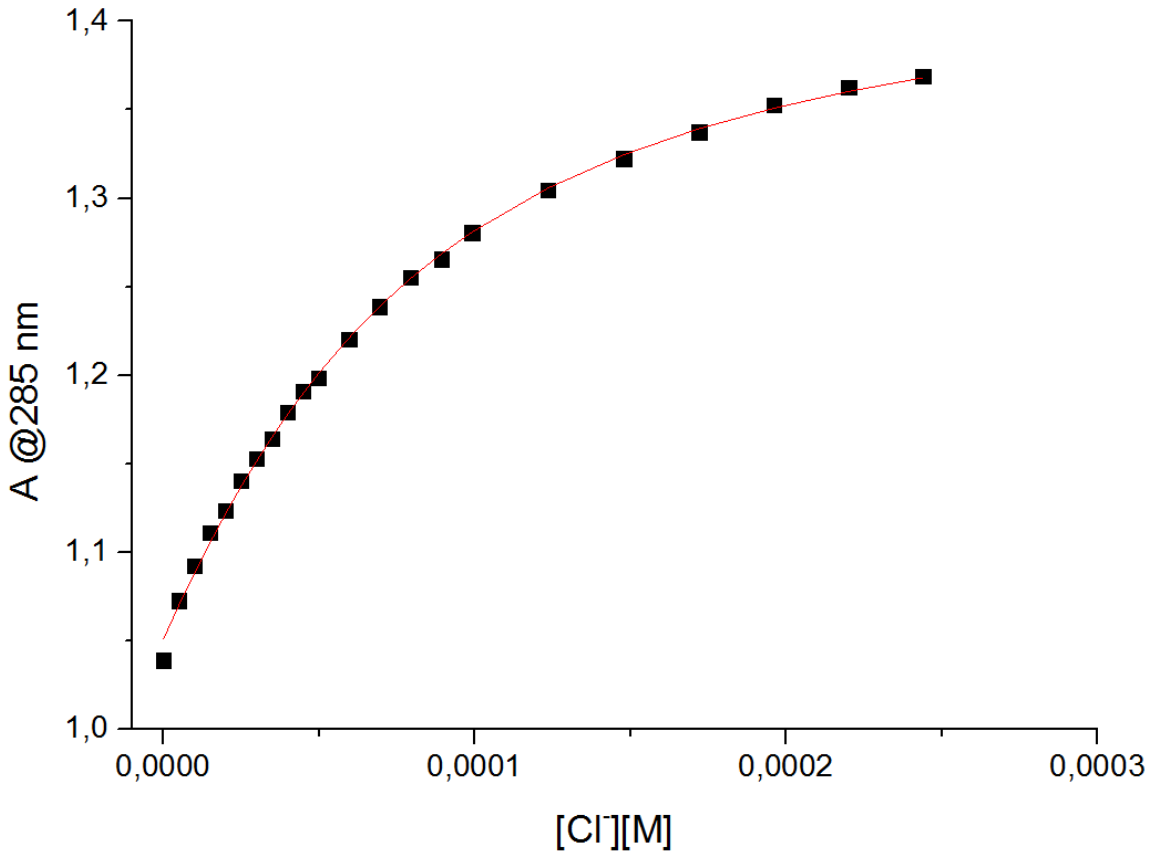
S-Cyclodiphosph(V)azane **16**



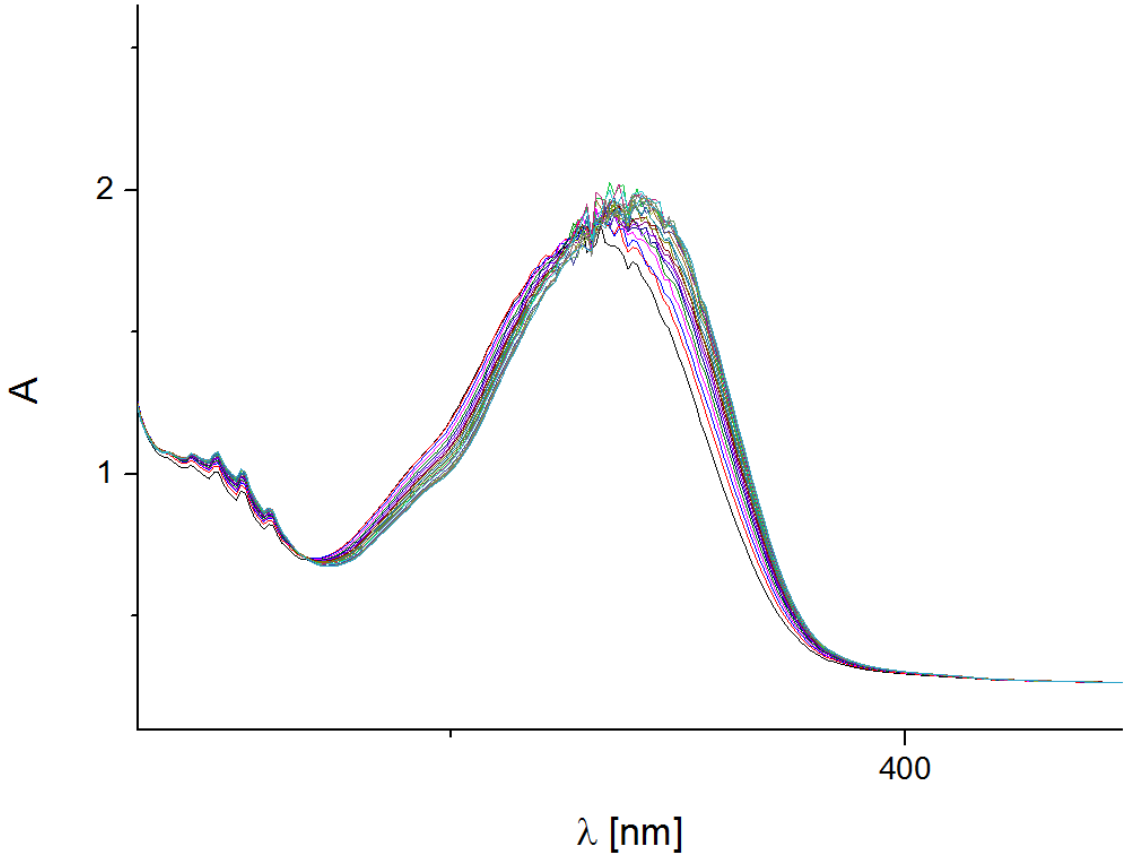


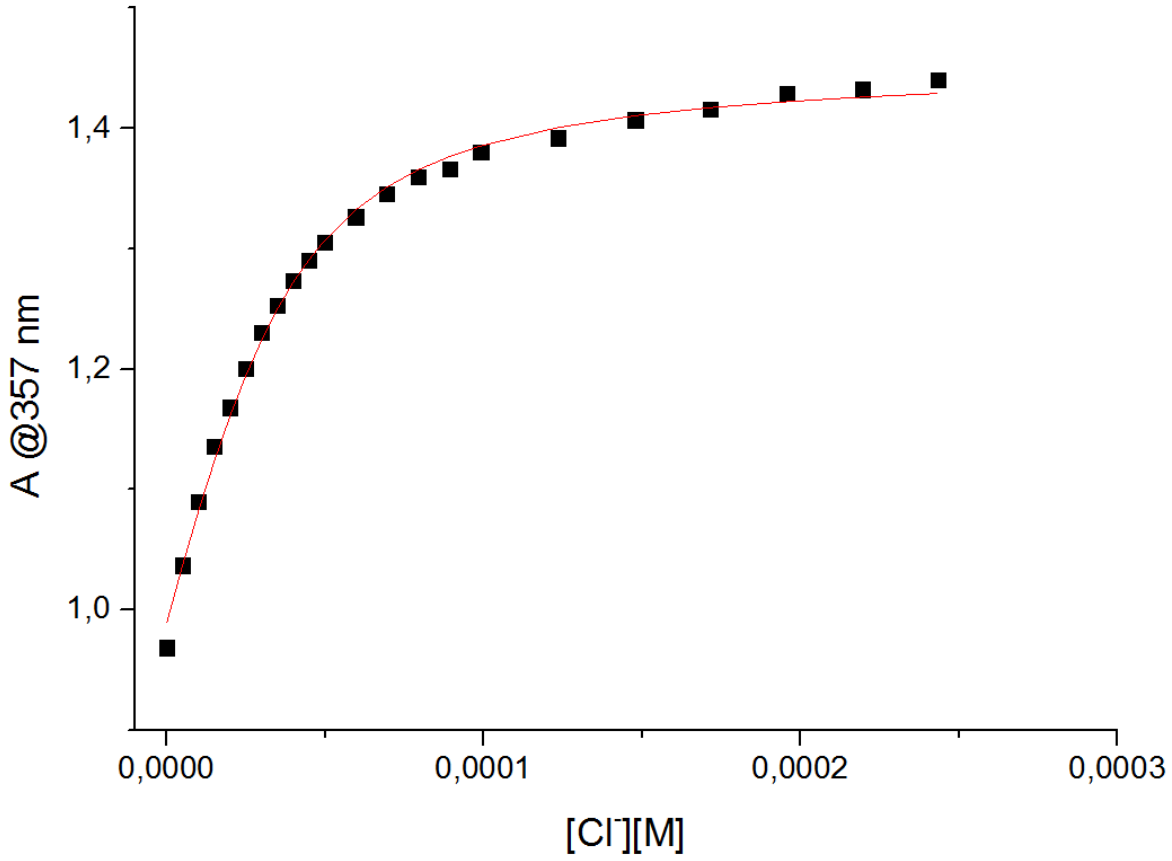
Thiourea **18**



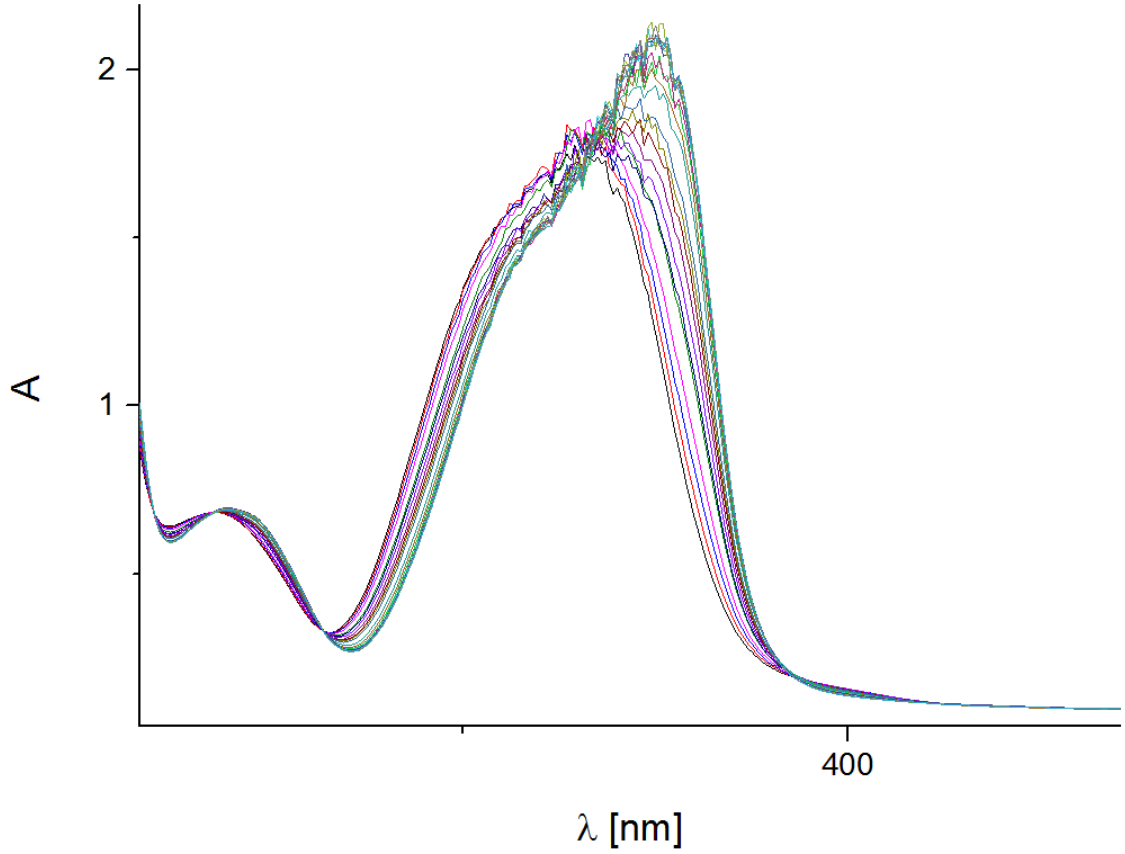


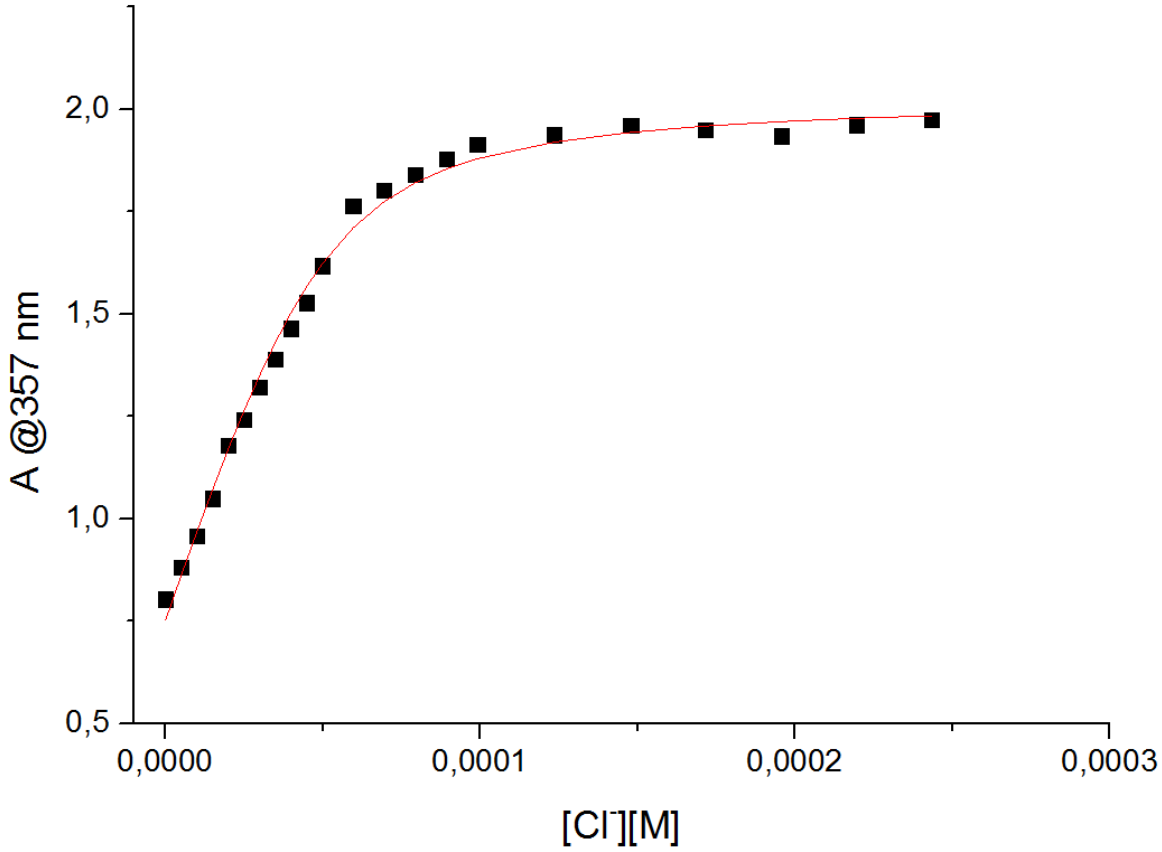
Squaramide **19**





Squaramide **20**



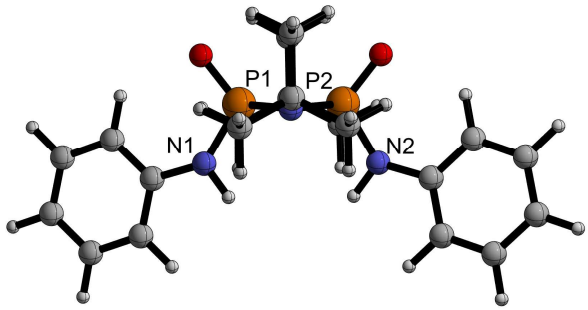


Geometries of computed structures (TPSS-D3/def2TZVP (pcm=acetonitrile))

O-cyclodiphosph(V)azane 4

"In-in"-conformation

Electronic energy =-1833.3057903, thermal correction to Gibbs free energy = 0.413309 NIMAG = 0



1	15	0	1.207027	0.412853	0.766227
2	7	0	-0.284168	1.167491	0.596634
3	7	0	0.292784	-1.028112	0.767586
4	15	0	-1.198725	-0.256046	0.818361
5	6	0	-0.703845	2.595883	0.727097
6	6	0	0.704809	-2.418687	1.126135
7	6	0	-0.794970	2.967248	2.217202
8	1	0	-1.517733	2.321947	2.725148
9	1	0	0.180162	2.848885	2.700102
10	1	0	-1.114647	4.009103	2.325444
11	6	0	-2.075452	2.736378	0.050907
12	1	0	-2.412440	3.775112	0.119584
13	1	0	-2.021084	2.452671	-1.004642
14	1	0	-2.823432	2.105502	0.544992
15	6	0	0.333023	3.474803	0.014956
16	1	0	0.405835	3.214463	-1.045241
17	1	0	0.033398	4.524083	0.098015
18	1	0	1.322812	3.366714	0.471741
19	6	0	2.090600	-2.663542	0.511547
20	1	0	2.829206	-1.961183	0.915107
21	1	0	2.422897	-3.677770	0.752521
22	1	0	2.060260	-2.552652	-0.576809
23	6	0	0.759733	-2.557171	2.657521
24	1	0	1.471000	-1.840432	3.078730
25	1	0	-0.226567	-2.367583	3.092632

26	1	0	1.075384	-3.569643	2.930560
27	6	0	-0.320790	-3.394733	0.533539
28	1	0	-0.357479	-3.309634	-0.556779
29	1	0	-0.038456	-4.419010	0.795857
30	1	0	-1.322915	-3.204373	0.933115
31	7	0	1.990462	0.622900	-0.694662
32	1	0	1.365081	0.612703	-1.495708
33	6	0	3.342883	0.380944	-1.038445
34	6	0	3.637479	0.100897	-2.382629
35	6	0	4.388100	0.431867	-0.103745
36	6	0	4.952160	-0.124307	-2.785133
37	1	0	2.830249	0.056479	-3.110455
38	6	0	5.698550	0.193973	-0.519651
39	1	0	4.169267	0.654496	0.933527
40	6	0	5.994082	-0.084009	-1.855677
41	1	0	5.158111	-0.338717	-3.830345
42	1	0	6.497436	0.233658	0.216282
43	1	0	7.018312	-0.264593	-2.168153
44	7	0	-1.984192	-0.694995	-0.588374
45	1	0	-1.360684	-0.837385	-1.377792
46	6	0	-3.341863	-0.548439	-0.960814
47	6	0	-3.654057	-0.593333	-2.329723
48	6	0	-4.376890	-0.381237	-0.027902
49	6	0	-4.974576	-0.473273	-2.756943
50	1	0	-2.856155	-0.720105	-3.058046
51	6	0	-5.693546	-0.254926	-0.471381
52	1	0	-4.146570	-0.353914	1.030134
53	6	0	-6.006277	-0.299617	-1.831374
54	1	0	-5.193307	-0.510870	-3.820728
55	1	0	-6.483572	-0.123856	0.263530
56	1	0	-7.035132	-0.202474	-2.164967

57	8	0	2.109714	0.668145	1.915692
58	8	0	-2.098825	-0.327774	1.995886

“In-out”-conformation

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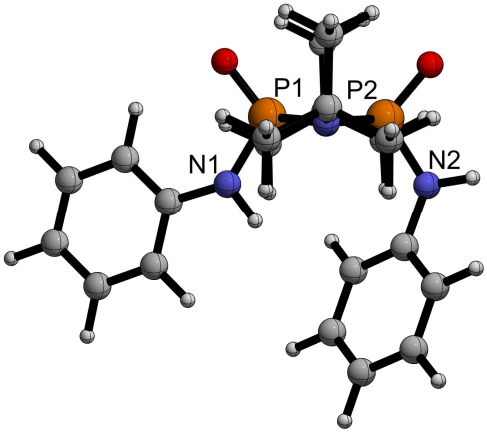


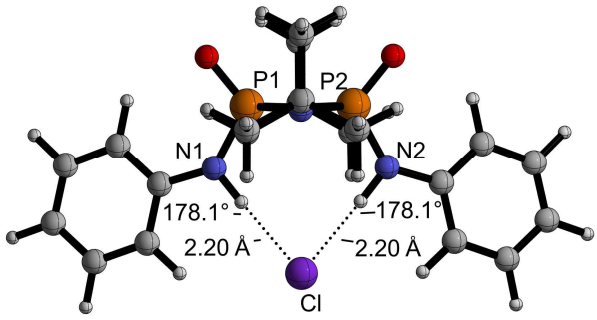
1	15	0	1.919270	-0.956031	0.373959
2	7	0	0.362060	-1.246318	0.941045
3	7	0	1.143833	-0.623836	-1.103551
4	15	0	-0.382849	-1.107630	-0.586869
5	6	0	-0.125408	-1.900845	2.192487
6	6	0	1.713780	-0.478698	-2.479428
7	6	0	-0.040617	-3.428788	2.038093
8	1	0	-0.652821	-3.760364	1.194361
9	1	0	0.995293	-3.734155	1.861309
10	1	0	-0.400643	-3.917586	2.949698
11	6	0	-1.580589	-1.460414	2.409857
12	1	0	-1.970693	-1.918885	3.323498
13	1	0	-1.653491	-0.372423	2.507047
14	1	0	-2.215517	-1.778062	1.574751
15	6	0	0.757561	-1.431168	3.357140
16	1	0	0.712092	-0.344811	3.477820
17	1	0	0.410684	-1.899567	4.283187
18	1	0	1.801802	-1.721980	3.198595
19	6	0	2.986558	0.372549	-2.375193
20	1	0	3.738518	-0.118539	-1.747258
21	1	0	3.415969	0.505462	-3.372821
22	1	0	2.761324	1.357427	-1.955574
23	6	0	2.041024	-1.873055	-3.041141
24	1	0	2.762293	-2.382512	-2.394843
25	1	0	1.134665	-2.483417	-3.103190
26	1	0	2.470393	-1.781122	-4.044387
27	6	0	0.675663	0.229235	-3.360473

28	1	0	0.441097	1.223169	-2.967645
29	1	0	1.077895	0.338523	-4.372324
30	1	0	-0.251311	-0.351108	-3.423736
31	7	0	2.534108	0.446710	1.047785
32	1	0	3.549403	0.427834	1.084867
33	6	0	1.969969	1.748586	0.985705
34	6	0	2.759477	2.824401	0.554659
35	6	0	0.644725	1.983726	1.375976
36	6	0	2.224914	4.111022	0.503755
37	1	0	3.789180	2.646909	0.255186
38	6	0	0.112953	3.272294	1.304374
39	1	0	0.041992	1.165295	1.751276
40	6	0	0.895758	4.341812	0.866334
41	1	0	2.849714	4.933860	0.167741
42	1	0	-0.915176	3.438555	1.613829
43	1	0	0.479414	5.343444	0.817993
44	7	0	-1.324305	0.266081	-0.688071
45	1	0	-0.801421	1.122886	-0.517103
46	6	0	-2.725829	0.429357	-0.600880
47	6	0	-3.218645	1.725734	-0.376299
48	6	0	-3.632330	-0.632592	-0.741600
49	6	0	-4.589898	1.954451	-0.289644
50	1	0	-2.521065	2.552905	-0.269274
51	6	0	-5.002891	-0.388572	-0.648119
52	1	0	-3.262674	-1.634025	-0.926572
53	6	0	-5.494729	0.898353	-0.421826
54	1	0	-4.948977	2.965106	-0.114955
55	1	0	-5.691962	-1.222038	-0.757110
56	1	0	-6.563704	1.076334	-0.352115
57	8	0	2.971378	-2.001591	0.449133
58	8	0	-1.079768	-2.299034	-1.130599

4•Cl

Electronic energy = -2293.7335075, thermal correction to Gibbs free energy = 0.410360 NIMAG = 0

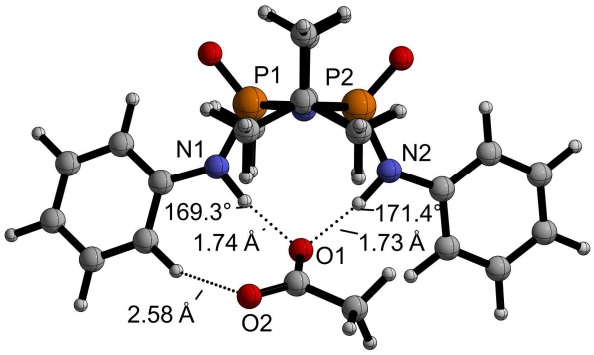
1	15	0	1.253838	-0.800534	0.723840
2	7	0	-0.000185	0.130308	1.377576
3	7	0	0.000105	-1.648595	-0.030501
4	15	0	-1.253930	-0.800771	0.723698
5	6	0	-0.000322	1.249526	2.353427
6	6	0	0.000321	-2.954664	-0.752501
7	6	0	-0.000269	0.676463	3.781609
8	1	0	-0.889034	0.057902	3.941294
9	1	0	0.888576	0.057995	3.941203
10	1	0	-0.000280	1.488357	4.517163
11	6	0	-1.260022	2.095437	2.112716
12	1	0	-1.288096	2.924878	2.826307
13	1	0	-1.266713	2.503550	1.097535
14	1	0	-2.167863	1.497185	2.253986
15	6	0	1.259247	2.095646	2.112810
16	1	0	1.265966	2.503837	1.097661
17	1	0	1.287121	2.925063	2.826441
18	1	0	2.167177	1.497547	2.254137
19	6	0	1.258061	-3.018781	-1.630487
20	1	0	2.166914	-2.959734	-1.021445
21	1	0	1.271932	-3.969846	-2.172043
22	1	0	1.267431	-2.197780	-2.353187
23	6	0	0.000523	-4.100660	0.274825
24	1	0	0.889360	-4.041134	0.910782
25	1	0	-0.888373	-4.041422	0.910734
26	1	0	0.000693	-5.068060	-0.239194
27	6	0	-1.257365	-3.019304	-1.630489
28	1	0	-1.267082	-2.198321	-2.353194
29	1	0	-1.270825	-3.970371	-2.172053



30	1	0	-2.166261	-2.960650	-1.021475
31	7	0	2.035237	0.022210	-0.489260
32	1	0	1.400188	0.347090	-1.242393
33	6	0	3.328484	0.574620	-0.545939
34	6	0	3.632028	1.401766	-1.643936
35	6	0	4.319761	0.341792	0.422778
36	6	0	4.893637	1.978400	-1.767297
37	1	0	2.863573	1.587033	-2.390632
38	6	0	5.578423	0.928477	0.284884
39	1	0	4.100160	-0.296961	1.269945
40	6	0	5.880340	1.748455	-0.804387
41	1	0	5.103759	2.614083	-2.623870
42	1	0	6.331689	0.736970	1.045285
43	1	0	6.863660	2.199462	-0.901543
44	7	0	-2.035341	0.021772	-0.489574
45	1	0	-1.400182	0.346931	-1.242477
46	6	0	-3.328537	0.574350	-0.546192
47	6	0	-3.631782	1.402151	-1.643776
48	6	0	-4.320057	0.340998	0.422147
49	6	0	-4.893336	1.978919	-1.767105
50	1	0	-2.863131	1.587841	-2.390164
51	6	0	-5.578645	0.927855	0.284315
52	1	0	-4.100695	-0.298195	1.269040
53	6	0	-5.880272	1.748468	-0.804562
54	1	0	-5.103222	2.615115	-2.623354
55	1	0	-6.332102	0.735960	1.044430
56	1	0	-6.863554	2.199568	-0.901687
57	8	0	2.194087	-1.476545	1.656411
58	8	0	-2.194219	-1.477020	1.656057
59	17	0	0.000095	1.042638	-2.789693

4•OAc “one-binding”-mode

Electronic energy = -2062.0888437, thermal correction to Gibbs free energy = 0.455853 NIMAG = 0



1	15	0	-1.256123	-0.907340	0.887381
2	7	0	-0.039564	-1.649221	-0.028951
3	7	0	0.034885	-0.157694	1.678031
4	15	0	1.254026	-0.958041	0.818815
5	6	0	-0.092510	-2.685903	-1.088664
6	6	0	0.093017	0.639531	2.936493
7	6	0	-0.095380	-4.077772	-0.431785
8	1	0	0.809667	-4.212869	0.168843
9	1	0	-0.966837	-4.184700	0.221808
10	1	0	-0.130521	-4.861147	-1.197034
11	6	0	1.140427	-2.520720	-1.990307
12	1	0	1.122498	-3.280210	-2.778265
13	1	0	1.154740	-1.529981	-2.454558
14	1	0	2.065685	-2.649993	-1.417195
15	6	0	-1.376218	-2.475132	-1.906606
16	1	0	-1.382311	-1.486042	-2.374583
17	1	0	-1.441371	-3.236145	-2.690633
18	1	0	-2.265868	-2.565622	-1.272088
19	6	0	-1.152271	1.534482	3.002858
20	1	0	-2.069440	0.935268	2.999348
21	1	0	-1.128991	2.118327	3.928424
22	1	0	-1.180778	2.221075	2.152933
23	6	0	0.127918	-0.320911	4.138971
24	1	0	-0.769798	-0.947300	4.151829
25	1	0	1.006217	-0.971439	4.080112
26	1	0	0.173485	0.246783	5.074874
27	6	0	1.360024	1.507002	2.904578
28	1	0	1.348032	2.185487	2.046814
29	1	0	1.414105	2.097842	3.824766

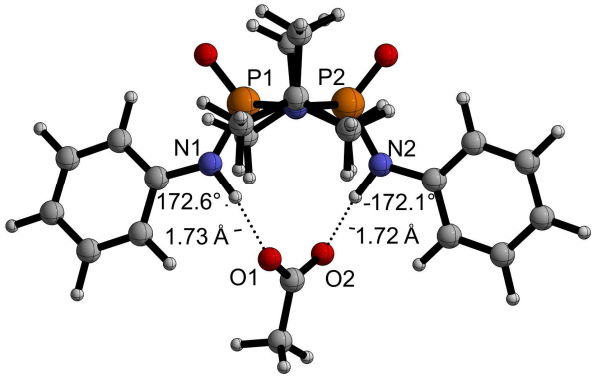
30	1	0	2.260282	0.884899	2.847015
31	7	0	-1.997065	0.295334	0.012661
32	1	0	-1.307098	0.977967	-0.383665
33	6	0	-3.257723	0.312956	-0.610275
34	6	0	-3.432069	1.181907	-1.704182
35	6	0	-4.346380	-0.468887	-0.186029
36	6	0	-4.662778	1.270699	-2.350221
37	1	0	-2.588755	1.779626	-2.039396
38	6	0	-5.570713	-0.375735	-0.848956
39	1	0	-4.223902	-1.140304	0.655760
40	6	0	-5.744384	0.491264	-1.930506
41	1	0	-4.772656	1.949732	-3.192145
42	1	0	-6.401002	-0.989040	-0.507127
43	1	0	-6.703090	0.558192	-2.436706
44	7	0	1.996150	0.208077	-0.094327
45	1	0	1.334114	0.955330	-0.421583
46	6	0	3.275363	0.257931	-0.669566
47	6	0	3.602778	1.409737	-1.412317
48	6	0	4.229533	-0.768415	-0.553117
49	6	0	4.846826	1.522020	-2.028105
50	1	0	2.871650	2.212560	-1.477083
51	6	0	5.472998	-0.637759	-1.173241
52	1	0	3.995126	-1.655195	0.024326
53	6	0	5.794635	0.499649	-1.917073
54	1	0	5.077580	2.419623	-2.596964
55	1	0	6.196819	-1.443101	-1.072787
56	1	0	6.764605	0.589788	-2.397802
57	8	0	-2.217142	-1.774962	1.619996
58	8	0	2.211381	-1.864205	1.509244
59	6	0	-1.199435	3.971473	-0.393957
60	1	0	-1.953608	3.371238	0.125281

61	1	0	-1.050060	4.916270	0.133387
62	1	0	-1.590083	4.183983	-1.396343
63	6	0	0.116748	3.196727	-0.524803
64	8	0	0.010023	1.969806	-0.906496
65	8	0	1.198205	3.778046	-0.281937

4•OAc “two-binding”-mode

Electronic energy = -2062.0885446, thermal correction to Gibbs free energy = 0.455394 NIMAG = 0

1	15	0	-1.181807	-1.309752	-0.098965
2	7	0	0.262690	-1.335753	-0.956660
3	7	0	-0.176742	-1.031811	1.248530
4	15	0	1.271069	-1.200401	0.412574
5	6	0	0.578788	-1.718056	-2.358559
6	6	0	-0.502884	-0.949299	2.697741
7	6	0	0.733501	-3.246745	-2.450242
8	1	0	1.533881	-3.586409	-1.785861
9	1	0	-0.198399	-3.739507	-2.154744
10	1	0	0.976994	-3.542701	-3.476567
11	6	0	1.888484	-1.019177	-2.753795
12	1	0	2.142143	-1.269842	-3.788718
13	1	0	1.788134	0.066882	-2.666421
14	1	0	2.716440	-1.344684	-2.113892
15	6	0	-0.564467	-1.240335	-3.265967
16	1	0	-0.678533	-0.153930	-3.209725
17	1	0	-0.344641	-1.520603	-4.301127
18	1	0	-1.514005	-1.706817	-2.980583
19	6	0	-1.797854	-0.135461	2.846891
20	1	0	-2.632496	-0.624561	2.331449
21	1	0	-2.058991	-0.052609	3.906797
22	1	0	-1.671400	0.868654	2.431594
23	6	0	-0.692992	-2.371370	3.254875
24	1	0	-1.493154	-2.886215	2.714297



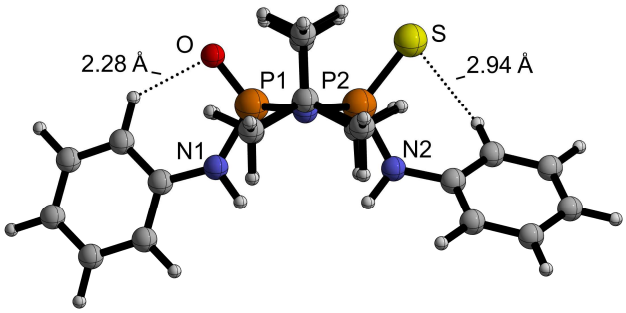
25	1	0	0.230188	-2.949274	3.143903
26	1	0	-0.955244	-2.330020	4.317833
27	6	0	0.647451	-0.236669	3.423031
28	1	0	0.773981	0.779863	3.041263
29	1	0	0.423348	-0.190262	4.493626
30	1	0	1.590225	-0.780509	3.295577
31	7	0	-1.965954	0.077183	-0.556794
32	1	0	-1.325585	0.868593	-0.806117
33	6	0	-3.324244	0.429370	-0.469796
34	6	0	-3.687163	1.730070	-0.872941
35	6	0	-4.330728	-0.437334	-0.006252
36	6	0	-5.014562	2.146957	-0.812277
37	1	0	-2.911515	2.400933	-1.232590
38	6	0	-5.656335	-0.004451	0.046668
39	1	0	-4.071184	-1.443666	0.300557
40	6	0	-6.014348	1.285064	-0.351974
41	1	0	-5.266753	3.156252	-1.128581
42	1	0	-6.417592	-0.691657	0.408360
43	1	0	-7.049265	1.611680	-0.305568
44	7	0	2.008660	0.281330	0.470792
45	1	0	1.343074	1.092210	0.564198
46	6	0	3.348115	0.640013	0.245199
47	6	0	3.667716	2.012582	0.259214
48	6	0	4.378784	-0.288168	0.008021
49	6	0	4.975669	2.438646	0.041475
50	1	0	2.874584	2.732007	0.443500
51	6	0	5.683910	0.154996	-0.208543
52	1	0	4.153462	-1.348074	0.004483
53	6	0	5.998461	1.515533	-0.195458
54	1	0	5.194620	3.503633	0.056526
55	1	0	6.463859	-0.580718	-0.390221

56	1	0	7.017786	1.850024	-0.365738
57	8	0	-2.080319	-2.495713	-0.053660
58	8	0	2.202805	-2.330070	0.681998
59	6	0	-0.492296	4.474019	-0.223252
60	1	0	-1.579932	4.574403	-0.120813
61	1	0	-0.009489	5.018471	0.591597
62	1	0	-0.213783	4.915938	-1.185086
63	6	0	-0.134453	2.985936	-0.201882
64	8	0	-0.450180	2.304556	-1.228020
65	8	0	0.427494	2.523908	0.838247

O/S-cyclodiphosph(V)azane 13

“In-in”conformation

Electronic energy = -2156.2531573, thermal correction to Gibbs free energy = 0.411557 NIMAG = 0



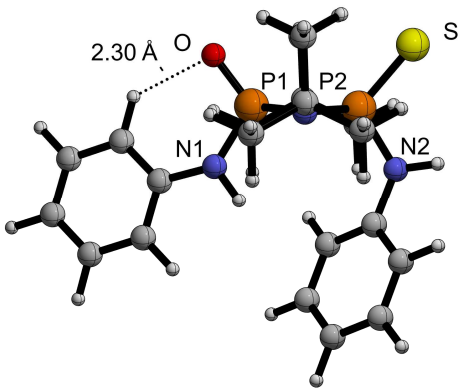
1	15	0	1.312386	0.203416	0.753185
2	7	0	-0.057376	1.179956	0.632566
3	7	0	0.218445	-1.072271	0.534156
4	15	0	-1.177957	-0.116151	0.636922
5	6	0	-0.252124	2.624780	0.971196
6	6	0	0.424307	-2.547093	0.622218
7	6	0	-0.293245	2.797436	2.499129
8	1	0	-1.118223	2.219064	2.924706
9	1	0	0.643603	2.451149	2.946498
10	1	0	-0.433430	3.853809	2.751401
11	6	0	-1.572487	3.085221	0.337631
12	1	0	-1.740668	4.139169	0.579248
13	1	0	-1.541685	2.977991	-0.750753
14	1	0	-2.418417	2.507547	0.726100
15	6	0	0.922591	3.413374	0.374698
16	1	0	0.962231	3.295780	-0.712512
17	1	0	0.796586	4.475312	0.607533

18	1	0	1.877242	3.083222	0.798683
19	6	0	1.759575	-2.868396	-0.065378
20	1	0	2.593600	-2.370532	0.442786
21	1	0	1.938903	-3.947140	-0.026671
22	1	0	1.746930	-2.549980	-1.112236
23	6	0	0.461602	-2.975476	2.099062
24	1	0	1.280886	-2.471283	2.620675
25	1	0	-0.479697	-2.715421	2.592539
26	1	0	0.611522	-4.058092	2.171068
27	6	0	-0.730664	-3.241456	-0.112482
28	1	0	-0.784131	-2.915019	-1.155172
29	1	0	-0.575662	-4.324397	-0.086904
30	1	0	-1.688596	-3.025143	0.372914
31	7	0	2.190011	0.487397	-0.638441
32	1	0	1.620581	0.714608	-1.448460
33	6	0	3.550579	0.267638	-0.948355
34	6	0	3.959489	0.497086	-2.273253
35	6	0	4.496953	-0.163835	-0.006046
36	6	0	5.286310	0.299132	-2.647336
37	1	0	3.231087	0.830801	-3.009001
38	6	0	5.822736	-0.357569	-0.396037
39	1	0	4.194744	-0.338281	1.019448
40	6	0	6.230659	-0.130270	-1.711648
41	1	0	5.579720	0.482011	-3.677576
42	1	0	6.542860	-0.692923	0.345796
43	1	0	7.265023	-0.285081	-2.003809
44	7	0	-1.916336	-0.122090	-0.866484
45	1	0	-1.321385	0.256449	-1.599709
46	6	0	-3.297640	-0.141579	-1.201223
47	6	0	-3.788378	0.811601	-2.104414
48	6	0	-4.161582	-1.117270	-0.689222

49	6	0	-5.129684	0.791530	-2.485021
50	1	0	-3.116999	1.566891	-2.504801
51	6	0	-5.506821	-1.115091	-1.057768
52	1	0	-3.780510	-1.871875	-0.011486
53	6	0	-5.998852	-0.165058	-1.955681
54	1	0	-5.495784	1.534323	-3.188423
55	1	0	-6.169066	-1.874484	-0.650969
56	1	0	-7.045553	-0.174709	-2.245381
57	8	0	2.180953	0.195798	1.956444
58	16	0	-2.423932	-0.346769	2.103019

“In-out-S”-conformation

Electronic energy = -2156.2607621, thermal correction to Gibbs free energy = 0.4737989 NIMAG = 0



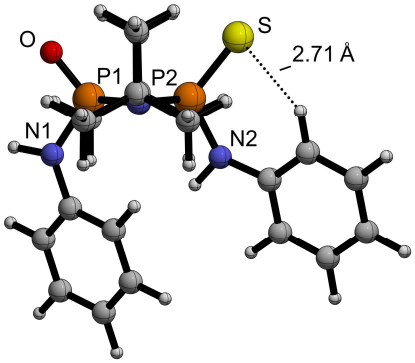
1	15	0	1.948760	-0.622478	0.223427
2	7	0	0.476015	-1.179963	0.840045
3	7	0	1.026090	-0.279948	-1.174413
4	15	0	-0.376574	-1.033860	-0.628509
5	6	0	0.155614	-2.011810	2.041298
6	6	0	1.455734	0.098101	-2.558121
7	6	0	0.430547	-3.493314	1.734086
8	1	0	-0.174484	-3.821328	0.883741
9	1	0	1.486537	-3.641164	1.489410
10	1	0	0.180512	-4.107762	2.605484
11	6	0	-1.332189	-1.797178	2.357793
12	1	0	-1.608153	-2.389837	3.235158
13	1	0	-1.545158	-0.744171	2.567563
14	1	0	-1.962238	-2.119918	1.521137
15	6	0	1.025667	-1.529641	3.210116
16	1	0	0.838298	-0.475179	3.433899
17	1	0	0.792043	-2.121648	4.100253
18	1	0	2.089573	-1.656707	2.983696
19	6	0	2.632751	1.075970	-2.439315

20	1	0	3.482272	0.608690	-1.929331
21	1	0	2.958509	1.370901	-3.441339
22	1	0	2.336977	1.974394	-1.889496
23	6	0	1.872881	-1.167534	-3.326036
24	1	0	2.698459	-1.669612	-2.813282
25	1	0	1.031135	-1.863227	-3.398015
26	1	0	2.195379	-0.900332	-4.337929
27	6	0	0.272994	0.784197	-3.256002
28	1	0	-0.032168	1.684876	-2.714786
29	1	0	0.573024	1.069378	-4.269093
30	1	0	-0.587841	0.111299	-3.333004
31	7	0	2.379582	0.803690	0.993435
32	1	0	3.386821	0.935203	1.008255
33	6	0	1.616877	2.002284	1.061077
34	6	0	2.204999	3.214100	0.672162
35	6	0	0.299414	1.997963	1.537268
36	6	0	1.476922	4.400696	0.746259
37	1	0	3.229545	3.221422	0.309355
38	6	0	-0.428212	3.188128	1.588114
39	1	0	-0.144703	1.072025	1.882844
40	6	0	0.152975	4.393842	1.191642
41	1	0	1.945916	5.332425	0.442702
42	1	0	-1.449388	3.168941	1.958586
43	1	0	-0.414488	5.318327	1.239049
44	7	0	-1.519557	0.175833	-0.548984
45	1	0	-1.125256	1.088785	-0.332247
46	6	0	-2.928915	0.126655	-0.467662
47	6	0	-3.608784	1.334853	-0.238168
48	6	0	-3.668225	-1.057737	-0.610279
49	6	0	-4.998602	1.357422	-0.150447
50	1	0	-3.042252	2.256668	-0.129548

