

Supporting information

A Reactivity Profile of a Peri-substitution Stabilized Phosphanlydene-Phosphorane; Synthetic, Structural and Computational Study

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Table S1 Computed P-P distances [in Å] and WBIs for selected compounds (B3LYP level) forming datapoints in Figure 11.

Compd.	d(P-P)	WBI
1	2.165	1.13
2	2.263	0.88
3	2.289	0.84
3	2.898 ^a	0.15
4	2.205 ^b	1.00
4	3.480 ^a	0.03
5	2.257	0.93
6	3.248	0.08
6	2.159 ^c	1.30
8	3.388	0.01
9	2.376	0.62
10	2.374	0.63
11	2.286	0.84
13	2.260	0.94
PhP=PPh	2.058	1.82

^a P1...P1ⁱ distance ^b Mean value ^c Central P=P bond.

Cartesian coordinates of all computed structures, xyz format in Å (B3LYP optimized).

42				C	-2.445992	7.358481	-2.949515
compd. 1				C	0.281256	3.875779	3.031804
P	1.687304	0.156034	-0.063591	C	0.583580	2.557949	3.764873
P	1.052874	2.192091	-0.438597	C	-1.191760	4.289733	3.178888
C	-0.703119	1.650944	-0.318619	C	2.690070	3.651005	1.163383
C	-1.824366	2.474085	-0.462922	C	3.409082	4.409827	2.293455
H	-1.683389	3.533680	-0.666137	C	3.223313	4.072181	-0.216165
C	-3.164375	1.991538	-0.353039	H	1.248952	6.899284	1.520333
H	-3.980900	2.700515	-0.478488	H	0.285885	8.760260	0.225594
C	-3.406723	0.657000	-0.089847	H	-3.157064	4.508421	-3.600666
C	-2.282893	-0.183455	0.057569	H	-2.238063	2.576308	-2.381805
C	-2.609863	-1.524077	0.336821	H	-0.942005	8.967201	-2.646777
C	-1.584349	-2.438928	0.514087	H	-2.286848	9.052283	-1.518032
H	-1.786161	-3.484159	0.737737	H	-3.523568	7.546826	-2.872397
C	-0.231676	-2.004402	0.405799	H	-2.183491	7.471790	-4.008117
H	0.557689	-2.737122	0.556367	H	0.909272	4.674819	3.451590
C	0.080043	-0.677458	0.122936	H	0.388097	2.697742	4.834821
C	-0.961789	0.269658	-0.051961	H	1.615634	2.216021	3.646424
C	-4.659824	-0.185762	0.097023	H	-0.074104	1.758607	3.407832
H	-5.297967	-0.173882	-0.795891	H	-1.863003	3.530865	2.763015
H	-5.279152	0.178275	0.926678	H	-1.406956	5.249892	2.699851
C	-4.126349	-1.639740	0.387423	H	-1.422168	4.384199	4.246779
H	-4.464619	-2.001626	1.366485	H	2.859166	2.574744	1.302920
H	-4.496866	-2.358025	-0.354603	H	4.486647	4.243441	2.182847
C	2.671521	-0.622415	-1.466227	H	3.129563	4.054861	3.289013
H	3.499652	0.083876	-1.620842	H	3.237869	5.492177	2.240742
C	1.823644	-0.650694	-2.748147	H	3.119654	5.151421	-0.375240
H	2.450048	-0.953453	-3.596438	H	2.723836	3.546676	-1.035866
H	1.398689	0.333846	-2.966726	H	4.287529	3.816651	-0.270026
H	1.000904	-1.369846	-2.661695	Au	-1.270390	-1.186178	-1.365542
C	3.253463	-2.009627	-1.146747	Au	1.776917	-1.123254	1.157038
H	2.461843	-2.740751	-0.944600	Cl	-2.779821	-0.048993	-2.770105
H	3.938398	-1.998045	-0.292885	Cl	3.289075	0.158511	2.447590
H	3.817683	-2.376117	-2.013688	P	-0.830700	-3.832600	1.246084
C	2.699139	-0.116078	1.491991	P	0.257766	-2.352864	-0.076278
H	2.879179	-1.198293	1.553499	C	-0.257766	-5.338363	0.413715
