Supporting information for:

Synthesis, reactivity and computational analysis of halophosphines supported by dianionic guanidinate ligands

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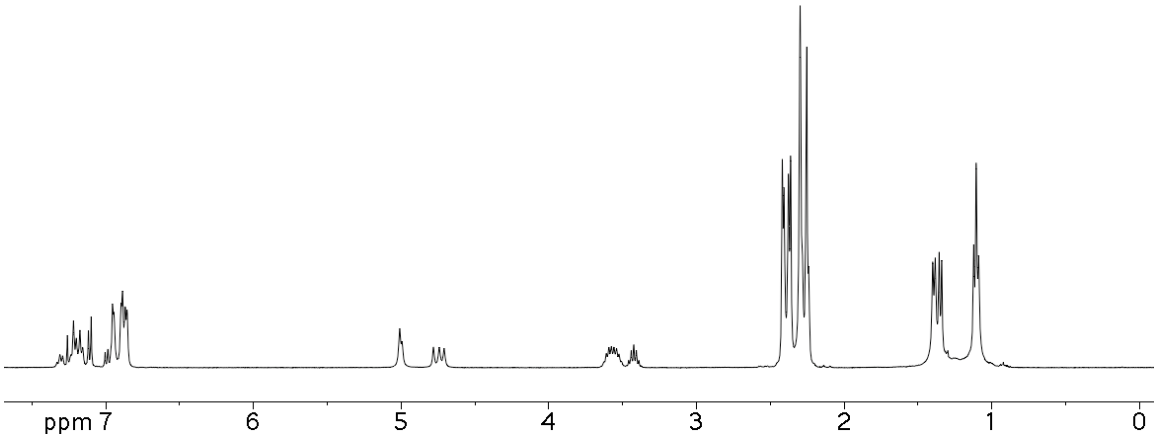

Figure S-1: ^{1}H NMR spectrum of **3**.

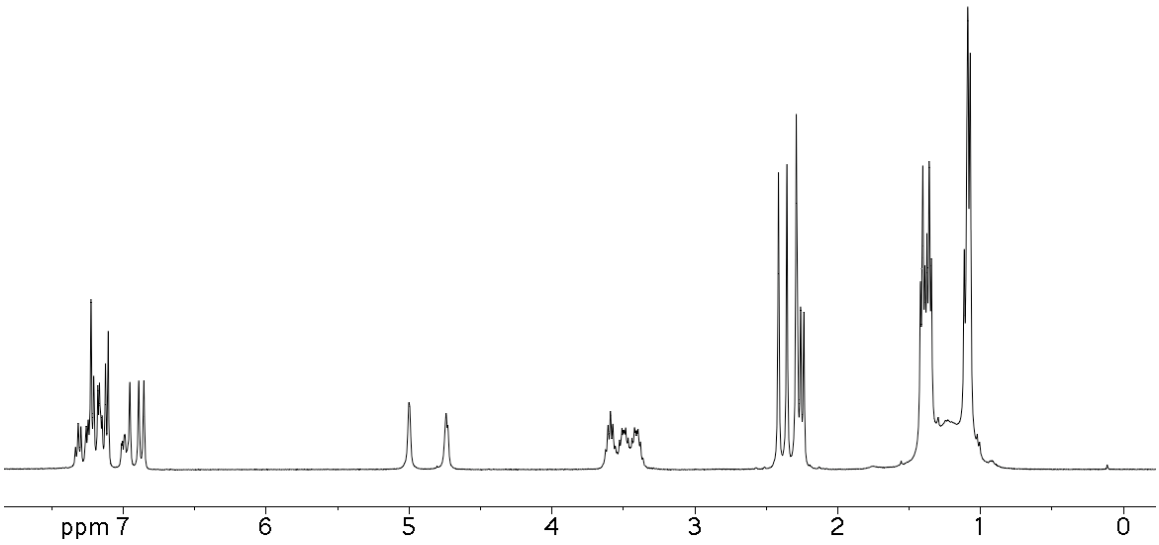

Figure S-2: ^{1}H NMR spectrum of **4**.

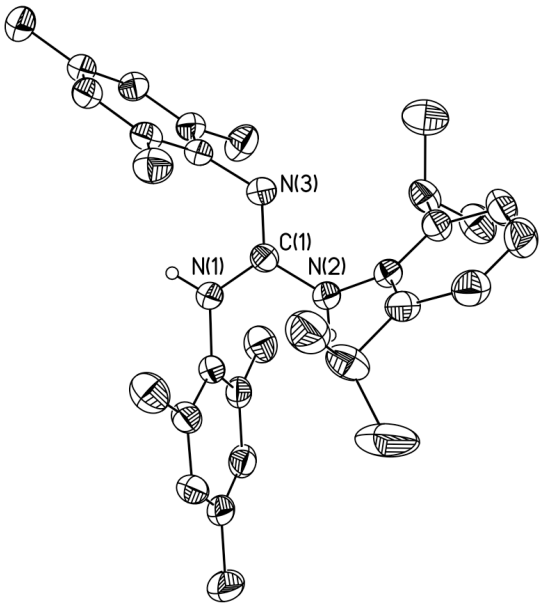

Figure S-3: Solid-state structure of **3**. Ellipsoids are drawn to 50% probability. Selected hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): C(1)–N(1) 1.376(2), C(1)–N(2) 1.375(2), C(1)–N(3) 1.287(2), N(1)–C(1)–N(2) 114.50(14), N(1)–C(1)–N(3) 125.75(15), N(2)–C(1)–N(3) 120.73(15).