51	6	0	-5.060102	-1.019039	-0.519379
52	1	0	-3.156276	-1.994132	-0.797031
53	6	0	-5.737323	0.179890	-0.289427
54	1	0	-5.503143	2.303185	0.027968
55	1	0	-5.617908	-1.945147	-0.631362
56	1	0	-6.820932	0.197472	-0.221074
57	16	0	3.511632	-1.773391	0.132208
58	8	0	-0.919322	-2.268607	-1.246390

“In-S-out”-conformation

Electronic energy = -2156.2578827, thermal correction to Gibbs free energy = 0.4739318 NIMAG = 0



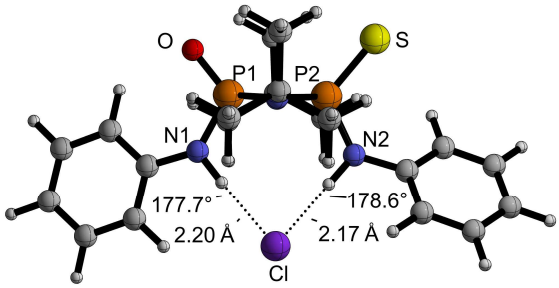
1	15	0	2.000485	-0.801824	0.369397
2	7	0	0.490975	-1.175797	1.016064
3	7	0	1.142246	-0.562754	-1.075574
4	15	0	-0.340816	-1.133103	-0.482946
5	6	0	0.127591	-1.774534	2.338130
6	6	0	1.650647	-0.421451	-2.477533
7	6	0	0.356409	-3.295077	2.303583
8	1	0	-0.267517	-3.759528	1.534902
9	1	0	1.405645	-3.515518	2.084437
10	1	0	0.100510	-3.730110	3.275597
11	6	0	-1.348117	-1.454353	2.611519
12	1	0	-1.634910	-1.856096	3.587946
13	1	0	-1.523902	-0.373830	2.613481
14	1	0	-1.991917	-1.914222	1.854680
15	6	0	1.018629	-1.129909	3.410347
16	1	0	0.873542	-0.046474	3.449777
17	1	0	0.764201	-1.551884	4.387337
18	1	0	2.077296	-1.334043	3.216699
19	6	0	2.853842	0.531886	-2.439460
20	1	0	3.664401	0.119789	-1.827953
21	1	0	3.235938	0.670153	-3.455526

22	1	0	2.566743	1.507582	-2.036191
23	6	0	2.073087	-1.799543	-3.014015
24	1	0	2.851293	-2.231763	-2.377723
25	1	0	1.218097	-2.481877	-3.033629
26	1	0	2.465503	-1.697878	-4.031328
27	6	0	0.533773	0.177697	-3.343174
28	1	0	0.243506	1.168556	-2.980431
29	1	0	0.893403	0.275936	-4.372020
30	1	0	-0.350342	-0.468512	-3.351151
31	7	0	2.563035	0.653694	0.969770
32	1	0	3.578214	0.675960	1.004127
33	6	0	1.943707	1.928083	0.894889
34	6	0	2.690484	3.032404	0.459184
35	6	0	0.606162	2.110008	1.270976
36	6	0	2.101228	4.293778	0.389231
37	1	0	3.729205	2.896004	0.169565
38	6	0	0.018538	3.372619	1.176614
39	1	0	0.035266	1.270990	1.649951
40	6	0	0.758922	4.470154	0.734741
41	1	0	2.693407	5.139362	0.050579
42	1	0	-1.020698	3.495539	1.468610
43	1	0	0.299880	5.452000	0.669530
44	7	0	-1.309152	0.225051	-0.589886
45	1	0	-0.747818	1.074928	-0.605754
46	6	0	-2.693827	0.476842	-0.473848
47	6	0	-3.111572	1.808165	-0.646500
48	6	0	-3.651477	-0.506991	-0.190804
49	6	0	-4.457038	2.147077	-0.534702
50	1	0	-2.373321	2.575969	-0.865825
51	6	0	-4.998141	-0.154477	-0.089107
52	1	0	-3.350161	-1.538787	-0.060189

53	6	0	-5.413551	1.167246	-0.256420
54	1	0	-4.756101	3.183167	-0.668028
55	1	0	-5.726990	-0.930100	0.130582
56	1	0	-6.463505	1.430734	-0.170789
57	8	0	3.114989	-1.781737	0.430970
58	16	0	-1.179332	-2.755459	-1.127519

13•Cl

Electronic energy = -2616.6814056, thermal correction to Gibbs free energy = 0.407593 NIMAG = 0



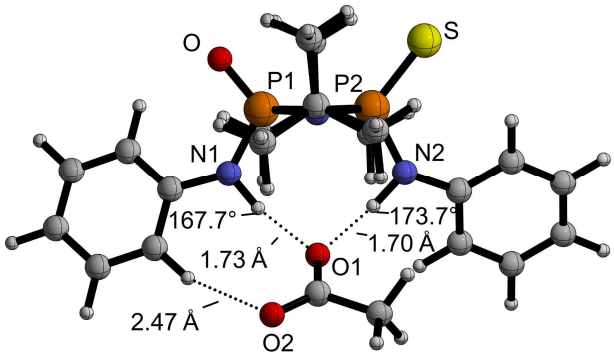
1	15	0	-1.189615	-0.780988	0.521346
2	7	0	0.181487	-1.406502	-0.257798
3	7	0	-0.037615	0.043628	1.470060
4	15	0	1.315185	-0.678950	0.773832
5	6	0	0.351933	-2.481017	-1.271694
6	6	0	-0.204899	0.887692	2.689112
7	6	0	0.413216	-3.847439	-0.566906
8	1	0	1.254378	-3.873243	0.132683
9	1	0	-0.510565	-4.023860	-0.007425
10	1	0	0.540695	-4.648687	-1.302990
11	6	0	1.661633	-2.205381	-2.026954
12	1	0	1.822240	-2.985839	-2.777372
13	1	0	1.623634	-1.234084	-2.529467
14	1	0	2.518886	-2.211804	-1.343483
15	6	0	-0.836126	-2.426355	-2.242832
16	1	0	-0.896938	-1.448624	-2.729871
17	1	0	-0.714472	-3.197373	-3.010122
18	1	0	-1.778126	-2.615883	-1.716683
19	6	0	-1.491912	1.711405	2.531236
20	1	0	-2.366741	1.059604	2.427326
21	1	0	-1.633600	2.332751	3.421260
22	1	0	-1.427618	2.358691	1.651950
23	6	0	-0.290080	-0.018430	3.929730

24	1	0	-1.146482	-0.694995	3.851468
25	1	0	0.621104	-0.617386	4.027352
26	1	0	-0.405220	0.592797	4.831652
27	6	0	1.004230	1.828337	2.794722
28	1	0	1.071922	2.468445	1.910605
29	1	0	0.891743	2.457103	3.683856
30	1	0	1.937703	1.263156	2.894007
31	7	0	-1.881463	0.362902	-0.467713
32	1	0	-1.238370	1.158549	-0.664111
33	6	0	-3.224817	0.616113	-0.818844
34	6	0	-3.640322	1.955993	-0.906114
35	6	0	-4.134573	-0.403560	-1.135471
36	6	0	-4.942336	2.265791	-1.294217
37	1	0	-2.926847	2.743500	-0.678400
38	6	0	-5.441597	-0.082010	-1.502627
39	1	0	-3.818784	-1.439144	-1.095978
40	6	0	-5.856252	1.249332	-1.585020
41	1	0	-5.244967	3.307727	-1.359560
42	1	0	-6.135865	-0.883645	-1.741399
43	1	0	-6.873456	1.491286	-1.879532
44	7	0	2.123603	0.541732	-0.008538
45	1	0	1.495399	1.278756	-0.379948
46	6	0	3.461721	0.655856	-0.425653
47	6	0	3.801643	1.775639	-1.208412
48	6	0	4.462486	-0.276776	-0.103516
49	6	0	5.108331	1.956187	-1.654251
50	1	0	3.025721	2.494027	-1.462272
51	6	0	5.767179	-0.081081	-0.558558
52	1	0	4.214680	-1.139837	0.503081
53	6	0	6.105135	1.030134	-1.334025
54	1	0	5.346471	2.828354	-2.258030

55	1	0	6.527887	-0.813457	-0.299357
56	1	0	7.123990	1.171835	-1.682700
57	8	0	2.223353	-1.563696	1.550552
58	17	0	0.095186	2.801817	-1.123052
59	16	0	-2.458537	-1.990992	1.364560

13•OAc “one-binding”-mode 1

Electronic energy = -2385.0368897, thermal correction to Gibbs free energy = 0.452593 NIMAG = 0



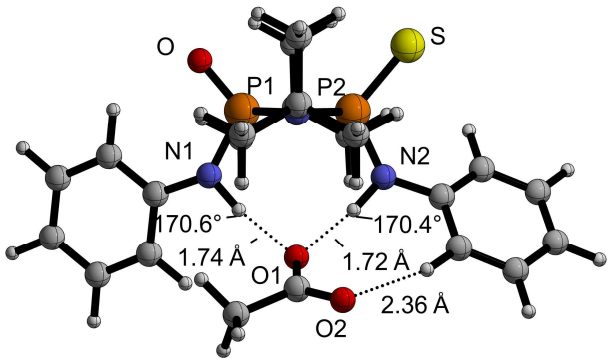
1	15	0	1.228767	-1.048832	-0.501290
2	7	0	0.019752	-1.463534	0.627066
3	7	0	-0.094526	-0.627438	-1.475262
4	15	0	-1.290620	-1.147224	-0.393903
5	6	0	0.095254	-2.080364	1.975910
6	6	0	-0.191774	-0.264112	-2.917771
7	6	0	0.119500	-3.612984	1.838590
8	1	0	-0.790382	-3.962328	1.340267
9	1	0	0.984173	-3.925502	1.245380
10	1	0	0.180170	-4.081435	2.827193
11	6	0	-1.139404	-1.634995	2.775424
12	1	0	-1.103607	-2.077781	3.775965
13	1	0	-1.170100	-0.545688	2.871368
14	1	0	-2.064695	-1.968300	2.291204
15	6	0	1.374124	-1.579652	2.664701
16	1	0	1.355701	-0.491515	2.775334
17	1	0	1.457244	-2.033047	3.657445
18	1	0	2.264036	-1.856184	2.087414
19	6	0	1.069140	0.515919	-3.314984
20	1	0	1.970103	-0.089799	-3.169240
21	1	0	1.004771	0.785707	-4.373858
22	1	0	1.162643	1.429589	-2.722461
23	6	0	-0.318455	-1.546429	-3.759677
24	1	0	0.562044	-2.181061	-3.619839

25	1	0	-1.206631	-2.111407	-3.459910
26	1	0	-0.404727	-1.292245	-4.821831
27	6	0	-1.432381	0.623889	-3.103675
28	1	0	-1.355788	1.533164	-2.500274
29	1	0	-1.519207	0.903948	-4.158593
30	1	0	-2.346019	0.091626	-2.816595
31	7	0	1.920900	0.404329	-0.085220
32	1	0	1.174733	1.109795	0.161974
33	6	0	3.185216	0.705999	0.469307
34	6	0	3.230932	1.602628	1.551341
35	6	0	4.387740	0.206631	-0.052755
36	6	0	4.452798	1.983027	2.102903
37	1	0	2.299071	1.999832	1.944637
38	6	0	5.604340	0.578207	0.520672
39	1	0	4.361863	-0.465006	-0.902494
40	6	0	5.649059	1.465907	1.598509
41	1	0	4.467092	2.680062	2.936909
42	1	0	6.527248	0.179443	0.106936
43	1	0	6.601133	1.756009	2.033744
44	7	0	-2.090370	0.206485	0.120577
45	1	0	-1.455846	1.033290	0.246507
46	6	0	-3.428557	0.412536	0.492806
47	6	0	-3.837884	1.742115	0.714490
48	6	0	-4.360560	-0.625262	0.669507
49	6	0	-5.144551	2.019637	1.108962
50	1	0	-3.118643	2.543545	0.554566
51	6	0	-5.667862	-0.328324	1.057362
52	1	0	-4.058870	-1.651587	0.496060
53	6	0	-6.073358	0.988933	1.283802
54	1	0	-5.439972	3.053018	1.274784
55	1	0	-6.374850	-1.144058	1.188975

56	1	0	-7.092660	1.208622	1.588616
57	8	0	-2.202087	-2.262450	-0.766827
58	16	0	2.479297	-2.439817	-1.047888
59	6	0	-0.221101	3.260221	-0.192340
60	6	0	1.115210	3.911469	-0.562042
61	1	0	1.638948	4.208686	0.353606
62	1	0	1.758609	3.190398	-1.077355
63	1	0	0.966478	4.789837	-1.193728
64	8	0	-0.139182	2.143776	0.449668
65	8	0	-1.292466	3.824849	-0.505964

13•OAc “one-binding”-mode 2

Electronic energy = -2385.0373311, thermal correction to Gibbs free energy = 0.450404 NIMAG = 0



1	15	0	-1.203698	-1.012877	0.545893
2	7	0	0.177970	-1.622513	-0.232175
3	7	0	-0.061006	-0.246365	1.552989
4	15	0	1.301795	-0.914206	0.822843
5	6	0	0.362102	-2.627540	-1.310556
6	6	0	-0.238501	0.515511	2.823268
7	6	0	0.400041	-4.037359	-0.694150
8	1	0	1.226802	-4.115041	0.018838
9	1	0	-0.536475	-4.242218	-0.166328
10	1	0	0.537239	-4.790848	-1.477601
11	6	0	1.688689	-2.317981	-2.022036
12	1	0	1.856890	-3.052038	-2.816397
13	1	0	1.670324	-1.317296	-2.464529
14	1	0	2.532373	-2.375016	-1.324023
15	6	0	-0.805115	-2.504752	-2.300684
16	1	0	-0.855323	-1.496671	-2.723041
17	1	0	-0.668747	-3.223416	-3.114926
18	1	0	-1.757896	-2.726555	-1.808269
19	6	0	-1.530628	1.339773	2.721098

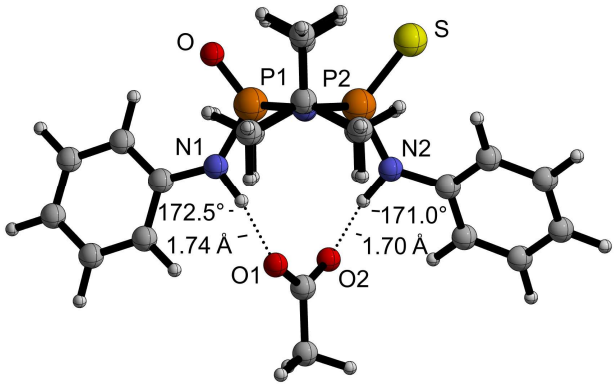
20	1	0	-2.400239	0.687248	2.584051
21	1	0	-1.670506	1.901341	3.650723
22	1	0	-1.481502	2.043984	1.885531
23	6	0	-0.319733	-0.474358	3.998964
24	1	0	-1.164367	-1.156510	3.862793
25	1	0	0.599732	-1.065117	4.064066
26	1	0	-0.453561	0.070557	4.939999
27	6	0	0.965236	1.451910	2.997893
28	1	0	1.030609	2.157144	2.165937
29	1	0	0.850546	2.013730	3.930434
30	1	0	1.902354	0.886847	3.052728
31	7	0	-1.862690	0.199426	-0.371268
32	1	0	-1.194232	1.004976	-0.507913
33	6	0	-3.159849	0.425172	-0.870982
34	6	0	-3.560481	1.763654	-1.041242
35	6	0	-4.038999	-0.603346	-1.245790
36	6	0	-4.816141	2.058845	-1.568293
37	1	0	-2.871200	2.556331	-0.753714
38	6	0	-5.300660	-0.292360	-1.755045
39	1	0	-3.738109	-1.638280	-1.137335
40	6	0	-5.700695	1.035301	-1.921864
41	1	0	-5.108161	3.098720	-1.694329
42	1	0	-5.969912	-1.101668	-2.036645
43	1	0	-6.682248	1.268277	-2.325106
44	7	0	2.077986	0.357753	0.087147
45	1	0	1.406511	1.068741	-0.286572
46	6	0	3.368519	0.422854	-0.469480
47	6	0	3.590519	1.359599	-1.496390
48	6	0	4.439261	-0.381527	-0.042316
49	6	0	4.850294	1.491463	-2.075533
50	1	0	2.761184	1.974694	-1.834914

51	6	0	5.693335	-0.244805	-0.638598
52	1	0	4.279560	-1.104693	0.748966
53	6	0	5.914022	0.688713	-1.654216
54	1	0	4.997114	2.222366	-2.866846
55	1	0	6.509328	-0.876904	-0.296677
56	1	0	6.895461	0.788917	-2.108717
57	8	0	2.228835	-1.812806	1.561728
58	16	0	-2.492078	-2.264492	1.302259
59	6	0	-0.004514	3.309595	-0.291856
60	6	0	1.314863	4.075343	-0.145553
61	1	0	2.071691	3.451421	0.341222
62	1	0	1.696182	4.326491	-1.142400
63	1	0	1.174489	4.997349	0.422781
64	8	0	0.094237	2.110727	-0.755551
65	8	0	-1.077987	3.872195	0.020615

13•OAc “two-binding”-mode

Electronic energy = -2385.0365214, thermal correction to Gibbs free energy = 0.452866 NIMAG = 0

1	15	0	-1.210285	-1.129684	-0.246372
2	7	0	0.194012	-0.960073	-1.172379
3	7	0	-0.105433	-1.269659	1.053419
4	15	0	1.282422	-1.247540	0.100280
5	6	0	0.413671	-0.920973	-2.643274
6	6	0	-0.308512	-1.608557	2.489662
7	6	0	0.472418	-2.357021	-3.193196
8	1	0	1.287091	-2.911488	-2.716946
9	1	0	-0.468811	-2.877785	-2.990807
10	1	0	0.642174	-2.340411	-4.275432
11	6	0	1.743754	-0.194005	-2.894446
12	1	0	1.935976	-0.146648	-3.971115
13	1	0	1.710298	0.823379	-2.493571
14	1	0	2.578301	-0.728025	-2.425491



15	6	0	-0.739165	-0.141154	-3.292769
16	1	0	-0.781870	0.880321	-2.904923
17	1	0	-0.583507	-0.105047	-4.375873
18	1	0	-1.700360	-0.631032	-3.101717
19	6	0	-1.633897	-0.982115	2.945256
20	1	0	-2.475378	-1.407971	2.388870
21	1	0	-1.790410	-1.191296	4.008182
22	1	0	-1.624727	0.101333	2.794480
23	6	0	-0.349932	-3.137798	2.657880
24	1	0	-1.166293	-3.562773	2.066125
25	1	0	0.592380	-3.582741	2.322646
26	1	0	-0.504145	-3.396832	3.711210
27	6	0	0.853249	-1.013246	3.299832
28	1	0	0.892506	0.073286	3.182241
29	1	0	0.710439	-1.252644	4.358653
30	1	0	1.813671	-1.434008	2.982359
31	7	0	-1.912119	0.370773	-0.231897
32	1	0	-1.216081	1.148685	-0.396301
33	6	0	-3.248667	0.805931	-0.157065
34	6	0	-3.542049	2.082319	-0.675541
35	6	0	-4.285708	0.063324	0.431224
36	6	0	-4.836440	2.592505	-0.612333
37	1	0	-2.736855	2.665564	-1.113102
38	6	0	-5.581424	0.580223	0.474669
39	1	0	-4.082590	-0.916116	0.845849
40	6	0	-5.870932	1.843811	-0.043563
41	1	0	-5.037098	3.581439	-1.017052
42	1	0	-6.368989	-0.013712	0.931951
43	1	0	-6.881236	2.240506	-0.000121
44	7	0	2.102922	0.134584	0.501650
45	1	0	1.484048	0.929346	0.799136

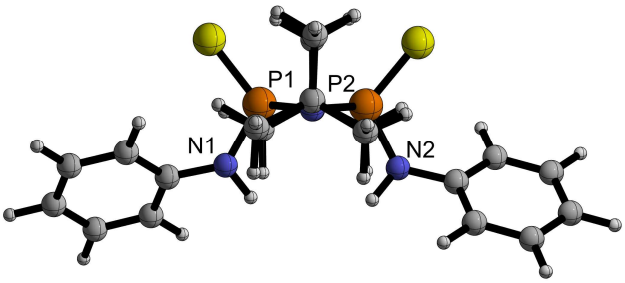
46	6	0	3.452584	0.480799	0.313594
47	6	0	3.839852	1.796431	0.638033
48	6	0	4.427429	-0.405903	-0.179190
49	6	0	5.159878	2.208341	0.471844
50	1	0	3.089589	2.483248	1.020167
51	6	0	5.745693	0.022468	-0.339086
52	1	0	4.148543	-1.423011	-0.427755
53	6	0	6.127570	1.327068	-0.018932
54	1	0	5.431538	3.229475	0.728450
55	1	0	6.481960	-0.680012	-0.722461
56	1	0	7.156352	1.650638	-0.148565
57	8	0	2.166112	-2.440947	-0.002744
58	16	0	-2.437493	-2.608110	-0.582851
59	6	0	0.167930	3.032610	0.420356
60	6	0	0.152703	4.555390	0.569206
61	1	0	0.696183	5.009172	-0.266899
62	1	0	-0.880828	4.916021	0.518706
63	1	0	0.603646	4.873262	1.511954
64	8	0	-0.309497	2.558806	-0.658922
65	8	0	0.649212	2.341136	1.369872

S-cyclodiphosph(V)azane 11

“In-in”-conformation

Electronic energy = -2479.2007788, thermal correction to Gibbs free energy = 0.407939 NIMAG = 0

1	15	0	1.263317	-0.064963	-0.603747
2	7	0	-0.057516	-1.133231	-0.501223
3	7	0	0.057465	1.131650	-0.502981
4	15	0	-1.263300	0.063169	-0.604388
5	16	0	2.475593	-0.150936	-2.112632
6	16	0	-2.475218	0.147627	-2.113625



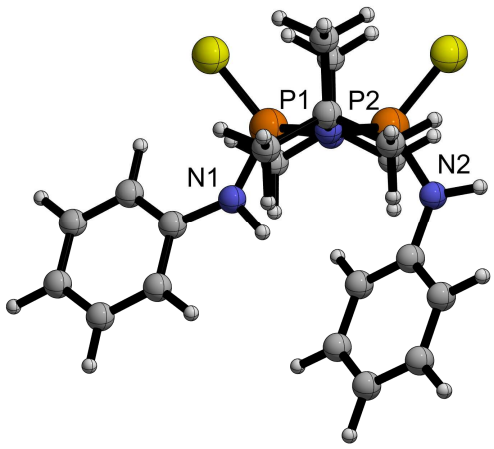
7	6	0	-0.143199	-2.613421	-0.698267
8	6	0	0.143335	2.611495	-0.702204
9	6	0	-0.198750	-2.945330	-2.199479
10	1	0	-1.073818	-2.480075	-2.662402
11	1	0	0.700370	-2.581093	-2.704891
12	1	0	-0.263671	-4.030308	-2.334230
13	6	0	-1.413073	-3.112548	0.007030
14	1	0	-1.503894	-4.193141	-0.140134
15	1	0	-1.370469	-2.910742	1.081575
16	1	0	-2.309460	-2.636972	-0.406376
17	6	0	1.098466	-3.248807	-0.056916
18	1	0	1.165004	-2.998711	1.005879
19	1	0	1.040334	-4.336581	-0.161887
20	1	0	2.011210	-2.909448	-0.557998
21	6	0	1.412705	3.111567	0.003327
22	1	0	2.309396	2.635565	-0.408933
23	1	0	1.503586	4.191989	-0.145058
24	1	0	1.369392	2.910965	1.078065
25	6	0	0.200037	2.941156	-2.203858
26	1	0	1.075270	2.474852	-2.665400
27	1	0	-0.698833	2.576426	-2.709355
28	1	0	0.265424	4.025905	-2.340208
29	6	0	-1.098783	3.247857	-0.062692
30	1	0	-1.166152	2.999255	1.000405
31	1	0	-1.040581	4.335481	-0.169131
32	1	0	-2.011125	2.907792	-0.564028
33	7	0	2.050315	-0.071933	0.876896
34	1	0	1.463574	0.272485	1.633162
35	6	0	3.438507	-0.042671	1.176615
36	6	0	3.904711	0.888658	2.115548
37	6	0	4.336594	-0.947977	0.598305

38	6	0	5.254031	0.917102	2.465353
39	1	0	3.207629	1.589014	2.568661
40	6	0	5.688511	-0.896938	0.937908
41	1	0	3.977926	-1.686563	-0.108365
42	6	0	6.155721	0.031556	1.870887
43	1	0	5.600148	1.642222	3.196753
44	1	0	6.376667	-1.601989	0.479559
45	1	0	7.208280	0.059665	2.137137
46	7	0	-2.050607	0.070907	0.876167
47	1	0	-1.464464	-0.275031	1.632190
48	6	0	-3.438726	0.044288	1.176087
49	6	0	-3.906057	-0.884973	2.116553
50	6	0	-4.335751	0.949895	0.596578
51	6	0	-5.255314	-0.911060	2.466715
52	1	0	-3.209868	-1.585622	2.570591
53	6	0	-5.687646	0.901228	0.936632
54	1	0	-3.976346	1.686894	-0.111366
55	6	0	-6.155939	-0.025177	1.871143
56	1	0	-5.602229	-1.634610	3.199291
57	1	0	-6.374938	1.606517	0.477351
58	1	0	-7.208473	-0.051419	2.137680

“In-out”-conformation

Electronic energy = -2479.2079829, thermal correction to Gibbs free energy = 0.411252 NIMAG = 0

1	15	0	2.027681	-0.389327	0.260572
2	7	0	0.632242	-1.057692	0.945524
3	7	0	1.051987	-0.229377	-1.128956
4	15	0	-0.276793	-1.081669	-0.507625
5	6	0	0.431090	-1.782632	2.240222
6	6	0	1.422730	0.093564	-2.545080
7	6	0	0.889668	-3.244040	2.104221
8	1	0	0.314383	-3.755249	1.327464



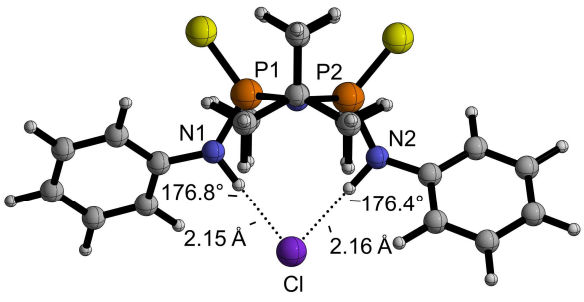
9	1	0	1.950391	-3.285465	1.839962
10	1	0	0.741936	-3.766969	3.055219
11	6	0	-1.064728	-1.715491	2.579439
12	1	0	-1.243225	-2.210529	3.538674
13	1	0	-1.408761	-0.678926	2.652848
14	1	0	-1.661488	-2.228796	1.818204
15	6	0	1.252192	-1.067311	3.323239
16	1	0	0.937998	-0.025938	3.440008
17	1	0	1.107184	-1.583081	4.277448
18	1	0	2.320426	-1.087207	3.083005
19	6	0	2.483911	1.202070	-2.510081
20	1	0	3.387349	0.865395	-1.989773
21	1	0	2.761330	1.464997	-3.535377
22	1	0	2.097385	2.096286	-2.012391
23	6	0	1.976962	-1.162389	-3.237789
24	1	0	2.855488	-1.533657	-2.702336
25	1	0	1.221033	-1.952501	-3.259116
26	1	0	2.264876	-0.920601	-4.266368
27	6	0	0.164053	0.596617	-3.266536
28	1	0	-0.225605	1.502285	-2.791822
29	1	0	0.417777	0.830042	-4.305256
30	1	0	-0.622811	-0.165124	-3.269973
31	7	0	2.328139	1.119397	0.927269
32	1	0	3.319519	1.341601	0.929064
33	6	0	1.458744	2.244871	0.936598
34	6	0	1.927193	3.480820	0.468837
35	6	0	0.150625	2.146212	1.427891
36	6	0	1.090139	4.595469	0.479389
37	1	0	2.943830	3.562427	0.093543
38	6	0	-0.687585	3.262432	1.413515
39	1	0	-0.202492	1.205478	1.832194

40	6	0	-0.225394	4.490584	0.937994
41	1	0	1.466849	5.547046	0.114993
42	1	0	-1.701334	3.167808	1.792419
43	1	0	-0.878027	5.358342	0.934594
44	7	0	-1.478283	0.076932	-0.457087
45	1	0	-1.084568	1.014826	-0.392152
46	6	0	-2.887135	0.058304	-0.357246
47	6	0	-3.546922	1.293746	-0.479599
48	6	0	-3.643562	-1.099432	-0.127784
49	6	0	-4.932966	1.368140	-0.373232
50	1	0	-2.965538	2.195630	-0.656160
51	6	0	-5.033216	-1.011771	-0.033339
52	1	0	-3.153896	-2.060334	-0.031838
53	6	0	-5.689300	0.214214	-0.152150
54	1	0	-5.421381	2.334166	-0.467694
55	1	0	-5.604134	-1.919427	0.143547
56	1	0	-6.770778	0.271066	-0.072385
57	16	0	3.696803	-1.382701	0.209812
58	16	0	-0.845841	-2.784006	-1.234377

11•Cl

Electronic energy = -2939.6289646, thermal correction to Gibbs free energy = 0.404810 NIMAG = 0

1	15	0	1.267892	-0.887644	0.142221
2	7	0	-0.117982	-0.838370	1.114504
3	7	0	0.142459	-0.723319	-1.131113
4	15	0	-1.245603	-0.859387	-0.167693
5	6	0	-0.308133	-1.058088	2.576684
6	6	0	0.326392	-0.777121	-2.608075
7	6	0	-0.398835	-2.565361	2.871076
8	1	0	-1.229686	-3.009506	2.315160
9	1	0	0.527229	-3.066506	2.573330
10	1	0	-0.559782	-2.728128	3.942412



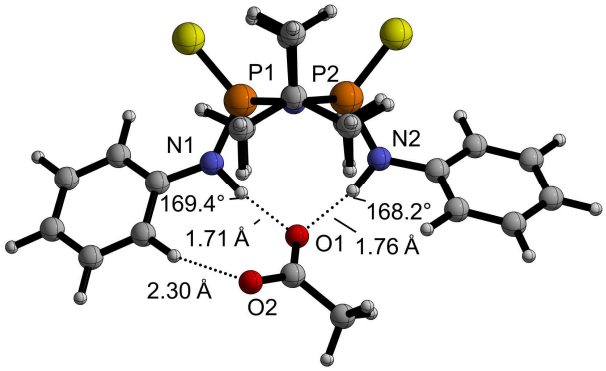
11	6	0	-1.604508	-0.346392	2.993161
12	1	0	-1.764619	-0.485357	4.067009
13	1	0	-1.541307	0.724971	2.780889
14	1	0	-2.470200	-0.758838	2.462834
15	6	0	0.885546	-0.438022	3.317880
16	1	0	0.959177	0.633384	3.110804
17	1	0	0.752340	-0.584086	4.394615
18	1	0	1.825254	-0.916478	3.021015
19	6	0	1.664171	-0.098075	-2.938897
20	1	0	2.497369	-0.612803	-2.446779
21	1	0	1.831821	-0.134408	-4.019882
22	1	0	1.659314	0.947914	-2.618899
23	6	0	0.331243	-2.239642	-3.085832
24	1	0	1.150066	-2.791758	-2.614793
25	1	0	-0.613676	-2.725664	-2.824561
26	1	0	0.459182	-2.276986	-4.173290
27	6	0	-0.827430	-0.003587	-3.263902
28	1	0	-0.850638	1.031839	-2.912240
29	1	0	-0.692386	-0.008699	-4.350250
30	1	0	-1.792866	-0.469885	-3.038424
31	7	0	2.037628	0.563281	0.400691
32	1	0	1.370164	1.362869	0.370223
33	6	0	3.386725	0.946265	0.203196
34	6	0	3.643993	2.133220	-0.502445
35	6	0	4.460178	0.220959	0.739093
36	6	0	4.953687	2.575917	-0.681103
37	1	0	2.807796	2.704642	-0.896285
38	6	0	5.768276	0.661547	0.535393
39	1	0	4.265720	-0.678349	1.311117
40	6	0	6.025722	1.836877	-0.174414
41	1	0	5.135032	3.497713	-1.227683

42	1	0	6.591375	0.086808	0.952275
43	1	0	7.046675	2.177337	-0.321980
44	7	0	-2.013759	0.612698	-0.211162
45	1	0	-1.375998	1.397852	0.039133
46	6	0	-3.386216	0.950532	-0.163565
47	6	0	-3.786552	1.987888	0.694629
48	6	0	-4.341435	0.332664	-0.983206
49	6	0	-5.120841	2.389338	0.738546
50	1	0	-3.040795	2.478401	1.314269
51	6	0	-5.677828	0.727022	-0.915171
52	1	0	-4.034907	-0.447984	-1.669210
53	6	0	-6.077901	1.753997	-0.056827
54	1	0	-5.413140	3.195985	1.405787
55	1	0	-6.407959	0.236098	-1.553488
56	1	0	-7.118981	2.061313	-0.015251
57	17	0	-0.018877	3.019627	0.442928
58	16	0	2.445701	-2.436930	0.138106
59	16	0	-2.434508	-2.388668	-0.357689

11•OAc “one-atom”-mode

Electronic energy = -2707.9839372, thermal correction to Gibbs free energy = 0.450594 NIMAG = 0

1	15	0	-1.250284	-1.043078	0.364914
2	7	0	0.088124	-1.587230	-0.524070
3	7	0	-0.062405	-0.349580	1.364878
4	15	0	1.276312	-0.988888	0.545191
5	6	0	0.192926	-2.495793	-1.698800
6	6	0	-0.167990	0.362630	2.670285
7	6	0	0.237429	-3.960591	-1.229206
8	1	0	1.101893	-4.125439	-0.579174
9	1	0	-0.672022	-4.207233	-0.672811
10	1	0	0.314158	-4.628614	-2.094322
11	6	0	1.476614	-2.138893	-2.462862



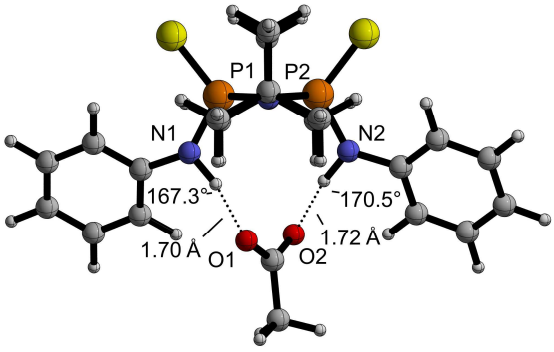
12	1	0	1.564646	-2.781929	-3.344259
13	1	0	1.461788	-1.093614	-2.785585
14	1	0	2.361187	-2.299526	-1.837574
15	6	0	-1.029099	-2.264163	-2.599738
16	1	0	-1.093327	-1.218028	-2.912414
17	1	0	-0.946173	-2.896615	-3.489357
18	1	0	-1.953725	-2.532750	-2.077906
19	6	0	-1.442621	1.219300	2.646994
20	1	0	-2.334919	0.598980	2.506307
21	1	0	-1.539643	1.744750	3.602412
22	1	0	-1.393806	1.957310	1.841822
23	6	0	-0.230622	-0.667073	3.811714
24	1	0	-1.100273	-1.319717	3.688079
25	1	0	0.672469	-1.285126	3.812542
26	1	0	-0.308407	-0.153240	4.776280
27	6	0	1.059647	1.272555	2.828763
28	1	0	1.099439	2.015947	2.026918
29	1	0	0.995226	1.789290	3.792231
30	1	0	1.986513	0.687970	2.817588
31	7	0	-1.969819	0.204752	-0.467380
32	1	0	-1.317464	1.009495	-0.609880
33	6	0	-3.340079	0.498565	-0.652529
34	6	0	-3.787712	1.804633	-0.399114
35	6	0	-4.253893	-0.454839	-1.124944
36	6	0	-5.120791	2.150426	-0.615839
37	1	0	-3.084242	2.543037	-0.029300
38	6	0	-5.590951	-0.106606	-1.317989
39	1	0	-3.915043	-1.461038	-1.341259
40	6	0	-6.033691	1.194831	-1.068363
41	1	0	-5.446857	3.168200	-0.417823
42	1	0	-6.287225	-0.857656	-1.682132

43	1	0	-7.074351	1.461499	-1.229395
44	7	0	2.029093	0.316262	-0.139454
45	1	0	1.340311	1.094007	-0.340015
46	6	0	3.365526	0.604419	-0.473232
47	6	0	3.708673	1.961549	-0.625772
48	6	0	4.347629	-0.373923	-0.698349
49	6	0	5.002479	2.323248	-0.994306
50	1	0	2.946635	2.717126	-0.441954
51	6	0	5.643471	0.004712	-1.052510
52	1	0	4.101291	-1.423126	-0.592056
53	6	0	5.983914	1.350053	-1.206177
54	1	0	5.246133	3.376839	-1.108817
55	1	0	6.389663	-0.767987	-1.221100
56	1	0	6.993568	1.634940	-1.488474
57	6	0	-1.012261	4.276908	-0.961922
58	1	0	-1.640456	4.541965	-0.102562
59	1	0	-0.603636	5.208624	-1.364353
60	1	0	-1.635007	3.788079	-1.714756
61	6	0	0.128211	3.371677	-0.483099
62	8	0	0.040865	2.121041	-0.775249
63	8	0	1.065109	3.893620	0.164858
64	16	0	-2.509268	-2.338421	1.093407
65	16	0	2.454121	-2.262542	1.434643

11•OAc “two-atom”-mode

Electronic energy = -2707.9838133, thermal correction to Gibbs free energy = 0.450207 NIMAG = 0

1	15	0	-1.280566	-1.141426	-0.017623
2	7	0	0.136229	-1.328134	-0.923026
3	7	0	-0.193002	-0.761615	1.246978
4	15	0	1.219170	-1.083927	0.379313
5	6	0	0.357229	-1.839693	-2.305883
6	6	0	-0.433460	-0.509282	2.695744



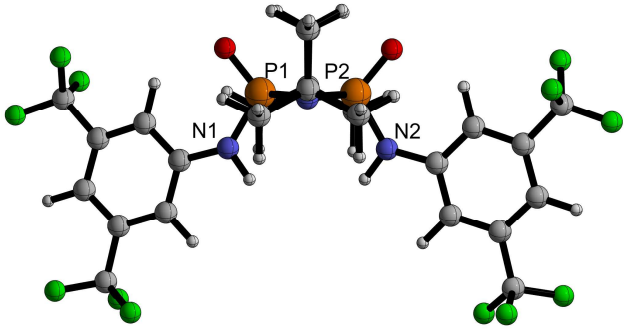
7	6	0	0.406298	-3.377680	-2.296972
8	1	0	1.219061	-3.729328	-1.654593
9	1	0	-0.537954	-3.784896	-1.922189
10	1	0	0.572773	-3.751544	-3.313359
11	6	0	1.686621	-1.262526	-2.813321
12	1	0	1.857485	-1.592718	-3.842846
13	1	0	1.670489	-0.168886	-2.788848
14	1	0	2.523565	-1.615964	-2.202214
15	6	0	-0.793595	-1.350381	-3.198317
16	1	0	-0.835625	-0.257936	-3.217740
17	1	0	-0.634261	-1.719413	-4.216731
18	1	0	-1.757219	-1.731121	-2.842892
19	6	0	-1.755354	0.264483	2.824457
20	1	0	-2.591514	-0.313394	2.414259
21	1	0	-1.961016	0.455245	3.882688
22	1	0	-1.699373	1.221493	2.298340
23	6	0	-0.518611	-1.846413	3.452013
24	1	0	-1.319577	-2.464999	3.036745
25	1	0	0.425163	-2.393271	3.365540
26	1	0	-0.723864	-1.663336	4.512573
27	6	0	0.720341	0.345410	3.241718
28	1	0	0.781779	1.296978	2.706640
29	1	0	0.546290	0.543311	4.304573
30	1	0	1.677957	-0.177871	3.144505
31	7	0	-1.994468	0.226111	-0.618497
32	1	0	-1.296790	0.970434	-0.897910
33	6	0	-3.307222	0.725471	-0.429883
34	6	0	-3.459255	2.055726	-0.003556
35	6	0	-4.451287	-0.035842	-0.709079
36	6	0	-4.730204	2.608650	0.145286
37	1	0	-2.573200	2.645711	0.210759

38	6	0	-5.719611	0.519768	-0.536342
39	1	0	-4.339914	-1.054453	-1.061131
40	6	0	-5.869817	1.841882	-0.110729
41	1	0	-4.827953	3.640298	0.473512
42	1	0	-6.596938	-0.084148	-0.754147
43	1	0	-6.860358	2.270443	0.013314
44	7	0	1.981035	0.380435	0.223091
45	1	0	1.317601	1.195774	0.304904
46	6	0	3.331787	0.754496	0.090983
47	6	0	3.671358	2.080468	0.424897
48	6	0	4.341557	-0.100033	-0.381410
49	6	0	4.983445	2.529653	0.297056
50	1	0	2.887544	2.748140	0.771520
51	6	0	5.654668	0.359185	-0.491618
52	1	0	4.104745	-1.120912	-0.653503
53	6	0	5.990311	1.671908	-0.155431
54	1	0	5.219248	3.558086	0.559354
55	1	0	6.419891	-0.321446	-0.856761
56	1	0	7.014270	2.021994	-0.249696
57	6	0	0.229270	4.523059	-1.084677
58	1	0	-0.358009	5.125952	-0.382656
59	1	0	1.277333	4.820671	-0.970888
60	1	0	-0.103526	4.730119	-2.104177
61	6	0	0.074200	3.043535	-0.729981
62	8	0	-0.441607	2.269972	-1.594000
63	8	0	0.472285	2.683627	0.423091
64	16	0	-2.495502	-2.638267	0.279829
65	16	0	2.384054	-2.560242	0.896761

O-cyclodiphosph(V)azane 5

“In-in”-conformation

Electronic energy = -3182.2040385, thermal correction to Gibbs free energy = 0.403243 NIMAG = 0