C	1.907029	0.322810	2.732663	C	-0.568261	-6.663500	0.705952
H	2.515234	0.159112	3.631306	C	-0.011999	-7.741672	-0.037818
H	0.976593	-0.242944	2.844553	C	0.864371	-7.469995	-1.075210
H	1.653578	1.387142	2.675606	C	1.177979	-6.127930	-1.363165
C	4.047143	0.620337	1.400675	C	2.085515	-5.975102	-2.431113
H	3.892582	1.701144	1.297613	C	2.460492	-4.694235	-2.786920
H	4.661138	0.280090	0.559179	C	1.928591	-3.574733	-2.080378
H	4.623261	0.452290	2.318901	C	1.033157	-3.732438	-1.029544
				C	0.640906	-5.043354	-0.650024
92				C	1.627119	-8.354647	-2.048108
complex 2				C	2.445992	-7.358481	-2.949515
Au	1.270390	1.186178	-1.365542	C	-0.281256	-3.875779	3.031804
Au	-1.776917	1.123254	1.157038	C	-0.583580	-2.557949	3.764873
Cl	2.779821	0.048993	-2.770105	C	1.191760	-4.289733	3.178888
Cl	-3.289075	-0.158511	2.447590	C	-2.690070	-3.651005	1.163383
P	0.830700	3.832600	1.246084	C	-3.409082	-4.409827	2.293455
P	-0.257766	2.352864	-0.076278	C	-3.223313	-4.072181	-0.216165
C	0.257766	5.338363	0.413715	H	-1.248952	-6.899284	1.520333
C	0.568261	6.663500	0.705952	H	-0.285885	-8.760260	0.225594
C	0.011999	7.741672	-0.037818	H	3.157064	-4.508421	-3.600666
C	-0.864371	7.469995	-1.075210	H	2.238063	-2.576308	-2.381805
C	-1.177979	6.127930	-1.363165	H	0.942005	-8.967201	-2.646777
C	-2.085515	5.975102	-2.431113	H	2.286848	-9.052283	-1.518032
C	-2.460492	4.694235	-2.786920	H	3.523568	-7.546826	-2.872397
C	-1.928591	3.574733	-2.080378	H	2.183491	-7.471790	-4.008117
C	-1.033157	3.732438	-1.029544	H	-0.909272	-4.674819	3.451590
C	-0.640906	5.043354	-0.650024	H	-0.388097	-2.697742	4.834821
C	-1.627119	8.354647	-2.048108	H	-1.615634	-2.216021	3.646424

H	0.074104	-1.758607	3.407832	H	0.493257	-4.916948	0.140462
H	1.863003	-3.530865	2.763015	H	3.406642	-2.503676	-4.676145
H	1.406956	-5.249892	2.699851	H	2.572629	-3.889547	-3.965032
H	1.422168	-4.384199	4.246779	H	1.741813	-2.843503	-5.143057
H	-2.859166	-2.574744	1.302920	H	3.980925	-1.461594	-2.461664
H	-4.486647	-4.243441	2.182847	H	2.757493	-1.195514	-1.228271
H	-3.129563	-4.054861	3.289013	H	3.276862	-2.858312	-1.629240
H	-3.237869	-5.492177	2.240742	H	-1.893563	0.901696	3.552951
H	-3.119654	-5.151421	-0.375240	H	1.042993	3.734827	1.297037
H	-2.723836	-3.546676	-1.035866	H	-2.572629	3.889547	3.965032
H	-4.287529	-3.816651	-0.270026	H	-3.406642	2.503676	4.676145
90				H	-1.741813	2.843503	5.143057
complex 3				H	-2.757493	1.195514	1.228271
Pt	1.110283	1.103254	-0.861971	H	-3.980925	1.461594	2.461664
Cl	1.501902	1.587964	-3.188893	H	-3.276862	2.858312	1.629240
Cl	2.798323	2.670911	-0.155771	H	0.280855	5.975741	2.016759
P	-0.492053	-0.497087	-1.269114	H	-1.008821	5.287174	3.009653
P	0.269247	-2.244463	-2.537217	H	0.699419	5.003997	3.426709
C	-1.797464	-0.129820	-2.501502	H	-0.882201	3.205380	-0.225621
C	-2.731764	0.890140	-2.386833	H	-1.919036	4.311601	0.719538
C	-3.719619	1.130558	-3.382788	H	-0.493257	4.916948	-0.140462