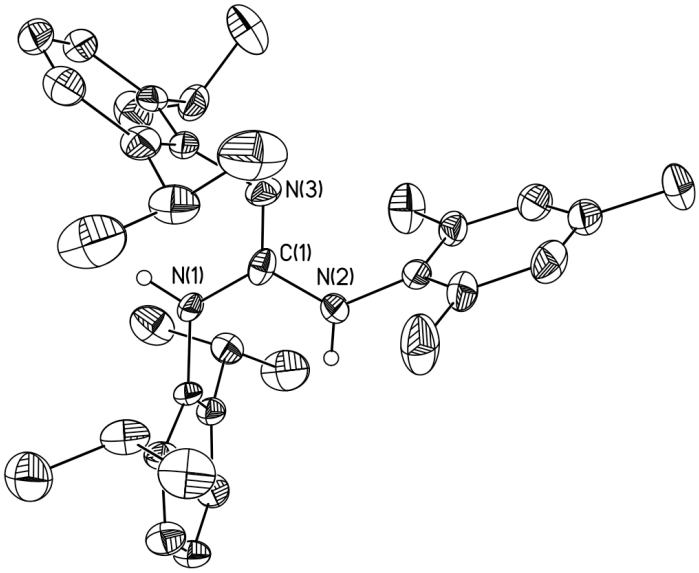

Figure S-4: Solid-state structure of **4**. Ellipsoids are drawn to 50% probability. Selected hydrogen atoms have been omitted for clarity. Because the data from the best of the examined crystals was of low quality, the metrical parameters will not be discussed. However, the solution and refinement of the structure confirms the identity and connectivity of **4**.

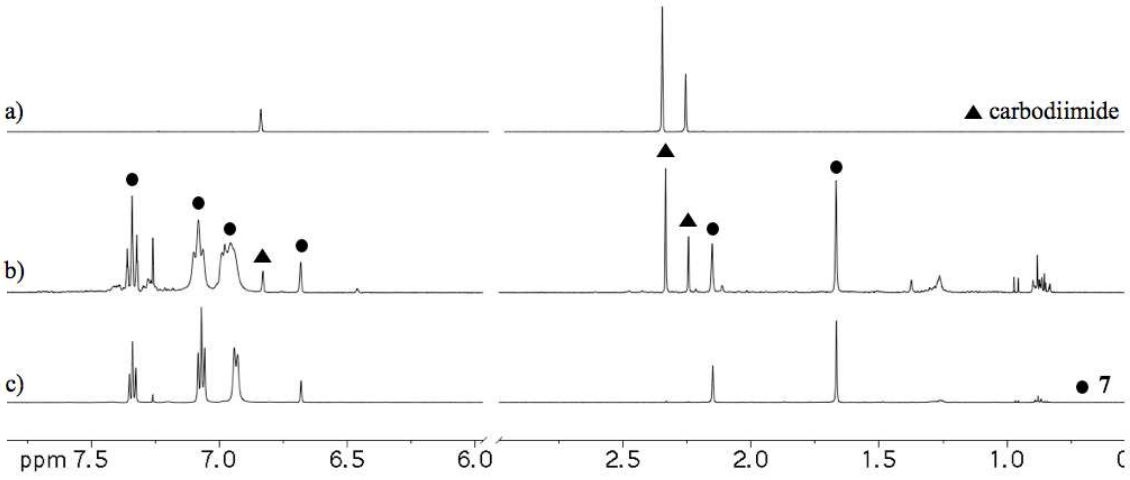

Figure S-5: Stacked plot of the ^{1}H NMR spectra for a) pure *N,N′*-bis(Mes)carbodiimide, b) crude **7**, and c) purified **7**.

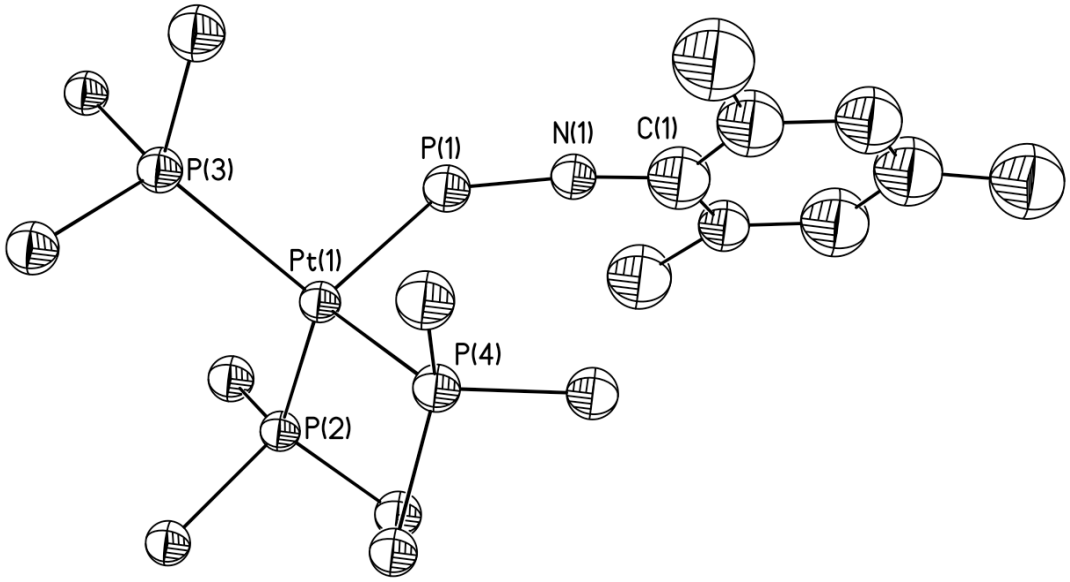

Figure S-6: Isotropic solid-state structure of cation **7**. Ellipsoids are drawn to 30% probability. Hydrogen atoms and all but the *ipso*-carbons on PPh_3 have been omitted for clarity. Because the data from the best of the examined crystals gave a highly disordered anion that could not be modeled appropriately, a high amount of electron density was unaccounted for. Therefore, the metrical parameters will not be discussed. However, the solution and refinement of the cationic portion of the molecule confirms the identity and connectivity of **7**.

