

## Supplementary Data

**An aromatic-antiaromatic switch in P-heteroles. A small change in delocalisation makes a big reactivity difference.**

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**The Supplementary Data contains the following information**

**A./ A detailed description of the experimental procedure**

**B./ Total energies (in hartree) and optimized structures (in cartesian coordinates) of compounds 2a,c; 3a,c; 4a-e, 5a-e, 6a-e and 7a-e at the given levels of the theory. NIMAG=1 indicates that the structure is a first order saddle point.**

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**A./ The detailed description of the experimental procedure for the diethylamine catalysed transformation of 2b. The same procedure holds for 2a:**

A xylene solution (10 mL) of 1,2,5-triphenylthiophosphole **2b** (100 mg; 2.5 mmol) and diethylamine (1 mL) was refluxed for 4 hours under an inert atmosphere of argon. The solution was subjected to column chromatography on silica gel. Xylene was first eluted with pentane, then a pentane (80)/ether (20) was used affording the corresponding phospholene **3b** (96 mg, 2.4 mmol, yield 96 %) as a pale brownish oil.

**2a** *B3LYP/6-31+G\*\*/B3LYP/3-21G\** : -2385.722799

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.485583
C	1.304742	0.000000	2.259728
C	2.529506	0.386493	1.400900
C	2.515943	-0.408926	0.085252
C	1.306827	0.028798	-0.769443
C	-1.241690	-0.030152	2.064897
C	-1.629969	-0.072070	3.452483
S	-0.510726	-0.346424	4.793248
C	-1.787604	-0.267482	5.954995
C	-3.005559	-0.047808	5.362574
C	-2.920001	0.060297	3.947716
C	-1.240179	-0.013724	-0.581189
C	-1.619567	0.054895	-1.972783
S	-0.538362	0.599900	-3.260854
C	-1.778032	0.432691	-4.453601
C	-2.954573	-0.015947	-3.908498
C	-2.869522	-0.226964	-2.504448
P	-2.507633	-0.073874	0.739756
S	-3.775485	-1.558189	0.756364
C	-3.275374	1.579649	0.730714
C	-2.479667	2.735523	0.792472
C	-3.078309	3.993802	0.778861
C	-4.470655	4.108498	0.704090
C	-5.263200	2.961671	0.642499
C	-4.667987	1.697734	0.654545
H	1.217988	-0.610419	-1.655509
H	1.488443	1.053978	-1.127510
H	-3.680715	-0.603582	-1.898092
H	-3.849791	-0.195506	-4.486556
H	-1.575552	0.662123	-5.488151
H	-1.577198	-0.383110	7.006780
H	-3.931724	0.032914	5.913299
H	-3.776163	0.217314	3.309408
H	1.466870	-1.010010	2.666436
H	1.220629	0.680097	3.116011
H	3.443236	0.184353	1.970580
H	2.504614	1.460861	1.176977
H	3.437482	-0.238423	-0.482286
H	2.447936	-1.481832	0.304644
H	-5.270509	0.797308	0.607820
H	-6.341939	3.047663	0.583882
H	-4.932654	5.088929	0.694419
H	-2.462451	4.884267	0.827828
H	-1.401313	2.648210	0.854385