C	-3.759292	0.329782	-4.507086	H	0.384513	3.612101	5.262183
C	-2.808900	-0.704676	-4.622062	H	2.116692	3.110955	6.926334
C	-2.939947	-1.455194	-5.806518	H	2.717608	-1.532755	1.510856
C	-2.061431	-2.499236	-6.029316	H	4.425958	-1.944266	3.237370
C	-1.057979	-2.785066	-5.062034	H	4.871030	1.648846	6.782850
C	-0.928582	-2.042098	-3.891570	H	3.770019	0.543422	7.593885
C	-1.826605	-0.961406	-3.650432	H	5.701853	-0.140121	5.465034
C	-4.651481	0.299770	-5.737073	H	4.609822	-1.248272	6.285868
C	-4.100494	-0.888541	-6.606680	H	-0.384513	-3.612101	-5.262183
C	2.002622	-1.921185	-3.158565	H	-2.116692	-3.110955	-6.926334
C	3.055063	-1.868122	-2.038921	H	-2.717608	1.532755	-1.510856
C	2.438318	-2.855303	-4.300117	H	-4.425958	1.944266	-3.237370
C	-0.017457	-3.873818	-1.665891	H	-3.770019	-0.543422	-7.593885
C	0.887570	-4.074592	-0.439368	H	-4.871030	-1.648846	-6.782850
C	0.011085	-5.094462	-2.600526	H	-4.609822	1.248272	-6.285868
Pt	-1.110283	-1.103254	0.861971	H	-5.701853	0.140121	-5.465034
Cl	-1.501902	-1.587964	3.188893	93			
Cl	-2.798323	-2.670911	0.155771	complex 4			
P	0.492053	0.497087	1.269114	Mo	0.007140	-1.255752	-1.351068
P	-0.269247	2.244463	2.537217	P	-1.774426	-0.364765	0.435928
C	1.797464	0.129820	2.501502	P	-3.862037	-1.062583	0.283756
C	2.731764	-0.890140	2.386833	P	2.932673	-0.602178	1.660869
C	3.719619	-1.130558	3.382788	P	1.630308	0.279127	0.116488
C	3.759292	-0.329782	4.507086	8	0.190391	-3.910373	0.430313
C	2.808900	0.704676	4.622062	8	-0.581593	1.269960	-3.249401
C	2.939947	1.455194	5.806518	8	2.450719	-2.144876	-3.136758
C	2.061431	2.499236	6.029316	8	-1.806809	-2.945746	-3.294209
C	1.057979	2.785066	5.062034	C	1.550753	-1.812711	-2.472434
C	0.928582	2.042098	3.891570	C	4.485490	0.239563	1.232611
C	1.826605	0.961406	3.650432	C	-0.343105	0.382074	-2.541213
C	4.651481	-0.299770	5.737073	C	6.876950	2.820441	-1.980418
C	4.100494	0.888541	6.606680	C	6.841983	0.921694	1.349119
C	-2.002622	1.921185	3.158565	C	7.704134	2.366927	-0.719311
C	-3.055063	1.868122	2.038921	C	5.711803	0.245617	1.891377
C	-2.438318	2.855303	4.300117	C	0.158652	-2.928788	-0.198744
C	0.017457	3.873818	1.665891	C	3.221442	-2.457732	1.666803
C	-0.887570	4.074592	0.439368	C	4.345065	0.927300	-0.002584
C	-0.011085	5.094462	2.600526	C	3.116474	0.983324	-0.725781
H	-1.042993	-3.734827	-1.297037	C	4.295781	2.304534	-2.458441
H	1.893563	-0.901696	-3.552951	C	1.042459	-0.788900	3.729407
H	1.008821	-5.287174	-3.009653	C	6.723189	1.578367	0.135205
H	-0.280855	-5.975741	-2.016759	C	3.127731	1.663937	-1.942038
H	-0.699419	-5.003997	-3.426709	C	-5.809878	4.708974	0.627959
H	1.919036	-4.311601	-0.719538	C	5.478605	2.268191	-1.747469
H	0.882201	-3.205380	0.225621	C	5.477309	1.572203	-0.520566

C	-1.564907	2.523697	0.254583	70			
C	-4.345936	-0.839291	-2.464771	complex	5		
C	-2.368462	1.385784	0.318464	Rh	-1.961853	-0.169406	-0.218523
C	3.976488	-2.966618	2.906916	Cl	-2.014941	2.214548	-0.776132