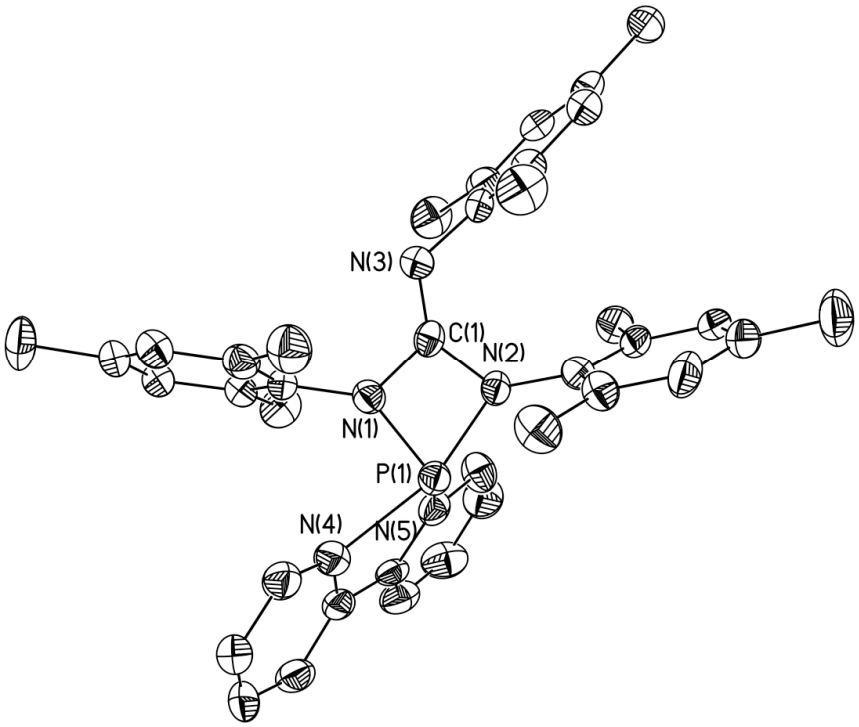

Figure S-7: Anisotropic solid-state structure of cation **8**. Ellipsoids are drawn to 50% probability. Hydrogen atoms have been omitted for clarity. Because the data from the best of the examined crystals gave a highly disordered anion that could not be modeled appropriately, a high amount of electron density was unaccounted for. Therefore, the metrical parameters will not be discussed. However, the solution and refinement of the cationic portion of the molecule confirms the identity and connectivity of **8**.

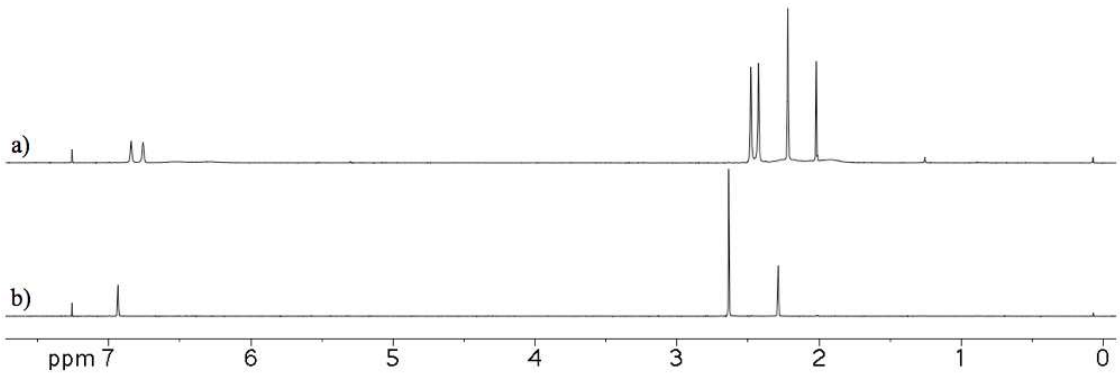

Figure S-8: Stacked plot of the ^{1}H NMR spectra for a) **1PCl** and b) **10**.

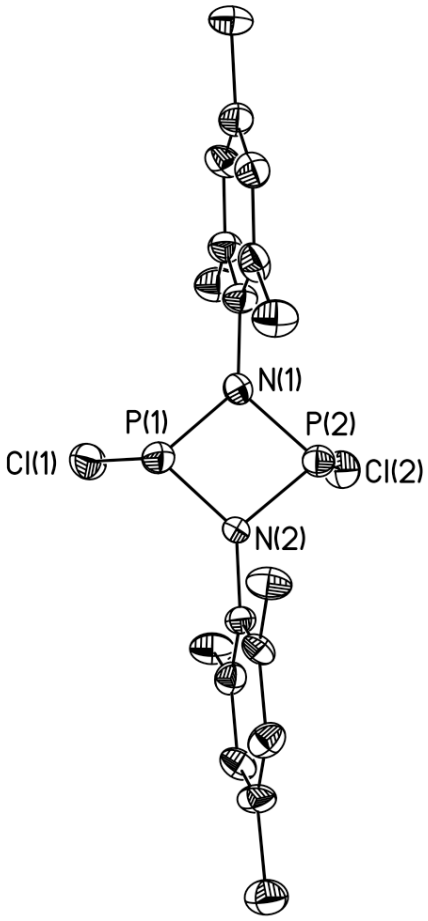

Figure S-9: Solid-state structure of **10**. Ellipsoids are drawn to 50% probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): P(1)–N(1) 1.705(4), P(1)–N(2) 1.694(4), P(2)–N(1) 1.711(4), P(2)–N(2) 1.705(4), P(1)–Cl(1) 2.110(2), P(2)–Cl(2) 2.1112(19), P(1)–N(1)–P(2) 97.4(2), P(1)–N(2)–P(2) 98.1(2), N(1)–P(1)–N(2) 82.0(2), N(1)–P(2)–N(2) 81.47(19), N(1)–P(1)–Cl(1) 103.86(17), N(2)–P(1)–Cl(1) 104.23(16), N(1)–P(2)–Cl(2) 104.37(16), N(2)–P(2)–Cl(2) 103.00(16).