2c B3LYP/6-31+G\*\*/B3LYP/3-21G\* : -1776.290451

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.409320
N	1.168169	0.000000	2.106324
C	2.331364	-0.006778	1.429992
C	2.407255	-0.018973	0.037833
C	1.211429	-0.010907	-0.684283
C	-1.250829	-0.015019	2.174371
C	-1.417761	0.210792	3.512181
C	-2.824212	0.032479	4.005377
C	-3.161346	0.308191	5.457797
C	-1.931956	0.316283	6.387607
C	-0.831330	1.206403	5.788044
C	-0.310565	0.578540	4.480378
C	-3.721199	-0.341138	3.041497
C	-5.152480	-0.628901	3.185641
N	-5.708809	-0.545688	4.423774
C	-7.014453	-0.828033	4.577799
C	-7.846373	-1.201503	3.523019
C	-7.285880	-1.286526	2.246738
C	-5.935034	-1.003086	2.073770
P	-2.863579	-0.423538	1.434308
S	-3.540794	0.718140	-0.007793
C	-2.760975	-2.192079	1.000667
C	-2.342954	-3.134129	1.955475
C	-2.261142	-4.482479	1.613145
C	-2.594470	-4.900595	0.320243
C	-3.009504	-3.966809	-0.629981
C	-3.092374	-2.613624	-0.292119
H	-3.931628	-0.391859	5.781480
H	-3.636866	1.301006	5.493816
H	-5.493507	-1.045126	1.088759
H	-7.893049	-1.567946	1.394720
H	-8.893645	-1.413848	3.695226
H	-7.407158	-0.747952	5.586055
H	-0.937075	0.040931	-0.538442
H	1.221410	-0.007031	-1.767748
H	3.367654	-0.030429	-0.461411
H	3.235474	-0.004593	2.029985
H	0.245681	-0.339434	4.717693
H	0.408105	1.224977	3.974038
H	0.006134	1.318517	6.486189
H	-1.238809	2.206330	5.590230
H	-2.237308	0.681306	7.374898
H	-1.546589	-0.704219	6.514514
H	-3.413727	-1.876244	-1.019505
H	-3.267885	-4.287880	-1.632355
H	-2.529877	-5.950264	0.057937
H	-1.938969	-5.207206	2.351743
H	-2.086052	-2.812634	2.958029

**3a** B3LYP/6-31+G\*\*/B3LYP/3-21G\* : -2385.721418

S	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.749238
C	1.284616	0.000000	2.235961
C	2.274990	-0.007727	1.202102
C	1.731875	-0.009090	-0.055694
C	-1.284492	0.044950	2.512107
C	-1.455596	-1.014586	3.607283
C	-2.285120	-0.536202	4.725375
C	-2.728901	-1.567799	5.741480
C	-1.595961	-2.601259	5.972127
C	-1.188628	-3.279240	4.645094
C	-0.962562	-2.261313	3.548063
C	-2.538425	0.805270	4.753197
C	-3.346407	1.565986	5.693803
S	-4.805152	0.921304	6.441046
C	-5.118470	2.416687	7.254662
C	-4.163304	3.358659	6.971533
C	-3.159063	2.880360	6.078909
P	-1.615685	1.667264	3.431131
S	-0.085263	2.749755	3.964978
C	-2.839509	2.539087	2.406999
C	-4.119932	1.994278	2.210942
C	-5.037125	2.644598	1.386188
C	-4.684107	3.839569	0.751832
C	-3.414685	4.386867	0.949116
C	-2.494452	3.741729	1.777429
H	-1.510043	4.161224	1.950493
H	-3.141419	5.315796	0.462500
H	-5.398842	4.343452	0.111463
H	-6.026173	2.224988	1.243487
H	-4.401790	1.076646	2.715547
H	-2.313928	3.464038	5.741536
H	-4.170363	4.357799	7.383250
H	-5.979126	2.521244	7.896612
H	-2.998373	-1.082973	6.683652
H	-3.619455	-2.091165	5.363059
H	-1.926405	-3.353482	6.696477
H	-0.727040	-2.081669	6.391620
H	-0.368759	-2.560040	2.689936
H	-0.276110	-3.870364	4.792513
H	-1.974633	-3.983943	4.330777
H	-2.132797	-0.050922	1.818930
H	1.508826	0.021126	3.291781
H	3.338937	-0.006682	1.392030
H	2.252378	-0.014532	-1.000291