1	15	0	-1.216284	1.481904	0.271538
2	7	0	0.237291	1.394548	1.107152
3	7	0	-0.244403	1.342104	-1.118323
4	15	0	1.208941	1.467353	-0.287532
5	6	0	0.583350	1.679573	2.535785
6	6	0	-0.590993	1.548699	-2.560202
7	6	0	0.619523	3.201672	2.751978
8	1	0	1.355539	3.662450	2.086502
9	1	0	-0.361840	3.639484	2.544447
10	1	0	0.891973	3.425329	3.788561
11	6	0	1.960669	1.058863	2.810036
12	1	0	2.241875	1.242692	3.851045
13	1	0	1.944977	-0.021458	2.636566
14	1	0	2.729445	1.509423	2.171539
15	6	0	-0.483160	1.029870	3.427270
16	1	0	-0.508417	-0.054355	3.282273
17	1	0	-0.250363	1.236492	4.476205
18	1	0	-1.477671	1.436819	3.213717
19	6	0	-1.967116	0.911007	-2.799729
20	1	0	-2.737830	1.398084	-2.191087
21	1	0	-2.246216	1.031409	-3.850463
22	1	0	-1.950851	-0.156913	-2.561255
23	6	0	-0.630457	3.056670	-2.858516
24	1	0	-1.369955	3.550773	-2.221436
25	1	0	0.349171	3.507816	-2.672250
26	1	0	-0.900201	3.223225	-3.906551
27	6	0	0.476347	0.853915	-3.416023

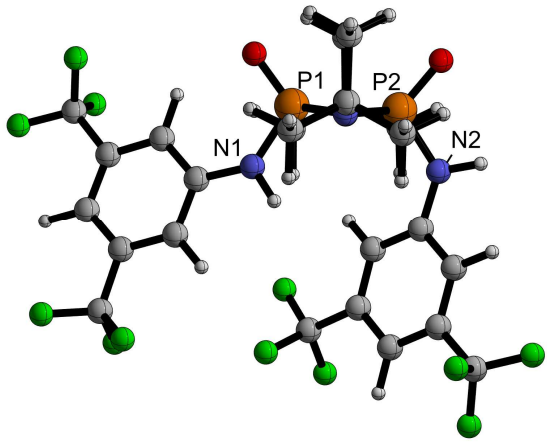
28	1	0	0.512600	-0.218831	-3.203827
29	1	0	0.235249	0.992467	-4.474201
30	1	0	1.468284	1.282440	-3.235316
31	7	0	-2.007849	0.037468	0.585492
32	1	0	-1.391962	-0.754641	0.743204
33	6	0	-3.357283	-0.311060	0.421334
34	6	0	-3.702808	-1.669790	0.512970
35	6	0	-4.367118	0.631481	0.183976
36	6	0	-5.028317	-2.065947	0.369986
37	1	0	-2.933279	-2.412213	0.700578
38	6	0	-5.686799	0.205847	0.036298
39	1	0	-4.118854	1.684009	0.129395
40	6	0	-6.041747	-1.137829	0.122917
41	1	0	-7.071764	-1.453845	0.012849
42	7	0	1.998937	0.007786	-0.525437
43	1	0	1.382363	-0.791644	-0.637007
44	6	0	3.353033	-0.328972	-0.379937
45	6	0	3.705468	-1.686993	-0.457619
46	6	0	4.360941	0.622633	-0.172454
47	6	0	5.035446	-2.073170	-0.330738
48	1	0	2.937652	-2.436464	-0.623163
49	6	0	5.685681	0.207029	-0.041988
50	1	0	4.107632	1.674425	-0.128673
51	6	0	6.047413	-1.135554	-0.114992
52	1	0	7.081140	-1.443732	-0.018310
53	8	0	-2.142870	2.633984	0.376484
54	8	0	2.137138	2.611411	-0.449604
55	6	0	-6.733804	1.247154	-0.263541
56	6	0	-5.371409	-3.531733	0.426387
57	6	0	5.387515	-3.537270	-0.372277
58	6	0	6.730843	1.259206	0.224570

59	9	0	-6.581588	2.365817	0.498217
60	9	0	-6.674098	1.662413	-1.565230
61	9	0	-7.997667	0.796642	-0.058592
62	9	0	-6.604462	-3.752713	0.954969
63	9	0	-5.379833	-4.098259	-0.818487
64	9	0	-4.485603	-4.248559	1.167400
65	9	0	5.433776	-4.082840	0.881033
66	9	0	4.487720	-4.272654	-1.077279
67	9	0	6.607704	-3.758317	-0.930161
68	9	0	7.994249	0.812357	0.009163
69	9	0	6.687419	1.696938	1.519517
70	9	0	6.561067	2.363576	-0.554285

“In-out”-conformantion

Electronic energy = -3182.2081798, thermal correction to Gibbs free energy = 0.407045 NIMAG = 0

1	15	0	-1.826010	2.831054	0.260602
2	7	0	-0.376969	2.403632	1.004801
3	7	0	-1.051605	2.338873	-1.170754
4	15	0	0.461771	2.168439	-0.459453
5	6	0	0.148827	2.738887	2.369182
6	6	0	-1.457755	2.530436	-2.602262
7	6	0	0.656365	4.189955	2.385161
8	1	0	1.455054	4.324459	1.650163
9	1	0	-0.159702	4.879418	2.148238
10	1	0	1.045977	4.435338	3.378534
11	6	0	1.288582	1.758643	2.678309
12	1	0	1.683925	1.961282	3.678004
13	1	0	0.939006	0.721996	2.646539
14	1	0	2.111456	1.874584	1.964205
15	6	0	-0.999006	2.560894	3.372554
16	1	0	-1.368786	1.531209	3.375876
17	1	0	-0.638396	2.802634	4.376712



18	1	0	-1.831622	3.233641	3.139527
19	6	0	-2.959005	2.229811	-2.707300
20	1	0	-3.544516	2.922162	-2.092280
21	1	0	-3.278228	2.352088	-3.746427
22	1	0	-3.175499	1.203995	-2.393928
23	6	0	-1.162458	3.980835	-3.019169
24	1	0	-1.718394	4.680372	-2.387812
25	1	0	-0.093614	4.196127	-2.923964
26	1	0	-1.459281	4.135226	-4.061570
27	6	0	-0.658881	1.546397	-3.467165
28	1	0	-0.877916	0.510274	-3.191190
29	1	0	-0.932351	1.690437	-4.516639
30	1	0	0.418775	1.717661	-3.371628
31	7	0	-3.042400	1.758000	0.682228
32	1	0	-3.954485	2.205110	0.656390
33	6	0	-3.075256	0.352186	0.623525
34	6	0	-4.236835	-0.281596	0.164680
35	6	0	-1.995765	-0.430376	1.059754
36	6	0	-4.312988	-1.673201	0.146922
37	1	0	-5.079399	0.313706	-0.173043
38	6	0	-2.092503	-1.819081	1.028715
39	1	0	-1.106759	0.045128	1.452851
40	6	0	-3.244722	-2.460108	0.570395
41	1	0	-3.312976	-3.541637	0.560124
42	7	0	0.852769	0.557560	-0.691400
43	1	0	0.052294	-0.052730	-0.824390
44	6	0	2.085903	-0.104864	-0.607275
45	6	0	2.099796	-1.495951	-0.798070
46	6	0	3.292498	0.557155	-0.344240
47	6	0	3.293733	-2.202561	-0.707767
48	1	0	1.176637	-2.020894	-1.018811

49	6	0	4.475944	-0.175831	-0.259229
50	1	0	3.305702	1.633617	-0.226893
51	6	0	4.500414	-1.557672	-0.430028
52	1	0	5.427511	-2.113181	-0.362219
53	8	0	-2.386254	4.198805	0.374900
54	8	0	1.618392	3.049026	-0.747141
55	6	0	5.744931	0.566508	0.071489
56	6	0	3.273750	-3.701224	-0.859386
57	6	0	-5.558593	-2.327482	-0.395017
58	6	0	-0.955560	-2.675507	1.526689
59	9	0	0.071291	-1.950381	2.036951
60	9	0	-0.434204	-3.451533	0.530307
61	9	0	-1.360238	-3.534095	2.503175
62	9	0	-5.728312	-3.589707	0.074453
63	9	0	-5.526199	-2.419648	-1.758200
64	9	0	-6.683117	-1.628899	-0.084723
65	9	0	3.120951	-4.330267	0.345180
66	9	0	2.254376	-4.132536	-1.648540
67	9	0	4.426132	-4.181056	-1.398207
68	9	0	6.862103	-0.151643	-0.209669
69	9	0	5.811336	0.886840	1.399465
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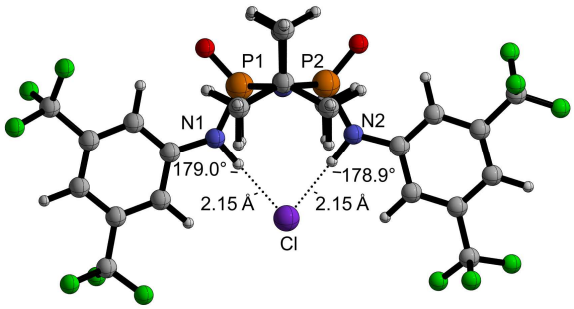
5•Cl

Electronic energy = -3642.6365135, thermal correction to Gibbs free energy = 0.398407 NIMAG = 0



1	15	0	1.250572	-1.664780	0.496252
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3	7	0	0.009912	-1.697182	-0.650488
4	15	0	-1.249397	-1.667162	0.475260
5	6	0	-0.021318	-1.577614	3.104958
6	6	0	0.025474	-1.911337	-2.123302
7	6	0	-0.014237	-3.048614	3.554526

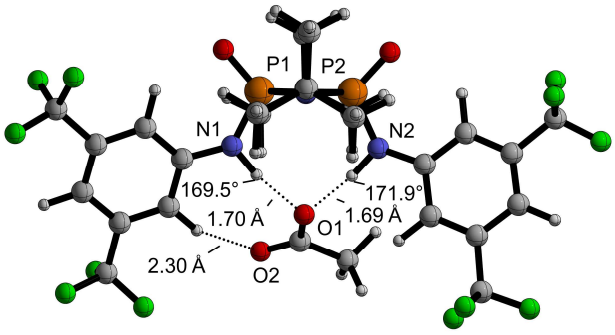
8	1	0	-0.895815	-3.570697	3.169391
9	1	0	0.881597	-3.557363	3.184794
10	1	0	-0.023311	-3.106601	4.648211
11	6	0	-1.289125	-0.866715	3.598959
12	1	0	-1.316709	-0.899073	4.692450
13	1	0	-1.299037	0.178088	3.275438
14	1	0	-2.191284	-1.361102	3.221543
15	6	0	1.226447	-0.847376	3.621268
16	1	0	1.226495	0.197018	3.296098
17	1	0	1.234261	-0.877821	4.715161
18	1	0	2.142806	-1.328573	3.261497
19	6	0	1.269110	-1.212800	-2.693801
20	1	0	2.187150	-1.635139	-2.268134
21	1	0	1.304476	-1.358191	-3.777778
22	1	0	1.245254	-0.139587	-2.482316
23	6	0	0.072343	-3.421173	-2.413562
24	1	0	0.970801	-3.864663	-1.973057
25	1	0	-0.806073	-3.917543	-1.989452
26	1	0	0.087554	-3.597159	-3.494441
27	6	0	-1.249911	-1.287176	-2.709220
28	1	0	-1.289915	-0.213674	-2.502009
29	1	0	-1.264600	-1.437487	-3.792930
30	1	0	-2.146261	-1.761098	-2.291942
31	7	0	2.005237	-0.178411	0.473543
32	1	0	1.359480	0.625926	0.610386
33	6	0	3.316382	0.179057	0.161906
34	6	0	3.633697	1.551276	0.164393
35	6	0	4.324644	-0.747153	-0.148053
36	6	0	4.925822	1.971068	-0.129022
37	1	0	2.857065	2.272310	0.401932
38	6	0	5.611868	-0.296101	-0.439739

39	1	0	4.100588	-1.806479	-0.144263
40	6	0	5.937665	1.058235	-0.438655
41	1	0	6.943691	1.393167	-0.660454
42	7	0	-2.004625	-0.181436	0.440470
43	1	0	-1.361014	0.622729	0.587602
44	6	0	-3.312441	0.177312	0.117082
45	6	0	-3.628485	1.548420	0.114264
46	6	0	-4.317104	-0.748841	-0.209971
47	6	0	-4.914413	1.970783	-0.207746
48	1	0	-2.852568	2.269932	0.354212
49	6	0	-5.595578	-0.295986	-0.530086
50	1	0	-4.091231	-1.807517	-0.213741
51	6	0	-5.921278	1.060059	-0.531525
52	1	0	-6.918429	1.396268	-0.787711
53	8	0	2.219795	-2.788193	0.547000
54	8	0	-2.217968	-2.791683	0.510855
55	17	0	-0.003755	2.268386	0.871154
56	6	0	-6.666425	-1.309622	-0.836253
57	6	0	-5.231135	3.441713	-0.156584
58	6	0	5.239725	3.442993	-0.163614
59	6	0	6.655362	-1.315348	-0.813420
60	9	0	-6.170682	-2.439931	-1.408405
61	9	0	-7.326836	-1.711544	0.293541
62	9	0	-7.617520	-0.823316	-1.679197
63	9	0	-6.255665	3.783740	-0.983424
64	9	0	-4.167674	4.217260	-0.500548
65	9	0	-5.603276	3.839444	1.099260
66	9	0	5.211566	3.939715	-1.438832
67	9	0	4.362194	4.188126	0.557148
68	9	0	6.483740	3.716099	0.320253
69	9	0	7.923376	-0.858483	-0.638126

70	9	0	6.557440	-1.684697	-2.128161
71	9	0	6.544642	-2.463486	-0.089769

5•OAc “one-atom”-mode

Electronic energy = -3410.9937424, thermal correction to Gibbs free energy = 0.445459 NIMAG = 0



1	15	0	1.301317	-1.749628	0.673049
2	7	0	-0.030411	-1.554292	1.686079
3	7	0	0.139724	-1.921755	-0.545810
4	15	0	-1.195020	-1.784777	0.479999
5	6	0	-0.155795	-1.479680	3.171380
6	6	0	0.260200	-2.233450	-1.994627
7	6	0	-0.236111	-2.908970	3.734252
8	1	0	-1.104787	-3.431656	3.321799
9	1	0	0.665843	-3.471906	3.473510
10	1	0	-0.328948	-2.880186	4.825201
11	6	0	-1.429039	-0.690569	3.510335
12	1	0	-1.534723	-0.629538	4.598134
13	1	0	-1.382084	0.322790	3.100949
14	1	0	-2.319457	-1.189454	3.111143
15	6	0	1.076541	-0.751605	3.725201
16	1	0	1.133750	0.267530	3.334383
17	1	0	1.008261	-0.706761	4.816453
18	1	0	1.999302	-1.280908	3.462262
19	6	0	1.536232	-1.563149	-2.526228
20	1	0	2.423817	-1.936963	-2.002007
21	1	0	1.653721	-1.791213	-3.590041
22	1	0	1.487614	-0.477027	-2.402884
23	6	0	0.337916	-3.759506	-2.172459
24	1	0	1.207136	-4.158412	-1.640249
25	1	0	-0.563767	-4.233676	-1.772340
26	1	0	0.427476	-4.014628	-3.233954
27	6	0	-0.973534	-1.666931	-2.713173

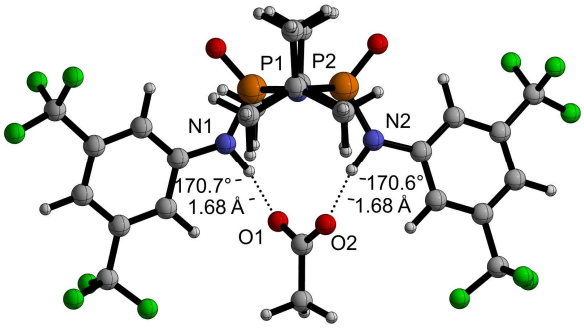
28	1	0	-1.044537	-0.584571	-2.570571
29	1	0	-0.901761	-1.878292	-3.784414
30	1	0	-1.893285	-2.131536	-2.339379
31	7	0	2.005623	-0.241270	0.576457
32	1	0	1.300751	0.540775	0.582109
33	6	0	3.276484	0.123525	0.136768
34	6	0	3.463756	1.452779	-0.285126
35	6	0	4.376666	-0.750854	0.111318
36	6	0	4.715596	1.890064	-0.705427
37	1	0	2.618226	2.132853	-0.277908
38	6	0	5.617568	-0.288209	-0.323694
39	1	0	4.254265	-1.776722	0.436837
40	6	0	5.813549	1.029206	-0.737962
41	1	0	6.786297	1.374709	-1.064620
42	7	0	-1.922337	-0.306390	0.260447
43	1	0	-1.272242	0.511380	0.404594
44	6	0	-3.237552	0.020659	-0.059226
45	6	0	-3.627617	1.364136	0.099856
46	6	0	-4.175038	-0.904553	-0.547824
47	6	0	-4.918480	1.759212	-0.236413
48	1	0	-2.909165	2.074079	0.507019
49	6	0	-5.463674	-0.479660	-0.869185
50	1	0	-3.894073	-1.942581	-0.673925
51	6	0	-5.860338	0.849003	-0.721507
52	1	0	-6.861961	1.166188	-0.984354
53	8	0	2.297498	-2.833346	0.873625
54	8	0	-2.172385	-2.901264	0.555567
55	6	0	-6.458588	-1.500643	-1.351427
56	6	0	-5.321464	3.191578	-0.010948
57	6	0	4.858772	3.308959	-1.186963
58	6	0	6.763143	-1.263691	-0.381471

59	9	0	-5.880750	-2.482209	-2.097916
60	9	0	-7.086590	-2.134563	-0.312584
61	9	0	-7.443633	-0.953605	-2.113838
62	9	0	-6.325055	3.588853	-0.840836
63	9	0	-4.291244	4.061234	-0.192071
64	9	0	-5.776302	3.400462	1.263935
65	9	0	4.459939	3.448188	-2.488889
66	9	0	4.101590	4.181179	-0.464897
67	9	0	6.140925	3.756012	-1.129661
68	9	0	7.976370	-0.650343	-0.368014
69	9	0	6.728607	-2.022854	-1.520245
70	9	0	6.752254	-2.142515	0.658609
71	6	0	-0.174347	2.523086	1.507372
72	8	0	0.005222	1.623189	0.597844
73	8	0	-1.293541	2.906175	1.912051
74	6	0	1.094489	3.154906	2.084009
75	1	0	0.872843	3.722422	2.990130
76	1	0	1.847488	2.390181	2.300602
77	1	0	1.525990	3.834711	1.339573

5•OAc “two-atom”-mode

Electronic energy = -3410.9938991, thermal correction to Gibbs free energy = 0.441993 NIMAG = 0

1	15	0	1.228669	-1.781961	-0.238351
2	7	0	0.204943	-1.727057	1.117892
3	7	0	-0.201917	-1.722304	-1.115606
4	15	0	-1.225444	-1.786232	0.240635
5	6	0	0.502950	-1.851889	2.572644
6	6	0	-0.497617	-1.859112	-2.569730
7	6	0	0.652478	-3.340550	2.930228
8	1	0	-0.276570	-3.878106	2.715245
9	1	0	1.460458	-3.792330	2.346615
10	1	0	0.882799	-3.451577	3.995378



11	6	0	-0.650744	-1.219332	3.364072
12	1	0	-0.441512	-1.305804	4.434861
13	1	0	-0.763602	-0.161816	3.109112
14	1	0	-1.596989	-1.733331	3.160379
15	6	0	1.809747	-1.094813	2.854473
16	1	0	1.717104	-0.042224	2.570816
17	1	0	2.043861	-1.155002	3.921761
18	1	0	2.647839	-1.536103	2.302667
19	6	0	0.631312	-1.186078	-3.363712
20	1	0	1.595176	-1.668265	-3.165201
21	1	0	0.421237	-1.275956	-4.434102
22	1	0	0.709582	-0.126203	-3.105277
23	6	0	-0.595484	-3.352413	-2.925870
24	1	0	0.351920	-3.857080	-2.711257
25	1	0	-1.386379	-3.831112	-2.340237
26	1	0	-0.823382	-3.472776	-3.990533
27	6	0	-1.831010	-1.148934	-2.848964
28	1	0	-1.774851	-0.092633	-2.569261
29	1	0	-2.066458	-1.220068	-3.915183
30	1	0	-2.650974	-1.617914	-2.292934
31	7	0	1.967138	-0.310001	-0.469964
32	1	0	1.307310	0.495110	-0.649406
33	6	0	3.305467	0.051775	-0.331462
34	6	0	3.643854	1.403910	-0.542728
35	6	0	4.328723	-0.847124	0.014185
36	6	0	4.959492	1.829282	-0.402537
37	1	0	2.859707	2.105842	-0.807089
38	6	0	5.640443	-0.391731	0.146067
39	1	0	4.093630	-1.891887	0.175716
40	6	0	5.983750	0.942720	-0.059079
41	1	0	7.005224	1.284336	0.054083

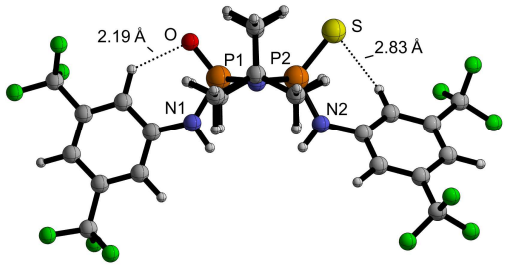
42	7	0	-1.966256	-0.316647	0.479321
43	1	0	-1.306945	0.488081	0.665148
44	6	0	-3.303714	0.046000	0.335805
45	6	0	-3.641492	1.398991	0.542882
46	6	0	-4.326742	-0.852859	-0.010423
47	6	0	-4.956155	1.825373	0.396728
48	1	0	-2.857599	2.100465	0.809525
49	6	0	-5.637454	-0.396420	-0.148478
50	1	0	-4.091978	-1.898380	-0.167551
51	6	0	-5.980012	0.939011	0.051489
52	1	0	-7.000654	1.281435	-0.066444
53	8	0	2.178108	-2.920467	-0.349926
54	8	0	-2.172163	-2.927666	0.346163
55	6	0	-6.702665	-1.404451	-0.488138
56	6	0	-5.293684	3.267417	0.664731
57	6	0	5.297662	3.270270	-0.675419
58	6	0	6.706273	-1.399663	0.484083
59	9	0	-6.295090	-2.287109	-1.443876
60	9	0	-7.055154	-2.160033	0.597390
61	9	0	-7.846956	-0.831144	-0.944262
62	9	0	-6.317403	3.714363	-0.113944
63	9	0	-4.241848	4.103344	0.453294
64	9	0	-5.686757	3.467684	1.961051
65	9	0	5.691259	3.465782	-1.972348
66	9	0	4.246335	4.107395	-0.467054
67	9	0	6.321572	3.719326	0.101907
68	9	0	7.849283	-0.826270	0.943496
69	9	0	7.061345	-2.151280	-0.603409
70	9	0	6.298608	-2.285832	1.436381
71	6	0	-0.007158	2.501200	0.012824
72	8	0	0.482950	1.920131	-1.005365

73	8	0	-0.482052	1.905476	1.031017
74	6	0	-0.059859	4.027975	0.010505
75	1	0	-1.082085	4.341929	-0.234792
76	1	0	0.174148	4.418787	1.004955
77	1	0	0.622586	4.450389	-0.730557

O/S-cyclodiphosph(V)azane 14

“In-in” conformation

Electronic energy = -3505.1507168, thermal correction to Gibbs free energy = 0.400292 NIMAG = 0



1	15	0	-1.305707	1.126205	0.814506
2	7	0	0.024618	0.631827	1.725133
3	7	0	-0.159374	1.483628	-0.374622
4	15	0	1.190469	1.209512	0.618020
5	6	0	0.138326	0.332896	3.191439
6	6	0	-0.319758	2.203742	-1.674775
7	6	0	0.136438	1.647158	3.990125
8	1	0	0.988966	2.270507	3.705751
9	1	0	-0.785686	2.206234	3.804019
10	1	0	0.203206	1.428180	5.060920
11	6	0	1.446187	-0.437295	3.418373
12	1	0	1.559218	-0.644993	4.486535
13	1	0	1.439560	-1.389467	2.879310
14	1	0	2.311778	0.150809	3.093679
15	6	0	-1.064674	-0.535373	3.585707
16	1	0	-1.079664	-1.469037	3.015655
17	1	0	-0.997059	-0.776364	4.650903
18	1	0	-2.008282	-0.004439	3.418240
19	6	0	-1.612730	1.690986	-2.326335
20	1	0	-2.484486	1.912651	-1.699092
21	1	0	-1.758069	2.192516	-3.287804
22	1	0	-1.565004	0.611170	-2.496317

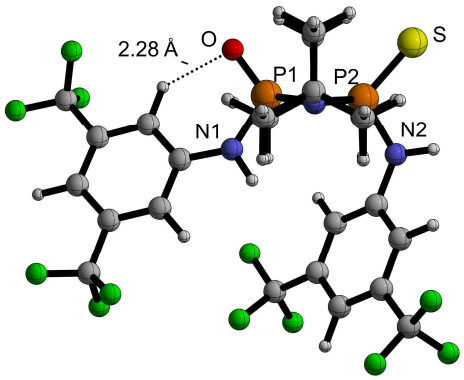
23	6	0	-0.408673	3.717222	-1.417673
24	1	0	-1.264657	3.943810	-0.774911
25	1	0	0.501533	4.073528	-0.926548
26	1	0	-0.529242	4.249793	-2.366789
27	6	0	0.889443	1.872718	-2.559099
28	1	0	0.981515	0.793311	-2.711589
29	1	0	0.770069	2.357923	-3.532307
30	1	0	1.814238	2.248886	-2.108661
31	7	0	-2.142846	-0.271885	0.419967
32	1	0	-1.555068	-1.083125	0.253464
33	6	0	-3.491960	-0.474356	0.093579
34	6	0	-3.874537	-1.752223	-0.347412
35	6	0	-4.466290	0.529266	0.192728
36	6	0	-5.200506	-2.011976	-0.677555
37	1	0	-3.134284	-2.542566	-0.424204
38	6	0	-5.787316	0.242186	-0.148142
39	1	0	-4.189651	1.514147	0.546255
40	6	0	-6.178410	-1.020192	-0.589014
41	1	0	-7.210106	-1.229299	-0.844458
42	7	0	1.989396	-0.166987	0.068489
43	1	0	1.434451	-1.014339	0.154094
44	6	0	3.358971	-0.403079	-0.157062
45	6	0	3.898146	-1.641606	0.218043
46	6	0	4.183230	0.538795	-0.783814
47	6	0	5.239639	-1.923102	-0.029215
48	1	0	3.268676	-2.383856	0.698343
49	6	0	5.528228	0.243597	-1.002227
50	1	0	3.776775	1.486233	-1.110753
51	6	0	6.076327	-0.982103	-0.629360
52	1	0	7.119323	-1.205092	-0.817792
53	8	0	-2.232071	2.188815	1.273119

54	16	0	2.391735	2.658149	1.059844
55	6	0	-6.803000	1.353455	-0.080800
56	6	0	-5.581685	-3.376335	-1.189694
57	6	0	6.401969	1.291691	-1.640861
58	6	0	5.809511	-3.244180	0.417402
59	9	0	-6.565761	2.214008	0.945413
60	9	0	-6.802176	2.108577	-1.221535
61	9	0	-8.071787	0.891617	0.072703
62	9	0	-6.837058	-3.736520	-0.810768
63	9	0	-5.563350	-3.427968	-2.556215
64	9	0	-4.739854	-4.352219	-0.757982
65	9	0	4.886724	-4.242742	0.392416
66	9	0	6.279521	-3.186610	1.700036
67	9	0	6.852871	-3.644982	-0.355685
68	9	0	7.507573	0.762443	-2.226136
69	9	0	6.846547	2.206260	-0.727401
70	9	0	5.742918	1.999114	-2.598757

“In-out-S” conformation

Electronic energy = -3505.1575086, thermal correction to Gibbs free energy = 0.404027 NIMAG = 0

1	15	0	-2.135526	-2.569332	-0.109388
2	7	0	-0.665100	-2.373531	-0.930261
3	7	0	-1.247534	-2.012076	1.240161
4	15	0	0.246576	-2.061540	0.469942
5	6	0	-0.207446	-2.884568	-2.265329
6	6	0	-1.596431	-1.977798	2.698928
7	6	0	0.178447	-4.368576	-2.153405
8	1	0	0.978729	-4.500270	-1.419422
9	1	0	-0.684358	-4.965695	-1.844253
10	1	0	0.527804	-4.731995	-3.125391
11	6	0	1.007692	-2.042481	-2.680656
12	1	0	1.360057	-2.373185	-3.662061



13	1	0	0.753825	-0.979885	-2.742159
14	1	0	1.833549	-2.165781	-1.970991
15	6	0	-1.355097	-2.698308	-3.267002
16	1	0	-1.629981	-1.643924	-3.366954
17	1	0	-1.037773	-3.067226	-4.246813
18	1	0	-2.239972	-3.264660	-2.958399
19	6	0	-3.059593	-1.532939	2.826055
20	1	0	-3.731167	-2.239212	2.325934
21	1	0	-3.333456	-1.497913	3.884572
22	1	0	-3.203607	-0.536423	2.397678
23	6	0	-1.396263	-3.376870	3.303450
24	1	0	-2.043559	-4.104093	2.805281
25	1	0	-0.355982	-3.696837	3.188920
26	1	0	-1.642610	-3.357808	4.370066
27	6	0	-0.675232	-0.958961	3.384513
28	1	0	-0.806224	0.040340	2.958525
29	1	0	-0.922242	-0.917181	4.449558
30	1	0	0.377439	-1.247740	3.292588
31	7	0	-3.213544	-1.379484	-0.616173
32	1	0	-4.178761	-1.680528	-0.513420
33	6	0	-3.024137	0.020047	-0.624925
34	6	0	-3.994162	0.849370	-0.048225
35	6	0	-1.902502	0.598086	-1.232995
36	6	0	-3.829907	2.233107	-0.072012
37	1	0	-4.866612	0.412621	0.426603
38	6	0	-1.752319	1.983396	-1.236255
39	1	0	-1.165449	-0.031365	-1.713187
40	6	0	-2.708296	2.818247	-0.657200
41	1	0	-2.582453	3.894698	-0.661850
42	7	0	0.795491	-0.480108	0.479172
43	1	0	0.055805	0.215369	0.510170

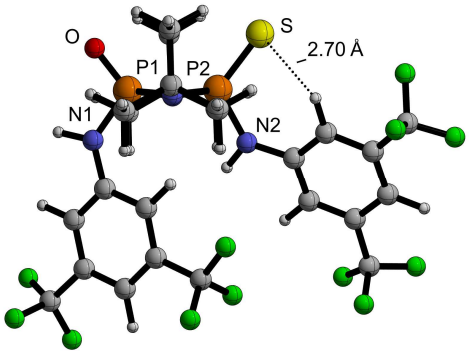
44	6	0	2.093789	0.048490	0.479360
45	6	0	2.240537	1.431255	0.673622
46	6	0	3.238419	-0.736351	0.286607
47	6	0	3.505217	2.009833	0.658667
48	1	0	1.365754	2.051354	0.841468
49	6	0	4.495393	-0.132276	0.285575
50	1	0	3.145447	-1.807684	0.159135
51	6	0	4.652849	1.240372	0.462052
52	1	0	5.635256	1.695509	0.458653
53	16	0	-3.074187	-4.261481	-0.064195
54	8	0	1.325836	-3.007418	0.838271
55	6	0	5.699810	-1.004328	0.040926
56	6	0	3.627984	3.503551	0.808903
57	6	0	-0.568372	2.607918	-1.931232
58	6	0	-4.902025	3.112172	0.522044
59	9	0	5.639228	-2.172333	0.738510
60	9	0	5.813061	-1.353298	-1.276392
61	9	0	6.865235	-0.397782	0.382318
62	9	0	4.822387	3.874911	1.339965
63	9	0	3.524815	4.143303	-0.395326
64	9	0	2.657168	4.027945	1.604094
65	9	0	0.423378	1.711165	-2.176571
66	9	0	-0.020343	3.614929	-1.196819
67	9	0	-0.913616	3.150389	-3.132801
68	9	0	-5.851945	3.442106	-0.401880
69	9	0	-4.402755	4.281724	0.998896
70	9	0	-5.555527	2.506685	1.548151

“In-S-out” conformation

Electronic energy = -3505.155317, thermal correction to Gibbs free energy = 0.403134 NIMAG = 0

1	15	0	1.887844	-2.786160	0.042478
2	7	0	0.473814	-2.459766	0.897989

3	7	0	1.017114	-2.226379	-1.300578
4	15	0	-0.477176	-2.170613	-0.498263
5	6	0	0.092753	-2.831182	2.301241
6	6	0	1.343075	-2.337724	-2.762079
7	6	0	-0.285639	-4.319717	2.366351
8	1	0	-1.137002	-4.528559	1.712853
9	1	0	0.558667	-4.941512	2.053772
10	1	0	-0.556447	-4.585282	3.393542
11	6	0	-1.092565	-1.949579	2.715734
12	1	0	-1.353894	-2.158711	3.757070
13	1	0	-0.848521	-0.886591	2.624697
14	1	0	-1.972249	-2.165627	2.101077
15	6	0	1.304241	-2.550433	3.202306
16	1	0	1.588225	-1.494182	3.172368
17	1	0	1.048550	-2.810488	4.233720
18	1	0	2.166799	-3.155962	2.903780
19	6	0	2.811357	-1.923648	-2.936415
20	1	0	3.480577	-2.606218	-2.400979
21	1	0	3.071597	-1.962598	-3.998301
22	1	0	2.977536	-0.905081	-2.572468
23	6	0	1.129686	-3.786580	-3.230047
24	1	0	1.760997	-4.470168	-2.654715
25	1	0	0.084367	-4.081161	-3.099590
26	1	0	1.390220	-3.874447	-4.289876
27	6	0	0.427618	-1.378593	-3.534500
28	1	0	0.601942	-0.339432	-3.238234
29	1	0	0.637185	-1.470058	-4.604356
30	1	0	-0.628059	-1.622016	-3.372869
31	7	0	3.104831	-1.711531	0.455639
32	1	0	4.019696	-2.150060	0.403482
33	6	0	3.122982	-0.309286	0.522119

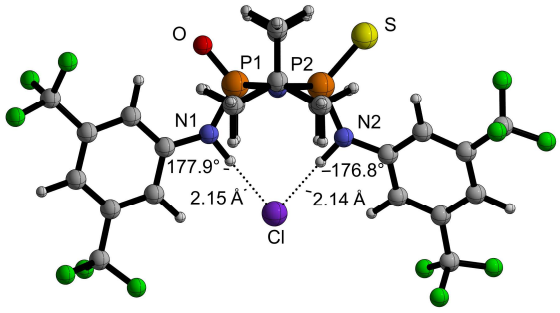


34	6	0	4.305397	0.368889	0.195114
35	6	0	2.006691	0.428993	0.941207
36	6	0	4.361637	1.757738	0.286301
37	1	0	5.175605	-0.189568	-0.134927
38	6	0	2.085006	1.817122	1.020738
39	1	0	1.098859	-0.081637	1.233536
40	6	0	3.256232	2.501600	0.695045
41	1	0	3.307300	3.582104	0.762655
42	7	0	-0.871279	-0.538278	-0.597916
43	1	0	-0.074724	0.031712	-0.869559
44	6	0	-2.075465	0.173481	-0.500161
45	6	0	-2.080209	1.502521	-0.954940
46	6	0	-3.248778	-0.360096	0.043947
47	6	0	-3.233115	2.272007	-0.859331
48	1	0	-1.178523	1.931454	-1.379091
49	6	0	-4.398258	0.428011	0.114988
50	1	0	-3.276201	-1.383088	0.394538
51	6	0	-4.412531	1.748175	-0.324933
52	1	0	-5.311324	2.349145	-0.260488
53	6	0	-5.630142	-0.176794	0.737524
54	6	0	-3.202208	3.713101	-1.296974
55	6	0	0.891947	2.620709	1.472550
56	6	0	5.658266	2.461581	-0.024285
57	9	0	-5.839806	-1.456678	0.321516
58	9	0	-5.533767	-0.230712	2.100371
59	9	0	-6.758058	0.523176	0.455814
60	9	0	-4.371182	4.100172	-1.874978
61	9	0	-2.998509	4.557363	-0.241041
62	9	0	-2.211507	3.968696	-2.190716
63	9	0	-0.128040	1.845735	1.922080
64	9	0	0.386866	3.386786	0.460049

65	9	0	1.211041	3.481747	2.477359
66	9	0	6.456758	2.558424	1.080156
67	9	0	5.463712	3.728933	-0.472538
68	9	0	6.386696	1.810152	-0.969331
69	16	0	-1.950036	-3.355775	-0.892277
70	8	0	2.491539	-4.140275	0.035995

14•Cl

Electronic energy = -3965.5838615, thermal correction to Gibbs free energy = 0.397686 NIMAG = 0



1	15	0	1.187527	-1.645561	0.647141
2	7	0	-0.030753	-1.317774	1.786691
3	7	0	-0.115973	-1.795373	-0.430348
4	15	0	-1.320643	-1.572936	0.734247
5	6	0	0.016072	-1.196401	3.276720
6	6	0	-0.199447	-2.211062	-1.857844
7	6	0	-0.028146	-2.603482	3.894936
8	1	0	-0.950014	-3.116991	3.603561
9	1	0	0.824724	-3.196765	3.551838
10	1	0	0.005433	-2.533840	4.987378
11	6	0	-1.198228	-0.369224	3.722617
12	1	0	-1.182649	-0.270879	4.812614
13	1	0	-1.169023	0.627808	3.273467
14	1	0	-2.136944	-0.858677	3.439262
15	6	0	1.311068	-0.467378	3.661583
16	1	0	1.338029	0.528308	3.209358
17	1	0	1.353456	-0.363644	4.750271
18	1	0	2.193960	-1.030002	3.338753
19	6	0	1.050076	-1.695980	-2.586008
20	1	0	1.955793	-2.157707	-2.178009
21	1	0	0.988390	-1.958417	-3.646530
22	1	0	1.134818	-0.608942	-2.495641
23	6	0	-0.280295	-3.744763	-1.936928

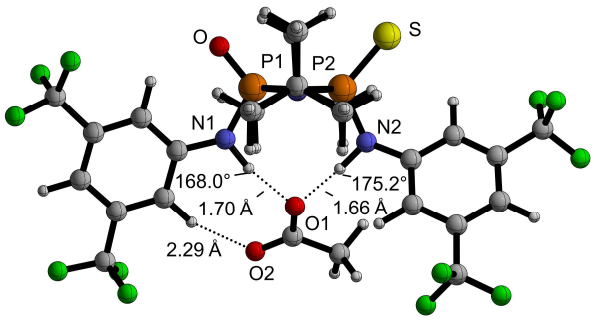
24	1	0	0.605588	-4.192924	-1.476787
25	1	0	-1.168881	-4.105280	-1.409498
26	1	0	-0.336627	-4.065712	-2.982616
27	6	0	-1.461344	-1.571675	-2.457360
28	1	0	-1.412294	-0.480093	-2.400036
29	1	0	-1.554985	-1.865789	-3.507118
30	1	0	-2.361619	-1.912284	-1.932399
31	7	0	1.926647	-0.166416	0.406283
32	1	0	1.292691	0.638078	0.607872
33	6	0	3.223825	0.214351	0.055346
34	6	0	3.605172	1.539234	0.339059
35	6	0	4.143478	-0.628547	-0.584695
36	6	0	4.874722	1.991742	-0.003219
37	1	0	2.893594	2.200445	0.824560
38	6	0	5.416061	-0.154264	-0.902954
39	1	0	3.874248	-1.649194	-0.822361
40	6	0	5.803841	1.154486	-0.625134
41	1	0	6.794705	1.510826	-0.878258
42	7	0	-2.036551	-0.077107	0.558625
43	1	0	-1.373774	0.719316	0.653220
44	6	0	-3.316253	0.278242	0.134546
45	6	0	-3.577753	1.644662	-0.078146
46	6	0	-4.343788	-0.650941	-0.096281
47	6	0	-4.832913	2.057962	-0.512095
48	1	0	-2.783586	2.366950	0.087612
49	6	0	-5.591114	-0.207446	-0.533006
50	1	0	-4.159024	-1.705983	0.063387
51	6	0	-5.862127	1.143479	-0.744592
52	1	0	-6.834557	1.472403	-1.089562
53	8	0	-2.318768	-2.653159	0.940223
54	17	0	0.022669	2.332375	0.915658

55	16	0	2.413827	-3.130507	0.880004
56	6	0	5.236216	3.428428	0.264451
57	6	0	6.358349	-1.083719	-1.620656
58	6	0	-6.682248	-1.225324	-0.735042
59	6	0	-5.096441	3.529429	-0.691822
60	9	0	6.571605	3.601077	0.458942
61	9	0	4.892843	4.242362	-0.780899
62	9	0	4.607376	3.931467	1.360271
63	9	0	6.053038	-1.190324	-2.950667
64	9	0	6.315349	-2.350778	-1.121819
65	9	0	7.652272	-0.675855	-1.554939
66	9	0	-6.209085	-2.407312	-1.217481
67	9	0	-7.326023	-1.523057	0.435611
68	9	0	-7.641126	-0.800298	-1.600368
69	9	0	-6.050684	3.775856	-1.629893
70	9	0	-3.984910	4.218163	-1.066039
71	9	0	-5.537035	4.113730	0.464746

14•OAc “one-binding”-mode 1

Electronic energy = -3733.9411619, thermal correction to Gibbs free energy = 0.442134 NIMAG = 0

1	15	0	1.260731	-1.814295	0.210666
2	7	0	-0.065815	-1.807236	1.265963
3	7	0	0.063311	-1.667661	-0.991772
4	15	0	-1.251793	-1.774770	0.059639
5	6	0	-0.175118	-2.063559	2.731721
6	6	0	0.141820	-1.644664	-2.478001
7	6	0	-0.316274	-3.576802	2.969974
8	1	0	-1.201847	-3.959568	2.453165
9	1	0	0.563995	-4.104834	2.590781
10	1	0	-0.416725	-3.782252	4.041148
11	6	0	-1.413556	-1.317559	3.251861
12	1	0	-1.507586	-1.484742	4.329492



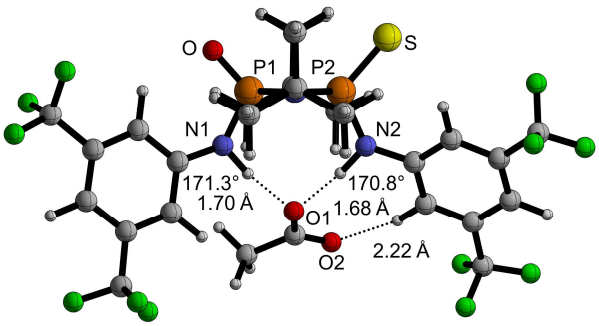
13	1	0	-1.329243	-0.242674	3.065843
14	1	0	-2.327281	-1.685255	2.771514
15	6	0	1.086817	-1.522185	3.417623
16	1	0	1.185118	-0.445218	3.256843
17	1	0	1.020939	-1.713564	4.493132
18	1	0	1.986707	-2.017401	3.036603
19	6	0	1.435268	-0.921253	-2.882674
20	1	0	2.315680	-1.437326	-2.482795
21	1	0	1.518005	-0.905747	-3.973736
22	1	0	1.435484	0.110140	-2.517635
23	6	0	0.137143	-3.087483	-3.012039
24	1	0	1.000607	-3.638488	-2.627632
25	1	0	-0.774952	-3.604668	-2.697809
26	1	0	0.179940	-3.083711	-4.106598
27	6	0	-1.077429	-0.873128	-3.006481
28	1	0	-1.089644	0.150059	-2.619619
29	1	0	-1.037008	-0.837400	-4.099530
30	1	0	-2.012673	-1.368099	-2.719904
31	7	0	1.975653	-0.325142	0.443183
32	1	0	1.241630	0.439208	0.499446
33	6	0	3.249146	0.153245	0.113393
34	6	0	3.340884	1.449017	-0.419933
35	6	0	4.431517	-0.565187	0.350257
36	6	0	4.584737	2.005260	-0.709746
37	1	0	2.430518	2.015089	-0.590966
38	6	0	5.662505	0.003416	0.030185
39	1	0	4.381515	-1.552422	0.790419
40	6	0	5.762924	1.289428	-0.503994
41	1	0	6.727359	1.724419	-0.735247
42	7	0	-1.995449	-0.291830	0.152615
43	1	0	-1.326890	0.497085	0.355521