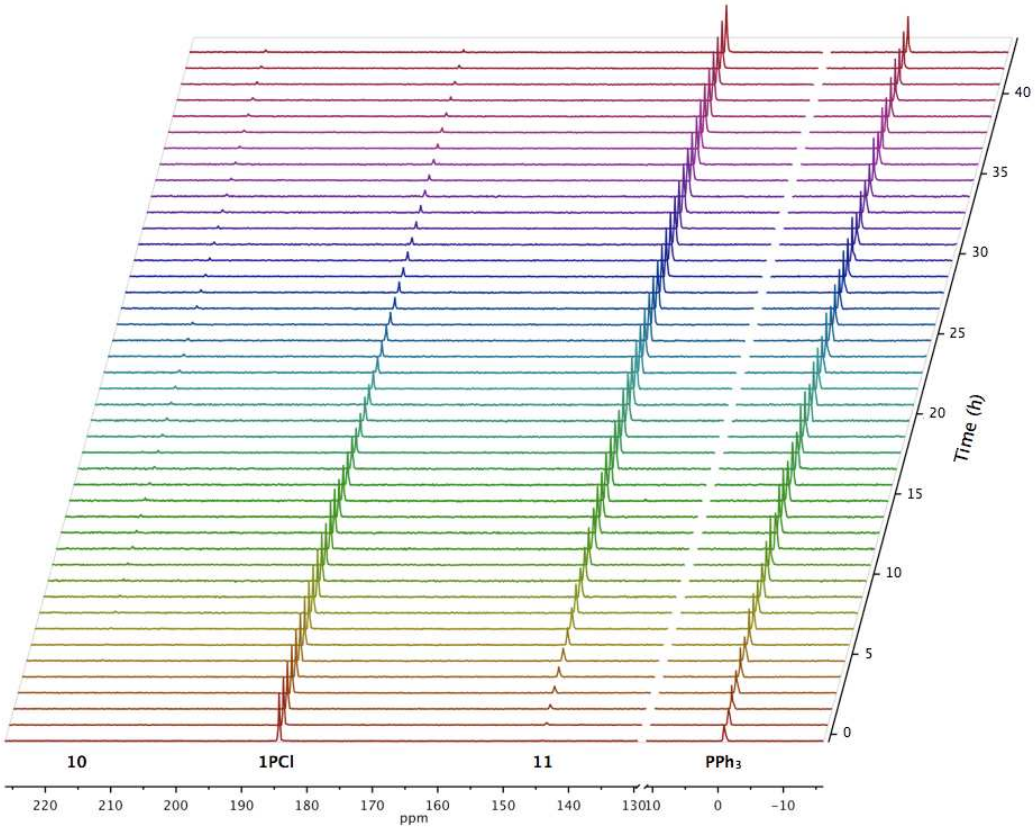

Figure S-10: Stacked plot of $^{31}P\{^{1}H\}$ NMR spectra showing all time points for monitoring the production of **11** from **1PCl**.

Table S1. LUMO energies (in a.u.) of $\mathbf{5P^+}$ and $\mathbf{12P^+}$−$\mathbf{19P^+}$.

Cation	E(LUMO)
$\mathbf{5P^+}$	-0.255723
$\mathbf{12P^+}$	-0.268399
$\mathbf{13P^+}$	-0.266101
$\mathbf{14P^+}$	-0.263908
$\mathbf{15P^+}$	-0.253984
$\mathbf{16P^+}$	-0.229327
$\mathbf{17P^+}$	-0.245803
$\mathbf{18P^+}$	-0.231882
$\mathbf{19P^+}$	-0.217149

Coordinates of optimized structures for **5PCl**, **12PCl−19PCl**, **5P$^+$**, **12P$^+$−19P$^+$** and **12PCl(bpy)**.

5PCl

C	-3.45924	-7.62730	3.28564
C	-4.42115	-6.45720	3.43944
C	-4.56620	-5.68794	2.12806
C	-5.00862	-6.61283	1.00236
C	-4.05205	-7.78650	0.84123
C	-3.89109	-8.54691	2.15094
N	-4.00463	-5.61081	4.53219
P	-2.54655	-5.18613	5.28749
Cl	-1.48359	-4.06356	3.84265
N	-3.68342	-4.04557	5.90109
C	-3.68370	-3.37059	7.18450
C	-2.31138	-2.75931	7.43715
C	-2.27252	-2.01956	8.76778
C	-2.69399	-2.91654	9.92385
C	-4.06221	-3.53399	9.66886
C	-4.09276	-4.27917	8.34134
C	-4.75816	-4.64112	5.19824
N	-6.00022	-4.48432	5.10821
C	-6.72909	-3.44194	5.79414
H	-4.40382	-2.54591	7.11473
H	-1.56185	-3.56283	7.44592
H	-2.05007	-2.09385	6.61030
H	-1.26938	-1.61922	8.93889
H	-2.94618	-1.15500	8.71689
H	-1.95470	-3.71766	10.04761
H	-2.69963	-2.35059	10.85995
H	-4.33710	-4.20956	10.48397
H	-4.82099	-2.74109	9.65629
H	-3.39578	-5.12640	8.37626
H	-5.08660	-4.69665	8.15188
H	-5.40861	-6.84762	3.71696
H	-2.45425	-7.23785	3.07422
H	-3.39613	-8.17967	4.22821
H	-3.16725	-9.35898	2.03641
H	-4.84626	-9.01763	2.41492
H	-3.07269	-7.41183	0.51862
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H	-3.60103	-5.23161	1.88125
H	-5.28238	-4.87458	2.26904
C	-8.19404	-3.84876	5.90669
H	-6.35408	-3.29158	6.81872
C	-9.03468	-2.76490	6.56585
H	-8.56564	-4.05286	4.89561
H	-8.26495	-4.78999	6.45980
C	-8.90464	-1.43736	5.83113
H	-10.08261	-3.07655	6.60874
H	-8.71008	-2.63324	7.60638
C	-7.44518	-1.02070	5.70817
H	-9.33505	-1.53840	4.82698
H	-9.48132	-0.65948	6.34095
C	-6.60766	-2.11058	5.05290
H	-7.35886	-0.09016	5.13893
H	-7.04701	-0.80774	6.70896
H	-6.93907	-2.26737	4.01953
H	-5.55542	-1.81295	5.00004

5P$^+$

C	-3.57374	-7.80150	2.81739
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C	-4.49476	-5.49201	2.43961
C	-3.15124	-5.04981	1.87688
C	-2.39465	-6.21602	1.25742
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C	-3.03061	-4.38606	8.76062
C	-3.14232	-4.09100	7.27186
C	-4.38165	-4.73948	6.66837
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C	-10.44538	-10.22219	4.09711
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H	-2.24926	-4.46242	6.75480
H	-5.28435	-4.31352	7.12301
H	-4.44023	-4.53795	5.59505
H	-8.49724	-7.54338	3.78228
H	-9.51374	-8.85538	6.34683
H	-9.92387	-7.23114	5.77870
H	-11.70913	-8.88429	5.23738
H	-11.02922	-8.17217	3.78759
H	-10.34348	-10.91957	4.93729
H	-11.25679	-10.60551	3.47401
H	-8.87216	-11.19343	2.97350
H	-9.28060	-9.58920	2.39952
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H	-3.43916	-8.59459	3.55912