**3c** *B3LYP/6-31+G\*\*//B3LYP/3-21G\** : -1776.292505

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.408732
N	1.167260	0.000000	2.105083
C	2.331110	0.009183	1.428759
C	2.407209	0.026052	0.036996
C	1.211491	0.015680	-0.684893
C	-1.261569	0.008529	2.169504
C	-1.434566	-0.310747	3.486516
C	-2.808206	-0.198706	4.000969
C	-3.156903	-0.596554	5.235120
C	-2.179951	-1.228849	6.201189
C	-0.956148	-1.802872	5.455622
C	-0.375831	-0.760354	4.472049
C	-3.800415	0.408431	3.007490
C	-4.337263	1.747421	3.465622
C	-5.684868	2.074887	3.275148
C	-6.154545	3.311370	3.718126
C	-5.265313	4.189789	4.339744
C	-3.936033	3.792351	4.482340
N	-3.472331	2.599582	4.057730
P	-2.844116	0.456866	1.386066
S	-3.598248	-0.728442	0.018092
C	-2.638975	2.173461	0.819434
C	-3.273812	2.596036	-0.356567
C	-3.102742	3.902953	-0.815309
C	-2.290295	4.791272	-0.107067
C	-1.651235	4.373037	1.063340
C	-1.822748	3.069766	1.529985
H	-6.348363	1.369694	2.789780
H	-4.178792	-0.454007	5.576445
H	-0.936835	-0.042011	-0.539398
H	1.220802	0.014042	-1.768347
H	3.367675	0.042140	-0.462065
H	3.234857	0.006275	2.029272
H	-4.633850	-0.277071	2.823828
H	-7.195051	3.581784	3.583042
H	-5.591072	5.156697	4.701295
H	-3.212713	4.451121	4.950578
H	-1.849052	-0.470196	6.928230
H	-2.684059	-2.018539	6.772346
H	0.497569	-1.130157	3.938008
H	-0.048638	0.126781	5.035446
H	-1.262939	-2.693567	4.894722
H	-0.183328	-2.102249	6.172075
H	-1.345415	2.751733	2.446913
H	-1.017504	5.060644	1.611383
H	-2.151423	5.804284	-0.467501
H	-3.595248	4.223048	-1.726164
H	-3.881101	1.887532	-0.908245

**4a** *B3LYP/6-311+G\*\** : -536.142401 *ccsd(t)/cc-PVDZ//B3LYP/6-311+G\*\** : -535.010357

C	-1.240255	-0.040521	-0.977335
C	-1.240217	-0.040305	0.374127
C	0.088199	-0.040562	0.993432
C	0.255698	-0.035410	2.487064
P	0.453853	0.168483	-1.597965
C	1.095115	-0.045113	0.084847
H	-2.124376	-0.028055	-1.600586
H	-2.144545	-0.038479	0.975372
H	2.148028	-0.026796	0.335211
H	0.687268	-1.121664	-2.153233
H	1.308039	-0.091738	2.770352
H	-0.166265	0.874408	2.927542
H	-0.267180	-0.883457	2.942011

*B3LYP/6-31+G\*\*//B3LYP/3-21G\** : -536.070518

C	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.818413
C	1.814494	0.000000	1.815088
C	2.307857	-0.167708	0.560439
C	3.764197	-0.340872	0.198764
C	1.257022	-0.166495	-0.475247
H	-0.892577	0.028629	-0.610952
H	1.501452	-0.284288	-1.525504
H	2.425288	0.021721	2.708596
H	-0.233185	1.386616	2.030637
H	4.400815	-0.258489	1.084148
H	3.935907	-1.322810	-0.260703
H	4.074652	0.423128	-0.525179

**4b** *B3LYP/6-311+G\*\**: -934.368542 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -932.690891

C	0.080133	-0.610909	-1.039087
P	0.079564	-0.599077	0.777385
S	1.767711	-0.588384	1.780573
C	-0.680159	0.394796	-1.508173
C	-1.305678	1.220056	-0.437971
C	-1.023276	0.853792	0.819075
H	0.642202	-1.317940	-1.632977
C	-0.916020	0.727533	-2.950229
H	-1.936574	2.066041	-0.693013
H	-1.362994	1.332761	1.726195
H	-0.795640	-1.665476	1.116937
H	-0.378132	0.048864	-3.612772
H	-1.983228	0.672796	-3.190141
H	-0.592473	1.751641	-3.165861