44	6	0	-3.330160	0.074614	-0.004743
45	6	0	-3.690085	1.388505	0.346518
46	6	0	-4.320823	-0.786911	-0.508818
47	6	0	-5.004887	1.819026	0.184370
48	1	0	-2.930417	2.050459	0.762499
49	6	0	-5.628026	-0.328292	-0.653859
50	1	0	-4.061538	-1.801899	-0.781319
51	6	0	-5.996705	0.974501	-0.313889
52	1	0	-7.015997	1.317988	-0.437625
53	8	0	-2.218972	-2.894400	-0.081331
54	16	0	2.487780	-3.318207	0.123103
55	6	0	-0.099635	2.347025	1.602222
56	6	0	1.220774	2.789214	2.235549
57	1	0	1.867465	1.924938	2.419625
58	1	0	1.751497	3.447175	1.537531
59	1	0	1.048927	3.327660	3.169662
60	8	0	0.000994	1.530456	0.603823
61	8	0	-1.181321	2.788773	2.044529
62	6	0	6.915753	-0.804042	0.241560
63	6	0	4.629411	3.391435	-1.294515
64	6	0	-5.333125	3.235478	0.573413
65	6	0	-6.678450	-1.285563	-1.148872
66	9	0	6.795943	-1.702411	1.255311
67	9	0	7.249955	-1.526018	-0.872365
68	9	0	7.994843	-0.025441	0.527066
69	9	0	5.870237	3.941447	-1.251649
70	9	0	3.791642	4.249539	-0.645335
71	9	0	4.242587	3.406131	-2.606396
72	9	0	-4.591239	4.145227	-0.125816
73	9	0	-5.076641	3.478211	1.893306
74	9	0	-6.637119	3.554982	0.365557

75	9	0	-7.696940	-0.655705	-1.795754
76	9	0	-6.178989	-2.214612	-2.008907
77	9	0	-7.255188	-1.987839	-0.123864

14•OAc “one-binding”-mode 2

Electronic energy = -3733.9419828, thermal correction to Gibbs free energy = 0.444502 NIMAG = 0



1	15	0	1.158186	-1.733833	0.588238
2	7	0	-0.007668	-1.369345	1.775829
3	7	0	-0.199980	-1.949275	-0.408102
4	15	0	-1.347333	-1.646724	0.797862
5	6	0	0.126306	-1.156222	3.247716
6	6	0	-0.357919	-2.428981	-1.808019
7	6	0	0.170005	-2.524830	3.948455
8	1	0	-0.752689	-3.081189	3.754295
9	1	0	1.015477	-3.113035	3.579282
10	1	0	0.277201	-2.390419	5.030222
11	6	0	-1.087174	-0.347153	3.726695
12	1	0	-1.015636	-0.200185	4.808851
13	1	0	-1.118473	0.631054	3.240314
14	1	0	-2.024033	-0.874651	3.515032
15	6	0	1.417276	-0.366791	3.509893
16	1	0	1.391446	0.604776	3.007676
17	1	0	1.524442	-0.206025	4.587437
18	1	0	2.295014	-0.921853	3.160708
19	6	0	0.852489	-1.956924	-2.626258
20	1	0	1.777594	-2.400541	-2.242477
21	1	0	0.734303	-2.273891	-3.667004
22	1	0	0.944400	-0.867224	-2.597023
23	6	0	-0.447021	-3.964764	-1.813412
24	1	0	0.461904	-4.397539	-1.384218
25	1	0	-1.306239	-4.297456	-1.222696
26	1	0	-0.562737	-4.331633	-2.839051

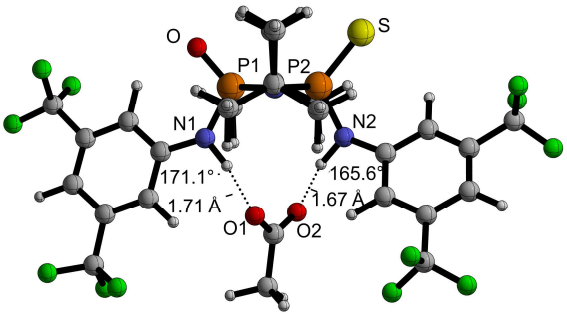
27	6	0	-1.648050	-1.813840	-2.372455
28	1	0	-1.592553	-0.720944	-2.375429
29	1	0	-1.798481	-2.161367	-3.399122
30	1	0	-2.520055	-2.120550	-1.782484
31	7	0	1.869449	-0.274089	0.223822
32	1	0	1.219726	0.549388	0.381736
33	6	0	3.183590	0.074903	-0.097613
34	6	0	3.618661	1.362929	0.262954
35	6	0	4.064278	-0.769557	-0.789637
36	6	0	4.907213	1.778283	-0.063455
37	1	0	2.934149	2.017360	0.803917
38	6	0	5.355358	-0.334216	-1.087386
39	1	0	3.746249	-1.759864	-1.088472
40	6	0	5.797820	0.940546	-0.737546
41	1	0	6.801110	1.269033	-0.977825
42	7	0	-2.035905	-0.145431	0.566322
43	1	0	-1.324267	0.627003	0.525895
44	6	0	-3.300092	0.196042	0.090096
45	6	0	-3.472070	1.488756	-0.438438
46	6	0	-4.405036	-0.671575	0.118297
47	6	0	-4.715843	1.899214	-0.906622
48	1	0	-2.620556	2.159893	-0.480679
49	6	0	-5.636581	-0.238949	-0.371176
50	1	0	-4.290157	-1.672314	0.516817
51	6	0	-5.819408	1.044785	-0.884481
52	1	0	-6.784407	1.367667	-1.254681
53	8	0	-2.354315	-2.695409	1.104038
54	16	0	2.403087	-3.204985	0.837593
55	6	0	0.149527	2.648074	1.385860
56	6	0	-1.129266	3.376036	1.804712
57	1	0	-1.497079	3.972629	0.961681

58	1	0	-1.915371	2.657963	2.061265
59	1	0	-0.943984	4.037987	2.652860
60	8	0	-0.002368	1.694516	0.527132
61	8	0	1.248500	3.004145	1.863687
62	6	0	6.253632	-1.262089	-1.859562
63	6	0	5.321929	3.176684	0.307445
64	6	0	-4.847335	3.272724	-1.508217
65	6	0	-6.809343	-1.179387	-0.283317
66	9	0	6.205584	-2.540294	-1.387438
67	9	0	5.898468	-1.335514	-3.179940
68	9	0	7.557012	-0.880190	-1.833324
69	9	0	6.667528	3.362212	0.245697
70	9	0	4.934605	3.515721	1.569030
71	9	0	4.765259	4.111838	-0.522786
72	9	0	-4.489253	3.287953	-2.829184
73	9	0	-4.053131	4.189676	-0.890022
74	9	0	-6.119746	3.748322	-1.452249
75	9	0	-7.803966	-0.861238	-1.153813
76	9	0	-6.459667	-2.470839	-0.536374
77	9	0	-7.374022	-1.176221	0.963633

14•OAc “two-binding”-mode

Electronic energy = -3733.9400984, thermal correction to Gibbs free energy = 0.441883 NIMAG = 0

1	15	0	-1.248528	-1.849750	0.086837
2	7	0	0.227883	-2.047161	-0.708067
3	7	0	-0.260461	-1.394775	1.411508
4	15	0	1.198241	-1.689765	0.639169
5	6	0	0.585486	-2.652056	-2.023422
6	6	0	-0.598241	-1.061886	2.825144
7	6	0	0.723156	-4.175719	-1.864419
8	1	0	1.489360	-4.412035	-1.119825
9	1	0	-0.227332	-4.609354	-1.538436



10	1	0	1.007591	-4.629047	-2.820220
11	6	0	1.918503	-2.032315	-2.470410
12	1	0	2.201220	-2.441134	-3.445435
13	1	0	1.832796	-0.944836	-2.553851
14	1	0	2.720870	-2.270179	-1.762644
15	6	0	-0.516190	-2.312762	-3.037029
16	1	0	-0.621808	-1.230303	-3.148783
17	1	0	-0.255625	-2.747176	-4.007452
18	1	0	-1.479387	-2.730276	-2.723505
19	6	0	-1.916774	-0.274019	2.827738
20	1	0	-2.730030	-0.864218	2.389628
21	1	0	-2.193431	-0.028401	3.857707
22	1	0	-1.810580	0.655646	2.261111
23	6	0	-0.737970	-2.362652	3.634251
24	1	0	-1.524602	-2.992718	3.209441
25	1	0	0.203391	-2.921377	3.619137
26	1	0	-0.991617	-2.131571	4.674446
27	6	0	0.527506	-0.191687	3.403660
28	1	0	0.631294	0.738970	2.839006
29	1	0	0.291618	0.050319	4.444808
30	1	0	1.485627	-0.723214	3.387433
31	7	0	-1.916626	-0.511739	-0.641998
32	1	0	-1.198635	0.195457	-0.980981
33	6	0	-3.196539	0.041848	-0.459021
34	6	0	-3.293768	1.408592	-0.153479
35	6	0	-4.373208	-0.701572	-0.622981
36	6	0	-4.542464	2.009617	-0.015622
37	1	0	-2.386522	1.987628	-0.020045
38	6	0	-5.612797	-0.084261	-0.456328
39	1	0	-4.312015	-1.749158	-0.889078
40	6	0	-5.719105	1.272235	-0.150900

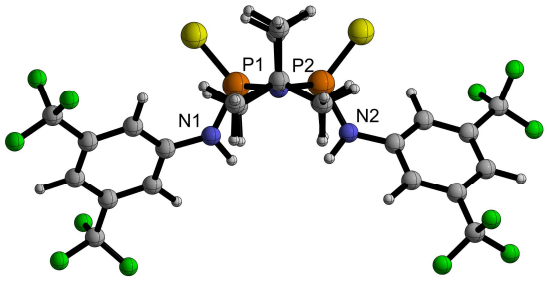
41	1	0	-6.687523	1.743599	-0.036978
42	7	0	1.919654	-0.200839	0.458579
43	1	0	1.247607	0.604829	0.376190
44	6	0	3.259584	0.138783	0.287588
45	6	0	3.575381	1.506011	0.152066
46	6	0	4.305421	-0.796781	0.238520
47	6	0	4.892046	1.908640	-0.033868
48	1	0	2.774521	2.236760	0.201602
49	6	0	5.618574	-0.363221	0.050648
50	1	0	4.088473	-1.851407	0.359098
51	6	0	5.939317	0.984223	-0.091909
52	1	0	6.963182	1.305914	-0.235495
53	8	0	2.153314	-2.728474	1.107745
54	16	0	-2.485483	-3.325046	0.368525
55	6	0	0.091872	2.278978	-0.994548
56	6	0	0.320025	3.694206	-1.520923
57	1	0	0.104745	3.766762	-2.589028
58	1	0	-0.328273	4.387962	-0.973549
59	1	0	1.355285	3.997165	-1.330513
60	8	0	-0.371560	1.405689	-1.790788
61	8	0	0.373911	2.062729	0.228250
62	6	0	-6.857521	-0.920114	-0.590431
63	6	0	-4.609432	3.467270	0.352491
64	6	0	5.188819	3.370291	-0.234833
65	6	0	6.695436	-1.414118	0.003813
66	9	0	-6.754390	-1.849598	-1.580125
67	9	0	-7.129978	-1.615324	0.556521
68	9	0	-7.963252	-0.176210	-0.858939
69	9	0	-5.784777	4.045531	-0.011657
70	9	0	-3.612839	4.193652	-0.223960
71	9	0	-4.488407	3.659147	1.702419

72	9	0	4.273342	4.180256	0.361185
73	9	0	5.194715	3.711451	-1.561168
74	9	0	6.409462	3.725265	0.252413
75	9	0	7.936125	-0.897951	-0.188468
76	9	0	6.748689	-2.145143	1.156976
77	9	0	6.485827	-2.315997	-1.001516

S-cyclodiphosph(V)azane 12

“In-in”-conformation

Electronic energy = -3828.0978348, thermal correction to Gibbs free energy = 0.400907 NIMAG = 0



1	15	0	1.259451	-1.362476	-0.046977
2	7	0	0.036487	-1.250933	1.134961
3	7	0	-0.036465	-1.250174	-1.135413
4	15	0	-1.259446	-1.362629	0.046459
5	16	0	2.478261	-2.862274	-0.053130
6	16	0	-2.478061	-2.862554	0.051604
7	6	0	0.084406	-1.450403	2.620111
8	6	0	-0.084304	-1.448667	-2.620692
9	6	0	0.062943	-2.951423	2.953998
10	1	0	-0.865952	-3.411602	2.605092
11	1	0	0.907228	-3.460596	2.480197
12	1	0	0.134723	-3.085335	4.038433
13	6	0	-1.134155	-0.746049	3.234111
14	1	0	-1.129277	-0.906142	4.316540
15	1	0	-1.105410	0.331120	3.043615
16	1	0	-2.070227	-1.153219	2.836358
17	6	0	1.379098	-0.805727	3.134697
18	1	0	1.430477	0.251222	2.857523
19	1	0	1.412396	-0.886893	4.225211
20	1	0	2.257261	-1.323327	2.734364
21	6	0	1.134454	-0.744154	-3.234127

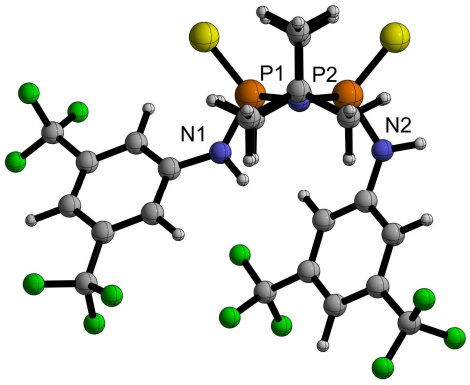
22	1	0	2.070410	-1.151757	-2.836547
23	1	0	1.129635	-0.903574	-4.316656
24	1	0	1.105916	0.332890	-3.042931
25	6	0	-0.063129	-2.949469	-2.955588
26	1	0	0.865603	-3.410101	-2.606847
27	1	0	-0.907606	-3.458774	-2.482270
28	1	0	-0.134779	-3.082646	-4.040124
29	6	0	-1.378812	-0.803359	-3.134951
30	1	0	-1.429978	0.253407	-2.857043
31	1	0	-1.412031	-0.883747	-4.225524
32	1	0	-2.257132	-1.321044	-2.735069
33	7	0	2.038248	0.128583	-0.138102
34	1	0	1.431122	0.870662	-0.475948
35	6	0	3.400233	0.476871	-0.121109
36	6	0	3.815286	1.574431	-0.889926
37	6	0	4.342020	-0.197624	0.665485
38	6	0	5.147932	1.977231	-0.872199
39	1	0	3.094766	2.115263	-1.495484
40	6	0	5.674922	0.210618	0.650911
41	1	0	4.038402	-1.026984	1.289312
42	6	0	6.099935	1.294800	-0.114471
43	1	0	7.136019	1.610505	-0.107462
44	7	0	-2.038294	0.128357	0.138680
45	1	0	-1.431342	0.870018	0.477750
46	6	0	-3.400268	0.476650	0.121638
47	6	0	-3.815359	1.574040	0.890717
48	6	0	-4.342028	-0.197563	-0.665220
49	6	0	-5.147970	1.976909	0.872973
50	1	0	-3.094902	2.114741	1.496466
51	6	0	-5.674918	0.210759	-0.650654
52	1	0	-4.038453	-1.026778	-1.289258

53	6	0	-6.099954	1.294740	0.114967
54	1	0	-7.136018	1.610514	0.107949
55	6	0	-6.673864	-0.566545	-1.467925
56	6	0	-5.576659	3.134156	1.736947
57	6	0	5.576494	3.134668	-1.735977
58	6	0	6.673931	-0.566890	1.467907
59	9	0	-6.147038	-1.013736	-2.640412
60	9	0	-7.119591	-1.674176	-0.801884
61	9	0	-7.774971	0.165253	-1.779235
62	9	0	-6.646589	3.795650	1.222508
63	9	0	-4.585390	4.049563	1.907171
64	9	0	-5.941772	2.725368	2.989558
65	9	0	4.585601	4.050834	-1.904576
66	9	0	5.939859	2.726353	-2.989244
67	9	0	6.647417	3.795162	-1.222400
68	9	0	7.774935	0.164913	1.779557
69	9	0	7.119828	-1.674206	0.801432
70	9	0	6.147115	-1.014626	2.640183

“In-out”-conformation

Electronic energy = -3828.1049194, thermal correction to Gibbs free energy = 0.402152 NIMAG = 0

1	15	0	-2.213664	-2.493927	-0.020724
2	7	0	-0.746125	-2.415727	-0.864303
3	7	0	-1.284625	-1.920429	1.288295
4	15	0	0.214092	-2.085485	0.512828
5	6	0	-0.372914	-2.958611	-2.214090
6	6	0	-1.621612	-1.810135	2.746913
7	6	0	-0.114742	-4.471512	-2.127190
8	1	0	0.703130	-4.683382	-1.433223
9	1	0	-1.012111	-4.993049	-1.782409
10	1	0	0.155564	-4.853264	-3.117282
11	6	0	0.892179	-2.220816	-2.673682



12	1	0	1.168463	-2.564298	-3.674868
13	1	0	0.733522	-1.138682	-2.709063
14	1	0	1.731940	-2.433247	-2.003899
15	6	0	-1.534536	-2.671243	-3.176471
16	1	0	-1.725411	-1.597772	-3.266548
17	1	0	-1.278501	-3.060221	-4.166492
18	1	0	-2.453258	-3.165119	-2.843185
19	6	0	-3.051722	-1.262191	2.852420
20	1	0	-3.770820	-1.942791	2.383658
21	1	0	-3.319468	-1.162471	3.908528
22	1	0	-3.129083	-0.278668	2.379104
23	6	0	-1.519318	-3.191723	3.413344
24	1	0	-2.209210	-3.895595	2.939588
25	1	0	-0.502623	-3.586124	3.327926
26	1	0	-1.774724	-3.106736	4.474607
27	6	0	-0.634508	-0.826048	3.390344
28	1	0	-0.720564	0.168778	2.942109
29	1	0	-0.860508	-0.743895	4.457614
30	1	0	0.399143	-1.173955	3.287998
31	7	0	-3.244127	-1.279219	-0.564765
32	1	0	-4.219913	-1.546865	-0.470595
33	6	0	-3.012124	0.110041	-0.644162
34	6	0	-3.985759	0.994675	-0.165605
35	6	0	-1.845602	0.625757	-1.226847
36	6	0	-3.784257	2.371377	-0.261141
37	1	0	-4.892047	0.607248	0.288936
38	6	0	-1.659181	2.003650	-1.300545
39	1	0	-1.102719	-0.046447	-1.634261
40	6	0	-2.620928	2.894315	-0.819783
41	1	0	-2.468139	3.965270	-0.882745
42	7	0	0.769063	-0.499785	0.432181

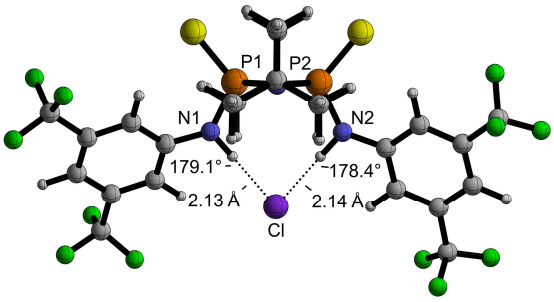
43	1	0	0.013905	0.170465	0.554650
44	6	0	2.046406	0.079048	0.423572
45	6	0	2.156787	1.415394	0.840142
46	6	0	3.193043	-0.593576	-0.014660
47	6	0	3.389532	2.057419	0.813320
48	1	0	1.275158	1.950375	1.177888
49	6	0	4.422196	0.065836	-0.012857
50	1	0	3.132787	-1.618649	-0.354226
51	6	0	4.543059	1.392027	0.395014
52	1	0	5.502763	1.894189	0.383353
53	16	0	-3.233845	-4.134754	0.105613
54	16	0	1.560146	-3.352593	1.068678
55	6	0	5.648459	-0.701404	-0.434967
56	6	0	3.475903	3.511730	1.196230
57	6	0	-0.424050	2.567276	-1.957842
58	6	0	-4.868935	3.294692	0.234241
59	9	0	6.153618	-1.451578	0.590273
60	9	0	5.390574	-1.569516	-1.450916
61	9	0	6.654579	0.110892	-0.850617
62	9	0	4.649640	3.813333	1.813328
63	9	0	3.396313	4.327535	0.101882
64	9	0	2.475434	3.893022	2.033021
65	9	0	-4.424864	4.560304	0.435550
66	9	0	-5.903526	3.377139	-0.652837
67	9	0	-5.405622	2.866364	1.409632
68	9	0	0.500714	1.613841	-2.241131
69	9	0	-0.717862	3.194283	-3.131673
70	9	0	0.190105	3.494815	-1.171113

12•Cl

Electronic energy = -4288.5314485, thermal correction to Gibbs free energy = 0.395549 NIMAG = 0

1	15	0	1.267686	-1.412785	0.852481

2	7	0	-0.059199	-0.839181	1.735132
3	7	0	0.080400	-1.898144	-0.263915
4	15	0	-1.250426	-1.440143	0.683138
5	6	0	-0.162014	-0.283854	3.119658
6	6	0	0.175257	-2.684986	-1.526976
7	6	0	-0.217935	-1.439890	4.131480
8	1	0	-1.089986	-2.071820	3.938801
9	1	0	0.683764	-2.055189	4.055450
10	1	0	-0.288709	-1.041290	5.149181
11	6	0	-1.436452	0.570368	3.192178
12	1	0	-1.531071	0.986273	4.200099
13	1	0	-1.385194	1.392057	2.471627
14	1	0	-2.329306	-0.031081	2.987414
15	6	0	1.067527	0.601219	3.372203
16	1	0	1.105245	1.421479	2.649209
17	1	0	1.003258	1.019980	4.381558
18	1	0	1.994143	0.020661	3.303468
19	6	0	1.472695	-2.279232	-2.241713
20	1	0	2.348528	-2.531463	-1.633884
21	1	0	1.551687	-2.826419	-3.186013
22	1	0	1.485349	-1.205803	-2.452815
23	6	0	0.185548	-4.187784	-1.200487
24	1	0	1.040027	-4.430923	-0.561797
25	1	0	-0.733731	-4.468100	-0.677327
26	1	0	0.257698	-4.770750	-2.124974
27	6	0	-1.036498	-2.331915	-2.401862
28	1	0	-1.066379	-1.259876	-2.616771
29	1	0	-0.971545	-2.881433	-3.346015
30	1	0	-1.971178	-2.620188	-1.908517
31	7	0	2.013227	-0.031160	0.280198
32	1	0	1.349278	0.768694	0.189903

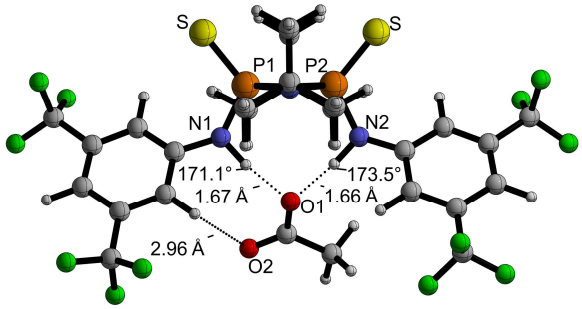


33	6	0	3.334469	0.299632	-0.028029
34	6	0	3.652273	1.667804	-0.110916
35	6	0	4.340352	-0.642727	-0.287131
36	6	0	4.944301	2.069954	-0.432890
37	1	0	2.874479	2.401933	0.077798
38	6	0	5.631067	-0.212783	-0.593813
39	1	0	4.121727	-1.701098	-0.236834
40	6	0	5.956845	1.139583	-0.675788
41	1	0	6.963647	1.459264	-0.914921
42	7	0	-1.946105	-0.087396	-0.010479
43	1	0	-1.296579	0.729780	-0.022365
44	6	0	-3.284711	0.252262	-0.237261
45	6	0	-3.662187	1.594092	-0.062300
46	6	0	-4.242408	-0.672179	-0.677139
47	6	0	-4.973343	1.989064	-0.313157
48	1	0	-2.916292	2.316348	0.255361
49	6	0	-5.553482	-0.255678	-0.904094
50	1	0	-3.963415	-1.702569	-0.851876
51	6	0	-5.941630	1.071239	-0.723221
52	1	0	-6.960769	1.384649	-0.914940
53	17	0	0.005681	2.421071	-0.052530
54	16	0	2.479220	-2.733756	1.595789
55	16	0	-2.527079	-2.777809	1.270497
56	6	0	-5.367627	3.422542	-0.076473
57	6	0	-6.575403	-1.276362	-1.329020
58	6	0	6.675331	-1.251888	-0.905584
59	6	0	5.240036	3.540245	-0.564749
60	9	0	-5.811648	3.624482	1.202384
61	9	0	-6.375904	3.825613	-0.896587
62	9	0	-4.334530	4.286327	-0.262102
63	9	0	-7.589688	-0.729703	-2.051340

64	9	0	-7.157828	-1.892165	-0.254669
65	9	0	-6.036553	-2.268307	-2.088982
66	9	0	4.484363	4.302648	0.270360
67	9	0	4.991037	3.997618	-1.830380
68	9	0	6.541937	3.834756	-0.302723
69	9	0	6.537041	-2.372842	-0.145685
70	9	0	6.608707	-1.665603	-2.208855
71	9	0	7.941428	-0.796549	-0.713281

12•OAc “one-atom”-mode

Electronic energy = -4056.8873682, thermal correction to Gibbs free energy = 0.438095 NIMAG = 0



1	15	0	1.251592	-1.657692	0.509374
2	7	0	-0.060683	-1.154321	1.461159
3	7	0	0.034664	-2.076475	-0.603530
4	15	0	-1.275801	-1.696591	0.403078
5	6	0	-0.130042	-0.620664	2.850164
6	6	0	0.103865	-2.807091	-1.902174
7	6	0	-0.146425	-1.788370	3.850866
8	1	0	-1.015924	-2.427660	3.671380
9	1	0	0.759923	-2.391619	3.742330
10	1	0	-0.195356	-1.404078	4.875383
11	6	0	-1.412286	0.217129	2.975518
12	1	0	-1.490744	0.606405	3.995299
13	1	0	-1.395492	1.060878	2.279553
14	1	0	-2.302998	-0.388831	2.773683
15	6	0	1.097645	0.273752	3.083912
16	1	0	1.111245	1.110735	2.379336
17	1	0	1.062498	0.673193	4.102389
18	1	0	2.027696	-0.295104	2.974374
19	6	0	1.383622	-2.365184	-2.627585
20	1	0	2.275007	-2.626128	-2.046087
21	1	0	1.445777	-2.879441	-3.591703

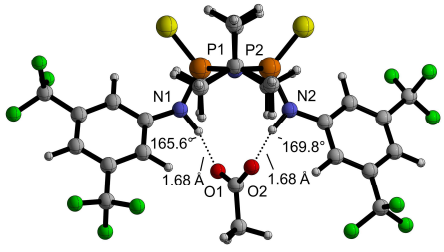
22	1	0	1.381812	-1.285136	-2.800573
23	6	0	0.125675	-4.322661	-1.641103
24	1	0	0.996202	-4.590599	-1.034839
25	1	0	-0.779324	-4.628166	-1.107273
26	1	0	0.175494	-4.865416	-2.591244
27	6	0	-1.128038	-2.422467	-2.734756
28	1	0	-1.154495	-1.344734	-2.918770
29	1	0	-1.088197	-2.945430	-3.695447
30	1	0	-2.053466	-2.714757	-2.226203
31	7	0	1.981763	-0.289293	-0.090127
32	1	0	1.269218	0.459496	-0.332720
33	6	0	3.304261	0.158595	-0.075337
34	6	0	3.519466	1.542212	0.053217
35	6	0	4.412901	-0.684580	-0.236996
36	6	0	4.812553	2.055552	0.045651
37	1	0	2.664334	2.202440	0.144808
38	6	0	5.700654	-0.147530	-0.226302
39	1	0	4.268464	-1.748016	-0.376115
40	6	0	5.924534	1.220583	-0.082611
41	1	0	6.929139	1.625258	-0.078867
42	7	0	-1.991303	-0.352205	-0.276420
43	1	0	-1.270077	0.400409	-0.472546
44	6	0	-3.303117	0.128332	-0.198064
45	6	0	-3.486628	1.504125	0.017565
46	6	0	-4.431120	-0.682981	-0.389182
47	6	0	-4.768838	2.045898	0.052108
48	1	0	-2.616413	2.140193	0.144088
49	6	0	-5.706122	-0.121780	-0.327057
50	1	0	-4.307785	-1.737907	-0.597383
51	6	0	-5.898129	1.241507	-0.102946
52	1	0	-6.893662	1.666382	-0.069713

53	6	0	-6.897807	-1.027932	-0.486259
54	6	0	-4.926999	3.518846	0.318163
55	6	0	5.009949	3.544861	0.129585
56	6	0	6.869059	-1.088697	-0.343412
57	9	0	-6.683868	-2.009654	-1.405420
58	9	0	-7.213234	-1.664775	0.683168
59	9	0	-8.016998	-0.360486	-0.872783
60	9	0	-6.117774	4.005080	-0.120789
61	9	0	-3.951018	4.259170	-0.276965
62	9	0	-4.861604	3.807193	1.654218
63	9	0	4.982711	4.134750	-1.105244
64	9	0	4.044252	4.159764	0.864890
65	9	0	6.205780	3.881646	0.685237
66	9	0	8.000245	-0.471816	-0.776891
67	9	0	6.623984	-2.116367	-1.203162
68	9	0	7.182378	-1.666285	0.857724
69	6	0	0.150013	1.941269	-1.944880
70	8	0	1.260787	2.169942	-2.462569
71	8	0	-0.015042	1.441573	-0.758782
72	6	0	-1.135794	2.255738	-2.711227
73	1	0	-1.763462	1.359563	-2.772862
74	1	0	-1.710815	3.016160	-2.171310
75	1	0	-0.915822	2.616319	-3.717925
76	16	0	2.468528	-3.005882	1.202093
77	16	0	-2.517124	-3.067302	0.999683

12•OAc “two-atom”-mode

Electronic energy = -4056.8877864, thermal correction to Gibbs free energy = 0.440076 NIMAG = 0

1	15	0	1.287010	-1.730574	0.294898
2	7	0	0.219893	-1.161543	1.501890
3	7	0	-0.140097	-2.071193	-0.545501
4	15	0	-1.199940	-1.618834	0.714194



5	6	0	0.477063	-0.673475	2.888487
6	6	0	-0.378916	-2.811747	-1.818868
7	6	0	0.629771	-1.872616	3.839819
8	1	0	-0.281479	-2.478861	3.832975
9	1	0	1.470803	-2.501293	3.533169
10	1	0	0.808607	-1.517671	4.860723
11	6	0	-0.702907	0.208176	3.323808
12	1	0	-0.521386	0.564261	4.342914
13	1	0	-0.806956	1.070038	2.659499
14	1	0	-1.640124	-0.359214	3.324004
15	6	0	1.762353	0.166779	2.854763
16	1	0	1.639261	1.020204	2.182262
17	1	0	1.981431	0.536388	3.861495
18	1	0	2.617907	-0.430901	2.519656
19	6	0	0.768854	-2.493758	-2.788537
20	1	0	1.732348	-2.811915	-2.375683
21	1	0	0.602992	-3.036148	-3.724786
22	1	0	0.815835	-1.422514	-3.002481
23	6	0	-0.437376	-4.322575	-1.536615
24	1	0	0.507968	-4.661826	-1.102035
25	1	0	-1.245137	-4.547676	-0.834122
26	1	0	-0.614622	-4.870798	-2.468191
27	6	0	-1.708135	-2.315854	-2.406180
28	1	0	-1.680084	-1.234491	-2.570472
29	1	0	-1.893599	-2.814990	-3.362339
30	1	0	-2.543219	-2.551294	-1.737849
31	7	0	1.964449	-0.454499	-0.528056
32	1	0	1.256974	0.252287	-0.885555
33	6	0	3.268727	0.061588	-0.435328
34	6	0	3.429039	1.434601	-0.191846
35	6	0	4.408286	-0.730488	-0.629804

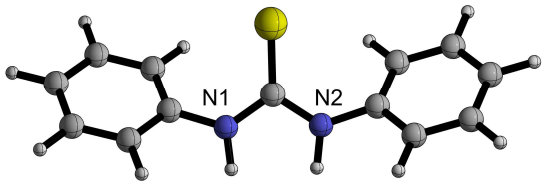
36	6	0	4.703971	1.992362	-0.131313
37	1	0	2.551806	2.053092	-0.039979
38	6	0	5.676015	-0.154732	-0.546350
39	1	0	4.297393	-1.784060	-0.852103
40	6	0	5.845085	1.206795	-0.296381
41	1	0	6.834563	1.643468	-0.237912
42	7	0	-1.938811	-0.177776	0.320739
43	1	0	-1.260699	0.635610	0.297206
44	6	0	-3.268364	0.187290	0.111112
45	6	0	-3.574408	1.561448	0.145041
46	6	0	-4.302998	-0.720746	-0.166653
47	6	0	-4.872761	2.000251	-0.091234
48	1	0	-2.777000	2.271047	0.342153
49	6	0	-5.599150	-0.255080	-0.384385
50	1	0	-4.100105	-1.782153	-0.212492
51	6	0	-5.910972	1.103030	-0.349095
52	1	0	-6.920061	1.451589	-0.531526
53	6	0	-6.692068	-1.261470	-0.627192
54	6	0	-5.164803	3.474887	-0.013138
55	6	0	4.842371	3.475665	0.081559
56	6	0	6.881772	-1.041499	-0.705835
57	9	0	-6.252006	-2.358836	-1.302426
58	9	0	-7.227237	-1.725677	0.544318
59	9	0	-7.728509	-0.746643	-1.341573
60	9	0	-6.235483	3.835360	-0.770860
61	9	0	-4.114125	4.237293	-0.423192
62	9	0	-5.448913	3.874220	1.265106
63	9	0	4.759868	4.170039	-1.094884
64	9	0	3.867167	3.978499	0.887113
65	9	0	6.034058	3.813995	0.642269
66	9	0	7.996535	-0.351876	-1.066026

67	9	0	6.692453	-2.008938	-1.645139
68	9	0	7.191679	-1.695294	0.455766
69	6	0	-0.043693	2.334333	-0.935320
70	8	0	0.451253	1.464946	-1.716663
71	8	0	-0.431867	2.096420	0.253804
72	6	0	-0.173831	3.771505	-1.433150
73	1	0	0.087973	3.856345	-2.489873
74	1	0	-1.195996	4.129156	-1.271803
75	1	0	0.493633	4.412579	-0.845432
76	16	0	2.546318	-3.128799	0.788831
77	16	0	-2.384764	-2.960720	1.474489

Thiourea 23

“In-in” conformation

Electronic energy = -1010.7087837, thermal correction to Gibbs free energy = 0.175702 NIMAG = 0



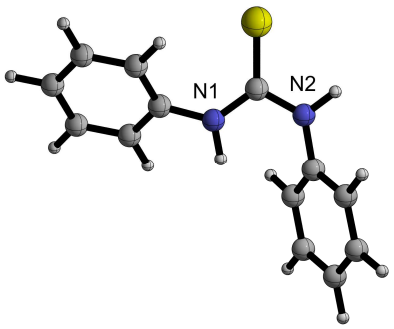
1	6	0	-3.428526	-0.854024	0.298842
2	16	0	-3.749943	-1.798480	-1.056624
3	7	0	-3.992484	0.372929	0.526383
4	1	0	-3.839251	0.784590	1.442572
5	7	0	-2.603055	-1.243031	1.322054
6	1	0	-2.659987	-0.708404	2.184260
7	6	0	-1.808886	-2.415724	1.417595
8	6	0	-1.791393	-3.102998	2.637666
9	6	0	-0.999739	-2.848899	0.360004
10	6	0	-0.978893	-4.226254	2.794443
11	1	0	-2.417545	-2.759807	3.457254
12	6	0	-0.203348	-3.981320	0.522366
13	1	0	-0.994744	-2.300117	-0.573747
14	6	0	-0.189043	-4.676037	1.735025
15	1	0	-0.972700	-4.752542	3.744689
16	1	0	0.420665	-4.313729	-0.302597

17	1	0	0.437661	-5.555026	1.854442
18	6	0	-4.926468	1.079267	-0.279107
19	6	0	-6.029004	1.667717	0.352621
20	6	0	-4.730539	1.256995	-1.653765
21	6	0	-6.940121	2.418366	-0.390997
22	1	0	-6.173091	1.530459	1.421184
23	6	0	-5.655136	1.996442	-2.390082
24	1	0	-3.862066	0.823398	-2.133888
25	6	0	-6.762494	2.577598	-1.766404
26	1	0	-7.793003	2.870110	0.107491
27	1	0	-5.499678	2.129207	-3.457135
28	1	0	-7.476209	3.155179	-2.346667

“In-out” conformation

Electronic energy = -1010.71222, thermal correction to Gibbs free energy = 0.176019 NIMAG = 0

1	6	0	-1.579710	0.807041	0.491557
2	16	0	-1.522690	2.418963	0.996588
3	7	0	-1.431872	0.367758	-0.786237
4	1	0	-1.436556	-0.642468	-0.906168
5	7	0	-1.793124	-0.172426	1.424846
6	1	0	-2.078347	0.187207	2.328543
7	6	0	-1.826711	-1.585078	1.238351
8	6	0	-2.935444	-2.301767	1.704819
9	6	0	-0.753926	-2.263289	0.642208
10	6	0	-2.973432	-3.688127	1.566160
11	1	0	-3.760538	-1.769186	2.168968
12	6	0	-0.813629	-3.648705	0.485567
13	1	0	0.130285	-1.715150	0.329236
14	6	0	-1.919905	-4.364683	0.946131
15	1	0	-3.834735	-4.238847	1.933026
16	1	0	0.018964	-4.168387	0.020521
17	1	0	-1.957754	-5.443679	0.830003

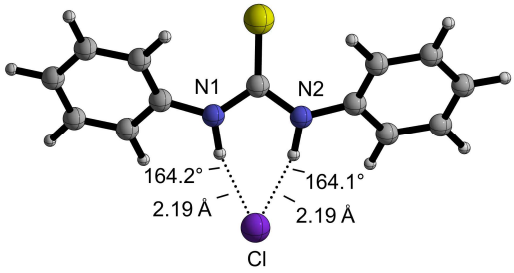


18	6	0	-1.112481	1.093175	-1.964810
19	6	0	-0.229998	0.488227	-2.869830
20	6	0	-1.691461	2.329447	-2.273850
21	6	0	0.085565	1.124522	-4.069187
22	1	0	0.210309	-0.475871	-2.628313
23	6	0	-1.358255	2.962613	-3.471706
24	1	0	-2.393362	2.782730	-1.585603
25	6	0	-0.470296	2.369488	-4.371691
26	1	0	0.772529	0.647743	-4.762503
27	1	0	-1.809736	3.922765	-3.705617
28	1	0	-0.219592	2.868950	-5.302974

23•Cl

Electronic energy = -1471.1343749, thermal correction to Gibbs free energy = 0.171769 NIMAG = 0

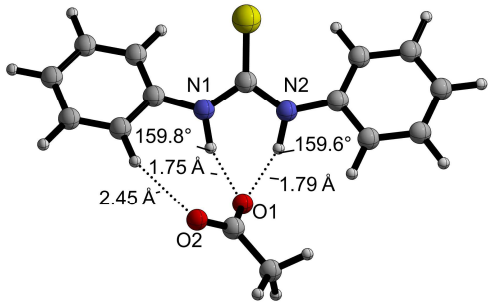
1	6	0	-2.415119	-0.588146	-1.081818
2	16	0	-2.515049	-1.446819	-2.534466
3	7	0	-3.120370	0.550729	-0.798972
4	1	0	-3.096031	0.834837	0.197590
5	7	0	-1.663923	-0.967313	-0.001839
6	1	0	-1.868864	-0.444039	0.869165
7	6	0	-0.814495	-2.077942	0.174153
8	6	0	-0.775683	-2.650295	1.456906
9	6	0	0.032277	-2.575849	-0.827444
10	6	0	0.082723	-3.713497	1.728526
11	1	0	-1.423708	-2.253531	2.234482
12	6	0	0.878901	-3.648079	-0.545744
13	1	0	0.026593	-2.123072	-1.810594
14	6	0	0.909268	-4.226257	0.725774
15	1	0	0.098474	-4.145313	2.725515
16	1	0	1.530288	-4.025857	-1.329522
17	1	0	1.573681	-5.059906	0.934223
18	6	0	-4.033957	1.277928	-1.587976



19	6	0	-5.116163	1.874240	-0.918812
20	6	0	-3.872434	1.494362	-2.964644
21	6	0	-6.030724	2.659298	-1.617602
22	1	0	-5.231093	1.715296	0.150537
23	6	0	-4.801414	2.273132	-3.654796
24	1	0	-3.026758	1.059629	-3.481808
25	6	0	-5.884938	2.856160	-2.992951
26	1	0	-6.862787	3.111335	-1.084652
27	1	0	-4.666509	2.433734	-4.721255
28	1	0	-6.601356	3.461982	-3.540301
29	17	0	-2.710211	0.933772	2.355549

23•OAc “one-atom”-mode

Electronic energy = -1239.4867279, thermal correction to Gibbs free energy = 0.214402 NIMAG = 0



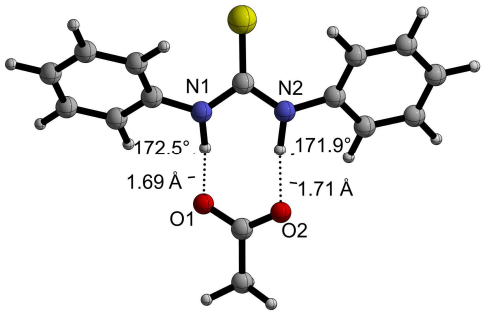
1	6	0	-0.508338	-0.718574	-0.149774
2	16	0	-0.530518	-2.291866	0.475478
3	7	0	-1.620254	0.042957	-0.409585
4	1	0	-1.397305	1.030707	-0.632079
5	7	0	0.622098	0.002197	-0.411792
6	1	0	0.444128	1.018153	-0.606203
7	6	0	1.978935	-0.352429	-0.290280
8	6	0	2.862568	0.673668	0.088743
9	6	0	2.487972	-1.622971	-0.601099
10	6	0	4.231401	0.425560	0.168601
11	1	0	2.452038	1.654924	0.321756
12	6	0	3.859989	-1.858620	-0.507448
13	1	0	1.814665	-2.410563	-0.915081
14	6	0	4.739418	-0.843788	-0.121234
15	1	0	4.902469	1.227467	0.465643
16	1	0	4.243968	-2.846099	-0.750664
17	1	0	5.806029	-1.038573	-0.052609
18	6	0	-2.993468	-0.212897	-0.258695