12PCl

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12P^{+}

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C	-7.74912	-4.18839	8.77732
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13PCl

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C	-4.18232	-5.27912	1.62440
P	-8.36919	-5.12202	3.99957
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C	-6.80260	-3.89559	6.02635
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H	-7.32954	-9.99781	0.02873
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H	-2.91015	-3.54993	3.30902
H	-2.30163	-4.74844	4.45879
Cl	-8.92782	-3.31600	3.10582

13P$^+$

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C	-6.78627	-3.92284	6.12886
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C	-5.46795	-3.03423	7.91314
C	-6.44691	-2.08129	8.15834
C	-7.59641	-2.04783	7.38132
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C	-7.65911	-7.70360	0.11734
C	-7.62382	-6.75768	1.12946
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H	-8.35601	-1.29706	7.56155	H	-1.37521	-0.01403	-2.48415
H	-4.57193	-3.06060	8.52131	H	-1.79252	-5.83718	0.60089
H	-6.36358	-10.35077	1.78842	H	-3.03463	-4.58272	0.76433
H	-8.04626	-7.43138	-0.85702	H	-3.50709	-6.28450	0.59654
C	-2.70004	-4.42094	3.38683	H	-2.48443	-6.63445	-2.98540
C	-3.33484	-6.83860	3.35421	H	-1.44394	-7.00808	-1.59358
C	-4.26162	-5.25877	1.62458	H	-3.14720	-7.48047	-1.58483
H	-2.45122	-7.03652	2.74529	H	-4.27360	-4.85664	-2.77983
H	-3.05696	-6.96118	4.40261	H	-4.96570	-5.71636	-1.39271
H	-4.09753	-7.57478	3.09691	H	-4.51625	-4.01085	-1.23860
H	-3.39232	-5.36442	0.97341	H	-1.36956	-1.29447	1.61942
H	-4.99032	-6.01587	1.33545	H	-1.65725	1.05696	2.31341
H	-4.68690	-4.26760	1.45222	H	-3.03262	2.60233	0.94679
H	-1.84315	-4.60732	2.73767	H	-4.11722	1.75990	-1.11725
H	-3.03669	-3.39543	3.22464	H	-3.81598	-0.58905	-1.81033
H	-2.37568	-4.51600	4.42426	Cl	-1.80133	-4.24819	-4.69756

14PCl

C	-3.32822	-0.21616	-0.91676
C	-2.53411	-1.08727	-0.16636
C	-1.95284	-0.61193	1.01179
C	-2.12494	0.70657	1.39985
C	-2.89440	1.57334	0.63689
C	-3.49968	1.09974	-0.51806
N	-2.44116	-2.42961	-0.49774
C	-1.77170	-3.01986	-1.38216
N	-1.85230	-4.38579	-1.66791
C	-2.83708	-5.37991	-1.24183
C	-2.44893	-6.70116	-1.89487
N	-0.77075	-2.70921	-2.32730
P	-0.67828	-4.32231	-2.89517
C	0.13661	-1.57658	-2.54852
C	0.81672	-1.16330	-1.24717
C	1.19848	-2.05309	-3.53678
C	-0.61823	-0.40252	-3.16522
C	-4.23524	-4.96153	-1.69365
C	-2.78853	-5.52592	0.27718
H	1.35109	-2.00834	-0.80633
H	0.09767	-0.78569	-0.51998
H	1.53912	-0.36829	-1.44660
H	0.74837	-2.38510	-4.47638
H	1.79338	-2.87134	-3.12335
H	1.87445	-1.22732	-3.76453
H	-1.10615	-0.70893	-4.09290
H	0.07890	0.40765	-3.39202

14P^{+}

C	0.60879	-1.99180	-4.13509
C	-0.16100	-1.46925	-2.92829
C	-1.33710	-0.61418	-3.38179
C	0.78245	-0.68397	-2.02647
N	-0.67137	-2.67419	-2.22026
C	-1.79288	-2.95711	-1.35243
N	-2.58037	-2.35782	-0.60485
C	-2.58429	-1.04799	-0.13659
P	-0.54728	-4.27104	-2.65463
N	-1.81593	-4.35995	-1.61428
C	-2.55054	-5.46094	-0.95869
C	-4.04263	-5.26810	-1.21038
C	-2.23995	-5.45759	0.53507
C	-2.05647	-6.74578	-1.60584
H	1.59776	-1.31436	-1.66577
H	0.25731	-0.25604	-1.17444
H	1.21725	0.13850	-2.59659
H	-0.04075	-2.54476	-4.82200
H	1.44654	-2.63090	-3.83795
H	1.02798	-1.15209	-4.69007
H	-2.01476	-1.18057	-4.02466
H	-0.95914	0.23426	-3.95450
H	-1.89895	-0.21737	-2.53540
H	-1.16924	-5.57690	0.71601
H	-2.58177	-4.53709	1.00826
H	-2.75672	-6.29387	1.00838
H	-2.25378	-6.75686	-2.68178

H	-0.98578	-6.89885	-1.43533
H	-2.57860	-7.59715	-1.16837
H	-4.26409	-5.27324	-2.27956
H	-4.59141	-6.08857	-0.74557
H	-4.39592	-4.33191	-0.77885
C	-3.75615	-0.30210	-0.26846
C	-3.80591	0.98518	0.23401
C	-2.72126	1.51312	0.92310
C	-1.57944	0.74683	1.10507
C	-1.49892	-0.52756	0.56885
H	-4.60773	-0.73509	-0.77912
H	-4.70678	1.57329	0.10641
H	-2.77556	2.51260	1.33691
H	-0.74515	1.14036	1.67377
H	-0.62447	-1.14397	0.74103