*B3LYP/6-31+G\*\*//B3LYP/3-21G\** : -934.272233

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.349349
C	1.211825	0.000000	2.243469
P	-1.700599	-0.015286	-0.630345
C	-2.383893	-0.026578	1.058671
C	-1.375168	-0.013119	1.947294
S	-2.270102	-1.338917	-1.933809
H	0.880743	-0.009757	-0.626629
H	-1.504800	-0.019728	3.023846
H	-3.438938	-0.052521	1.291080
H	-1.900221	1.334685	-1.012592
H	2.134848	-0.011397	1.658609
H	1.214038	0.890092	2.885644
H	1.200072	-0.880926	2.898303



**4c** *B3LYP/6-311+G\*\**: -611.396414 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\**: -610.056016

C	0.994959	0.096550	-0.454107
C	0.994955	0.096247	0.890174
C	2.199772	0.096347	1.780734
P	-0.712839	0.131119	-1.072230
C	-1.391327	0.077528	0.621817
C	-0.373285	0.087606	1.491076
O	-1.176211	-0.839590	-2.110930
H	1.873489	0.092747	-1.084717
H	-0.495550	0.085410	2.570104
H	-2.443576	0.063280	0.869259
H	-0.901426	1.495614	-1.433600
H	3.125617	0.072756	1.205256
H	2.210386	0.986915	2.418414
H	2.182886	-0.772449	2.448006

*B3LYP/6-31+G\*//B3LYP/3-21G\**: -611.305038

C	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.818437
O	1.287238	0.000000	2.590726
C	-0.816236	0.970548	-0.460541
C	-1.451871	1.782567	0.622609
C	-1.123349	1.439873	1.879956
C	-1.110783	1.281057	-1.899304
H	0.562989	-0.693159	-0.615364
H	-2.130624	2.595266	0.369304
H	-1.480011	1.917296	2.785526
H	-0.865518	-1.080537	2.146854
H	-0.552946	0.627518	-2.575827
H	-2.182005	1.165834	-2.112901
H	-0.850429	2.322841	-2.131122

**4d** *B3LYP/6-311+G\*\**: -575.396911 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -574.127405

C	-0.395940	0.802936	-2.599275
P	-0.395254	0.802082	-0.917439
C	1.244821	0.802218	-0.120317
C	1.256053	-0.048770	0.913791
C	-0.007006	-0.801940	1.153406
C	-0.076299	-1.816410	2.256749
C	-0.987277	-0.470268	0.296668
H	2.065880	1.418985	-0.456805
H	2.122578	-0.212426	1.547600
H	-1.979739	-0.903221	0.279716
H	-1.120922	1.927557	-0.466052
H	-1.311501	1.119041	-3.085551
H	0.197640	0.051945	-3.107411
H	-1.053725	-2.298804	2.295865
H	0.686010	-2.591741	2.119395
H	0.116467	-1.349162	3.228702

*B3LYP/6-31+G\*//B3LYP/3-21G\** : -575.312779

C	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.663089
C	1.411466	0.000000	2.872477
C	1.272508	0.989854	3.774177
C	2.204851	1.330892	4.909187
C	-0.720931	1.448445	2.507614
C	0.029458	1.805503	3.562421
H	-1.638330	1.922746	2.188802
H	-0.205895	2.624463	4.233772
H	2.240547	-0.696372	2.843566
H	-0.674589	-1.151540	2.121074
H	-0.019773	-0.946127	-0.528585
H	0.324552	0.876803	-0.548045
H	3.072855	0.666477	4.918444
H	2.557825	2.366782	4.817952
H	1.686869	1.242440	5.873213