19	6	0	-3.815624	0.916063	-0.078801
20	6	0	-3.589127	-1.481867	-0.343010
21	6	0	-5.196110	0.778875	0.030104
22	1	0	-3.357794	1.900791	-0.026147
23	6	0	-4.974205	-1.605370	-0.223346
24	1	0	-2.969819	-2.354763	-0.500687
25	6	0	-5.787270	-0.486197	-0.033287
26	1	0	-5.810062	1.664448	0.170522
27	1	0	-5.420047	-2.594477	-0.290501
28	1	0	-6.864038	-0.596156	0.057619
29	6	0	-0.183478	3.407918	-0.070733
30	6	0	-1.173380	4.577183	-0.036319
31	1	0	-1.317269	4.980382	-1.044133
32	1	0	-2.148483	4.213375	0.309505
33	1	0	-0.832062	5.369051	0.634612
34	8	0	-0.428347	2.499146	-0.952200
35	8	0	0.775587	3.388144	0.734622

23•OAc “two-atom”-mode

Electronic energy = -1239.4913833, thermal correction to Gibbs free energy = 0.213312 NIMAG = 0

1	6	0	-2.420404	-0.639875	-1.073407
2	16	0	-2.597652	-1.435685	-2.565723
3	7	0	-3.141288	0.466394	-0.716361
4	1	0	-3.236887	0.667300	0.317566
5	7	0	-1.606500	-1.055434	-0.061129
6	1	0	-1.656514	-0.513650	0.843926
7	6	0	-0.787928	-2.200754	0.025408
8	6	0	-0.664103	-2.794378	1.294521
9	6	0	-0.043074	-2.719366	-1.045951
10	6	0	0.166951	-3.896867	1.481762
11	1	0	-1.220331	-2.373413	2.127263
12	6	0	0.777921	-3.830069	-0.847822



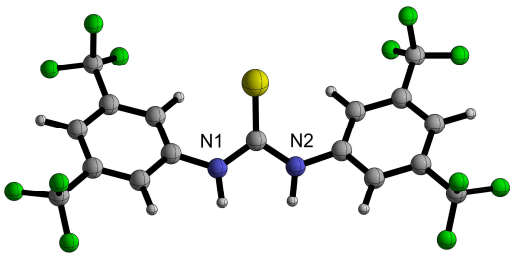
13	1	0	-0.109979	-2.252411	-2.019986
14	6	0	0.886359	-4.429971	0.409038
15	1	0	0.246000	-4.343689	2.469389
16	1	0	1.347304	-4.221442	-1.687114
17	1	0	1.528798	-5.294231	0.552460
18	6	0	-3.980076	1.253130	-1.529553
19	6	0	-5.174401	1.732667	-0.966453
20	6	0	-3.631299	1.646880	-2.831373
21	6	0	-6.010994	2.575007	-1.698491
22	1	0	-5.433048	1.442908	0.047755
23	6	0	-4.479960	2.480411	-3.557892
24	1	0	-2.698685	1.303420	-3.262651
25	6	0	-5.675027	2.947248	-3.001816
26	1	0	-6.932062	2.935116	-1.247588
27	1	0	-4.196948	2.777084	-4.564676
28	1	0	-6.329772	3.598042	-3.574507
29	6	0	-2.612758	0.845368	2.705575
30	6	0	-2.746570	1.327111	4.150684
31	1	0	-3.230405	2.307475	4.186293
32	1	0	-3.385441	0.622614	4.697295
33	1	0	-1.774403	1.368985	4.647429
34	8	0	-3.587650	1.075516	1.923125
35	8	0	-1.552666	0.226122	2.380428

Thiourea 18

“In-in” conformation

Electronic energy = -2359.6032341, thermal correction to Gibbs free energy = 0.164177 NIMAG = 0

1	6	0	-3.748512	-1.123615	0.364685
2	16	0	-3.994605	-2.034600	-1.019989
3	7	0	-4.325655	0.099841	0.596898
4	1	0	-4.222447	0.490582	1.529380

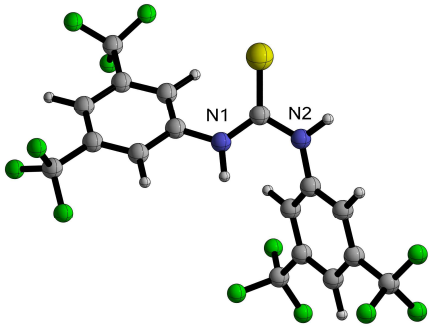


5	7	0	-2.976810	-1.533503	1.424917
6	1	0	-3.083817	-1.028740	2.300391
7	6	0	-2.202209	-2.709195	1.522994
8	6	0	-2.213029	-3.408948	2.732364
9	6	0	-1.382162	-3.142298	0.473968
10	6	0	-1.414881	-4.543588	2.884017
11	1	0	-2.840290	-3.070167	3.550860
12	6	0	-0.607395	-4.286865	0.642350
13	1	0	-1.337081	-2.579904	-0.448724
14	6	0	-0.617105	-5.004359	1.840073
15	1	0	-0.003729	-5.889070	1.960984
16	6	0	-5.235836	0.799527	-0.226144
17	6	0	-6.326773	1.424794	0.385297
18	6	0	-5.038616	0.933001	-1.604932
19	6	0	-7.222808	2.164774	-0.385441
20	1	0	-6.475438	1.332295	1.456580
21	6	0	-5.957477	1.662358	-2.357526
22	1	0	-4.172225	0.488404	-2.075563
23	6	0	-7.059178	2.278855	-1.764593
24	1	0	-7.762204	2.848649	-2.359913
25	6	0	-5.758310	1.759075	-3.848146
26	6	0	-8.416640	2.796450	0.282101
27	6	0	-1.468951	-5.304421	4.183321
28	6	0	0.242419	-4.775284	-0.502133
29	9	0	-6.379823	2.840081	-4.386484
30	9	0	-4.443945	1.842334	-4.188630
31	9	0	-6.253891	0.662818	-4.496357
32	9	0	-8.906193	3.849969	-0.421056
33	9	0	-8.128435	3.247475	1.532593
34	9	0	-9.447549	1.910012	0.421442
35	9	0	-2.549728	-6.138995	4.237894

36	9	0	-1.571097	-4.476794	5.258698
37	9	0	-0.371509	-6.079609	4.377533
38	9	0	-0.428585	-5.673852	-1.283357
39	9	0	0.634947	-3.767938	-1.325209
40	9	0	1.369287	-5.404791	-0.074849

“In-out” conformation

Electronic energy = -2359.6054216, thermal correction to Gibbs free energy = 0.166439 NIMAG = 0



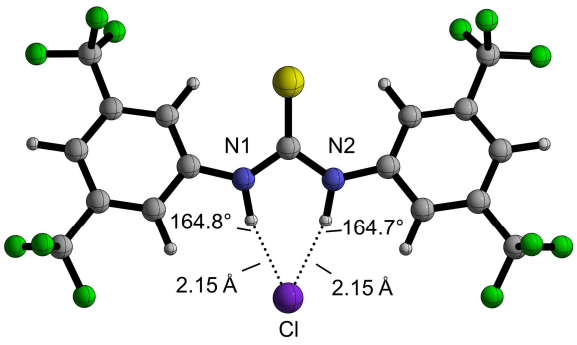
1	6	0	-0.064409	-2.017578	0.804570
2	16	0	0.855572	-3.375269	1.157176
3	7	0	0.423514	-0.754655	0.612315
4	1	0	-0.241129	0.006059	0.730796
5	7	0	-1.432106	-2.115753	0.750609
6	1	0	-1.790817	-2.984584	1.132301
7	6	0	-2.381282	-1.181549	0.279669
8	6	0	-3.615367	-1.094719	0.939070
9	6	0	-2.144830	-0.398602	-0.856967
10	6	0	-4.589061	-0.221547	0.465646
11	1	0	-3.806866	-1.709698	1.811885
12	6	0	-3.127399	0.488053	-1.296828
13	1	0	-1.218161	-0.497401	-1.410499
14	6	0	-4.353863	0.590740	-0.645700
15	1	0	-5.115122	1.274145	-1.002767
16	6	0	1.763740	-0.348767	0.464698
17	6	0	2.138583	0.883050	1.010483
18	6	0	2.694942	-1.105059	-0.256204
19	6	0	3.443644	1.344649	0.846135
20	1	0	1.415668	1.474996	1.562551
21	6	0	3.997483	-0.631389	-0.391395
22	1	0	2.402382	-2.043508	-0.707382
23	6	0	4.390432	0.591145	0.155361
24	1	0	5.406661	0.948964	0.039380

25	6	0	-5.906644	-0.101222	1.190338
26	6	0	-2.833002	1.359732	-2.492241
27	6	0	3.851147	2.648259	1.482553
28	6	0	4.988190	-1.425029	-1.204297
29	9	0	-6.174450	-1.180165	1.967915
30	9	0	-5.931097	0.989862	2.010801
31	9	0	-6.948956	0.042237	0.328931
32	9	0	-3.960873	1.802174	-3.102232
33	9	0	-2.095596	0.709508	-3.431573
34	9	0	-2.117364	2.468245	-2.139441
35	9	0	4.850653	3.265124	0.799722
36	9	0	2.818940	3.528730	1.564840
37	9	0	4.307986	2.468247	2.757981
38	9	0	5.017824	-1.014572	-2.508006
39	9	0	4.699239	-2.751855	-1.224421
40	9	0	6.257548	-1.297960	-0.733905

18•Cl

Electronic energy = -2820.0328733, thermal correction to Gibbs free energy = 0.160011 NIMAG = 0

1	6	0	-2.711661	-0.896779	-1.133917
2	16	0	-2.621542	-1.639127	-2.640832
3	7	0	-3.493839	0.190230	-0.832136
4	1	0	-3.562827	0.399197	0.184786
5	7	0	-2.060034	-1.318482	-0.001796
6	1	0	-2.372422	-0.847486	0.871860
7	6	0	-1.201403	-2.399706	0.216051
8	6	0	-1.156719	-2.897310	1.531418
9	6	0	-0.360419	-2.959532	-0.754377
10	6	0	-0.299971	-3.941609	1.855377
11	1	0	-1.794002	-2.453795	2.290289
12	6	0	0.482194	-4.016545	-0.404325
13	1	0	-0.360375	-2.567305	-1.761938



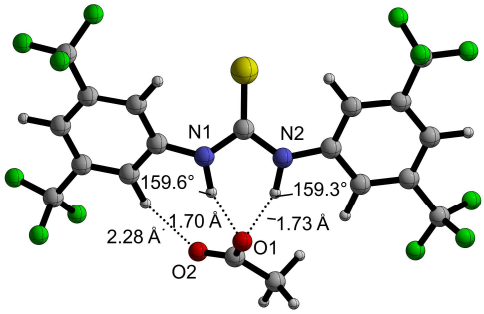
14	6	0	0.523864	-4.527043	0.890063
15	1	0	1.187080	-5.344699	1.145641
16	6	0	-4.367526	0.940282	-1.624765
17	6	0	-5.423171	1.578332	-0.949248
18	6	0	-4.217844	1.141059	-3.003689
19	6	0	-6.314491	2.384183	-1.647431
20	1	0	-5.531115	1.440174	0.122152
21	6	0	-5.134140	1.945799	-3.682339
22	1	0	-3.392289	0.683601	-3.530699
23	6	0	-6.192608	2.570050	-3.026470
24	1	0	-6.892206	3.195620	-3.568062
25	17	0	-3.409948	0.341401	2.325507
26	6	0	-7.465906	3.030072	-0.923006
27	6	0	-4.981034	2.108728	-5.172169
28	6	0	1.344588	-4.619802	-1.482268
29	6	0	-0.288600	-4.495628	3.255566
30	9	0	-7.714971	4.289813	-1.376004
31	9	0	-7.259357	3.122325	0.415694
32	9	0	-8.628340	2.329016	-1.089492
33	9	0	-5.567175	3.243842	-5.636265
34	9	0	-5.551736	1.071645	-5.857335
35	9	0	-3.676929	2.147681	-5.558654
36	9	0	-0.810034	-3.634579	4.166390
37	9	0	-1.015652	-5.650074	3.350881
38	9	0	0.969896	-4.805110	3.674121
39	9	0	0.619939	-5.414126	-2.326782
40	9	0	2.343366	-5.393953	-0.985069
41	9	0	1.929745	-3.670566	-2.265113

18•OAc “one-atom”-mode

Electronic energy = -2588.3875381, thermal correction to Gibbs free energy = 0.206248 NIMAG = 0

1	6	0	-0.621196	0.424486	0.133741

2	16	0	-0.606858	1.947429	0.855659
3	7	0	-1.747285	-0.307720	-0.163621
4	1	0	-1.539424	-1.285596	-0.456971
5	7	0	0.490382	-0.304816	-0.194961
6	1	0	0.282291	-1.297018	-0.485560
7	6	0	1.848481	-0.014981	-0.033832
8	6	0	2.696523	-1.121237	0.152656
9	6	0	2.401231	1.270964	-0.107639
10	6	0	4.068660	-0.929264	0.280435
11	1	0	2.256733	-2.117584	0.210484
12	6	0	3.780046	1.433387	0.034907
13	1	0	1.761338	2.127395	-0.271534
14	6	0	4.631685	0.347745	0.229877
15	1	0	5.699110	0.490862	0.343228
16	6	0	-3.106256	-0.045868	0.003822
17	6	0	-3.951639	-1.173613	-0.031380
18	6	0	-3.679056	1.223794	0.156830
19	6	0	-5.324202	-1.027883	0.106667
20	1	0	-3.517914	-2.159483	-0.163282
21	6	0	-5.063925	1.340777	0.298806
22	1	0	-3.047207	2.101359	0.172481
23	6	0	-5.904845	0.232728	0.280261
24	1	0	-6.976210	0.341768	0.399310
25	6	0	-0.329616	-3.672146	-0.070938
26	6	0	-1.474198	-4.643505	0.222286
27	1	0	-2.140622	-4.183783	0.963179
28	1	0	-2.064484	-4.829710	-0.679608
29	1	0	-1.100986	-5.585319	0.631103
30	8	0	-0.615045	-2.693167	-0.865274
31	8	0	0.785803	-3.846483	0.468190
32	6	0	-5.641499	2.725965	0.431018

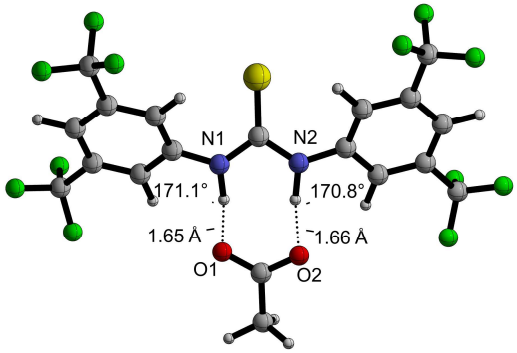


33	6	0	-6.222885	-2.234636	0.052165
34	6	0	4.959442	-2.132209	0.440957
35	6	0	4.342679	2.825374	-0.077779
36	9	0	-4.940663	3.493870	1.311576
37	9	0	-6.933074	2.720820	0.850437
38	9	0	-5.621586	3.399934	-0.758952
39	9	0	-7.114877	-2.252856	1.083334
40	9	0	-5.540161	-3.406793	0.098456
41	9	0	-6.968313	-2.260678	-1.093226
42	9	0	4.387647	-3.106329	1.198852
43	9	0	5.255643	-2.710905	-0.763586
44	9	0	6.151068	-1.826234	1.020900
45	9	0	3.614821	3.734409	0.630243
46	9	0	4.346569	3.270431	-1.371759
47	9	0	5.623957	2.914405	0.364128

18•OAc “two-atom”-mode

Electronic energy = -2588.3930697, thermal correction to Gibbs free energy = 0.204037 NIMAG = 0

1	6	0	-2.782218	-0.927491	-0.945584
2	16	0	-3.009719	-1.809063	-2.374382
3	7	0	-3.451083	0.228876	-0.646196
4	1	0	-3.493388	0.529818	0.375267
5	7	0	-1.974627	-1.313382	0.086696
6	1	0	-2.042978	-0.769622	0.998883
7	6	0	-1.153500	-2.443479	0.180603
8	6	0	-0.972186	-2.996809	1.458140
9	6	0	-0.448903	-2.990252	-0.903582
10	6	0	-0.126155	-4.090091	1.635393
11	1	0	-1.486539	-2.553906	2.304943
12	6	0	0.382249	-4.090612	-0.701738
13	1	0	-0.540687	-2.547651	-1.885523
14	6	0	0.549193	-4.664030	0.559452



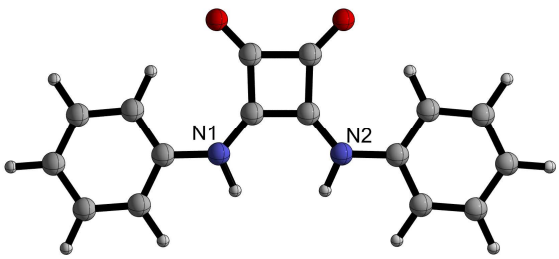
15	1	0	1.200208	-5.517731	0.702164
16	6	0	-4.294479	0.968448	-1.482206
17	6	0	-5.399870	1.602918	-0.894433
18	6	0	-4.038380	1.171393	-2.847000
19	6	0	-6.240630	2.402090	-1.667540
20	1	0	-5.584244	1.472938	0.166705
21	6	0	-4.900534	1.964656	-3.601286
22	1	0	-3.164601	0.728467	-3.304988
23	6	0	-6.015218	2.581834	-3.031671
24	1	0	-6.675271	3.199803	-3.628079
25	6	0	-2.942136	0.706385	2.758035
26	6	0	-3.094786	1.215550	4.188559
27	1	0	-3.621844	2.172168	4.212237
28	1	0	-3.682839	0.484805	4.757297
29	1	0	-2.119017	1.308099	4.672475
30	8	0	-3.776801	1.114733	1.890848
31	8	0	-2.002763	-0.117327	2.524181
32	6	0	-4.631406	2.127904	-5.073169
33	6	0	-7.446712	3.030218	-1.022741
34	6	0	0.009571	-4.682117	3.012605
35	6	0	1.091163	-4.691174	-1.886154
36	9	0	-3.301105	2.145470	-5.360678
37	9	0	-5.161346	3.274172	-5.577833
38	9	0	-5.165912	1.102983	-5.806064
39	9	0	-7.868987	4.144151	-1.678904
40	9	0	-7.216833	3.392406	0.268478
41	9	0	-8.514643	2.174304	-0.994228
42	9	0	0.072928	-3.727165	3.981531
43	9	0	-1.055969	-5.478387	3.333907
44	9	0	1.119368	-5.455378	3.143859
45	9	0	1.412393	-3.763616	-2.828104

46	9	0	0.321212	-5.628505	-2.520282
47	9	0	2.246298	-5.319962	-1.538073

Squaramide 19

“In-in” conformation

Electronic energy = -877.3725407, thermal correction to Gibbs free energy = 0.195376 NIMAG = 0

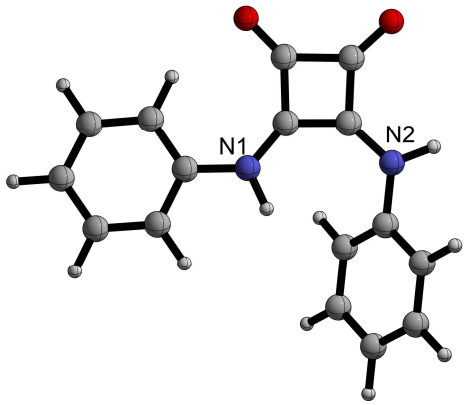


1	6	0	-0.758348	-1.910495	0.184302
2	6	0	0.758695	-1.909279	0.196550
3	6	0	-0.710872	-0.430419	0.077500
4	6	0	0.710549	-0.429010	0.092816
5	7	0	-1.563934	0.605846	-0.016740
6	1	0	-1.145347	1.525635	-0.120055
7	7	0	1.563137	0.610534	0.039077
8	1	0	1.144119	1.535493	0.011248
9	6	0	-2.978435	0.635914	-0.006765
10	6	0	-3.764290	-0.509513	0.168032
11	6	0	-3.588361	1.888321	-0.175901
12	6	0	-5.153428	-0.387069	0.169719
13	1	0	-3.296447	-1.480569	0.295195
14	6	0	-4.976674	1.992771	-0.169868
15	1	0	-2.975099	2.775917	-0.312532
16	6	0	-5.769170	0.855535	0.003024
17	1	0	-5.758628	-1.279226	0.305124
18	1	0	-5.437202	2.967611	-0.301657
19	1	0	-6.851887	0.937144	0.007860
20	6	0	2.977629	0.639555	0.025548
21	6	0	3.764029	-0.518713	0.014645
22	6	0	3.586975	1.903576	0.016190
23	6	0	5.153118	-0.397094	-0.003793
24	1	0	3.296640	-1.498213	0.025778
25	6	0	4.975248	2.006768	-0.004017

26	1	0	2.973298	2.801292	0.025748
27	6	0	5.768283	0.856881	-0.014133
28	1	0	5.758738	-1.299152	-0.011542
29	1	0	5.435322	2.990663	-0.011152
30	1	0	6.850969	0.937489	-0.030027
31	8	0	-1.612190	-2.788123	0.243143
32	8	0	1.612936	-2.786030	0.262295

“In-out” conformation

Electronic energy = -877.3744536, thermal correction to Gibbs free energy = 0.195821 NIMAG = 0



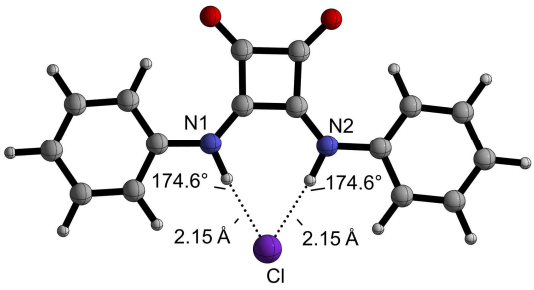
1	6	0	-2.010447	2.060659	1.932273
2	6	0	-0.688816	2.073488	1.175724
3	6	0	-2.663155	1.606165	0.696044
4	6	0	-1.448784	1.638623	-0.036378
5	7	0	-3.952622	1.343185	0.439881
6	1	0	-4.612482	1.610834	1.164888
7	7	0	-1.215670	1.420297	-1.345407
8	1	0	-2.041165	1.223145	-1.905761
9	6	0	-4.481942	0.743470	-0.732617
10	6	0	-3.806660	-0.313568	-1.357445
11	6	0	-5.700817	1.203777	-1.245950
12	6	0	-4.329614	-0.869477	-2.526116
13	1	0	-2.901874	-0.717785	-0.913509
14	6	0	-6.224535	0.622879	-2.398588
15	1	0	-6.221737	2.018120	-0.750306
16	6	0	-5.535851	-0.403791	-3.051429
17	1	0	-3.799679	-1.684307	-3.010410
18	1	0	-7.168444	0.984265	-2.795992
19	1	0	-5.943443	-0.844928	-3.955861
20	6	0	-0.004290	1.379886	-2.070246
21	6	0	1.252412	1.515694	-1.467464
22	6	0	-0.100256	1.181263	-3.456802

23	6	0	2.398157	1.459567	-2.260500
24	1	0	1.331286	1.674976	-0.397071
25	6	0	1.054113	1.123772	-4.233076
26	1	0	-1.077480	1.072380	-3.921657
27	6	0	2.311685	1.263556	-3.640712
28	1	0	3.370126	1.568101	-1.787088
29	1	0	0.967104	0.969092	-5.304720
30	1	0	3.211480	1.219106	-4.246845
31	8	0	-2.396152	2.335331	3.063038
32	8	0	0.472054	2.341564	1.459480

19•Cl

Electronic energy = -1337.8028471, thermal correction to Gibbs free energy = 0.190959 NIMAG = 0

1	6	0	-2.517086	2.292772	-0.771179
2	6	0	-1.004136	2.297331	-0.783823
3	6	0	-2.461979	1.321326	0.348134
4	6	0	-1.034667	1.325635	0.336240
5	7	0	-3.292857	0.632610	1.146018
6	1	0	-2.836718	0.019219	1.850774
7	7	0	-0.186518	0.642023	1.120197
8	1	0	-0.627326	0.026069	1.832575
9	6	0	-4.701568	0.607105	1.182343
10	6	0	-5.511194	1.358476	0.318957
11	6	0	-5.292697	-0.226629	2.147468
12	6	0	-6.898291	1.267318	0.430851
13	1	0	-5.059041	2.003961	-0.428151
14	6	0	-6.679286	-0.305125	2.244696
15	1	0	-4.655225	-0.805009	2.811993
16	6	0	-7.493106	0.440785	1.387680
17	1	0	-7.519672	1.852717	-0.241846
18	1	0	-7.124026	-0.953254	2.994904
19	1	0	-8.574657	0.378731	1.464474

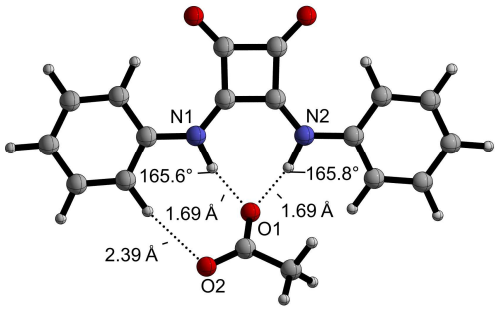


20	6	0	1.222722	0.624829	1.132859
21	6	0	2.013267	1.381391	0.256409
22	6	0	1.834931	-0.205758	2.087500
23	6	0	3.402563	1.298463	0.344952
24	1	0	1.544810	2.024438	-0.482713
25	6	0	3.223403	-0.275993	2.161416
26	1	0	1.212147	-0.788210	2.762309
27	6	0	4.018270	0.475110	1.291251
28	1	0	4.009064	1.887845	-0.337772
29	1	0	3.684527	-0.921771	2.903720
30	1	0	5.101310	0.419491	1.349863
31	8	0	-3.379678	2.869943	-1.432107
32	8	0	-0.156206	2.879636	-1.459058
33	17	0	-1.715742	-1.183286	3.232511

19•OAc “one-atom”-mode

Electronic energy = -1106.1577942, thermal correction to Gibbs free energy = 0.235731 NIMAG = 0

1	6	0	0.185495	-2.436022	0.250491
2	6	0	-1.325852	-2.401615	0.255011
3	6	0	0.177662	-0.982212	-0.043965
4	6	0	-1.252989	-0.949392	-0.032253
5	7	0	1.037900	0.024046	-0.251517
6	1	0	0.596367	0.961540	-0.434810
7	7	0	-2.068871	0.095871	-0.238132
8	1	0	-1.588126	1.012308	-0.417239
9	6	0	2.446269	0.011051	-0.284841
10	6	0	3.213104	-1.162329	-0.236319
11	6	0	3.082958	1.261059	-0.384094
12	6	0	4.604181	-1.073645	-0.286553
13	1	0	2.725414	-2.128360	-0.148612
14	6	0	4.472912	1.328607	-0.438046
15	1	0	2.477205	2.166336	-0.401181

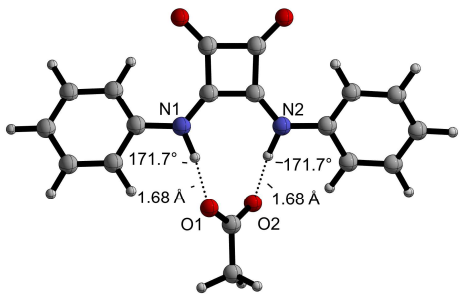


16	6	0	5.244670	0.163935	-0.390665
17	1	0	5.191944	-1.987207	-0.246899
18	1	0	4.955176	2.299804	-0.513421
19	1	0	6.328677	0.219952	-0.431768
20	6	0	-3.475046	0.148733	-0.244403
21	6	0	-4.295898	-0.934666	0.102344
22	6	0	-4.060234	1.371569	-0.617529
23	6	0	-5.681879	-0.781925	0.073282
24	1	0	-3.851540	-1.884985	0.382862
25	6	0	-5.445487	1.508587	-0.637339
26	1	0	-3.420449	2.204971	-0.893217
27	6	0	-6.268013	0.432984	-0.291417
28	1	0	-6.309737	-1.627285	0.342859
29	1	0	-5.881987	2.460682	-0.926778
30	1	0	-7.348698	0.539628	-0.307379
31	8	0	1.021376	-3.324254	0.423050
32	8	0	-2.200142	-3.252174	0.430288
33	6	0	-0.260708	3.340866	-0.020552
34	8	0	0.866922	3.843011	0.171153
35	8	0	-0.473073	2.249368	-0.681588
36	6	0	-1.506531	4.033239	0.536090
37	1	0	-2.074723	3.333720	1.159085
38	1	0	-1.239766	4.914063	1.123881
39	1	0	-2.159087	4.335514	-0.290937

19•OAc “two-atom”-mode

Electronic energy = -1106.1588856, thermal correction to Gibbs free energy = 0.233931 NIMAG = 0

1	6	0	-1.204236	4.302133	0.644425
2	6	0	0.307048	4.282279	0.548404
3	6	0	-1.144016	2.924199	1.192312
4	6	0	0.280721	2.904936	1.099688
5	7	0	-1.975709	1.997220	1.689052



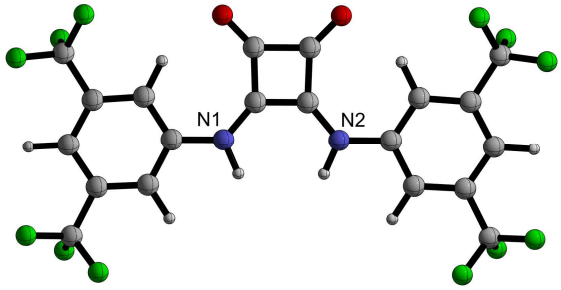
6	1	0	-1.540268	1.217942	2.258447
7	7	0	1.138328	1.909567	1.366132
8	1	0	0.728996	0.940853	1.491610
9	6	0	-3.381991	1.969518	1.622671
10	6	0	-4.123278	2.771728	0.741209
11	6	0	-4.052234	1.056023	2.456608
12	6	0	-5.513712	2.669688	0.717859
13	1	0	-3.618358	3.480252	0.094589
14	6	0	-5.441029	0.960656	2.414673
15	1	0	-3.471830	0.428678	3.127288
16	6	0	-6.183742	1.768141	1.548846
17	1	0	-6.076757	3.299354	0.033782
18	1	0	-5.944528	0.250803	3.065672
19	1	0	-7.266836	1.692771	1.518765
20	6	0	2.544333	1.972269	1.417921
21	6	0	3.252408	3.178865	1.530527
22	6	0	3.249595	0.755299	1.400165
23	6	0	4.644859	3.158922	1.600156
24	1	0	2.720234	4.122980	1.546174
25	6	0	4.640063	0.752376	1.479729
26	1	0	2.695031	-0.175843	1.326246
27	6	0	5.349537	1.952631	1.576140
28	1	0	5.181949	4.100249	1.683006
29	1	0	5.171030	-0.195777	1.463789
30	1	0	6.433965	1.947852	1.636730
31	8	0	-2.073006	5.129965	0.368436
32	8	0	1.156175	5.089527	0.169875
33	6	0	-0.383584	-0.902030	2.660603
34	8	0	-1.062265	-0.024083	3.280480
35	8	0	0.294008	-0.676039	1.609179
36	6	0	-0.408091	-2.332778	3.193573

37	1	0	-0.682043	-2.354444	4.251009
38	1	0	-1.160472	-2.900445	2.632133
39	1	0	0.558599	-2.820756	3.042632

Squaramide 20

"In-in" conformation

Electronic energy = -2226.2655203, thermal correction to Gibbs free energy = 0.184794 NIMAG = 0



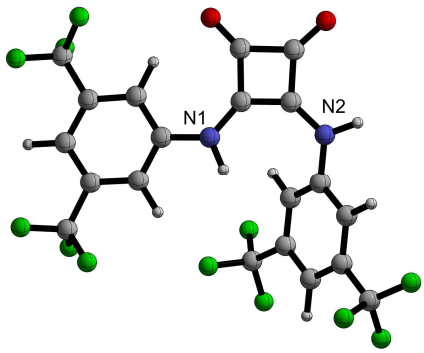
1	6	0	0.758285	-2.265741	0.049241
2	6	0	-0.761465	-2.265503	0.034612
3	6	0	0.707329	-0.780423	0.017221
4	6	0	-0.709379	-0.780311	-0.002317
5	7	0	1.570799	0.255708	0.016378
6	1	0	1.164443	1.186413	0.031928
7	7	0	-1.571938	0.255545	-0.047701
8	1	0	-1.164608	1.184471	-0.100107
9	6	0	2.978165	0.257414	0.001312
10	6	0	3.739475	-0.915215	-0.040092
11	6	0	3.616872	1.505238	0.017627
12	6	0	5.129283	-0.819553	-0.066789
13	1	0	3.255581	-1.887358	-0.055468
14	6	0	5.006166	1.570034	-0.010620
15	1	0	3.032132	2.419383	0.042629
16	6	0	5.782671	0.411763	-0.049821
17	1	0	6.864001	0.469964	-0.078788
18	6	0	-2.979400	0.259071	-0.040951
19	6	0	-3.742628	-0.910788	0.027969
20	6	0	-3.616182	1.506342	-0.110350
21	6	0	-5.132849	-0.813434	0.023758
22	1	0	-3.260131	-1.882865	0.072929
23	6	0	-5.005460	1.572771	-0.111340
24	1	0	-3.029759	2.417626	-0.172225

25	6	0	-5.784010	0.417068	-0.041251
26	1	0	-6.865572	0.476046	-0.049056
27	8	0	1.613779	-3.138711	0.074274
28	8	0	-1.617606	-3.138033	0.051453
29	6	0	5.685531	2.914518	0.047440
30	6	0	5.939864	-2.091446	-0.070142
31	6	0	-5.683824	2.918639	-0.142050
32	6	0	-5.942436	-2.080985	0.137120
33	9	0	6.168956	-2.546410	1.197944
34	9	0	7.158843	-1.926085	-0.646544
35	9	0	5.316733	-3.100163	-0.733762
36	9	0	6.869453	2.920758	-0.619004
37	9	0	4.921670	3.905500	-0.482535
38	9	0	5.962885	3.284794	1.332953
39	9	0	-4.926901	3.868794	-0.750444
40	9	0	-5.946452	3.379787	1.116996
41	9	0	-6.875725	2.877730	-0.793129
42	9	0	-6.097889	-2.465075	1.439331
43	9	0	-7.191887	-1.945429	-0.377515
44	9	0	-5.356356	-3.126357	-0.504069

“In-out” conformation

Electronic energy = -2226.2662923, thermal correction to Gibbs free energy = 0.186210 NIMAG = 0

1	6	0	-0.238316	-4.365979	-0.186449
2	6	0	1.093261	-3.624537	-0.059905
3	6	0	-0.916463	-3.061702	-0.074393
4	6	0	0.302019	-2.363734	0.084966
5	7	0	-2.226175	-2.757923	-0.081724
6	1	0	-2.867266	-3.542753	-0.002301
7	7	0	0.536279	-1.058450	0.346385
8	1	0	-0.287559	-0.491472	0.525077
9	6	0	-2.789502	-1.471026	-0.210236

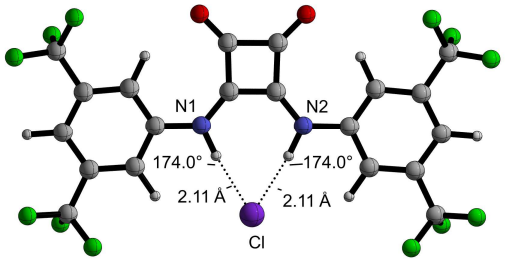


10	6	0	-2.181291	-0.506334	-1.021766
11	6	0	-3.981264	-1.172465	0.461635
12	6	0	-2.735473	0.771843	-1.099644
13	1	0	-1.309319	-0.758683	-1.614980
14	6	0	-4.532967	0.098666	0.339519
15	1	0	-4.463624	-1.926392	1.074716
16	6	0	-3.909535	1.089851	-0.422567
17	1	0	-4.342498	2.079941	-0.501147
18	6	0	1.743868	-0.340449	0.371488
19	6	0	2.991841	-0.937584	0.164163
20	6	0	1.659949	1.037586	0.614795
21	6	0	4.136853	-0.144559	0.210623
22	1	0	3.069506	-2.006130	-0.012229
23	6	0	2.819581	1.804532	0.652338
24	1	0	0.694798	1.507304	0.774375
25	6	0	4.073331	1.228025	0.448670
26	1	0	4.973910	1.829008	0.484254
27	8	0	-0.606556	-5.524298	-0.299528
28	8	0	2.272367	-3.941859	-0.072708
29	6	0	-5.793712	0.439409	1.095793
30	6	0	-2.028769	1.828670	-1.911598
31	6	0	2.708968	3.292637	0.865633
32	6	0	5.474806	-0.788259	-0.054422
33	9	0	-6.558217	-0.653367	1.346499
34	9	0	-6.568841	1.327591	0.420851
35	9	0	-5.514618	1.008005	2.305153
36	9	0	-2.878746	2.775058	-2.380773
37	9	0	-1.089139	2.483007	-1.163974
38	9	0	-1.374393	1.305315	-2.980167
39	9	0	1.622981	3.629853	1.610287
40	9	0	2.589063	3.964463	-0.318094

41	9	0	3.799746	3.805815	1.491658
42	9	0	6.493021	-0.138738	0.568335
43	9	0	5.517337	-2.083374	0.353814
44	9	0	5.776462	-0.792931	-1.387531

20•Cl

Electronic energy = -2686.7002962, thermal correction to Gibbs free energy = 0.180291 NIMAG = 0



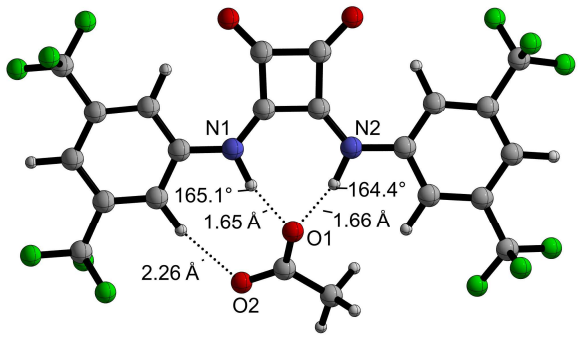
1	6	0	0.761215	-2.507972	-0.010602
2	6	0	-0.757308	-2.509017	-0.010537
3	6	0	0.711594	-1.024599	-0.021603
4	6	0	-0.709729	-1.025574	-0.021522
5	7	0	1.552258	0.024740	-0.028577
6	1	0	1.102872	0.966279	-0.032901
7	7	0	-1.551827	0.022616	-0.028488
8	1	0	-1.103725	0.964772	-0.032888
9	6	0	2.952135	0.045998	-0.033433
10	6	0	3.742039	-1.110528	-0.037832
11	6	0	3.565918	1.309661	-0.041086
12	6	0	5.130016	-0.984938	-0.052448
13	1	0	3.277481	-2.092780	-0.037518
14	6	0	4.953167	1.402619	-0.055577
15	1	0	2.950144	2.204369	-0.044751
16	6	0	5.756494	0.260684	-0.057997
17	1	0	6.836510	0.341921	-0.075970
18	6	0	-2.951733	0.041966	-0.032837
19	6	0	-3.740063	-1.115637	-0.037220
20	6	0	-3.567246	1.304787	-0.040046
21	6	0	-5.128213	-0.991938	-0.051335
22	1	0	-3.274167	-2.097255	-0.037253
23	6	0	-4.954629	1.395854	-0.054064
24	1	0	-2.952700	2.200339	-0.043731
25	6	0	-5.756397	0.252829	-0.056430

26	1	0	-6.836529	0.332587	-0.074016
27	8	0	1.621685	-3.382291	-0.003536
28	8	0	-1.616572	-3.384521	-0.003404
29	17	0	-0.001686	2.763795	-0.041053
30	6	0	5.966265	-2.238169	-0.016193
31	6	0	5.604961	2.760387	-0.020758
32	6	0	-5.962711	-2.246331	-0.015031
33	6	0	-5.608238	2.752739	-0.018764
34	9	0	6.791130	2.779793	-0.686385
35	9	0	6.151433	-2.687300	1.262259
36	9	0	7.206173	-2.052061	-0.540836
37	9	0	5.393344	-3.263381	-0.701599
38	9	0	4.824548	3.728570	-0.567617
39	9	0	5.876380	3.159687	1.258696
40	9	0	-5.879472	3.151584	1.260855
41	9	0	-4.829414	3.722019	-0.565994
42	9	0	-6.794790	2.770614	-0.683738
43	9	0	-7.203149	-2.061785	-0.538954
44	9	0	-6.146558	-2.696124	1.263383
45	9	0	-5.388720	-3.270531	-0.701068

20•OAc “one-atom”-mode

Electronic energy = -2455.0573423, thermal correction to Gibbs free energy = 0.225318 NIMAG = 0

1	6	0	0.747701	-2.690377	-0.105564
2	6	0	-0.769051	-2.686700	-0.114481
3	6	0	0.705753	-1.209586	-0.001303
4	6	0	-0.719957	-1.208923	-0.010744
5	7	0	1.545367	-0.165400	0.070168
6	1	0	1.077874	0.783767	0.153483
7	7	0	-1.560733	-0.161322	0.058955
8	1	0	-1.100685	0.782181	0.126897
9	6	0	2.944874	-0.154157	0.068806

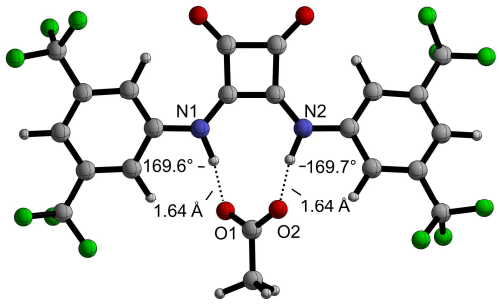


10	6	0	3.730629	-1.314954	0.099787
11	6	0	3.563761	1.106575	0.036388
12	6	0	5.118963	-1.196702	0.098329
13	1	0	3.261692	-2.294797	0.111535
14	6	0	4.953053	1.190176	0.044106
15	1	0	2.947921	2.005027	-0.015329
16	6	0	5.752243	0.046620	0.074835
17	1	0	6.832753	0.122167	0.076528
18	6	0	-2.958188	-0.147086	0.052799
19	6	0	-3.748067	-1.296642	-0.087350
20	6	0	-3.578833	1.105962	0.188582
21	6	0	-5.135992	-1.172179	-0.096342
22	1	0	-3.281103	-2.272174	-0.192527
23	6	0	-4.965778	1.200053	0.172799
24	1	0	-2.969722	1.996628	0.298361
25	6	0	-5.766778	0.065184	0.033270
26	1	0	-6.846924	0.146081	0.015575
27	8	0	1.604886	-3.568015	-0.161083
28	8	0	-1.629930	-3.560949	-0.182545
29	6	0	5.952562	-2.448564	0.180522
30	6	0	5.593379	2.550555	-0.043463
31	6	0	-5.972902	-2.421092	-0.201867
32	6	0	-5.617430	2.545059	0.359780
33	9	0	6.878100	2.553778	0.401599
34	9	0	6.175967	-2.827674	1.476434
35	9	0	7.178653	-2.295253	-0.388146
36	9	0	5.361155	-3.509601	-0.430214
37	9	0	5.630371	3.013304	-1.330543
38	9	0	4.920531	3.487537	0.677854
39	9	0	-5.904027	2.792030	1.673907
40	9	0	-4.829121	3.569911	-0.059584