C	2.387915	-0.125504	3.383526	Cl	-0.995896	-0.894539	-2.315067
C	-4.329211	-2.219954	1.673619	P	1.478878	1.781479	0.082474
C	-2.095577	3.849281	0.297912	P	0.127069	0.132717	0.821671
C	-3.776495	1.594276	0.424510	C	3.024637	0.818034	0.114461
C	2.325805	1.400514	3.550751	C	4.337793	1.251212	-0.040983
C	-5.648164	3.196533	0.604632	C	5.425421	0.332806	-0.095564
C	-6.550731	2.148664	0.679566	C	5.171593	-1.025626	-0.016454
C	3.928332	-2.884084	0.369655	C	3.840316	-1.456336	0.142292
C	-4.347841	5.279598	0.497735	C	3.701484	-2.858795	0.191945
C	-4.715282	0.529124	0.480452	C	2.426600	-3.370331	0.329567
C	-5.815075	-2.509633	-1.238957	C	1.312692	-2.484686	0.442249
C	-4.276356	2.903753	0.481785	C	1.443370	-1.100142	0.413066
C	-4.422389	-1.861430	-1.318946	C	2.754552	-0.571881	0.227705
C	-4.116761	-1.564507	3.046892	C	6.065256	-2.255465	-0.069091
C	-3.456293	4.049388	0.417573	C	5.083189	-3.479980	0.054230
C	-1.171269	-2.297466	-2.553421	C	-3.535727	-0.091189	1.346430
C	-3.564517	-3.550982	1.558014	C	-4.253821	-0.181633	0.076699
C	-6.072355	0.808945	0.611473	C	-3.888290	-1.392543	-0.551481
H	5.828284	-0.271820	2.840548	C	-2.941833	-2.086233	0.318493
H	7.781078	0.903156	1.897389	C	-2.804350	-1.313270	1.525172
H	8.104129	3.229365	-0.171600	C	-3.723929	1.000968	2.357534
H	8.566693	1.752531	-1.005507	C	-5.209581	0.857307	-0.423087
H	6.872652	3.913249	-2.077834	C	-4.358272	-1.929268	-1.868568
H	7.319403	2.426649	-2.903941	C	-2.446239	-3.477814	0.055738
H	4.225307	2.812938	-3.417795	C	-2.087452	-1.725838	2.776445
H	2.218072	1.718929	-2.533862	C	1.328912	2.578296	-1.614728
H	2.212260	-2.885141	1.668006	C	1.673903	1.564756	-2.716894
H	3.446218	-2.765090	3.843064	C	1.595678	3.128642	1.374305
H	4.095819	-4.054325	2.827209	C	2.006329	2.566683	2.745317
H	4.982093	-2.535323	2.975805	C	0.298301	3.949532	1.466875
H	3.421784	-2.507076	-0.522096	C	2.166817	3.861703	-1.746669
H	4.965754	-2.531483	0.350562	H	4.558386	2.312079	-0.131020
H	3.940408	-3.978837	0.309141	H	6.435612	0.718064	-0.213272
H	3.166024	-0.518486	4.052232	H	6.799132	-2.248568	0.746424
H	2.035412	1.638112	4.581912	H	6.638102	-2.293456	-1.003658
H	3.292289	1.874866	3.351954	H	5.335987	-4.105533	0.919281
H	1.585461	1.838241	2.873773	H	5.147175	-4.127656	-0.828914
H	0.754138	-0.515501	4.752054	H	2.244683	-4.442827	0.353080
H	0.246504	-0.450143	3.055758	H	0.324351	-2.920999	0.543922
H	1.086418	-1.882532	3.679161	H	0.263905	2.819918	-1.685670
H	-5.402878	-2.410774	1.540375	H	2.403568	3.779875	1.013880
H	-4.435944	-2.260680	3.832717	H	1.868140	4.645968	-1.044065
H	-3.060508	-1.324497	3.206274	H	3.240198	3.671535	-1.624708
H	-4.695266	-0.641426	3.155268	H	2.024746	4.261223	-2.758524
H	-3.887171	-4.228099	2.358375	H	2.736999	1.297901	-2.701874
H	-3.738931	-4.059681	0.603947	H	1.071179	0.656021	-2.639452
H	-2.485045	-3.398938	1.665652	H	1.452849	2.022394	-3.689117