**4e** *B3LYP/6-311+G\*\**: -591.478925 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -590.175561

C	1.020164	0.117952	-0.448213
C	1.019948	0.117039	0.896543
C	2.223905	0.118088	1.790367
P	-0.703695	0.136716	-1.068189
C	-1.363660	0.086158	0.618691
C	-0.347836	0.106492	1.490729
N	-1.350973	-0.939022	-2.014203
H	1.903483	0.119977	-1.073533
H	-0.478164	0.101426	2.568537
H	-2.417142	0.054210	0.856528
H	-0.815003	1.521241	-1.425178
H	-1.089851	-0.901965	-2.993584
H	3.150500	0.098235	1.215527
H	2.232911	1.007467	2.429824
H	2.210378	-0.752548	2.455434

*B3LYP/6-31+G\*\*//B3LYP/3-21G\** : HF=-591.388341

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.349170
C	1.206878	0.000000	2.251833
P	-1.717755	0.040901	-0.627258
C	-2.384490	-0.005692	1.052849
C	-1.378280	0.004449	1.943240
N	-2.388106	-1.002946	-1.569926
H	0.894646	0.001375	-0.609496
H	-1.510306	0.003666	3.019579
H	-3.438397	-0.022813	1.290849
H	-1.791165	1.442948	-0.923110
H	-2.116509	-1.137288	-2.546142
H	2.133189	-0.030953	1.672266
H	1.217422	0.899726	2.880869
H	1.182710	-0.870328	2.920823

**5a** *B3LYP/6-311+G\*\**: -536.134835 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -535.001991

C	-1.252614	0.013610	-0.882764
P	-1.357623	0.209703	0.943026
C	0.512721	-0.028697	1.066567
C	1.067329	-0.158978	-0.347663
C	-0.007254	-0.194738	-1.339053
H	-2.130659	0.017365	-1.517876
H	0.221267	-0.366586	-2.386841
C	2.370603	-0.248574	-0.647267
H	0.976485	0.790266	1.618908
H	-1.389213	1.638589	0.967792
H	3.137838	-0.201892	0.117128
H	2.703790	-0.371725	-1.671904
H	0.700133	-0.947305	1.628482

**5b** *B3LYP/6-311+G\*\**: -934.372212 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -932.690891

C	0.111791	-0.600244	-1.131554
P	0.112698	-0.599550	0.728539
S	1.820923	-0.598069	1.694974
C	-0.831814	0.516060	-1.556068
C	-1.332321	1.275406	-0.407418
C	-0.972164	0.853805	0.814941
C	-1.172335	0.783166	-2.822519
H	-0.192920	-1.574763	-1.517287
H	-1.968269	2.140302	-0.571052
H	-1.251855	1.322922	1.748694
H	-0.728301	-1.686991	1.078951
H	-0.786496	0.205373	-3.654182
H	-1.852435	1.594053	-3.058892
H	1.136085	-0.407701	-1.458192

**5c** *B3LYP/6-311+G\*\**: -611.402107 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -610.059050

C	0.456162	-0.695921	-0.831206
P	0.348932	-0.659101	1.017080
O	1.620188	-0.654124	1.805196
C	-0.462525	0.408512	-1.331137
C	-1.013880	1.200275	-0.226528
C	-0.715078	0.808115	1.023074
H	0.186420	-1.674921	-1.231374
C	-0.751752	0.641694	-2.616879
H	-1.640184	2.060045	-0.446473
H	-1.049384	1.306050	1.923945
H	-0.513790	-1.735339	1.361976
H	-0.331375	0.043598	-3.416931
H	-1.424845	1.443033	-2.901610
H	1.500107	-0.499008	-1.091245

**5d** *B3LYP/6-311+G\*\**: -575.400751 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -574.128188

C	-0.362384	0.721854	-2.608472
P	-0.362339	0.722114	-0.937363
C	1.252994	0.722049	-0.091161
C	1.276770	-0.071610	0.990023
C	0.046686	-0.804418	1.311080
C	-0.110766	-1.504789	2.441719
C	-0.991766	-0.642027	0.220740
H	2.082017	1.321656	-0.443846
H	2.147438	-0.177590	1.630938
H	-1.986844	-0.410074	0.605474
H	-1.082846	1.856104	-0.507082
H	-1.179309	1.219044	-3.113125
H	0.202843	-0.023700	-3.152047
H	-1.031158	-2.031210	2.666085
H	0.683931	-1.564488	3.178161
H	-1.070194	-1.547807	-0.387688