41	9	0	-6.795081	2.646186	-0.313134
42	9	0	-7.187433	-2.186838	-0.766682
43	9	0	-6.219391	-2.970502	1.026410
44	9	0	-5.371033	-3.390682	-0.940220
45	6	0	0.245673	3.115315	-0.365148
46	6	0	-0.977907	3.926271	-0.788762
47	1	0	-0.684214	4.853507	-1.284607
48	1	0	-1.593232	3.329857	-1.472008
49	1	0	-1.592774	4.159306	0.087427
50	8	0	-0.002898	2.021200	0.281974
51	8	0	1.393130	3.521126	-0.641873

20•OAc “two-atom”-mode

Electronic energy = -2455.0588816, thermal correction to Gibbs free energy = 0.224242 NIMAG = 0



1	6	0	0.748925	-2.624362	-0.057168
2	6	0	-0.765910	-2.618767	-0.005169
3	6	0	0.708262	-1.140087	-0.074276
4	6	0	-0.714533	-1.134572	0.003832
5	7	0	1.556361	-0.103777	-0.185015
6	1	0	1.137467	0.848197	-0.415645
7	7	0	-1.555103	-0.091943	0.111407
8	1	0	-1.129785	0.859744	0.331733
9	6	0	2.954907	-0.119999	-0.126751
10	6	0	3.704998	-1.258345	0.200288
11	6	0	3.620921	1.090524	-0.391517
12	6	0	5.095826	-1.172361	0.247728
13	1	0	3.210127	-2.206328	0.386997
14	6	0	5.008815	1.145910	-0.333090
15	1	0	3.040352	1.971209	-0.647309
16	6	0	5.769725	0.020232	-0.010435
17	1	0	6.850989	0.070249	0.027948
18	6	0	-2.954277	-0.101549	0.067395

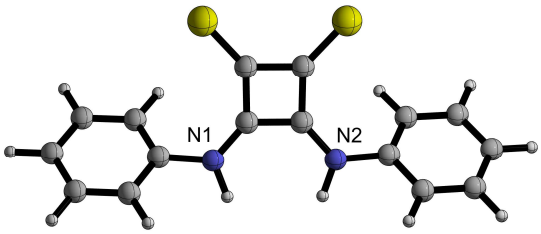
19	6	0	-3.712050	-1.235641	-0.257835
20	6	0	-3.612288	1.111990	0.336124
21	6	0	-5.101994	-1.141761	-0.301373
22	1	0	-3.222893	-2.183069	-0.459810
23	6	0	-5.000297	1.176021	0.279267
24	1	0	-3.025057	1.992135	0.578433
25	6	0	-5.768810	0.053471	-0.034348
26	1	0	-6.849385	0.112602	-0.080925
27	8	0	1.603343	-3.506963	-0.065618
28	8	0	-1.626549	-3.495219	0.008980
29	6	0	5.874465	-2.401826	0.637668
30	6	0	5.703313	2.460407	-0.573198
31	6	0	-5.897323	-2.385459	-0.601625
32	6	0	-5.688643	2.473367	0.612432
33	9	0	6.935993	2.301086	-1.126647
34	9	0	5.885443	-2.587470	1.993131
35	9	0	7.175004	-2.343454	0.247722
36	9	0	5.350311	-3.538546	0.103652
37	9	0	5.000531	3.281682	-1.397106
38	9	0	5.893399	3.154514	0.590699
39	9	0	-5.985461	2.564404	1.944990
40	9	0	-4.927389	3.560081	0.315847
41	9	0	-6.867238	2.620374	-0.050933
42	9	0	-7.123160	-2.108878	-1.120399
43	9	0	-6.115160	-3.132273	0.523986
44	9	0	-5.267679	-3.205391	-1.485811
45	6	0	0.013120	2.978490	-0.052099
46	6	0	0.052084	4.501953	-0.027320
47	1	0	0.752540	4.818418	0.755328
48	1	0	0.402723	4.900800	-0.981820
49	1	0	-0.931026	4.911864	0.218364

50	8	0	-0.741074	2.391123	0.786290
51	8	0	0.755329	2.375214	-0.889826

Thiosquaramide 21

“In-in” conformation

Electronic energy = -1523.2833342, thermal correction to Gibbs free energy = 0.189360 NIMAG = 0

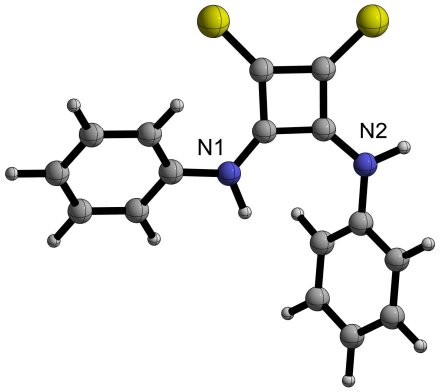


1	6	0	-2.497125	2.645000	0.162599
2	6	0	-1.007136	2.665120	0.178903
3	6	0	-2.458082	1.376152	0.888399
4	6	0	-1.026614	1.393126	0.897961
5	7	0	-3.338867	0.540025	1.440952
6	1	0	-2.970559	-0.188751	2.045124
7	7	0	-0.130413	0.578414	1.459861
8	1	0	-0.482316	-0.138835	2.087245
9	6	0	-4.754291	0.532428	1.275888
10	6	0	-5.334179	0.798932	0.032159
11	6	0	-5.548332	0.200144	2.379030
12	6	0	-6.722257	0.763163	-0.092102
13	1	0	-4.706762	1.017556	-0.823818
14	6	0	-6.933887	0.155544	2.238037
15	1	0	-5.082478	-0.007755	3.338300
16	6	0	-7.525090	0.444916	1.005542
17	1	0	-7.175086	0.971811	-1.056886
18	1	0	-7.550646	-0.097942	3.095146
19	1	0	-8.605308	0.412951	0.899031
20	6	0	1.278526	0.569620	1.255634
21	6	0	1.821517	0.845755	-0.003142
22	6	0	2.105564	0.222623	2.329835
23	6	0	3.204482	0.803630	-0.171812
24	1	0	1.169098	1.074054	-0.837771
25	6	0	3.485618	0.171537	2.144092

26	1	0	1.669771	0.006236	3.301319
27	6	0	4.039812	0.469552	0.896445
28	1	0	3.627416	1.018598	-1.148726
29	1	0	4.127554	-0.094971	2.978458
30	1	0	5.115829	0.431311	0.755297
31	16	0	-3.637965	3.718661	-0.354395
32	16	0	0.116647	3.774890	-0.298162

“In-out” conformation

Electronic energy = -1523.2880487, thermal correction to Gibbs free energy = 0.190348 NIMAG = 0

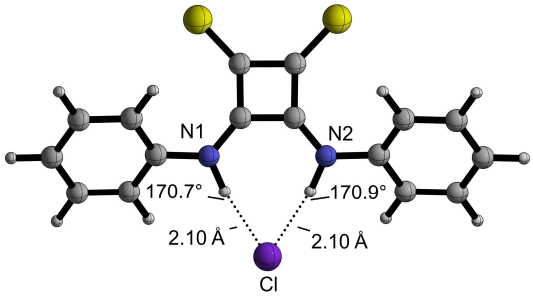


1	6	0	-1.890539	1.737729	1.871495
2	6	0	-0.617577	1.582911	1.117108
3	6	0	-2.622383	1.425004	0.659953
4	6	0	-1.409860	1.345206	-0.097632
5	7	0	-3.930026	1.306087	0.444655
6	1	0	-4.526693	1.573725	1.225866
7	7	0	-1.171950	1.121340	-1.391723
8	1	0	-1.974784	0.845418	-1.954123
9	6	0	-4.550230	0.825128	-0.740754
10	6	0	-4.019850	-0.286689	-1.407217
11	6	0	-5.702822	1.457629	-1.217819
12	6	0	-4.619301	-0.730425	-2.586485
13	1	0	-3.177778	-0.825019	-0.981031
14	6	0	-6.304839	0.989792	-2.384048
15	1	0	-6.109346	2.313031	-0.686471
16	6	0	-5.759223	-0.093450	-3.079133
17	1	0	-4.204629	-1.590142	-3.103986
18	1	0	-7.197275	1.482938	-2.757529
19	1	0	-6.228742	-0.446397	-3.992109
20	6	0	0.057814	1.252162	-2.093924
21	6	0	0.964098	2.270893	-1.783102
22	6	0	0.309624	0.371617	-3.152973

23	6	0	2.143278	2.380509	-2.518388
24	1	0	0.741595	2.973645	-0.989064
25	6	0	1.485947	0.500935	-3.888049
26	1	0	-0.406657	-0.410903	-3.388051
27	6	0	2.410065	1.499219	-3.568508
28	1	0	2.848431	3.170225	-2.276366
29	1	0	1.682140	-0.184451	-4.707258
30	1	0	3.327358	1.595952	-4.141606
31	16	0	-2.345980	2.084543	3.418133
32	16	0	0.973986	1.586164	1.550352

21•Cl

Electronic energy = -1983.7156565, thermal correction to Gibbs free energy = 0.186305 NIMAG = 0



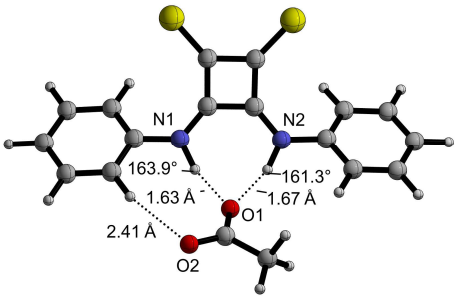
1	6	0	-0.739277	1.644892	0.633548
2	6	0	0.745234	1.634704	0.661412
3	6	0	-0.718148	0.232210	0.254910
4	6	0	0.720878	0.226923	0.268530
5	7	0	-1.574564	-0.765393	0.059583
6	1	0	-1.150512	-1.718131	-0.012417
7	7	0	1.576292	-0.772211	0.075224
8	1	0	1.151202	-1.723591	-0.006736
9	6	0	-2.983896	-0.704614	-0.067569
10	6	0	-3.624083	0.379759	-0.679010
11	6	0	-3.727319	-1.805053	0.380907
12	6	0	-5.012407	0.372056	-0.803396
13	1	0	-3.040662	1.211301	-1.056239
14	6	0	-5.113382	-1.804709	0.240263
15	1	0	-3.215141	-2.646047	0.839966
16	6	0	-5.762252	-0.713499	-0.343931
17	1	0	-5.507989	1.215751	-1.275229
18	1	0	-5.686759	-2.656973	0.593435
19	1	0	-6.843102	-0.714180	-0.450085

20	6	0	2.984487	-0.708513	-0.058910
21	6	0	3.619059	0.386516	-0.657563
22	6	0	3.732684	-1.815662	0.364445
23	6	0	5.006020	0.381618	-0.795485
24	1	0	3.032076	1.223447	-1.017053
25	6	0	5.117351	-1.812181	0.210433
26	1	0	3.225363	-2.664996	0.813431
27	6	0	5.760511	-0.711278	-0.361856
28	1	0	5.496590	1.233222	-1.258292
29	1	0	5.694268	-2.670209	0.543281
30	1	0	6.840197	-0.710136	-0.479191
31	17	0	-0.003958	-3.478078	-0.124639
32	16	0	-1.870735	2.791193	1.021465
33	16	0	1.877595	2.755873	1.115060

21•OAc “one-atom”-mode

Electronic energy = -1752.0717305, thermal correction to Gibbs free energy = 0.229912 NIMAG = 0

1	6	0	-0.357664	-2.008282	0.338505
2	6	0	-1.839362	-1.963448	0.348120
3	6	0	-0.337280	-0.596964	-0.055724
4	6	0	-1.781196	-0.559148	-0.046318
5	7	0	0.527451	0.385709	-0.269347
6	1	0	0.085084	1.351777	-0.358901
7	7	0	-2.612188	0.459252	-0.244045
8	1	0	-2.151366	1.403609	-0.321516
9	6	0	1.934695	0.323436	-0.388403
10	6	0	2.595866	-0.799262	-0.902383
11	6	0	2.658614	1.472975	-0.036067
12	6	0	3.984672	-0.780118	-1.021416
13	1	0	2.029005	-1.671759	-1.205189
14	6	0	4.045504	1.479690	-0.170223
15	1	0	2.120398	2.343576	0.334984

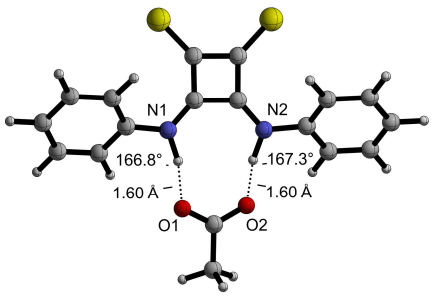


16	6	0	4.715969	0.352528	-0.654057
17	1	0	4.495698	-1.653812	-1.416457
18	1	0	4.604449	2.369163	0.107560
19	1	0	5.797462	0.360480	-0.755064
20	6	0	-4.019334	0.413612	-0.389673
21	6	0	-4.660009	-0.664402	-1.013329
22	6	0	-4.764614	1.518194	0.045741
23	6	0	-6.045346	-0.645579	-1.164812
24	1	0	-4.076770	-1.500031	-1.381851
25	6	0	-6.147968	1.529646	-0.120489
26	1	0	-4.258917	2.354406	0.518661
27	6	0	-6.795433	0.445543	-0.718988
28	1	0	-6.538284	-1.484968	-1.647157
29	1	0	-6.720144	2.386592	0.223386
30	1	0	-7.873954	0.455685	-0.846266
31	6	0	-0.757318	3.611023	0.321388
32	8	0	0.367155	3.945209	0.745370
33	8	0	-0.977009	2.587463	-0.443083
34	6	0	-1.992615	4.418556	0.719311
35	1	0	-1.714310	5.421117	1.051406
36	1	0	-2.704003	4.478615	-0.109233
37	1	0	-2.491341	3.906455	1.551888
38	16	0	0.735048	-3.186079	0.752563
39	16	0	-3.003623	-3.063613	0.782037

21•OAc “two-atom”-mode

Electronic energy = -1752.0740245, thermal correction to Gibbs free energy = 0.227876 NIMAG = 0

1	6	0	-1.172337	4.314060	1.518044
2	6	0	0.304930	4.319803	1.537535
3	6	0	-1.149851	2.852671	1.615797
4	6	0	0.294588	2.856870	1.603639
5	7	0	-2.024308	1.868359	1.772686



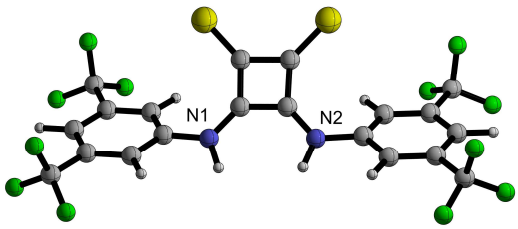
6	1	0	-1.677854	0.907394	2.099447
7	7	0	1.179066	1.875329	1.699257
8	1	0	0.843000	0.877246	1.902737
9	6	0	-3.426899	1.964259	1.589014
10	6	0	-3.978032	2.739605	0.560646
11	6	0	-4.261187	1.199536	2.416756
12	6	0	-5.360849	2.775221	0.390044
13	1	0	-3.326137	3.296753	-0.102371
14	6	0	-5.641818	1.237051	2.230810
15	1	0	-3.820259	0.584237	3.194763
16	6	0	-6.198628	2.030313	1.223720
17	1	0	-5.783222	3.380466	-0.407236
18	1	0	-6.284140	0.647000	2.878615
19	1	0	-7.275212	2.058389	1.082399
20	6	0	2.578628	1.991410	1.492114
21	6	0	3.106429	2.816133	0.490697
22	6	0	3.431394	1.192772	2.266305
23	6	0	4.485631	2.864675	0.294370
24	1	0	2.440305	3.400776	-0.133237
25	6	0	4.808063	1.244045	2.055941
26	1	0	3.007577	0.539825	3.022848
27	6	0	5.341975	2.084996	1.075566
28	1	0	4.890118	3.507761	-0.482277
29	1	0	5.464804	0.626920	2.662699
30	1	0	6.415393	2.123629	0.914074
31	6	0	-0.389555	-1.191768	2.614399
32	8	0	-1.497332	-0.574267	2.685336
33	8	0	0.699842	-0.692892	2.193719
34	6	0	-0.375187	-2.658410	3.037067
35	1	0	-1.137781	-2.853091	3.795078
36	1	0	-0.604572	-3.275387	2.159532

37	1	0	0.611032	-2.949596	3.406702
38	16	0	-2.311455	5.522606	1.527622
39	16	0	1.433353	5.535682	1.616556

Thiosquaramide 22

"In-in" conformation

Electronic energy = -2872.1744893, thermal correction to Gibbs free energy = 0.178192 NIMAG = 0



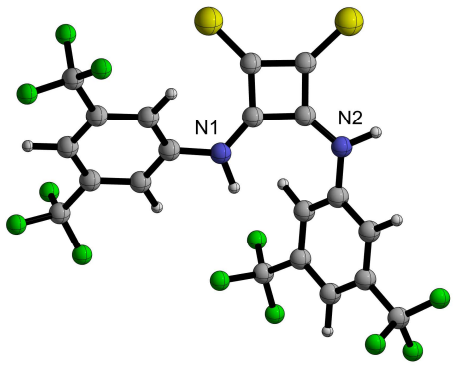
1	6	0	0.742969	-1.200202	1.173476
2	6	0	-0.750808	-1.182143	1.195663
3	6	0	0.708514	-0.081595	0.230576
4	6	0	-0.717143	-0.061158	0.257647
5	7	0	1.609258	0.709362	-0.363218
6	1	0	1.266900	1.537794	-0.840892
7	7	0	-1.621214	0.762873	-0.287775
8	1	0	-1.285041	1.623764	-0.709330
9	6	0	3.014881	0.523457	-0.387679
10	6	0	3.566644	-0.752192	-0.529557
11	6	0	3.837630	1.649826	-0.313325
12	6	0	4.953443	-0.889250	-0.554685
13	1	0	2.926563	-1.616780	-0.647474
14	6	0	5.220666	1.488615	-0.357604
15	1	0	3.401680	2.638634	-0.216569
16	6	0	5.792263	0.220702	-0.463378
17	1	0	6.868729	0.101903	-0.496337
18	6	0	-3.021129	0.556258	-0.337138
19	6	0	-3.545351	-0.727366	-0.514789
20	6	0	-3.868357	1.664502	-0.258624
21	6	0	-4.927656	-0.891415	-0.574354
22	1	0	-2.885676	-1.576785	-0.636869
23	6	0	-5.246440	1.476262	-0.338710
24	1	0	-3.455628	2.660275	-0.134421

25	6	0	-5.790520	0.199924	-0.482294
26	1	0	-6.863235	0.060937	-0.544296
27	6	0	6.110802	2.698619	-0.230809
28	6	0	5.551364	-2.269479	-0.654910
29	6	0	-6.164398	2.665303	-0.212794
30	6	0	-5.495733	-2.280567	-0.715891
31	9	0	5.695136	-2.846044	0.574485
32	9	0	6.785093	-2.257334	-1.222994
33	9	0	4.779312	-3.113260	-1.388832
34	9	0	7.297551	2.532847	-0.869933
35	9	0	5.533193	3.818602	-0.739244
36	9	0	6.407228	2.973426	1.073794
37	9	0	-5.597006	3.806791	-0.683417
38	9	0	-6.501764	2.907821	1.088349
39	9	0	-7.329994	2.488515	-0.887236
40	9	0	-5.668018	-2.879975	0.498842
41	9	0	-6.710811	-2.281516	-1.323308
42	9	0	-4.685245	-3.097995	-1.438085
43	16	0	1.882575	-2.046734	2.003897
44	16	0	-1.888967	-2.001290	2.055208

“In-out” conformation

Electronic energy = -2872.1772205, thermal correction to Gibbs free energy = 0.181235 NIMAG = 0

1	6	0	-1.974551	2.207063	2.005019
2	6	0	-0.700648	1.968211	1.262125
3	6	0	-2.706996	1.872844	0.796995
4	6	0	-1.498787	1.730341	0.052740
5	7	0	-4.022022	1.777831	0.581732
6	1	0	-4.614571	2.107869	1.342080
7	7	0	-1.248712	1.462108	-1.234388
8	1	0	-2.047756	1.239094	-1.821150
9	6	0	-4.647036	1.209734	-0.551485

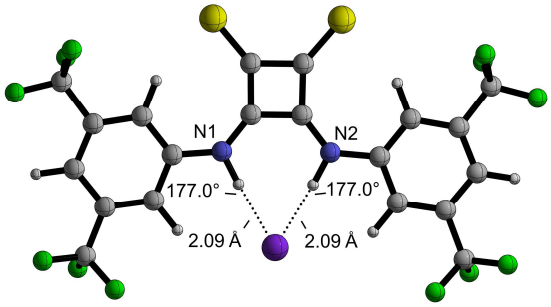


10	6	0	-4.105607	0.071635	-1.155871
11	6	0	-5.829172	1.776263	-1.041079
12	6	0	-4.718995	-0.457875	-2.292175
13	1	0	-3.245936	-0.424776	-0.717849
14	6	0	-6.440042	1.210720	-2.155175
15	1	0	-6.257933	2.647402	-0.557865
16	6	0	-5.885317	0.103794	-2.803699
17	1	0	-6.366515	-0.322713	-3.676039
18	6	0	0.008308	1.472642	-1.888602
19	6	0	0.972671	2.436319	-1.584084
20	6	0	0.237656	0.527498	-2.891691
21	6	0	2.186572	2.416714	-2.268662
22	1	0	0.768210	3.203288	-0.848587
23	6	0	1.452812	0.538842	-3.572648
24	1	0	-0.522065	-0.208672	-3.133619
25	6	0	2.442525	1.470991	-3.260593
26	1	0	3.384777	1.474339	-3.795359
27	6	0	-7.698505	1.828708	-2.715727
28	6	0	-4.088924	-1.647280	-2.975524
29	6	0	1.719701	-0.509548	-4.622364
30	6	0	3.247055	3.425810	-1.908037
31	9	0	-8.340119	2.608514	-1.810791
32	9	0	-8.582216	0.885106	-3.134431
33	9	0	-7.430316	2.616657	-3.796523
34	9	0	-4.986955	-2.370137	-3.687170
35	9	0	-3.114465	-1.258614	-3.851464
36	9	0	-3.497332	-2.490872	-2.090682
37	9	0	0.584613	-0.902027	-5.257999
38	9	0	2.270435	-1.636351	-4.081534
39	9	0	2.584887	-0.075579	-5.574962
40	9	0	4.083619	3.688039	-2.945498

41	9	0	2.715329	4.611673	-1.510893
42	9	0	4.029428	2.987514	-0.878478
43	16	0	-2.421240	2.632696	3.527644
44	16	0	0.884460	1.899106	1.694186

22•Cl

Electronic energy = -3332.6091119, thermal correction to Gibbs free energy = 0.174669 NIMAG = 0



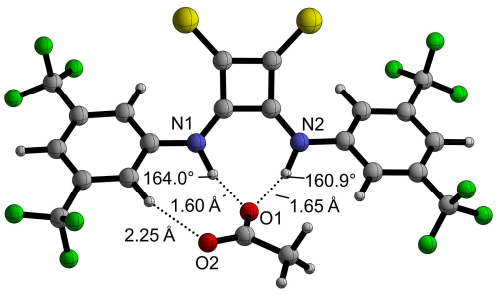
1	6	0	0.743838	-2.465832	-0.057058
2	6	0	-0.744097	-2.465429	-0.007384
3	6	0	0.720845	-1.003596	-0.054228
4	6	0	-0.720903	-1.003342	-0.027207
5	7	0	1.541258	0.052472	-0.065665
6	1	0	1.058376	0.981040	-0.065492
7	7	0	-1.541137	0.052866	-0.024186
8	1	0	-1.058190	0.981395	-0.032465
9	6	0	2.942841	0.163531	-0.055658
10	6	0	3.814768	-0.926671	-0.033431
11	6	0	3.458588	1.471112	-0.066012
12	6	0	5.190443	-0.697164	-0.021376
13	1	0	3.425055	-1.943340	-0.032775
14	6	0	4.833726	1.669297	-0.054770
15	1	0	2.775797	2.315741	-0.086666
16	6	0	5.720748	0.590268	-0.029472
17	1	0	6.791742	0.750760	-0.022980
18	6	0	-2.942723	0.163946	-0.022960
19	6	0	-3.814771	-0.926352	-0.044657
20	6	0	-3.458457	1.471302	-0.008032
21	6	0	-5.190369	-0.697026	-0.048342
22	1	0	-3.425182	-1.942890	-0.057374
23	6	0	-4.833804	1.669461	-0.015491
24	1	0	-2.775530	2.316082	0.001458
25	6	0	-5.720787	0.590511	-0.032223

26	1	0	-6.791674	0.751297	-0.041178
27	17	0	-0.000082	2.781712	-0.052928
28	6	0	6.101251	-1.898093	0.014639
29	6	0	5.382161	3.072433	-0.019108
30	6	0	-6.102374	-1.897629	-0.054341
31	6	0	-5.381221	3.072196	0.043677
32	9	0	6.557318	3.181290	-0.695589
33	9	0	5.956359	-2.607902	1.171800
34	9	0	7.413642	-1.566862	-0.080530
35	9	0	5.836587	-2.768873	-1.000373
36	9	0	4.526856	3.980774	-0.554496
37	9	0	5.635741	3.484077	1.259538
38	9	0	-5.628129	3.465535	1.329345
39	9	0	-4.526827	3.987424	-0.482045
40	9	0	-6.558896	3.192603	-0.625937
41	9	0	-7.408530	-1.565421	-0.212784
42	9	0	-6.014658	-2.605242	1.110179
43	9	0	-5.789775	-2.770457	-1.053356
44	16	0	1.821864	-3.716635	-0.104806
45	16	0	-1.822162	-3.715448	0.057397

22•OAc “one-atom”-mode

Electronic energy = -3100.9683698, thermal correction to Gibbs free energy = 0.219652 NIMAG = 0

1	6	0	0.696387	-2.097590	0.988767
2	6	0	-0.791008	-2.049481	1.011054
3	6	0	0.703077	-0.787085	0.332915
4	6	0	-0.734805	-0.750278	0.348778
5	7	0	1.560701	0.148463	-0.062081
6	1	0	1.105933	1.084946	-0.319973
7	7	0	-1.570391	0.219096	-0.026045
8	1	0	-1.109989	1.140535	-0.265223
9	6	0	2.961984	0.082609	-0.142522



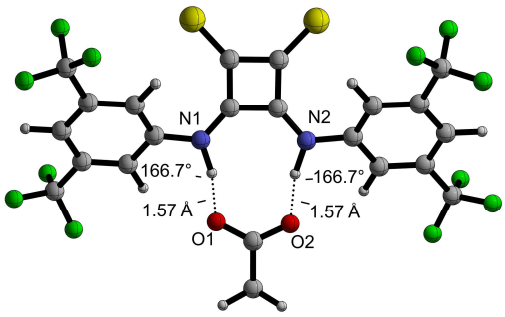
10	6	0	3.649070	-1.112637	-0.387859
11	6	0	3.664696	1.289343	-0.034880
12	6	0	5.038847	-1.091554	-0.475149
13	1	0	3.106975	-2.041182	-0.512469
14	6	0	5.054813	1.282031	-0.138773
15	1	0	3.110250	2.213967	0.129150
16	6	0	5.759805	0.097670	-0.348008
17	1	0	6.840157	0.100583	-0.424833
18	6	0	-2.969552	0.143615	-0.133941
19	6	0	-3.622411	-1.049915	-0.465438
20	6	0	-3.709477	1.320520	0.031965
21	6	0	-5.010736	-1.059530	-0.579497
22	1	0	-3.052561	-1.951275	-0.649110
23	6	0	-5.095011	1.289178	-0.104177
24	1	0	-3.203106	2.250457	0.264838
25	6	0	-5.764130	0.100170	-0.395431
26	1	0	-6.842411	0.082373	-0.499393
27	6	0	5.775760	-2.389860	-0.674640
28	6	0	5.780670	2.598032	-0.037050
29	6	0	-5.708927	-2.361166	-0.877508
30	6	0	-5.883472	2.553065	0.121122
31	9	0	7.129485	2.454631	0.009083
32	9	0	6.062217	-2.997948	0.516221
33	9	0	6.964184	-2.220245	-1.313067
34	9	0	5.058046	-3.288457	-1.399846
35	9	0	5.508296	3.410446	-1.101207
36	9	0	5.417471	3.297270	1.075381
37	9	0	-6.224731	2.711409	1.435222
38	9	0	-5.186518	3.666478	-0.230554
39	9	0	-7.045780	2.569322	-0.582390
40	9	0	-6.890798	-2.179657	-1.523720

41	9	0	-5.996058	-3.052751	0.265774
42	9	0	-4.955224	-3.189477	-1.647858
43	6	0	0.318881	3.373970	0.052989
44	6	0	-0.890219	4.234259	0.409428
45	1	0	-1.403345	3.778949	1.265711
46	1	0	-0.585116	5.245424	0.685752
47	1	0	-1.598757	4.268970	-0.423416
48	8	0	0.056562	2.269088	-0.577553
49	8	0	1.466546	3.735890	0.378111
50	16	0	-1.948525	-3.028075	1.674199
51	16	0	1.798786	-3.166168	1.602123

22•OAc “two-atom”-mode

Electronic energy = -3100.9713473, thermal correction to Gibbs free energy = 0.216797 NIMAG = 0

1	6	0	0.741168	-1.812475	1.102496
2	6	0	-0.740537	-1.831792	1.070901
3	6	0	0.719008	-0.523527	0.408085
4	6	0	-0.720095	-0.530460	0.397888
5	7	0	1.599184	0.389976	0.013655
6	1	0	1.259486	1.373043	-0.278149
7	7	0	-1.600631	0.389410	0.018047
8	1	0	-1.262261	1.389182	-0.212587
9	6	0	2.994138	0.206626	-0.065856
10	6	0	3.558857	-1.021985	-0.430695
11	6	0	3.818854	1.316954	0.153231
12	6	0	4.944347	-1.136168	-0.524676
13	1	0	2.923408	-1.866353	-0.663498
14	6	0	5.200665	1.180964	0.039925
15	1	0	3.372438	2.274443	0.398070
16	6	0	5.780625	-0.045835	-0.283922
17	1	0	6.855997	-0.144161	-0.372166
18	6	0	-2.995230	0.208411	-0.066799



19	6	0	-3.559096	-1.007694	-0.472338
20	6	0	-3.820815	1.309571	0.192363
21	6	0	-4.944681	-1.120639	-0.566449
22	1	0	-2.922513	-1.842836	-0.733823
23	6	0	-5.202737	1.175324	0.078132
24	1	0	-3.375296	2.258669	0.469458
25	6	0	-5.781855	-0.040407	-0.286179
26	1	0	-6.857363	-0.137062	-0.374419
27	6	0	5.549907	-2.472631	-0.863935
28	6	0	6.082011	2.369611	0.320111
29	6	0	-5.548933	-2.445996	-0.948584
30	6	0	-6.084493	2.352232	0.403049
31	9	0	7.265674	2.304487	-0.345346
32	9	0	5.787462	-3.220307	0.255633
33	9	0	6.744003	-2.353103	-1.503993
34	9	0	4.743326	-3.221746	-1.661413
35	9	0	5.492724	3.544708	-0.026782
36	9	0	6.392061	2.472285	1.648142
37	9	0	-6.383071	2.412403	1.736321
38	9	0	-5.500894	3.539206	0.088226
39	9	0	-7.273780	2.305077	-0.253800
40	9	0	-6.747681	-2.307888	-1.575917
41	9	0	-5.776415	-3.233409	0.145586
42	9	0	-4.745673	-3.164077	-1.777480
43	6	0	0.002339	3.476064	-0.721259
44	6	0	0.009873	4.979037	-0.972138
45	1	0	0.056896	5.492005	-0.003763
46	1	0	0.885102	5.273082	-1.555790
47	1	0	-0.907549	5.293287	-1.475571
48	8	0	-1.123307	2.922274	-0.519474
49	8	0	1.122746	2.877305	-0.705418

50	16	0	-1.877027	-2.860249	1.696492
51	16	0	1.876198	-2.791342	1.805804

Acetate

Electronic energy = -228.7482782, thermal correction to Gibbs free energy = 0.020278 NIMAG = 0

1	6	0	-1.228279	0.505629	0.242930
2	6	0	-2.774086	0.505644	0.252245
3	1	0	-3.170264	1.402200	0.739779
4	1	0	-3.133914	0.503846	-0.785273
5	1	0	-3.170284	-0.389193	0.742909
6	8	0	-0.657350	1.637304	0.222428
7	8	0	-0.657325	-0.626103	0.226771

Chloride

Electronic energy = -460.4033715

1	17	0	-0.311558	0.557789	0.000000

X-ray crystal structures

O(=P)-cyclodiphosph(V)azane 4

Identification code	fw_phos	
Empirical formula	C20 H30 N4 O2 P2	
Moiety formula	C20 H30 N4 O2 P2	
Formula weight	420.42	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.561(4) Å	α= 90°.
	b = 5.5343(7) Å	β= 105.037(13)°.
	c = 33.019(7) Å	γ = 90°.
Volume	4158.1(13) $Å^3$	
Z	8	
Density (calculated)	1.343 Mg/m^3	
Absorption coefficient	2.093 mm^{-1}	
F(000)	1792	
Crystal size	0.250 x 0.150 x 0.100 mm^3	
Theta range for data collection	2.771 to 72.280°.	
Index ranges	-28<=h<=28, -6<=k<=6, -32<=l<=40	
Reflections collected	26502	
Independent reflections	4075 [R(int) = 0.0329]	
Completeness to theta = 67.679°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6159	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4075 / 0 / 267	
Goodness-of-fit on F^2	1.246	
Final R indices [I>2sigma(I)]	R1 = 0.0432, wR2 = 0.0975	
R indices (all data)	R1 = 0.0449, wR2 = 0.0982	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.387 and -0.415 $e.Å^{-3}$	

S(=P)-cyclodiphosph(V)azane 11

Identification code	fwfr22	
Empirical formula	C20 H30 N4 P2 S2	
Moiety formula	C20 H30 N4 P2 S2	
Formula weight	452.54	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 15.3034(3) Å	α= 90°.
	b = 17.1558(3) Å	β= 90°.
	c = 17.7407(3) Å	γ = 90°.
Volume	4657.68(15) $Å^3$	
Z	8	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	3.471 mm^{-1}	
F(000)	1920	
Crystal size	0.400 x 0.300 x 0.070 mm^3	
Theta range for data collection	4.605 to 78.884°.	
Index ranges	-15<=h<=18, -21<=k<=21, -21<=l<=21	
Reflections collected	29498	
Independent reflections	4751 [R(int) = 0.0306]	
Completeness to theta = 67.679°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7542 and 0.4766	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4751 / 0 / 267	
Goodness-of-fit on F^2	1.080	
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0729	
R indices (all data)	R1 = 0.0306, wR2 = 0.0752	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.262 and -0.342 $e.Å^{-3}$	

cis-S(=P)-cyclodiphosph(V)azane 12

Identification code	fw_mjo4e	
Empirical formula	C28 H34 F12 N4 O2 P2 S2	
Moiety formula	C24 H26 F12 N4 P2 S2, C4 H8 O2	
Formula weight	812.65	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.1480(6) Å	α= 90°.
	b = 17.8831(19) Å	β= 93.484(9)°.
	c = 22.334(2) Å	γ = 90°.
Volume	3647.0(6) $Å^3$	
Z	4	
Density (calculated)	1.480 Mg/m^3	
Absorption coefficient	3.018 mm^{-1}	
F(000)	1664	
Crystal size	0.200 x 0.100 x 0.100 mm^3	
Theta range for data collection	3.168 to 72.160°.	
Index ranges	-11<=h<=11, -21<=k<=22, -27<=l<=27	
Reflections collected	101830	
Independent reflections	7192 [R(int) = 0.0346]	
Completeness to theta = 67.679°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.5937	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7192 / 0 / 467	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0884	
R indices (all data)	R1 = 0.0391, wR2 = 0.0897	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.959 and -0.812 $e.Å^{-3}$	

trans-S(=P)-cyclodiphosph(V)azane 12

Identification code	fw_mjo4d	
Empirical formula	C32 H45 F12 N6 P3 S3	
Moiety formula	C24 H26 F12 N4 P2 S2, 2(C20 H32 F6 N4 P2 S2)	
Formula weight	930.83	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.177(2) Å	α= 78.106(9)°.
	b = 13.8549(18) Å	β= 79.722(19)°.
	c = 14.3529(16) Å	γ = 75.226(15)°.
Volume	2084.4(6) $Å^3$	
Z	2	
Density (calculated)	1.483 Mg/m^3	
Absorption coefficient	3.499 mm^{-1}	
F(000)	960	
Crystal size	0.250 x 0.150 x 0.100 mm^3	
Theta range for data collection	3.175 to 72.237°.	
Index ranges	-13<=h<=13, -17<=k<=17, -17<=l<=17	
Reflections collected	43520	
Independent reflections	8088 [R(int) = 0.0264]	
Completeness to theta = 67.679°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.5635	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8088 / 0 / 556	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.0757	
R indices (all data)	R1 = 0.0321, wR2 = 0.0762	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.536 and -0.525 $e.Å^{-3}$	

O(=P)/S(=P)-cyclodiphosph(V)azane 13

Identification code	fwfr6_n	
Empirical formula	C21 H34 N4 O2 P2 S	
Moiety formula	C21 H34 N4 O2 P2 S	
Formula weight	468.52	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 21.6468(5) Å	α= 90°.
	b = 14.6286(3) Å	β= 112.6360(10)°.
	c = 16.9134(4) Å	γ = 90°.
Volume	4943.3(2) $Å^3$	
Z	8	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	2.580 mm^{-1}	
F(000)	2000	
Crystal size	0.150 x 0.150 x 0.030 mm^3	
Theta range for data collection	3.745 to 72.174°.	
Index ranges	-26<=h<=23, -18<=k<=17, -20<=l<=20	
Reflections collected	53551	
Independent reflections	9700 [R(int) = 0.0509]	
Completeness to theta = 67.679°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	.7536 and .5476	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9700 / 0 / 608	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.1247	
R indices (all data)	R1 = 0.0648, wR2 = 0.1314	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.712 and -0.785 $e.Å^{-3}$	

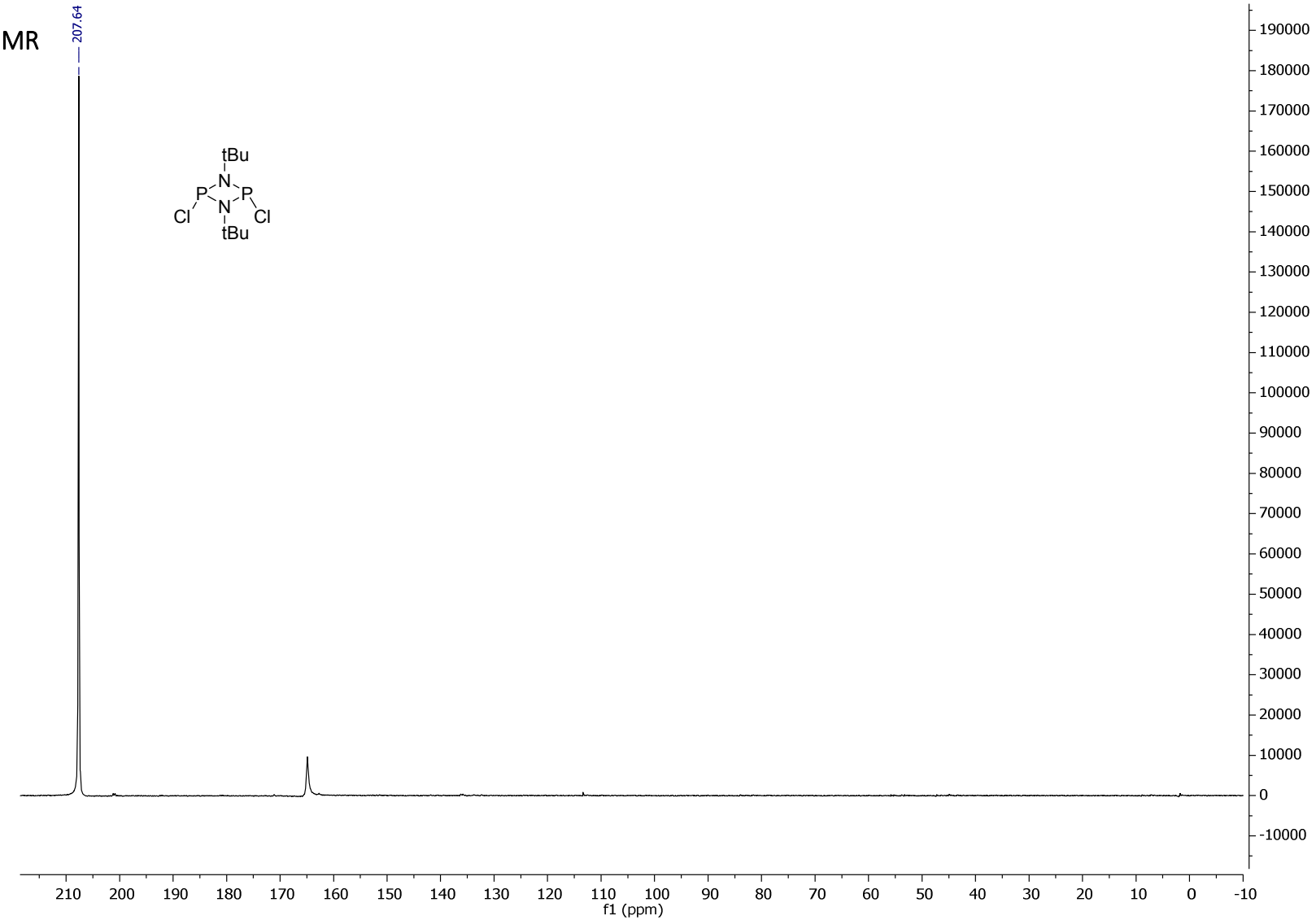
O(=P)/S(=P)-cyclodiphosph(V)azane 14

Identification code	fwfr11	
Empirical formula	C28 H36 F12 N4 O4 P2 S	
Moiety formula	?	
Formula weight	814.61	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 14.0313(4) Å	α= 90°.
	b = 21.6500(6) Å	β= 90°.
	c = 12.1766(3) Å	γ = 90°.
Volume	3698.98(17) $Å^3$	
Z	4	
Density (calculated)	1.463 Mg/m^3	
Absorption coefficient	2.504 mm^{-1}	
F(000)	1672	
Crystal size	0.300 x 0.200 x 0.150 mm^3	
Theta range for data collection	3.754 to 66.792°.	
Index ranges	-16<=h<=13, -24<=k<=25, -14<=l<=14	
Reflections collected	26645	
Independent reflections	6394 [R(int) = 0.0475]	
Completeness to theta = 66.792°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.5822	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6394 / 3 / 493	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2sigma(I)]	R1 = 0.0416, wR2 = 0.1115	
R indices (all data)	R1 = 0.0439, wR2 = 0.1129	
Absolute structure parameter	0.046(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.676 and -0.488 $e.Å^{-3}$	