H	-3.676036	-2.641957	-1.505524	H	0.442571	4.766642	2.184966
H	-5.117708	-0.068457	-2.359941	H	0.000050	4.384348	0.508737
H	-3.369891	-0.348895	-2.510348	H	-0.536256	3.331365	1.811010
H	-4.500997	-1.357046	-3.417879	H	2.115488	3.397753	3.453430
H	-6.595143	-1.774014	-1.009293	H	1.246233	1.881647	3.134268
H	-6.058312	-2.945562	-2.215706	H	2.958859	2.029132	2.703216
H	-5.868898	-3.315446	-0.500117	H	-4.728737	1.840962	-0.462462
H	-6.797940	0.000867	0.664070	H	-5.573620	0.623020	-1.426513
H	-7.619327	2.323140	0.782077	H	-6.077976	0.927660	0.246389
H	-0.486829	2.408291	0.181165	H	-3.758161	1.979987	1.869917
H	-1.402207	4.685755	0.236173	H	-4.663233	0.864751	2.913574
H	-4.093166	5.912487	1.357062	H	-2.906231	1.017865	3.084253
H	-4.249378	5.910479	-0.394470	H	-2.806168	-2.127171	3.504569
H	-6.289669	5.044217	1.555922	H	-1.341568	-2.501519	2.582847
H	-6.448821	5.053189	-0.194712	H	-1.572017	-0.882957	3.246716
				H	-1.732045	-3.807960	0.815277

H	-3.283588	-4.190169	0.063028	C	-6.297095	-2.798096	-1.572194
H	-1.960074	-3.540985	-0.923449	H	-6.751111	-3.710838	-1.167097
H	-4.998164	-1.214774	-2.392292	H	-6.384238	-2.864888	-2.664234
H	-3.504931	-2.153200	-2.518833	H	-6.996856	-1.512594	-1.024169
H	-4.931134	-2.855632	-1.723212	H	-7.492157	-0.945871	-1.822199
85				H	-7.773518	-1.760081	-0.289413
complex 6				C	-2.417330	3.131708	0.940925
Pd	-0.000054	0.449027	0.000094	H	-3.343610	3.289016	1.508151
P	0.707415	-1.685397	-0.815567	C	-2.671499	3.466955	-0.536213
P	1.896017	1.318593	-1.148621	H	-1.783092	3.254806	-1.141591
P	-0.707275	-1.685545	0.815441	H	-2.910377	4.533036	-0.647124
P	-1.895984	1.318581	1.148706	H	-3.501833	2.889734	-0.954074
C	2.318474	-1.899483	0.074001	C	-1.363548	4.074242	1.545401
C	2.535033	-3.112114	0.730318	H	-1.665382	5.116563	1.378446
H	1.704954	-3.810732	0.797780	H	-0.382991	3.932729	1.081813
C	3.773912	-3.500876	1.293265	H	-1.250361	3.936152	2.625615
H	3.859771	-4.460501	1.798788	C	-1.878191	1.168359	3.051621
C	4.848010	-2.656219	1.145961	H	-2.421333	2.055463	3.408180
C	4.659691	-1.419573	0.480355	C	-2.602180	-0.071618	3.598789
C	5.879980	-0.710968	0.384412	H	-2.563271	-0.056897	4.696431
C	5.886971	0.509834	-0.245886	H	-2.121327	-0.995884	3.261955
H	6.797844	1.090831	-0.373451	H	-3.653476	-0.103800	3.298618
C	4.655690	1.028863	-0.713390	C	-0.435977	1.227780	3.584526
H	4.696734	2.011154	-1.169612	H	0.128106	0.344509	3.266877
C	3.426867	0.375982	-0.610546	H	-0.444146	1.252271	4.682744
C	3.410129	-0.957892	-0.036225	H	0.106425	2.110838	3.231936
C	6.297059	-2.797820	1.572538	45			
H	6.751060	-3.711055	1.168553	compd. 8			
H	6.383944	-2.863419	2.664682	S	-0.667398	3.875089	-1.043882
C	6.997054	-1.512925	1.023412	S	-0.960106	2.166014	1.971569
H	7.493407	-0.946100	1.820703	S	-1.922062	0.763942	-1.111170
H	7.772924	-1.761235	0.288074	P	-0.515973	2.241938	0.043851
C	2.417410	3.131691	-0.940778	P	-1.502928	-0.993970	-0.137971