15PCl

C	0.99516	-2.48007	-3.49046
C	0.03143	-1.67444	-2.61785
N	0.79213	-1.22925	-1.43176
P	2.48447	-0.91659	-1.46894
N	1.90475	0.23091	-0.37179
C	2.56021	1.06843	0.63376
C	4.03894	1.13301	0.26709
C	-1.10744	-2.61451	-2.23628
C	-0.47342	-0.47453	-3.41645
C	0.56255	-0.19405	-0.45149
N	-0.34880	0.30356	0.24220
C	-1.72222	-0.00760	0.58370
C	-1.84831	-1.44931	1.07864
C	-2.07538	0.92109	1.75143
C	-2.70354	0.30128	-0.54689
C	2.39655	0.46569	2.02825
C	1.96636	2.47425	0.58528
H	0.36882	0.12092	-3.77807
H	-1.10923	0.17403	-2.81386
H	-1.05003	-0.80701	-4.28320
H	1.42677	-3.31409	-2.93174
H	1.80801	-1.86288	-3.87978
H	0.45084	-2.88811	-4.34415
H	-0.72509	-3.45286	-1.65032
H	-1.56812	-3.01207	-3.14353
H	-1.88802	-2.12228	-1.66264
H	2.10592	2.91435	-0.40503
H	0.90046	2.44820	0.80811
H	2.46744	3.11067	1.31871
H	4.50620	0.14546	0.30576
H	4.17762	1.54844	-0.73444
H	4.56189	1.77748	0.97610
H	2.82339	-0.53840	2.06695
H	2.90963	1.08898	2.76473
H	1.34178	0.40931	2.29810
H	-3.72916	0.20266	-0.18296
H	-2.56545	1.32914	-0.89105
H	-2.59180	-0.36127	-1.40267
H	-2.88174	-1.66328	1.36348
H	-1.54062	-2.17555	0.32906
H	-1.21743	-1.59316	1.95866
H	-3.09308	0.73329	2.10323
H	-1.38593	0.76307	2.58304
H	-2.00143	1.96613	1.44274
Cl	3.24911	-2.49924	-0.26734

15P^{+}

C	1.08556	-2.25777	-3.67479
C	0.03900	-1.63906	-2.75402
C	-0.75684	-2.75248	-2.08477
C	-0.84233	-0.69519	-3.56518
N	0.78795	-0.87249	-1.73339
C	0.51258	-0.15372	-0.47529
N	-0.38719	0.15960	0.28853
C	-1.80317	0.08949	0.60012
P	2.40600	-0.57525	-1.62597
N	1.91382	0.18000	-0.26679
C	2.58639	0.94559	0.79818
C	2.36940	0.24213	2.13480
C	2.02689	2.36486	0.82583
C	4.06657	0.96593	0.44498
H	-0.23304	0.04560	-4.08713
H	-1.56377	-0.17025	-2.94340
H	-1.39437	-1.26610	-4.31364
H	1.74821	-2.94134	-3.13545
H	1.68766	-1.49492	-4.17847
H	0.58365	-2.83427	-4.45273
H	-0.09566	-3.43089	-1.54171
H	-1.28225	-3.32917	-2.84742
H	-1.50118	-2.36692	-1.39068
H	2.17982	2.86573	-0.13253
H	0.96275	2.36445	1.05982
H	2.54590	2.93935	1.59470

H	4.48755	-0.04360	0.41065
H	4.24591	1.46172	-0.51399
H	4.61407	1.52171	1.20690
H	2.76819	-0.77431	2.11298
H	2.89061	0.79386	2.91869
H	1.31110	0.20194	2.39065
C	-2.09657	1.28309	1.51078
C	-2.72443	0.15299	-0.61088
C	-2.01086	-1.20836	1.38624
H	-3.75527	0.23592	-0.26276
H	-2.51157	1.03488	-1.21891
H	-2.66421	-0.73752	-1.23382
H	-3.05118	-1.25932	1.71160
H	-1.79696	-2.08865	0.77861
H	-1.37427	-1.23325	2.27190
H	-3.13564	1.25150	1.84214
H	-1.45242	1.26649	2.39104
H	-1.93893	2.22489	0.98101

16PCl

C	2.38715	-0.64689	0.00532
Si	0.52606	-0.73944	0.00489
N	-0.29766	0.28000	-1.14885
C	-0.34592	0.42936	-2.60234
C	-0.47810	-0.95515	-3.23040
P	-0.99273	1.29969	0.00891
N	-0.29795	0.27525	1.16265
C	-0.34638	0.41883	2.61674
C	-0.47983	-0.96808	3.23924
C	-0.00503	-2.52545	0.00117
C	0.93378	1.08549	3.12454
C	-1.55117	1.26727	3.01062
C	0.93378	1.09907	-3.10726
C	-1.55134	1.27836	-2.99307
H	2.72238	0.39206	0.00749
H	2.80306	-1.14815	0.88468
H	-1.09313	-2.61353	0.00078
H	0.38217	-3.04759	0.88039
H	1.05763	2.07174	2.67494
H	1.81023	0.48399	2.87028
H	0.90383	1.19657	4.21172
H	-2.48168	0.81541	2.65903
H	-1.47892	2.27544	2.59338
H	-1.60130	1.35999	4.09755
H	-1.38772	-1.46545	2.89095
H	-0.51985	-0.89422	4.32842
H	0.37775	-1.59731	2.98361
H	2.80328	-1.14455	-0.87597
H	0.38249	-3.04402	-0.88001
H	1.05675	2.08365	-2.65379
H	1.81068	0.49730	-2.85519
H	0.90394	1.21438	-4.19400
H	-2.48154	0.82430	-2.64349
H	-1.48006	2.28490	-2.57178
H	-1.60132	1.37540	-4.07964
H	-1.38561	-1.45471	-2.88426
H	-0.51802	-0.87696	-4.31928
H	0.37998	-1.58467	-2.97719
Cl	0.32542	3.04602	0.01278

16P$^+$

P	-1.09572	1.04240	0.00000
Si	0.72611	-0.69171	0.00000
C	2.51647	-0.25183	0.00000
H	2.67394	0.82785	0.00000
H	3.00964	-0.67457	0.87959
C	0.37414	-2.50141	0.00000
H	-0.69660	-2.71129	0.00000
H	0.82039	-2.97340	0.87960
N	-0.26664	0.25343	1.16281
C	-0.40073	0.38159	2.63018
C	0.93914	0.83669	3.19990
H	1.23670	1.80210	2.78572
H	1.72814	0.11008	2.99290
H	0.86354	0.93999	4.28356
C	-1.48043	1.40672	2.94379
H	-2.45372	1.10385	2.54619
H	-1.22877	2.39427	2.54560
H	-1.58688	1.50833	4.02434
C	-0.78519	-0.97975	3.20100
H	-1.73385	-1.32761	2.78729
H	-0.89209	-0.90879	4.28463
H	-0.01842	-1.72993	2.99447
H	3.00964	-0.67457	-0.87959
H	0.82039	-2.97340	-0.87960
N	-0.26664	0.25343	-1.16281
C	-0.40073	0.38159	-2.63018
C	0.93914	0.83669	-3.19990
H	1.23670	1.80210	-2.78572
H	1.72814	0.11008	-2.99290