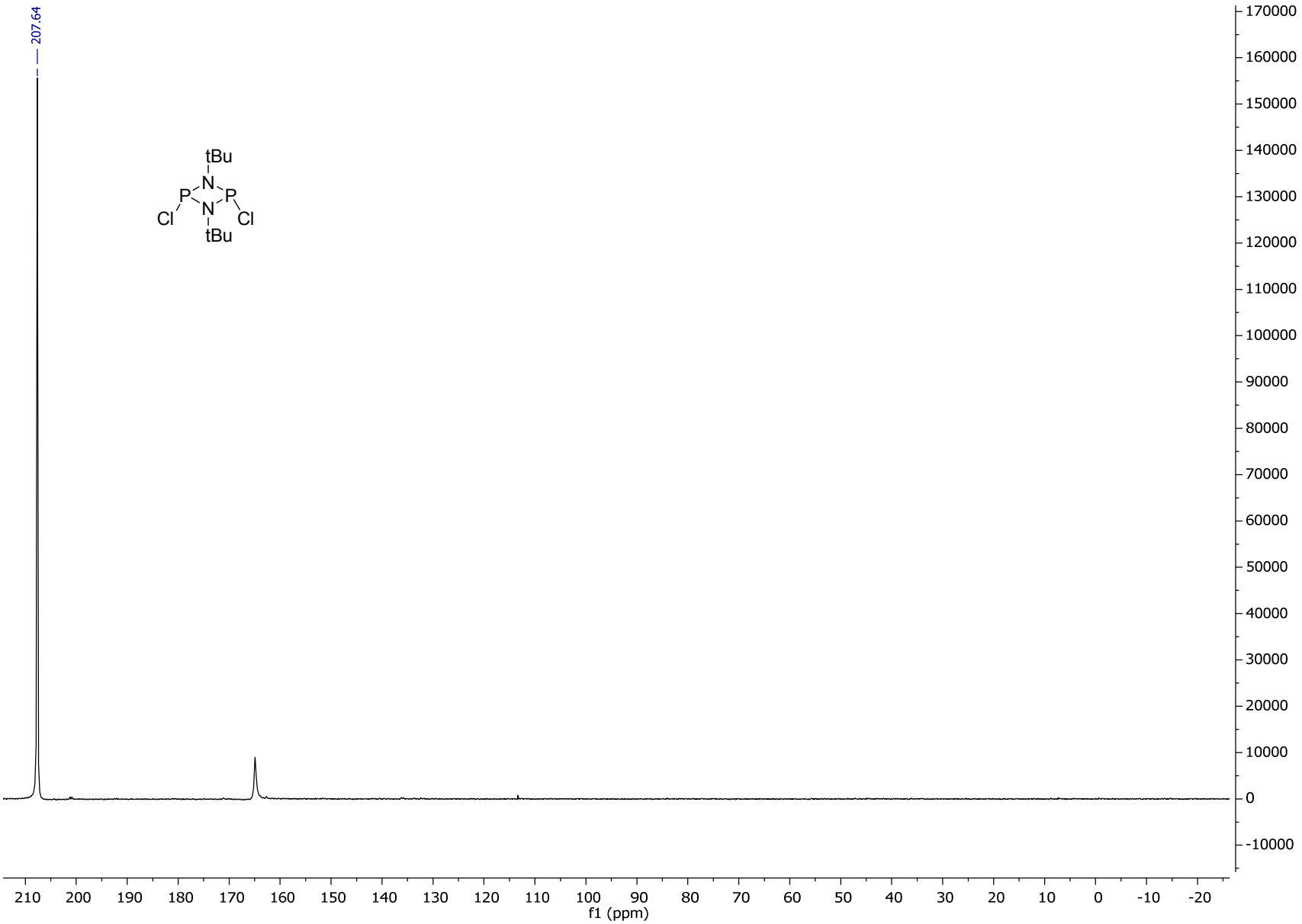
NMR-Spectra

1,3-di-tert-butyl-2,4-dichloro-1,3,2,4-diazadiphosphetidine (17)

$^{31}P\{^{1}H\}$-NMR

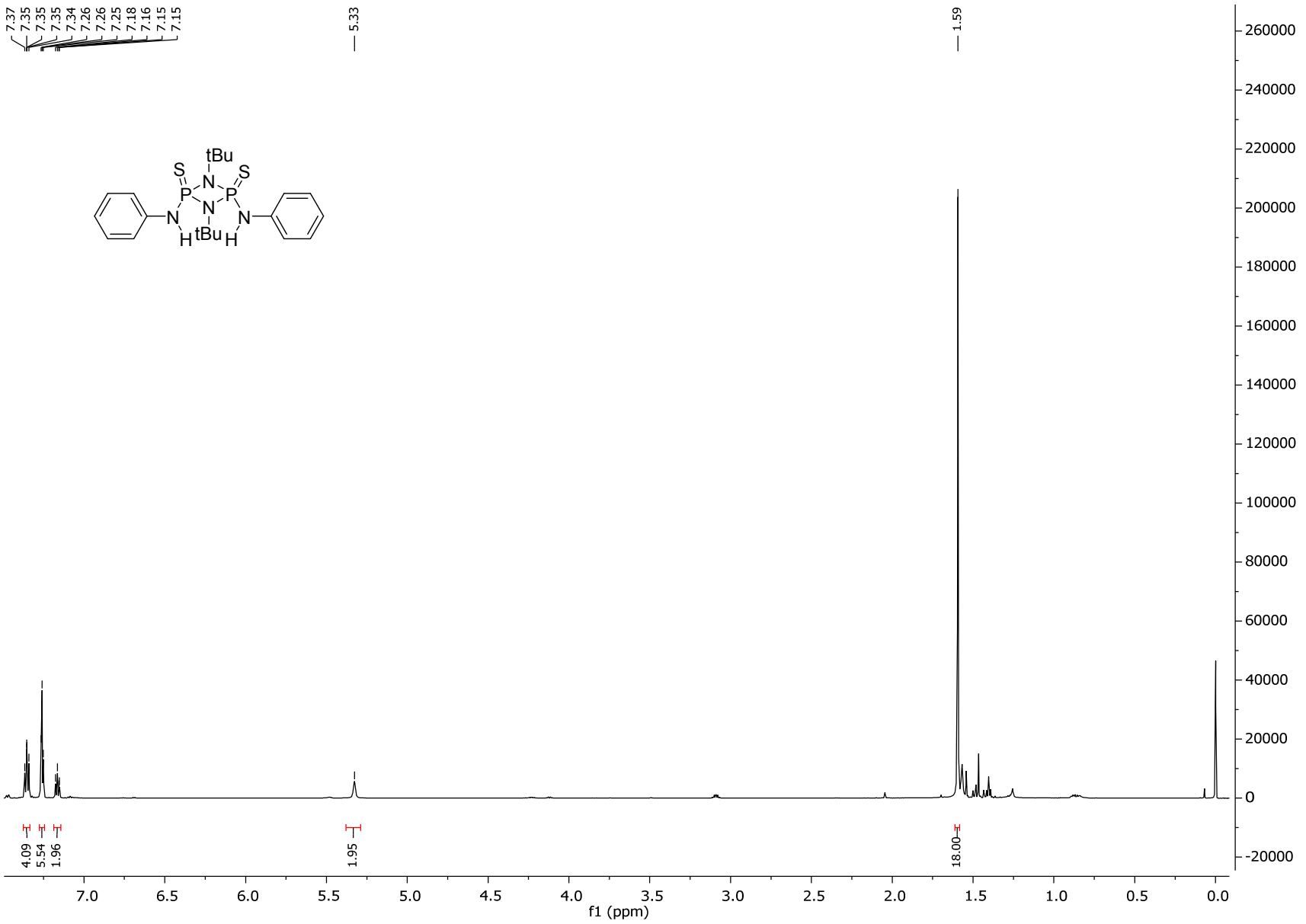


^{31}P-NMR

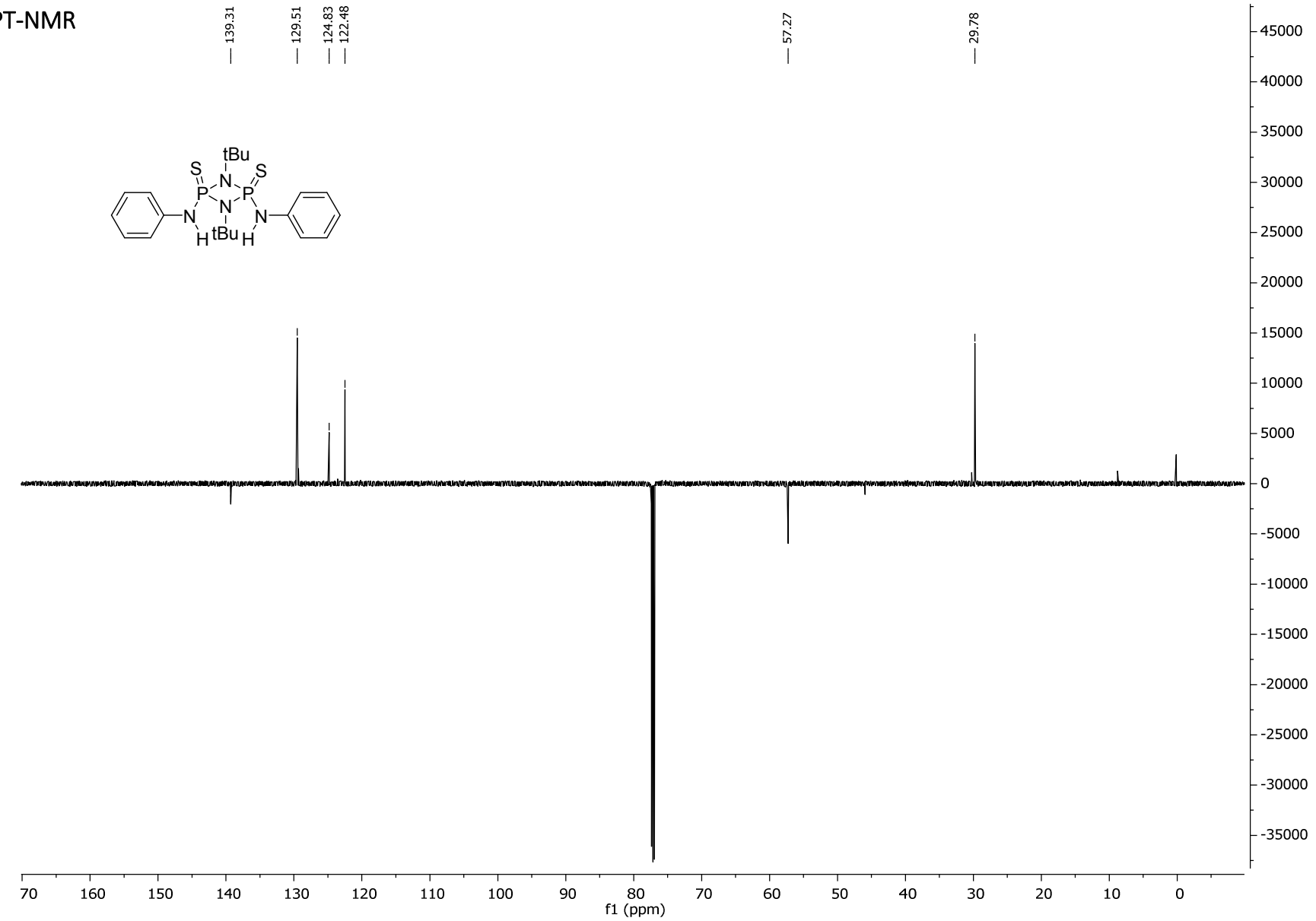

207.64
tBu
N
P
P
Cl
N
Cl
tBu
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

1,3-di-tert-butyl-2,4-bis(phenylamino)-1,3,2,4-diazadiphosphetidine 2,4-disulfide (11)

^{1}H-NMR

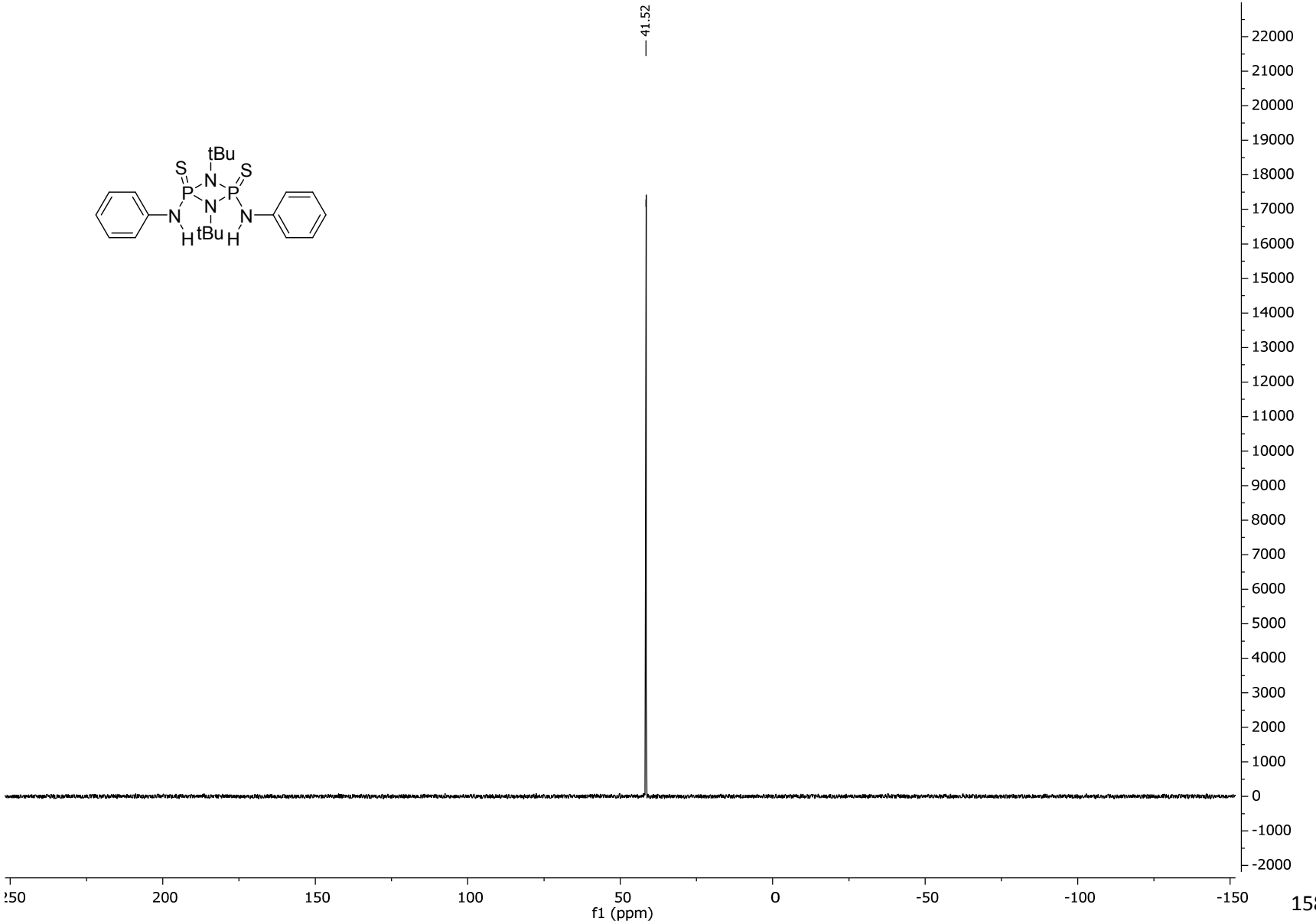


^{13}C-APT-NMR


139.31
129.51
124.83
122.48
57.27
29.78
tBu
S
S
N
P
P
N
N
H
tBu
H
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
-25000
-30000
-35000
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

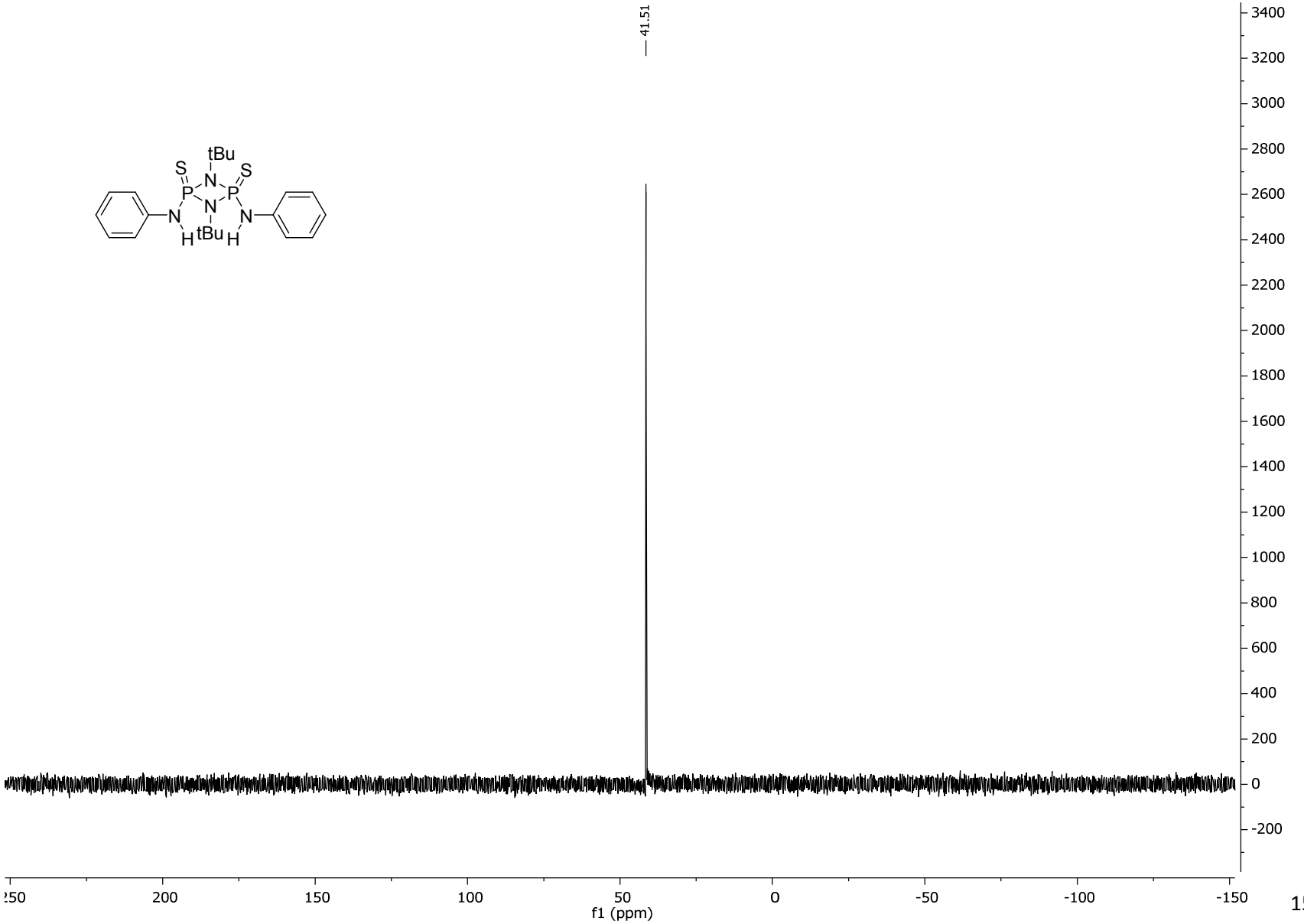
$^{31}P\{^{1}H\}$-NMR

tBu
S
S
N
P
P
N
N
N
H
tBu
H


41.52
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
250
200
150
100
50
0
-50
-100
-150
f1 (ppm)

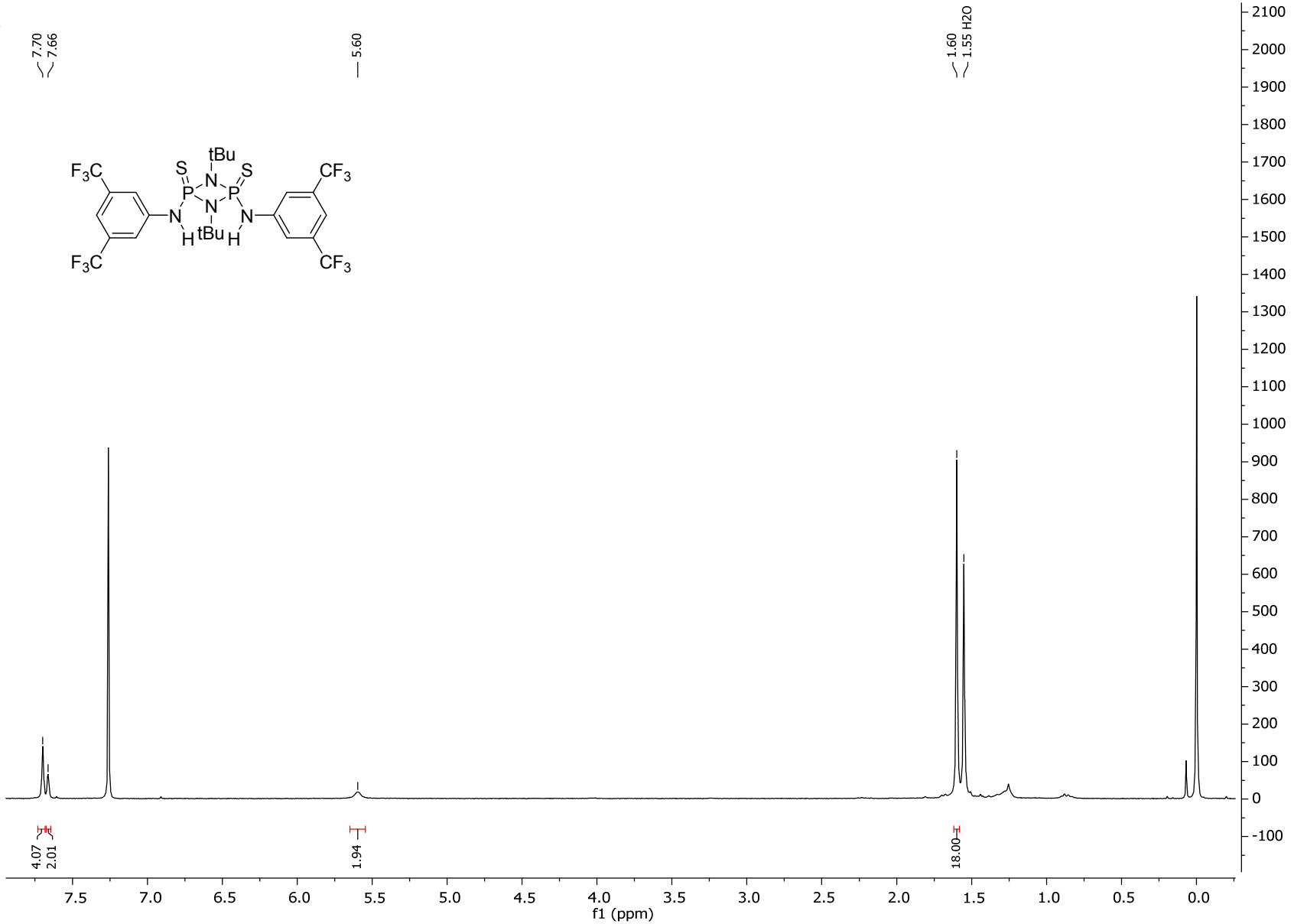
^{31}P-NMR

tBu
S
S
N
P
P
N
N
H
tBu
H


41.51
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
250
200
150
100
50
0
-50
-100
-150
f1 (ppm)

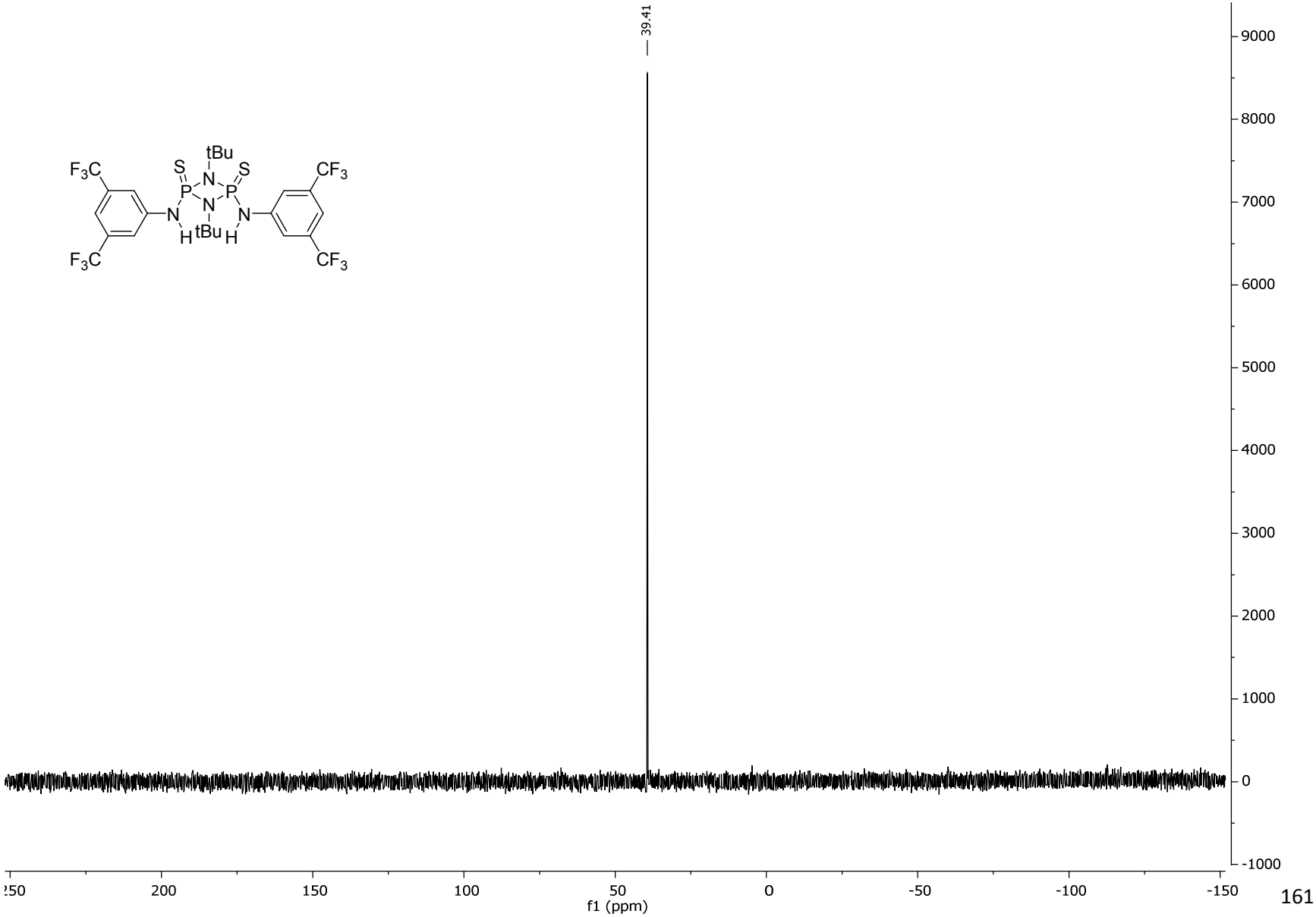
2,4-bis((3,5-bis(trifluoromethyl)phenyl)amino)-1,3-di-tert-butyl-1,3,2,4-diazadiphosphetidine 2,4-disulfide (12)

^{1}H-NMR



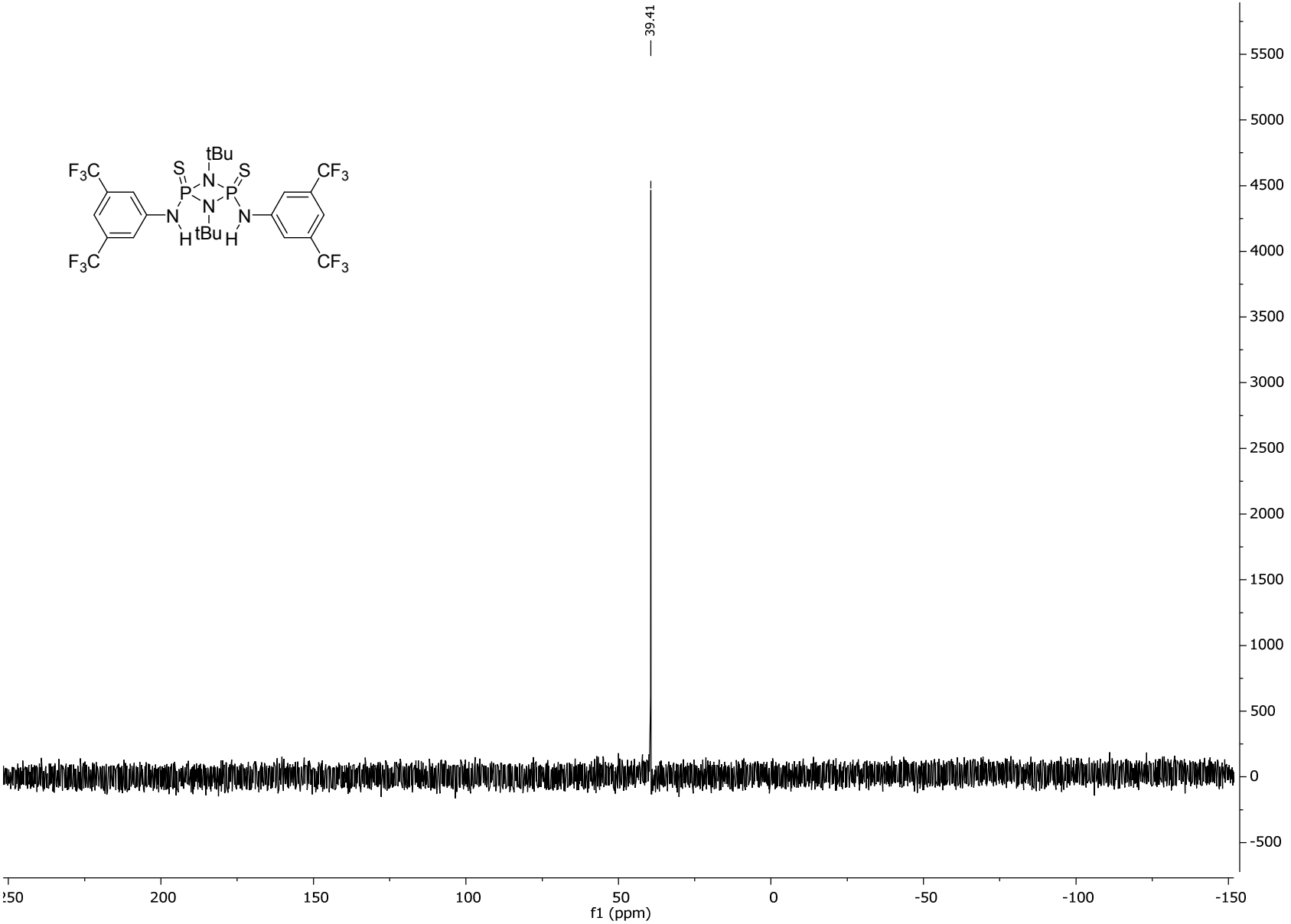
$^{31}P\{^{1}H\}$-NMR

tBu
S
S
F3C
CF3
P
N
P
N
N
H
tBu
H
F3C
CF3


39.41
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
250
200
150
100
50
0
-50
-100
-150
f1 (ppm)

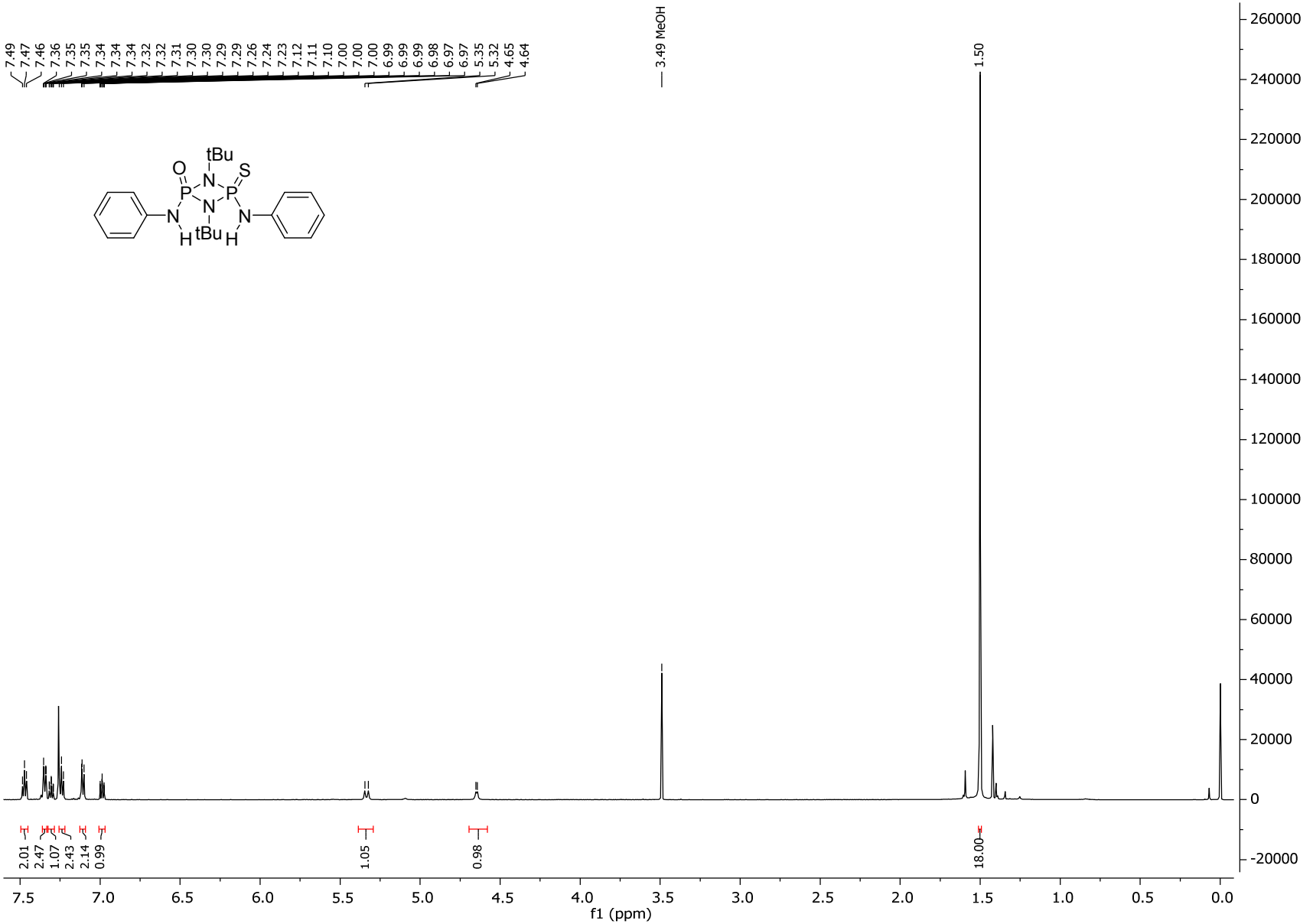
^{31}P-NMR

tBu
S
S
F3C
CF3
P
N
P
N
N
H
tBu
H
F3C
CF3

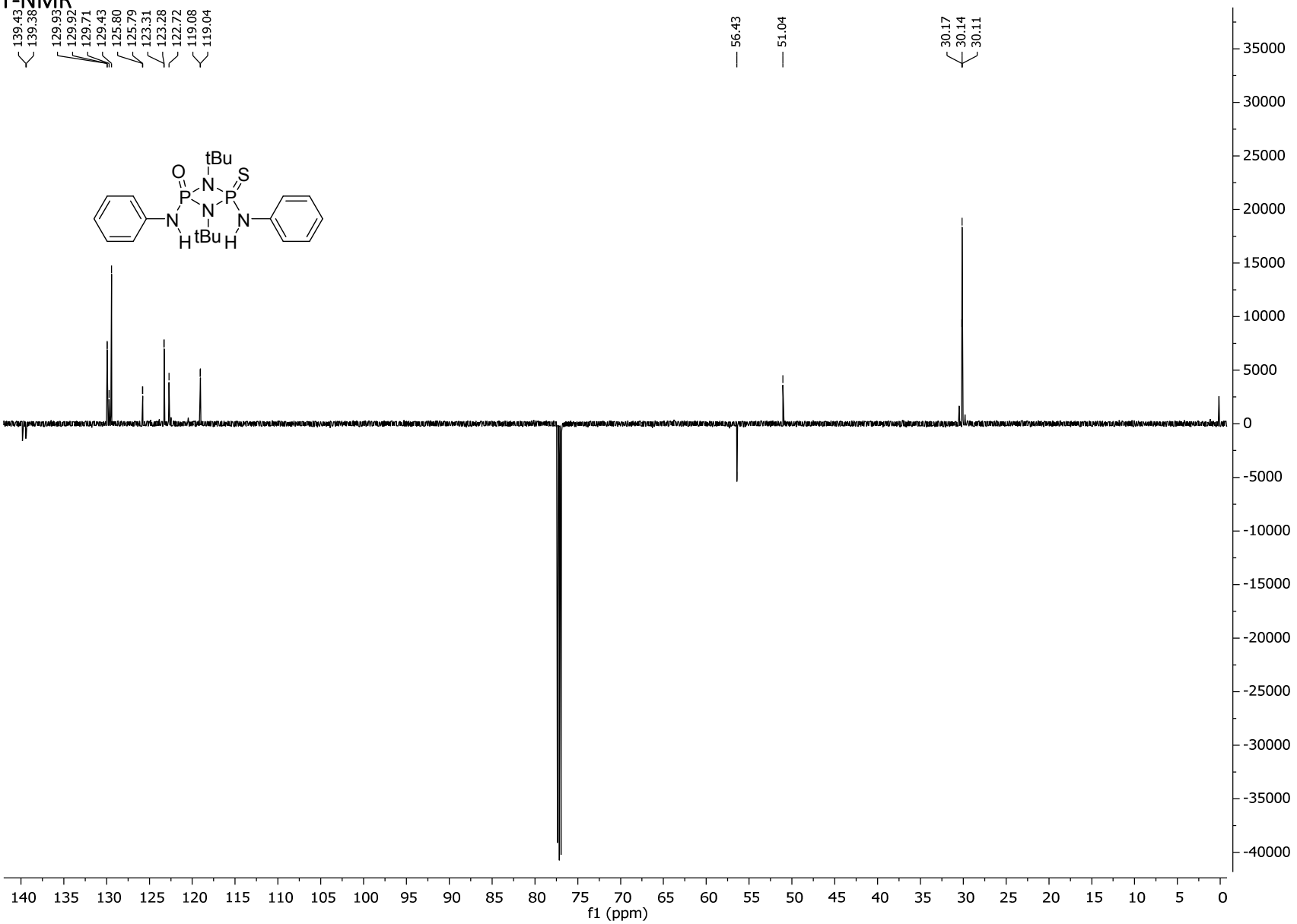

39.41
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
250
200
150
100
50
0
-50
-100
-150
f1 (ppm)

1,3-di-tert-butyl-2,4-bis(phenylamino)-1,3,2,4-diazadiphosphetidine 2-oxide 4-sulfide (13)

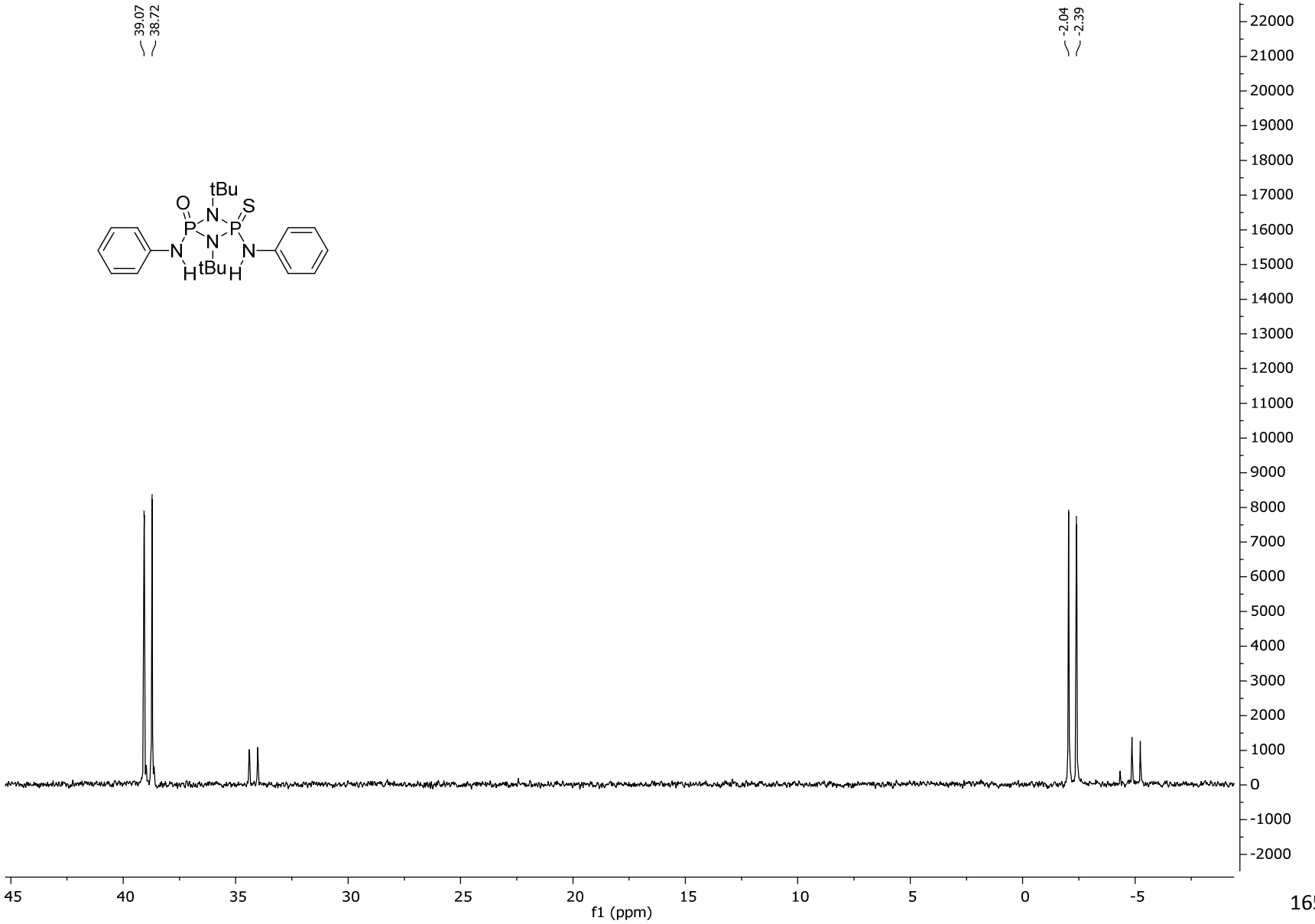
^{1}H-NMR



^{13}C-APT-NMR

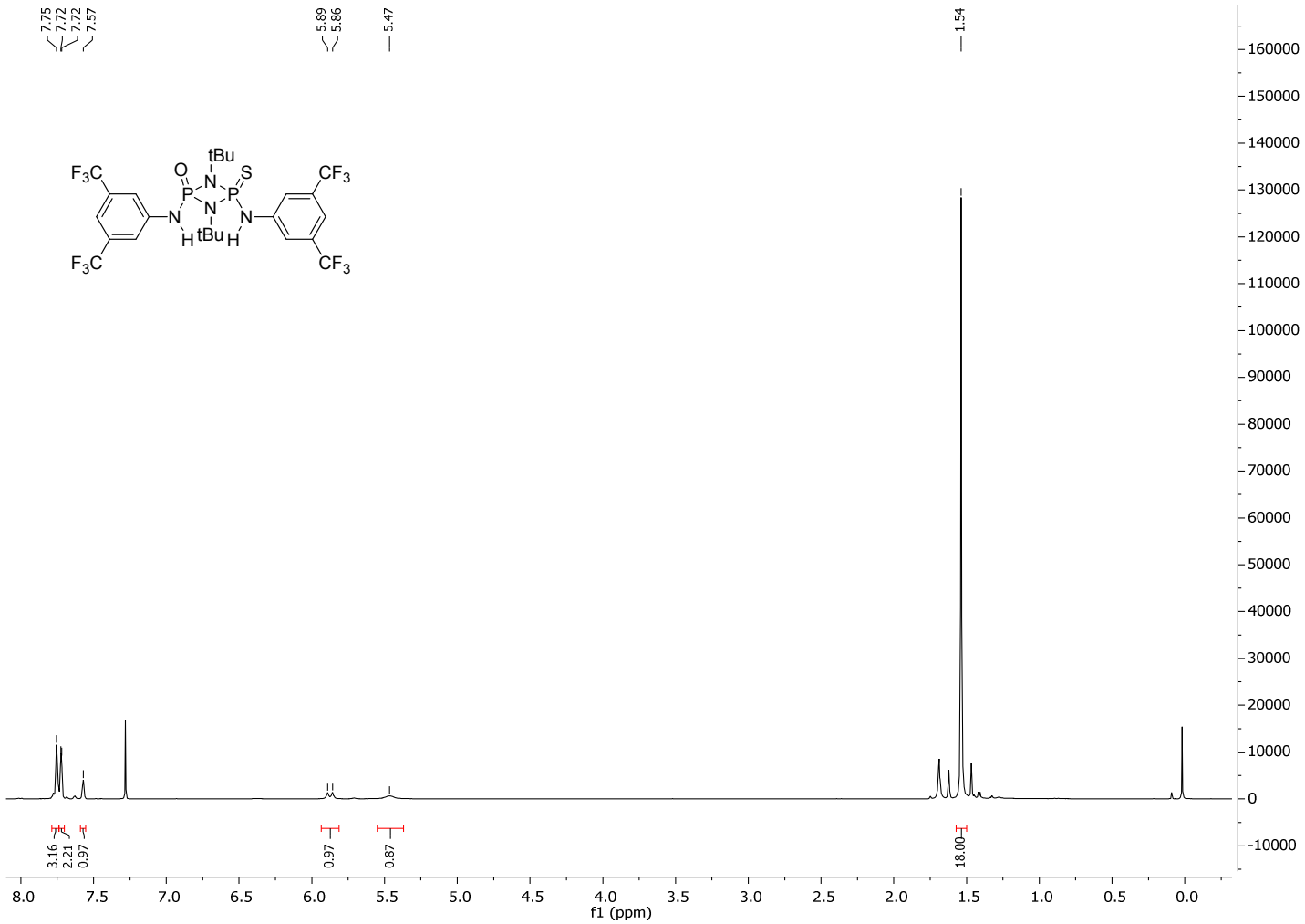

139.43
139.38
129.93
129.92
129.71
129.43
125.80
125.79
123.31
123.28
122.72
119.08
119.04
56.43
51.04
30.17
30.14
30.11
tBu
O
S
P
N
P
N
N
H
tBu
H
N
35000
30000
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
-25000
-30000
-35000
-40000
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