H	3.343611	3.289006	-1.508135	C	1.058654	1.315633	-0.242587
C	2.671757	3.466846	0.536345	C	2.164565	2.110484	-0.526284
H	1.783472	3.254500	1.141837	H	1.990603	3.160288	-0.743546
H	2.910481	4.532949	0.647326	C	3.498589	1.634283	-0.519420
H	3.502235	2.889707	0.954019	H	4.312585	2.318585	-0.745772
C	1.363552	4.074302	-1.545042	C	3.721883	0.319583	-0.189108
H	1.665393	5.116605	-1.377972	C	2.607634	-0.517725	0.067103
H	0.383063	3.932683	-1.081342	C	3.021553	-1.829908	0.390246
H	1.250220	3.936368	-2.625263	C	2.069367	-2.790002	0.655675
C	1.878009	1.168540	-3.051563	H	2.332906	-3.810049	0.922966
H	2.421318	2.055557	-3.408079	C	0.710768	-2.424642	0.534573
C	0.435731	1.228325	-3.584268	H	-0.026543	-3.209441	0.686626
H	-0.128396	0.345019	-3.266806	C	0.281539	-1.136110	0.209685
H	0.443752	1.253124	-4.682476	C	1.250835	-0.087122	0.010821
H	-0.106557	2.111318	-3.231345	C	5.003622	-0.476782	-0.041788
C	2.601613	-0.071536	-3.598979	H	5.669839	-0.030313	0.705888
H	2.562786	-0.056520	-4.696624	H	5.563915	-0.502489	-0.984543
H	2.120436	-0.995724	-3.262401	C	4.535204	-1.906139	0.382350
H	3.652880	-0.104143	-3.298755	H	4.892794	-2.677255	-0.310693
C	-2.318427	-1.899538	-0.074020	H	4.916965	-2.177217	1.374501
C	-2.535024	-3.112249	-0.730204	C	-1.917066	-2.363274	-1.351462
H	-1.704964	-3.810903	-0.797578	H	-1.704034	-3.289379	-0.798997
C	-3.773910	-3.501043	-1.293085	C	-3.410253	-2.350103	-1.725219
H	-3.859828	-4.460762	-1.798410	H	-3.676967	-1.430867	-2.257245
C	-4.847979	-2.656318	-1.145911	H	-4.068756	-2.447322	-0.856189
C	-4.659596	-1.419564	-0.480534	H	-3.617593	-3.195297	-2.392204
C	-5.879847	-0.710846	-0.384796	C	-1.029243	-2.315803	-2.604703
C	-5.886848	0.509953	0.245501	H	-1.272892	-3.170157	-3.247728
H	-6.797699	1.091004	0.372952	H	0.035941	-2.368730	-2.361592
C	-4.655585	1.028898	0.713169	H	-1.204643	-1.399162	-3.176685
H	-4.696640	2.011158	1.169467	C	-2.556410	-1.375201	1.384863
C	-3.426790	0.375984	0.610402	H	-2.920618	-2.391448	1.174645
C	-3.410031	-0.957899	0.036080	C	-1.770307	-1.404000	2.706027

H	-1.333827	-0.426112	2.924360	C	2.939199	-0.176830	-0.049463
H	-0.970042	-2.149203	2.705702	C	3.585718	-1.421911	0.088748
H	-2.465969	-1.661655	3.514193	C	2.803382	-2.548704	0.254093
C	-3.767128	-0.429220	1.473068	H	3.244077	-3.536205	0.368714
H	-4.416716	-0.769637	2.288677	C	1.385728	-2.422229	0.266480
H	-4.359375	-0.410375	0.553158	H	0.783835	-3.319560	0.383308
H	-3.443838	0.593273	1.688984	C	0.749238	-1.196197	0.126553
44				C	1.539938	-0.024801	-0.027751
compd. 9				C	5.251005	0.355310	-0.188960
S	-1.791120	2.245439	1.844385	H	5.837537	0.808190	0.619708
S	-1.666311	2.433437	-1.627565	H	5.779882	0.582253	-1.122675
P	-1.369498	-0.715026	0.000594	C	5.087012	-1.194714	0.016681
P	-1.084868	1.641584	0.094292	H	5.538741	-1.756353	-0.809919
C	0.385643	-1.131586	-0.135427	H	5.588033	-1.529919	0.932936
C	0.972548	-2.382914	-0.290546	C	-1.292943	2.153474	1.574621