H	0.86354	0.93999	-4.28356
C	-1.48043	1.40672	-2.94379
H	-2.45372	1.10385	-2.54619
H	-1.22877	2.39427	-2.54560
H	-1.58688	1.50833	-4.02434
C	-0.78519	-0.97975	-3.20100
H	-1.73385	-1.32761	-2.78729
H	-0.89209	-0.90879	-4.28463
H	-0.01842	-1.72993	-2.99447

17PCl

C	-1.81699	0.50533	3.14795
C	-0.73261	-0.12296	2.53302
C	0.27434	-0.65662	3.33996
C	0.20061	-0.55741	4.71863
C	-0.87439	0.07625	5.32409
C	-1.87914	0.60504	4.52752
N	-0.64368	-0.22489	1.14984
P	-1.67921	0.49286	-0.00021
N	-0.64350	-0.22476	-1.15026
C	-0.73238	-0.12295	-2.53347
C	0.27463	-0.65666	-3.34033
C	0.20093	-0.55754	-4.71901
C	-0.87401	0.07611	-5.32454
C	-1.87872	0.60509	-4.52807
C	-1.81672	0.50536	-3.14850
Si	0.40726	-1.02757	-0.00015
C	0.31296	-2.87984	-0.00029
C	2.16465	-0.42662	-0.00004
H	2.20506	0.66419	0.00016
H	2.70179	-0.79096	0.87988
H	-0.72866	-3.20638	-0.00053
H	0.80655	-3.29653	0.88231
H	2.70179	-0.79063	-0.88009
H	0.80692	-3.29643	-0.88273
H	1.12574	-1.15007	-2.88221
H	0.99489	-0.97994	-5.32470
H	-0.93011	0.15265	-6.40357
H	-2.73022	1.09757	-4.98404
H	-2.62189	0.90730	-2.54290
H	1.12547	-1.15006	2.88193
H	0.99461	-0.97963	5.32440
H	-0.93054	0.15287	6.40312
H	-2.73082	1.09724	4.98345
H	-2.62200	0.90748	2.54231
Cl	-3.36045	-0.80974	-0.00057

17P^{+}

C	3.14610	0.63708	-1.63598
C	2.55755	-0.00997	-0.55304
C	3.35171	-0.61220	0.41802
C	4.73076	-0.57262	0.29785
C	5.32023	0.05629	-0.78895
C	4.52476	0.65807	-1.75445
N	1.15519	-0.06995	-0.42475
P	-0.00000	0.00001	-1.58936
N	-1.15519	0.06995	-0.42474
C	-2.55756	0.00995	-0.55303
C	-3.35172	0.61221	0.41801
C	-4.73076	0.57270	0.29780
C	-5.32022	-0.05620	-0.78901
C	-4.52475	-0.65803	-1.75448
C	-3.14610	-0.63709	-1.63597
Si	-0.00000	-0.00003	0.95450
C	0.17331	1.55768	1.91664
C	-0.17331	-1.55777	1.91658
H	-0.12925	-2.43854	1.27369
H	0.60595	-1.63662	2.67885
H	0.12925	2.43848	1.27378
H	1.13769	1.55872	2.43416
H	-1.13769	-1.55883	2.43411
H	-0.60595	1.63650	2.67891
H	-2.89273	1.13366	1.25108
H	-5.34668	1.04404	1.05408
H	-6.39899	-0.08468	-0.88042
H	-4.98034	-1.16312	-2.59756
H	-2.53083	-1.14550	-2.37183
H	2.89273	-1.13368	1.25107
H	5.34668	-1.04393	1.05415
H	6.39899	0.08483	-0.88033
H	4.98034	1.16313	-2.59755
H	2.53083	1.14548	-2.37184

18PCl

C	2.43090	4.14134	3.19838
C	1.90360	3.07605	3.92426
C	1.53838	1.90922	3.25966
C	1.71578	1.80825	1.88886
C	2.23542	2.86992	1.16488

C	2.58474	4.03838	1.82663
N	1.74555	3.19502	5.31948
C	1.81386	2.11373	6.19755
C	1.56426	2.47938	7.45773
N	1.30145	3.84520	7.56023
C	0.94571	4.48134	8.76608
C	1.28002	5.81904	8.96290
C	0.93028	6.45629	10.14074
C	0.26323	5.76671	11.14306
C	-0.06414	4.43399	10.94867
C	0.26294	3.79291	9.76430
H	1.82648	6.35153	8.19283
H	-0.03503	2.76398	9.60404
H	1.09170	1.09095	3.81111
H	2.73104	5.04435	3.71768
P	1.06248	4.57533	6.04213
Cl	-1.05540	4.24326	5.71899
H	1.61960	1.86298	8.33989
H	2.11307	1.13967	5.84687
H	1.19587	7.49780	10.28068
H	-0.00054	6.26558	12.06788
H	-0.59554	3.88686	11.71899
H	1.42792	0.89409	1.38230
H	2.36606	2.78880	0.09242
H	2.99580	4.87500	1.27346

18P^{+}

C	2.50267	4.10830	3.20965
C	1.88567	3.07964	3.90667
C	1.40988	1.94835	3.25846
C	1.56362	1.84975	1.88609
C	2.17339	2.87395	1.17443
C	2.63845	4.00113	1.83458
N	1.72100	3.19881	5.32424
C	2.02958	2.20481	6.20020
C	1.77700	2.57735	7.48354
N	1.28355	3.84364	7.54561
C	0.92567	4.49127	8.77146
C	1.34478	5.79496	8.99397
C	0.97429	6.42843	10.16954
C	0.20741	5.75808	11.11030
C	-0.19885	4.45134	10.87695
C	0.15260	3.81014	9.70138
H	1.98028	6.29775	8.27317
H	-0.19287	2.80312	9.49776
H	0.90252	1.16842	3.81451
H	2.90170	4.96709	3.73821
P	1.09092	4.57254	6.04856
H	1.96080	2.01250	8.38466
H	2.45881	1.27754	5.85260
H	1.30119	7.44415	10.35500
H	-0.07397	6.25457	12.03095
H	-0.80452	3.93044	11.60837
H	1.19320	0.97293	1.36922
H	2.28779	2.79118	0.10050
H	3.12404	4.79606	1.28209