$^{31}P\{^{1}H\}$-NMR

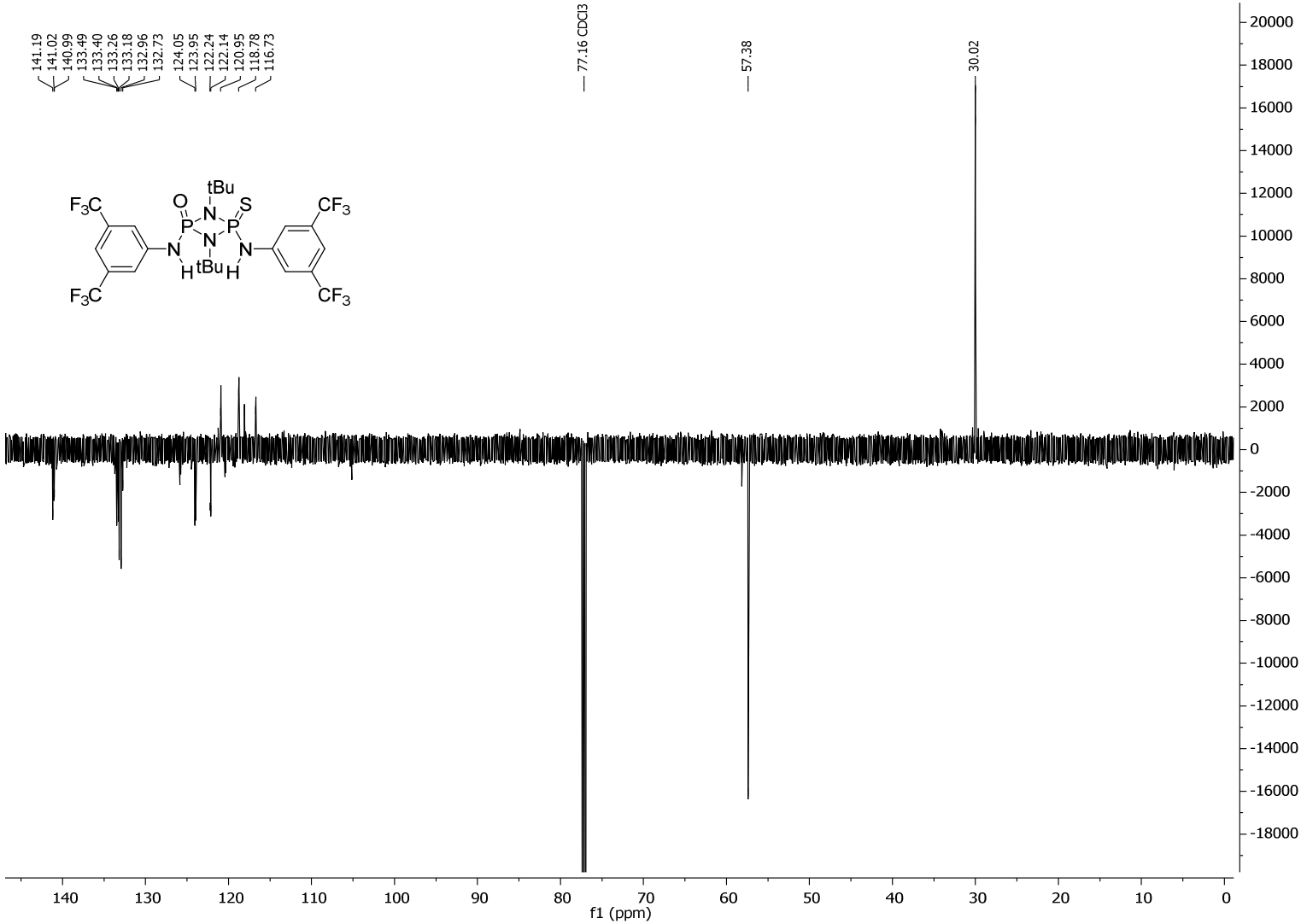

39.07
38.72
-2.04
-2.39
tBu
O
S
P
N
P
N
N
H
tBu
H
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
45
40
35
30
25
20
15
10
5
0
-5
f1 (ppm)

2,4-bis((3,5-bis(trifluoromethyl)phenyl)amino)-1,3-di-tert-butyl-1,3,2,4-diazadiphosphetidine 2-oxide 4-sulfide (14)

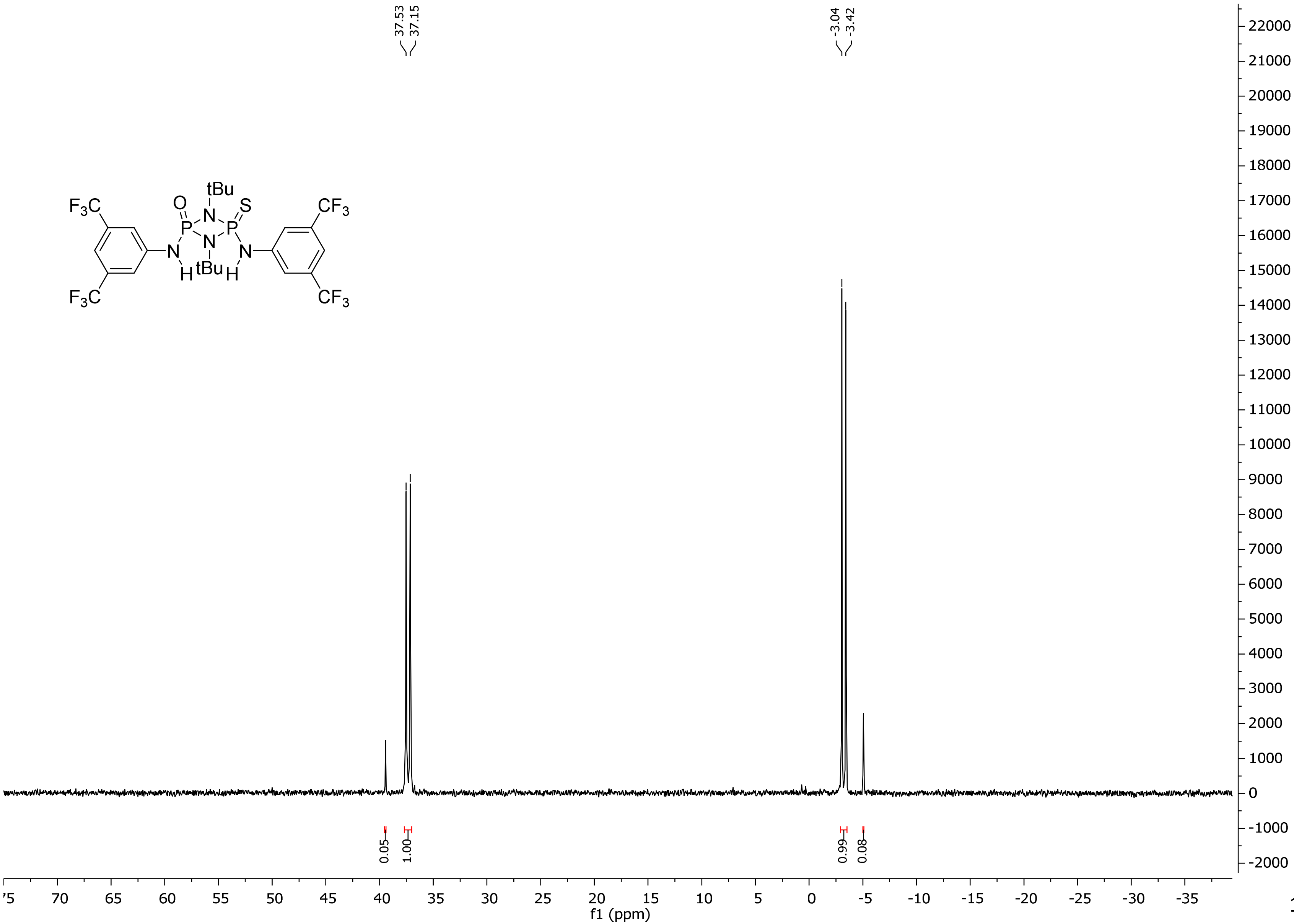
^{1}H-NMR



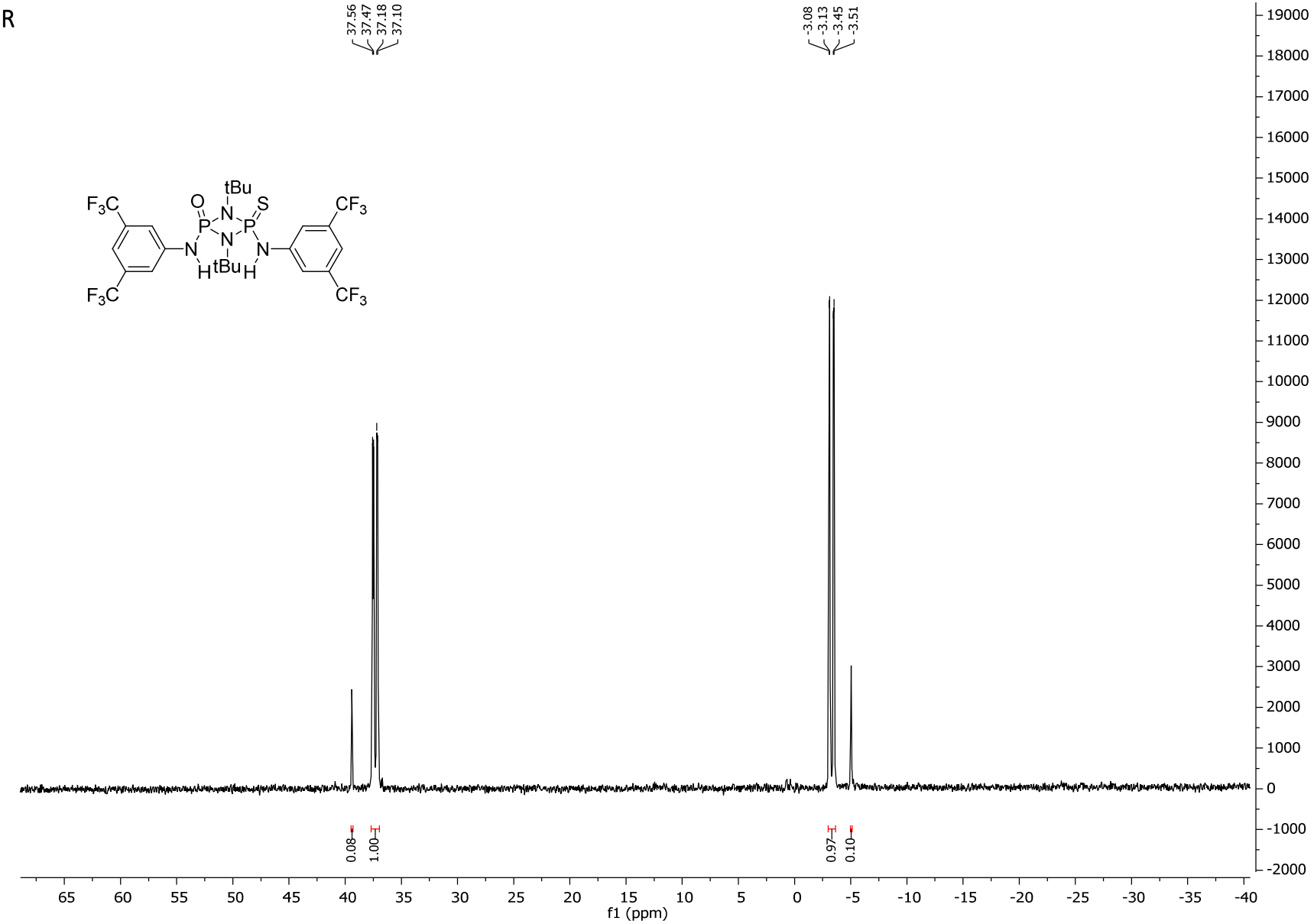
^{13}C-NMR


141.19
141.02
140.99
133.49
133.40
133.26
133.18
132.96
132.73
124.05
123.95
122.24
122.14
120.95
118.78
116.73
77.16 CDCl3
57.38
30.02
tBu
F3C
CF3
O
S
P
N
H
f1 (ppm)

$^{31}P\{^{1}H\}$-NMR

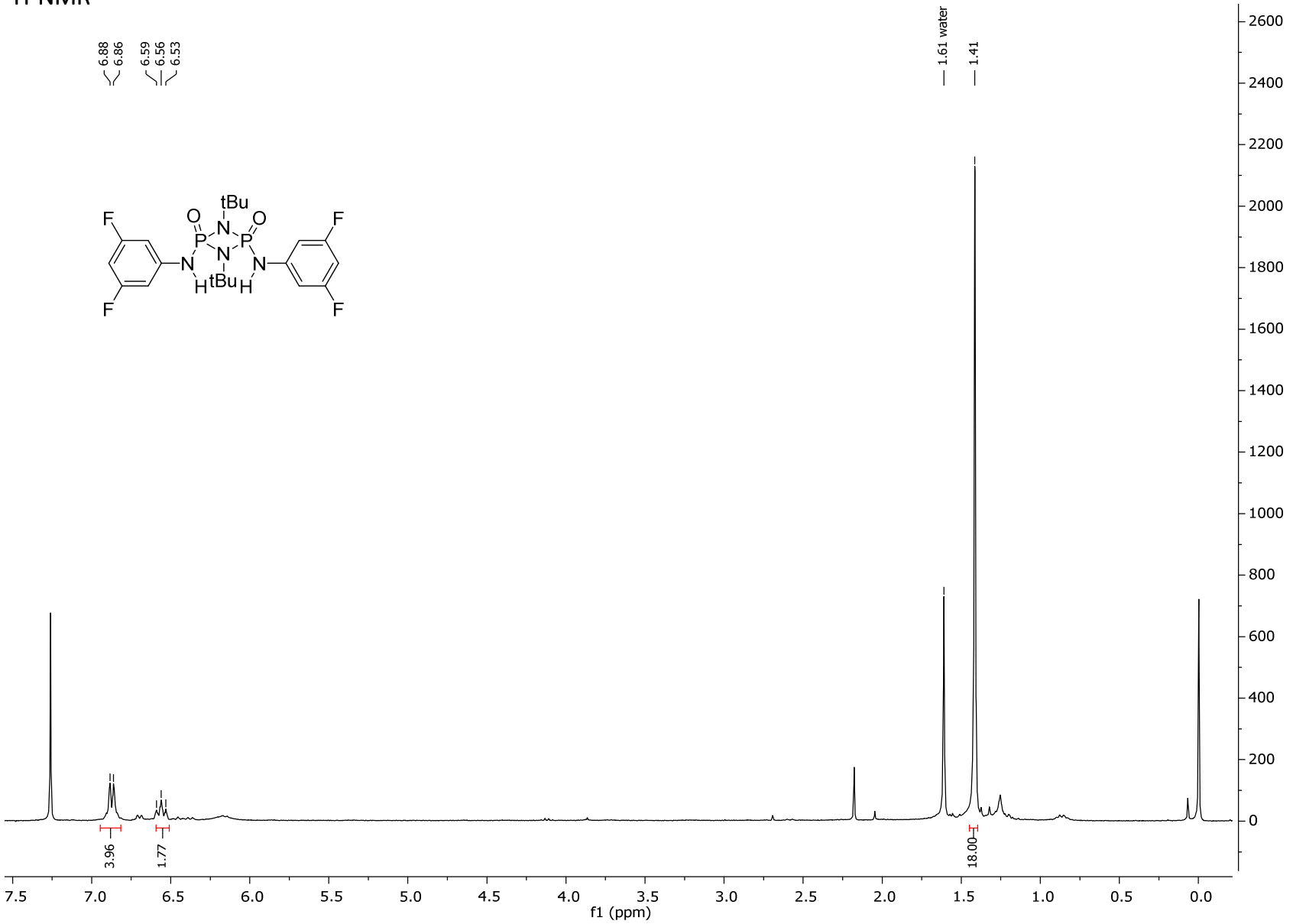


^{31}P-NMR


37.56
37.47
37.18
37.10
-3.08
-3.13
-3.45
-3.51
tBu
O
S
N
P
P
N
N
H
tBu
H
F3C
CF3
F3C
CF3
0.08
1.00
0.97
0.10
f1 (ppm)

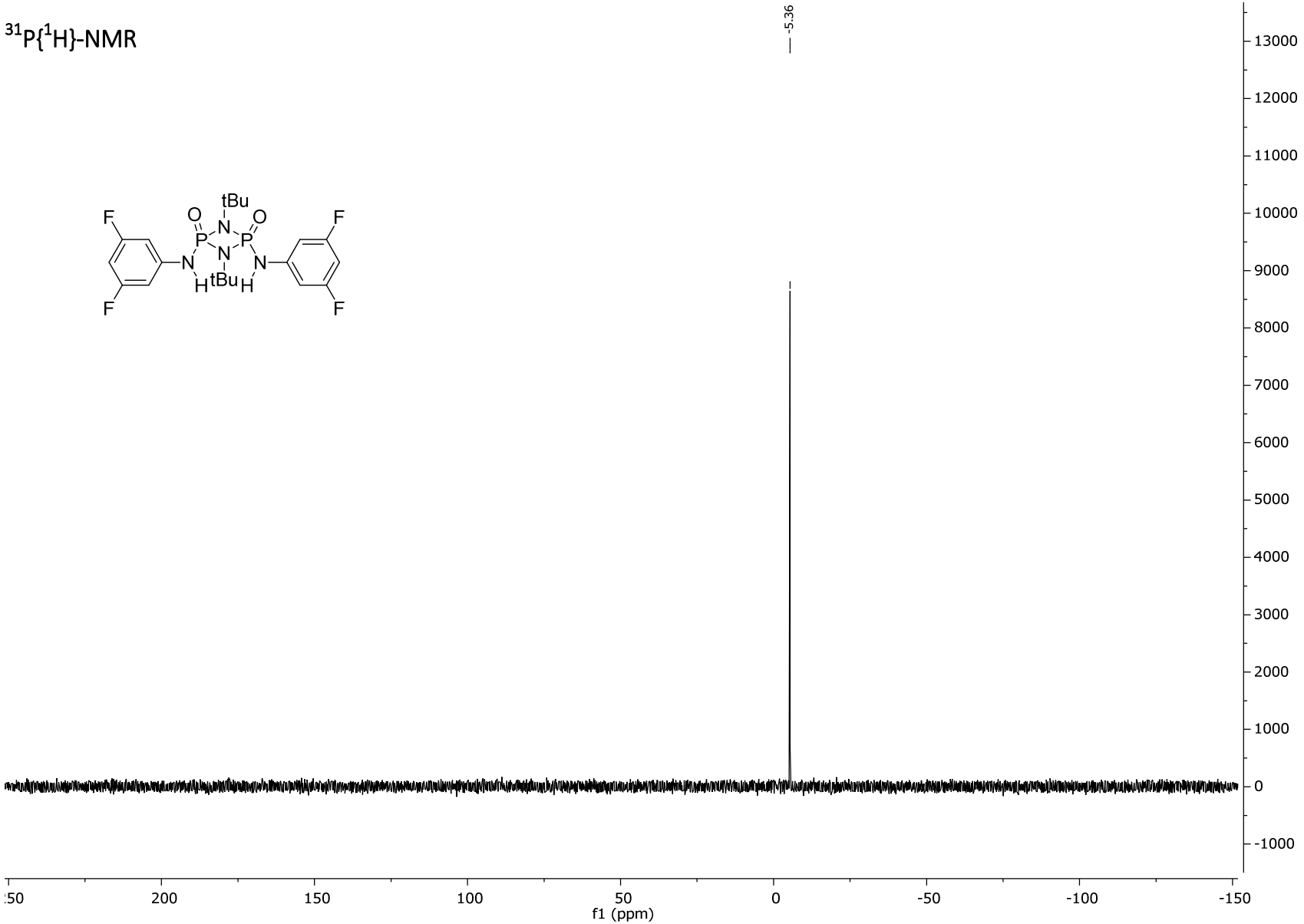
2,4-bis((3,5-bisfluorophenyl)amino)-1,3-di-tert-butyl-1,3,2,4-diazadiphosphetidine 2,4-dioxide (15)

^{1}H-NMR



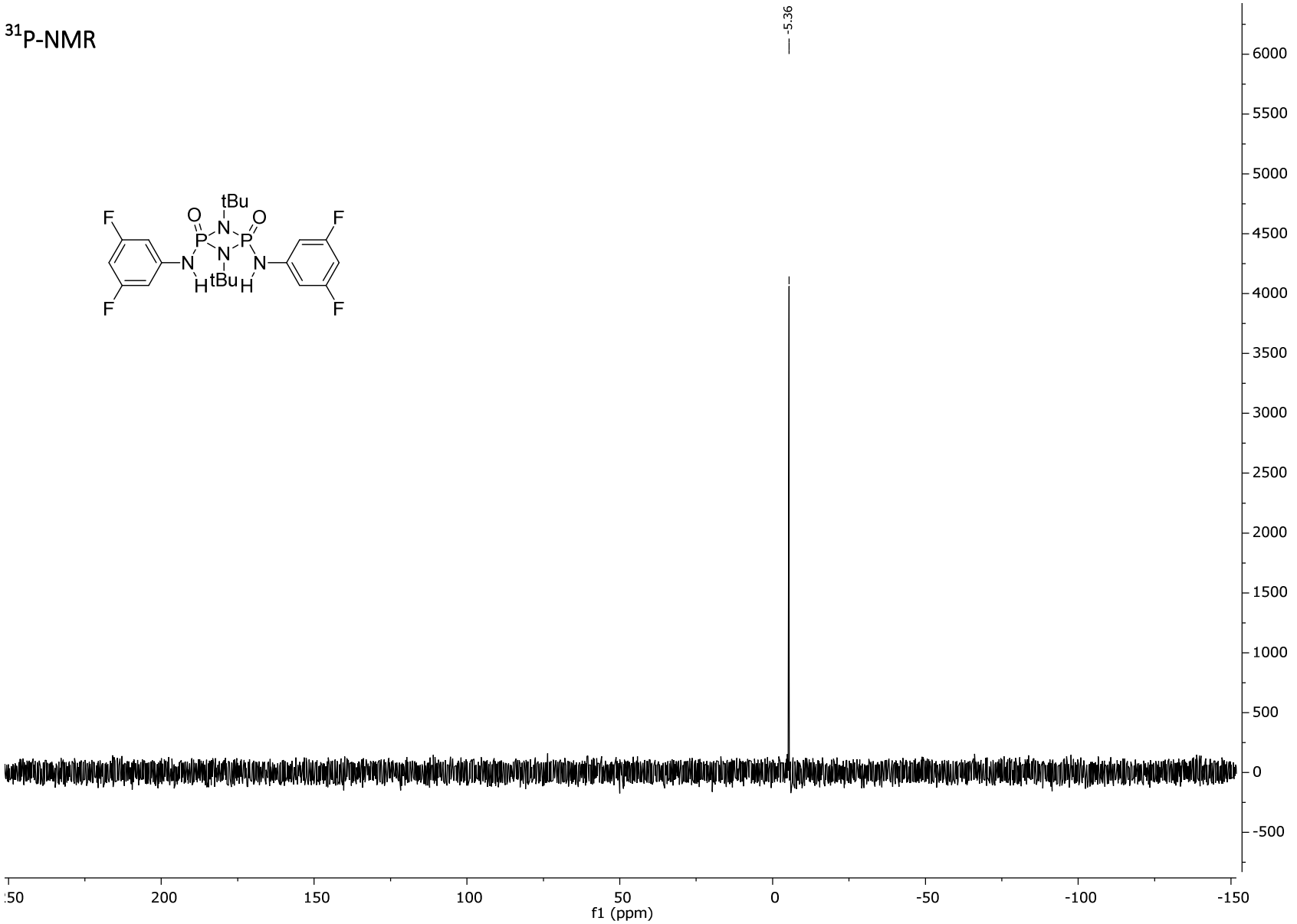
$^{31}P\{^{1}H\}$-NMR

tBu
O
O
F
F
P
N
P
N
N
H
tBu
H
F
F


-5.36
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
150
100
50
0
-50
-100
-150
f1 (ppm)

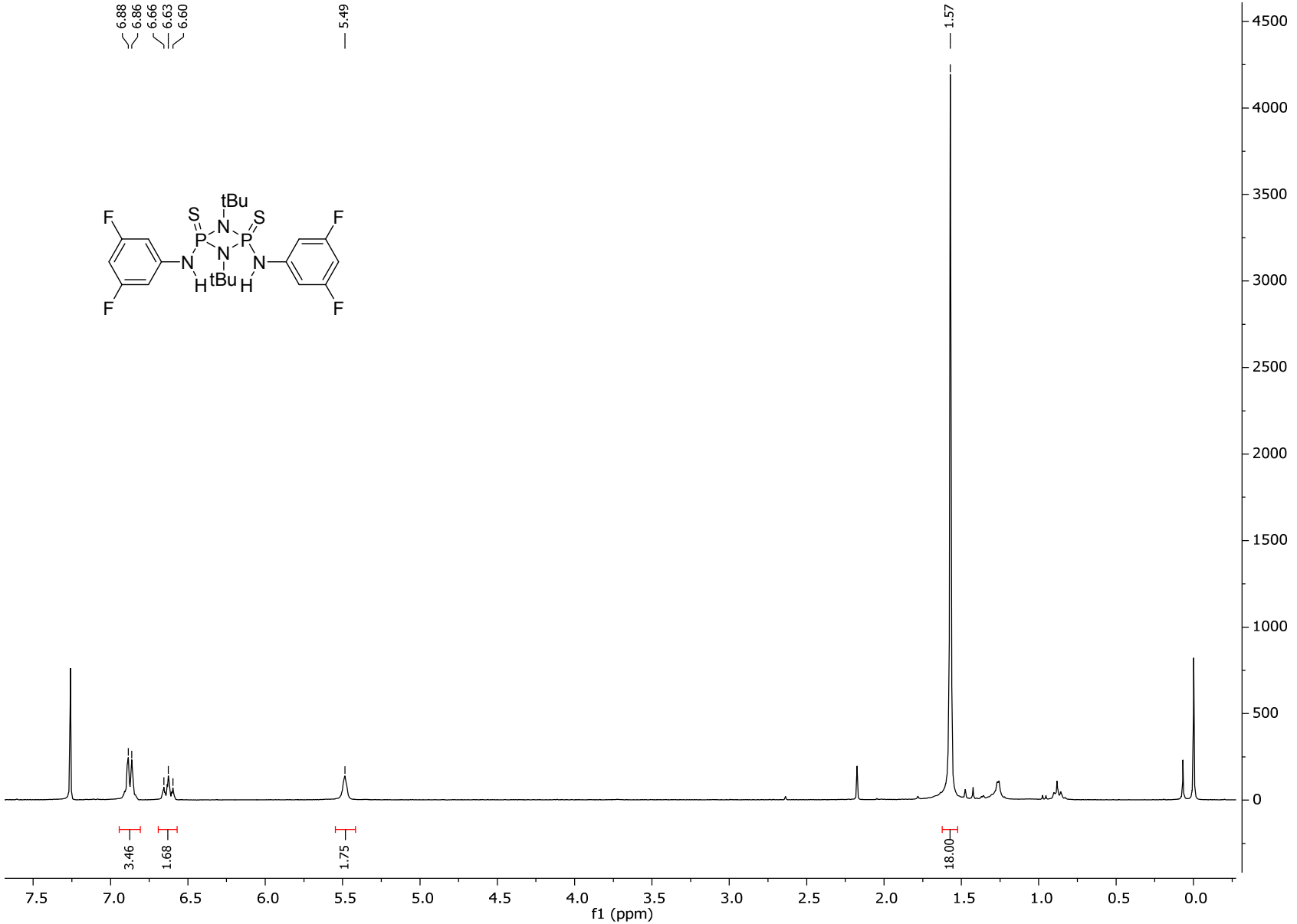
^{31}P-NMR

tBu
O
O
F
F
P
N
P
N
N
N
H
tBu
H
F
F

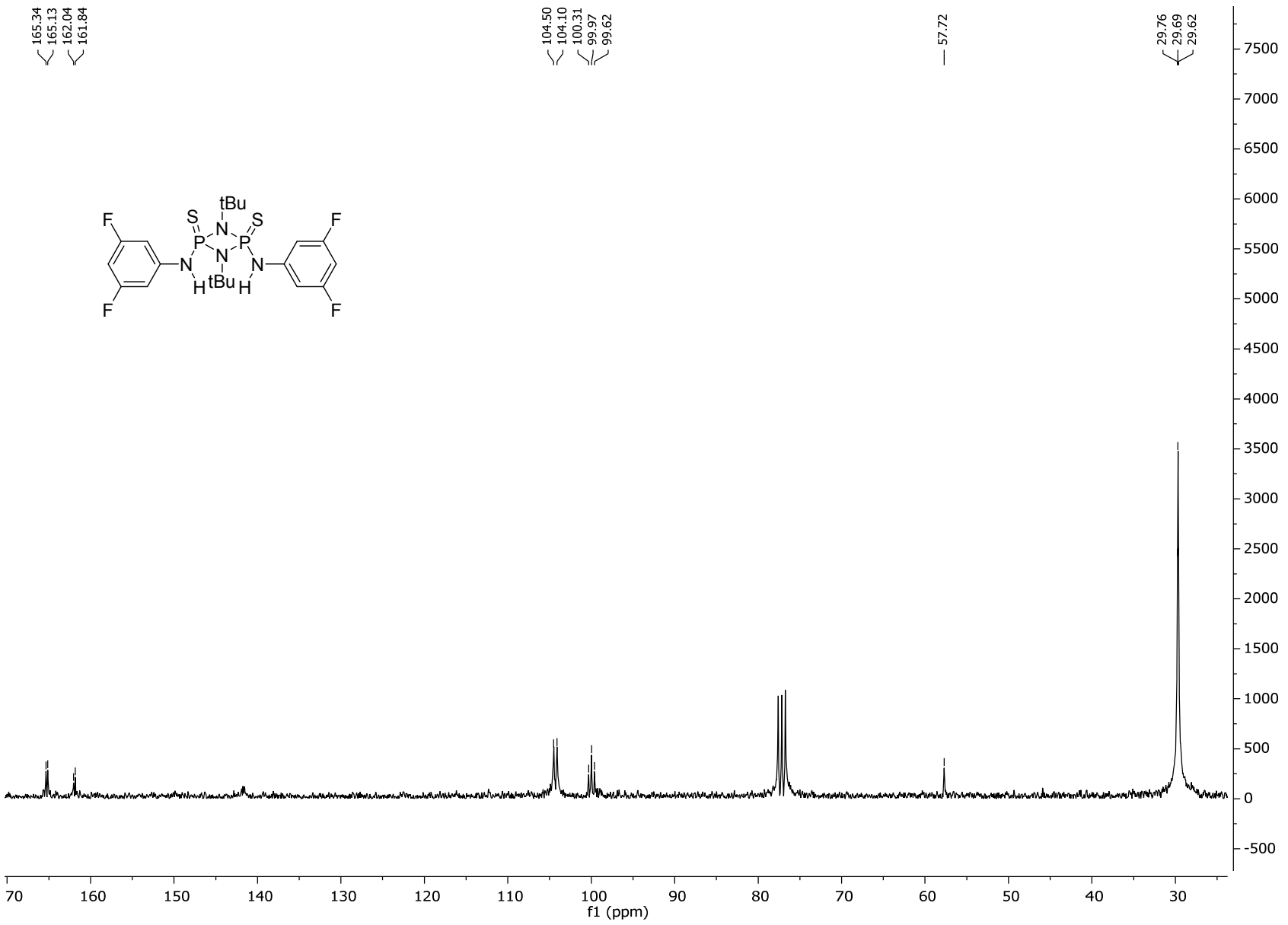

-5.36
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
150
100
50
0
-50
-100
-150
f1 (ppm)

2,4-bis((3,5-bisfluorophenyl)amino)-1,3-di-tert-butyl-1,3,2,4-diazadiphosphetidine 2,4-disulfide (16)

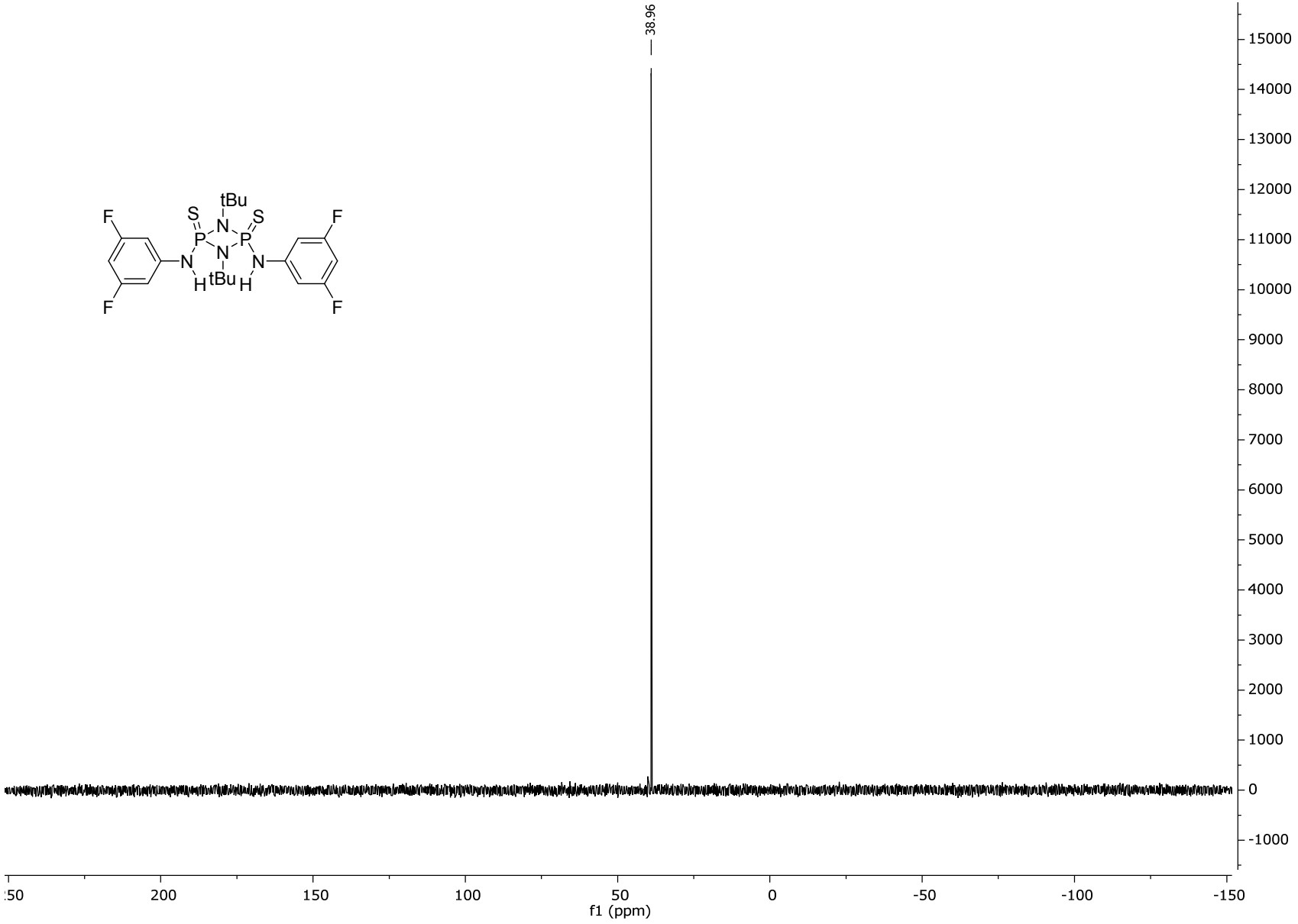
^{1}H-NMR



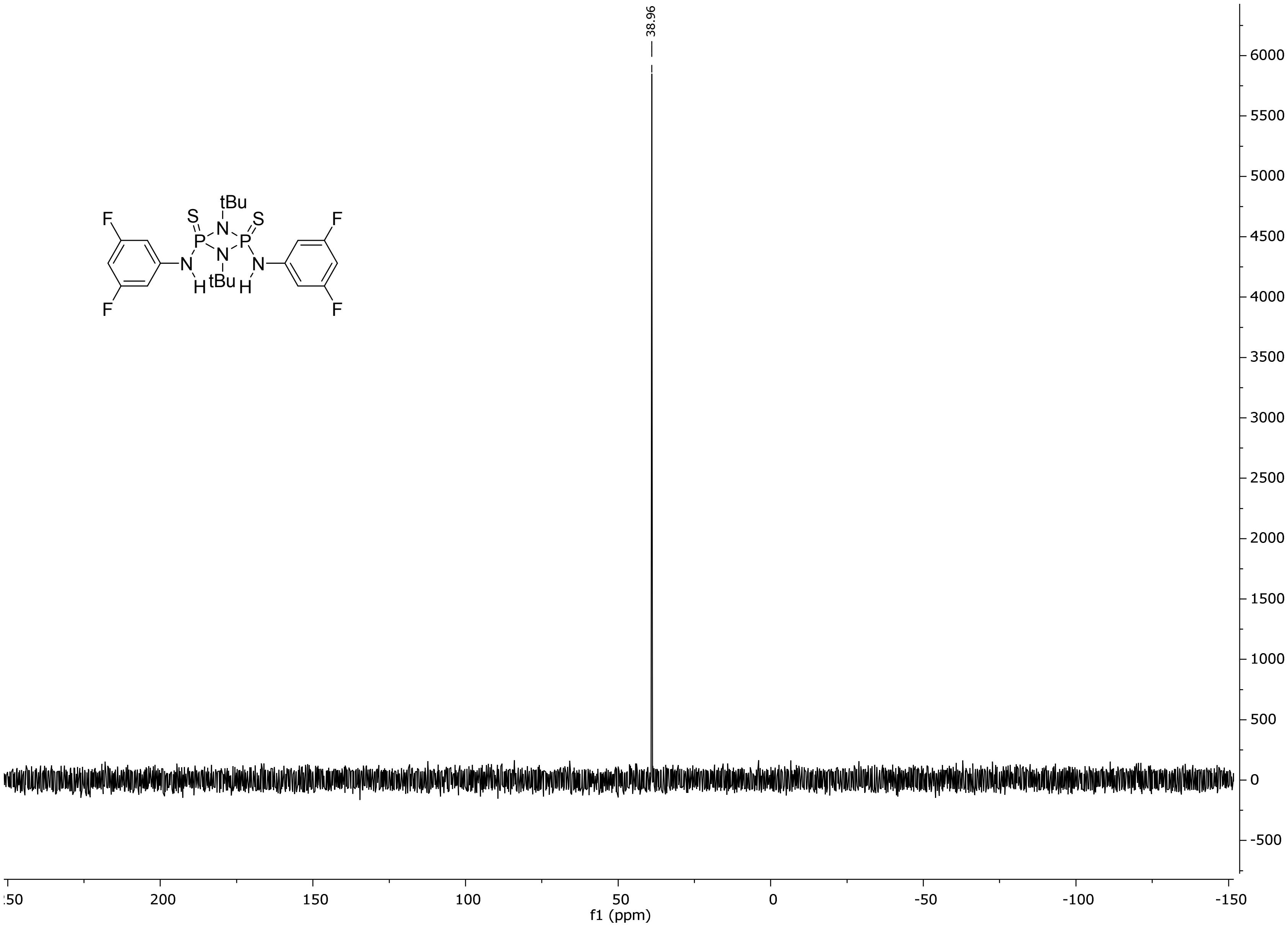
$^{13}C\{^{1}H\}$-NMR


165.34
165.13
162.04
161.84
104.50
104.10
100.31
99.97
99.62
57.72
29.76
29.69
29.62
tBu
S
S
P
P
N
N
N
N
H
H
tBu
F
F
F
F
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

$^{31}P\{^{1}H\}$-NMR


38.96
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
150
100
50
0
-50
-100
-150
f1 (ppm)
tBu
S
N
P
F
H

^{31}P-NMR



tBu
S
S
F
F
P
N
P
N
N
N
H
tBu
H
F
F
38.96
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
150
100
50
0
-50
-100
-150
f1 (ppm)

Product of the N-acyl-Mannich catalysis (10)

^{1}H-NMR