H	0.346599	-3.268269	-0.376693	H	-2.239832	1.649223	1.815874
C	2.384663	-2.552536	-0.341484	C	-0.291923	1.832026	2.698303
H	2.794215	-3.552019	-0.466114	H	0.676715	2.312291	2.521080
C	3.201148	-1.442158	-0.227232	H	-0.143428	0.755285	2.813015
C	2.606326	-0.173248	-0.073642	H	-0.693692	2.212720	3.645219
C	3.544835	0.873991	0.028497	C	-1.527707	3.669132	1.455515
C	3.071280	2.163084	0.177504	H	-1.837559	4.054235	2.434742
H	3.746150	3.011521	0.262727	H	-2.314617	3.926437	0.740495
C	1.666791	2.393467	0.213366	H	-0.612250	4.202901	1.171895
H	1.310050	3.414890	0.318190	C	-1.552983	2.252745	-1.462809
C	0.742442	1.362306	0.112450	H	-1.356769	3.312745	-1.249639
C	1.213733	0.028464	-0.029553	C	-3.077112	2.019956	-1.475856
C	4.710847	-1.266087	-0.234124	H	-3.525736	2.637786	-2.263217
H	5.148941	-1.632885	-1.170376	H	-3.554076	2.294107	-0.528139
H	5.181807	-1.837283	0.575183	H	-3.311381	0.972389	-1.688239
C	4.940929	0.279104	-0.058384	C	-0.899636	1.899734	-2.809719
H	5.525649	0.494128	0.844291	H	-1.030027	0.840786	-3.049443
H	5.503466	0.696945	-0.902004	H	0.170618	2.128825	-2.817028
C	-2.340608	-1.394254	-1.441889	H	-1.378750	2.494955	-3.597237
H	-2.394758	-2.476185	-1.257702	43			
C	-1.628560	-1.164280	-2.785830	compd. 11			
H	-2.227362	-1.623675	-3.582295	Te	2.709420	-1.820181	0.264547
H	-0.633949	-1.620820	-2.806666	P	1.064484	-0.641114	-1.078251
H	-1.527128	-0.097526	-3.003015	P	0.634855	1.385104	-0.111778
C	-3.767971	-0.811589	-1.440423	C	-0.672741	-1.143636	-0.618206
H	-3.749223	0.266263	-1.628676	C	-1.191211	-2.423718	-0.777198
H	-4.296558	-0.987362	-0.496747	C	-2.572441	-2.723977	-0.578681
H	-4.349824	-1.288047	-2.238754	C	-3.449425	-1.718493	-0.221740
C	-2.082862	-1.384360	1.597552	C	-2.925768	-0.421125	-0.045430
H	-2.894838	-0.678375	1.822033	C	-3.890673	0.529269	0.342079
C	-1.052859	-1.293710	2.737433	C	-3.488884	1.834714	0.568815
H	-1.543944	-1.570978	3.678114	C	-2.113602	2.175839	0.426532
H	-0.664817	-0.278723	2.853610	C	-1.164661	1.232964	0.043293
H	-0.215684	-1.981650	2.575423	C	-1.566846	-0.109081	-0.218469
C	-2.654590	-2.807503	1.475688	C	-4.942728	-1.672740	0.064199
H	-1.877835	-3.536988	1.215255	C	-5.238078	-0.170406	0.428546
H	-3.461489	-2.884588	0.740987	C	1.105478	2.762347	-1.274939
H	-3.067484	-3.105915	2.447122	C	0.315055	2.674703	-2.591355
44				C	1.419571	1.683774	1.555369
compd. 10				C	2.625757	2.748274	-1.525632
Se	-2.037736	-1.459307	1.930206	C	1.425456	3.161533	1.979387
Se	-1.840246	-1.716988	-1.819055	C	0.761643	0.785465	2.617110
P	-0.775710	1.338568	-0.031437	H	-0.521541	-3.233678	-1.056676
P	-1.090538	-1.013024	0.061344	H	-2.909167	-3.749256	-0.715598
C	1.028397	1.301468	-0.165190	H	-4.196134	2.605071	0.866844
C	1.909202	2.365129	-0.329969	H	-1.813728	3.200828	0.632754
H	1.523999	3.376627	-0.437391	H	-5.215109	-2.341088	0.890202
C	3.319605	2.176980	-0.360747	H	-5.531073	-1.993521	-0.804141