19PCl

C	1.92597	3.08367	3.86632
N	1.70837	3.14747	5.32412
C	2.51875	3.91562	6.15101
C	2.10970	3.87847	7.42432
N	0.98263	3.08158	7.58307
C	0.31274	2.93634	8.88941
P	0.31452	2.61583	6.10791
Cl	-1.15858	4.30507	5.68398
H	3.37155	4.44785	5.76223
H	2.56771	4.37481	8.26426
C	0.89653	2.14633	3.24769
C	1.76935	4.47906	3.26267
C	3.32633	2.53737	3.59990
C	-0.86905	1.98618	8.74246
C	1.30561	2.35145	9.89062
C	-0.18842	4.30020	9.36331
H	3.49765	2.46706	2.52362
H	4.10081	3.18442	4.01664
H	3.44100	1.54261	4.03568
H	1.07061	2.08520	2.17175
H	0.97346	1.13875	3.66270
H	-0.12187	2.51296	3.40037
H	1.90749	4.43545	2.17989
H	0.77603	4.87675	3.47692
H	2.51000	5.17256	3.66711
H	-1.35240	1.86499	9.71374
H	-1.61430	2.37868	8.04573
H	-0.54878	1.00077	8.39640
H	0.82019	2.22094	10.86015
H	1.66842	1.37936	9.55002
H	2.16737	3.00564	10.03742
H	-0.70487	4.19659	10.32035

H	0.63783	5.00085	9.50280
H	-0.87841	4.72649	8.63327

19P^{+}

C	1.90991	3.04973	3.86744
C	1.69432	3.16418	5.36802
C	2.78764	4.02278	5.99343
N	1.77671	1.79217	5.96681
P	2.06349	0.40120	5.08686
C	0.30857	3.72847	5.65954
C	1.62292	1.56227	7.29561
C	1.74031	0.24122	7.59505
N	1.98103	-0.50574	6.48766
C	2.15354	-1.99423	6.53737
C	0.87176	-2.60393	7.09322
C	2.40581	-2.49824	5.12541
C	3.34998	-2.30499	7.42939
H	1.43196	2.36560	7.98962
H	1.66060	-0.20725	8.57280
H	2.75298	5.02055	5.55396
H	2.65518	4.13401	7.07105
H	3.77698	3.60171	5.80438
H	1.85088	4.04508	3.42598
H	2.89656	2.64547	3.62436
H	1.14153	2.43655	3.38830
H	0.22607	4.72022	5.21293
H	-0.47283	3.09679	5.23265
H	0.12613	3.83464	6.73034
H	2.53255	-3.58090	5.15501
H	1.56478	-2.28842	4.45861
H	3.31924	-2.07669	4.69647
H	3.50120	-3.38484	7.46011
H	4.26108	-1.84452	7.04248
H	3.19543	-1.96593	8.45522
H	0.97492	-3.68956	7.11838
H	0.66720	-2.27008	8.11197
H	0.01300	-2.35802	6.46561

12PCl(bpy)

C	2.62167	1.35872	2.24521
N	1.30723	1.59243	1.92015
C	0.56573	2.53289	2.63491
C	1.18260	3.21425	3.71405
C	2.46747	2.94333	4.04394
C	3.20838	1.98352	3.28426
C	-0.68770	2.65853	2.10300
N	-0.83669	1.79712	0.97665
C	-2.10631	1.70457	0.39593
C	-3.11631	2.49645	0.78904
C	-2.93979	3.46754	1.83020
C	-1.74722	3.51778	2.46778
P	0.57252	1.04715	0.43994
N	-0.13810	0.22774	-0.99747
C	0.27156	-1.02044	-0.53826
N	0.18205	-2.22319	-0.90938
C	-0.62095	-2.68267	-1.94896
C	-1.94961	-2.28465	-2.11216
C	-2.72924	-2.83238	-3.11685
C	-2.20355	-3.78229	-3.98055
C	-0.88807	-4.19231	-3.81587
C	-0.10767	-3.65872	-2.80460
N	0.87498	-0.60333	0.65706
C	1.17950	-1.42543	1.76400
C	2.11669	-2.44097	1.61383
C	2.41880	-3.26230	2.68752
C	1.80301	-3.06561	3.91486
C	0.86846	-2.05136	4.06119
C	0.54518	-1.23873	2.98665
C	-0.19964	0.63751	-2.34205
C	-0.87321	1.81222	-2.66989
C	-0.92942	2.24361	-3.98496
C	-0.32536	1.50904	-4.99307
C	0.35549	0.34580	-4.66706
C	0.43140	-0.08395	-3.35354
H	-1.34319	2.40248	-1.89319
H	-0.37789	1.84339	-6.02251
H	0.98523	-0.98130	-3.11308
H	-2.37304	-1.55327	-1.43306
H	-2.81668	-4.20732	-4.76652
H	0.91379	-3.99087	-2.65773
H	2.58756	-2.58750	0.65019
H	2.04766	-3.70514	4.75504
H	-0.19930	-0.45880	3.09470
H	3.14395	-4.05858	2.56431
H	0.37621	-1.89715	5.01449
H	-1.45415	3.16298	-4.21869
H	0.84391	-0.23447	-5.44154
H	-3.75990	-2.51248	-3.22537
H	-0.46754	-4.94411	-4.47475
H	-1.57491	4.21177	3.28153

H	-3.75278	4.12294	2.11184
H	-4.08067	2.36446	0.31553
H	-2.21805	0.94440	-0.35950
H	0.60437	3.94829	4.26073
H	2.93987	3.45658	4.87189
H	4.23622	1.75318	3.52844
H	3.13975	0.63771	1.62842
Cl	2.02571	2.04093	-0.76669