H	3.966363	3.040764	-0.494121	H	-5.961362	0.274866	-0.265756
C	3.832784	0.901164	-0.213474	H	-5.671819	-0.078235	1.431755
				H	0.833595	3.696262	-0.764278

H	0.534171	1.743217	-3.124135	H	-4.080945	1.015261	-0.858978
H	0.602667	3.511811	-3.239306	C	-2.289370	-0.687493	1.643346
H	-0.765845	2.729690	-2.427544	H	-3.087207	0.051825	1.793017
H	2.451520	1.329410	1.414368	C	-1.261720	-0.531901	2.778557
H	2.891819	3.582486	-2.185838	H	-0.445420	-1.255401	2.676169
H	2.937222	1.818882	-2.014805	H	-1.764187	-0.721824	3.734720
H	3.207893	2.854114	-0.604244	H	-0.842873	0.475837	2.819699
H	1.973893	3.804769	1.283976	C	-2.894286	-2.102359	1.642027
H	1.914094	3.247430	2.957835	H	-3.318739	-2.303603	2.633179
H	0.407994	3.556665	2.088604	H	-2.132403	-2.867956	1.454252
H	-0.282558	1.067898	2.792002	H	-3.696962	-2.224478	0.910430
H	1.308768	0.898277	3.561034	B	-1.637628	2.986694	1.467639
H	0.809360	-0.270586	2.334863	B	-1.307366	2.563465	-1.951962
				H	-1.314231	4.125463	1.201676
				H	-1.119659	2.564953	2.476649
				H	-2.843066	2.831903	1.423274
				H	-2.511053	2.665526	-2.058255
				H	-0.739186	3.636204	-1.979872
				H	-0.805632	1.746359	-2.698365
50							
compd. 13				24			
P	-1.533264	-0.187600	0.006443	PhP=PPh			
P	-0.945363	1.992909	-0.091308	P	0.520366	0.887495	-0.067239
C	0.131144	-0.893722	-0.155647	C	2.265639	0.313277	0.003574
C	0.525334	-2.226140	-0.244914	C	3.216505	1.130868	-0.640380
H	-0.219793	-3.015585	-0.289584	C	4.571972	0.796820	-0.634677
C	1.898436	-2.599957	-0.276965	C	5.006373	-0.352558	0.031344
H	2.156003	-3.653622	-0.352119	C	4.077519	-1.162816	0.693165
C	2.871375	-1.618133	-0.203963	C	2.721858	-0.832878	0.684601
C	2.469129	-0.272005	-0.106859	H	5.287757	1.436067	-1.145427
C	3.546792	0.634155	-0.025464	H	4.410979	-2.050454	1.225244
C	3.256331	1.979368	0.083156	P	-0.520387	-0.887533	-0.067566
H	4.042706	2.727296	0.153197	C	-2.265641	-0.313285	0.003388
C	1.895432	2.409600	0.099087	C	-3.216626	-1.131005	-0.640227
H	1.692211	3.474616	0.173964	C	-4.572087	-0.796936	-0.634364
C	0.834115	1.518282	0.013011	C	-5.006359	0.352590	0.031487
C	1.123357	0.129690	-0.086262	C	-4.077383	1.162977	0.692975
C	4.390806	-1.662606	-0.199827	C	-2.721725	0.833022	0.684246
H	4.776231	-2.124596	-1.116905	H	-4.410739	2.050735	1.224919
H	4.769072	-2.264616	0.635370	H	-5.287968	-1.436283	-1.144855
C	4.842601	-0.160427	-0.078641	H	-2.889989	-2.031397	-1.156180
H	5.450676	0.000364	0.819762	H	-2.015530	1.463972	1.216579
H	5.461849	0.137816	-0.933215	H	-6.062349	0.610087	0.045282
C	-2.653165	-0.553964	-1.438292	H	2.015767	-1.463721	1.217199
H	-2.214052	0.083779	-2.215481	H	2.889767	2.031142	-1.156475
C	-2.631769	-2.007146	-1.939226	H	6.062369	-0.610037	0.045015
H	-3.247600	-2.069975	-2.844810				
H	-3.044853	-2.714985	-1.213182				
H	-1.622016	-2.331774	-2.208476				
C	-4.077626	-0.036080	-1.162540				
H	-4.594654	-0.625552	-0.397450				
H	-4.661341	-0.108622	-2.087572				