**5e** *B3LYP/6-311+G\*\** : -591.484060 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -590.178038

C	0.426494	-0.701578	-0.866322
P	0.264726	-0.695303	0.995575
N	1.501728	-0.741520	1.961366
C	-0.427887	0.453758	-1.360750
C	-0.853706	1.319075	-0.254413
C	-0.571378	0.906662	0.990678
H	0.139453	-1.658898	-1.304993
C	-0.768097	0.671367	-2.636981
H	-1.380233	2.244316	-0.468620
H	-0.816004	1.442320	1.898091
H	-0.774882	-1.656293	1.202303
H	1.862928	-1.654910	2.210950
H	-0.444573	0.014621	-3.436060
H	-1.386545	1.518224	-2.914447
H	1.484311	-0.524908	-1.083671

**6a** *B3LYP/6-311+G\*\** : -536.004874 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -534.870465  
*NIMAG=1*

C	-2.381315	-0.245508	0.170603
C	-1.046466	0.142190	-0.127792
C	-0.266747	-1.053040	-0.176363
P	1.536300	-0.568777	-0.014786
C	-0.312101	1.381846	-0.149688
C	1.016099	1.189314	0.058354
H	-1.584095	-1.566660	0.171233
H	-2.541250	-0.621837	1.176689
H	-3.256013	0.266417	-0.235003
H	1.795925	-0.727229	1.378810
H	-0.789715	2.355310	-0.144909
H	1.707079	1.990899	0.293026
H	-0.433251	-1.654061	-1.068732

**6b** *B3LYP/6-311+G\*\** : -934.233936 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -932.553706  
*NIMAG=1*

C	-0.841595	0.247852	-2.951011
C	-0.845979	0.227633	-1.535922
C	0.502436	0.199125	-1.093566
P	0.472927	-0.481559	0.619868
S	1.504202	0.387696	2.045944
C	-1.873378	0.049731	-0.512523
C	-1.371416	-0.384502	0.658977
H	0.632511	0.224617	-2.569854
H	-0.465556	-0.647954	-3.437038
H	-1.603135	0.762100	-3.539841
H	0.683546	-1.880882	0.500351
H	-2.933074	0.133647	-0.728873
H	-1.954041	-0.742601	1.498029
H	1.058214	1.132282	-1.151619

**6c** *B3LYP/6-311+G\*\** : -611.261816 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -609.918699  
*NIMAG=1*

C	0.554066	-0.449318	-2.624634
C	0.547119	-0.427055	-1.210100
C	1.591335	-0.436668	-0.181310
C	1.170866	0.070362	0.992298
P	-0.619884	0.532245	0.924786
O	-1.539348	0.070563	2.009874
C	-0.772590	-0.153904	-0.767610
H	-0.893786	-0.172235	-2.254957
H	0.340080	0.495650	-3.116288
H	1.228457	-1.082825	-3.203786
H	-0.548619	1.946499	0.781619
H	2.619334	-0.704422	-0.402567
H	1.815545	0.315082	1.827349
H	-1.492740	-0.966429	-0.834016

**6d** *B3LYP/6-311+G\*\** : -575.259117 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -573.986120  
*NIMAG=1*

C	-0.592282	0.422936	-2.639882
C	-0.607816	0.327460	-1.225539
C	0.746011	0.223054	-0.787217
P	0.656990	-0.515106	0.886650
C	1.499319	0.325964	2.072774
C	-1.632272	0.183226	-0.203398
C	-1.156089	-0.294099	0.968983
H	0.877113	0.309437	-2.257699
H	-0.274931	-0.471722	-3.167797
H	-1.319068	1.011314	-3.203234
H	0.740362	-1.939676	0.631745
H	-2.685340	0.346448	-0.405811
H	-1.773462	-0.616754	1.797848
H	1.309953	1.153948	-0.790069
H	1.197274	0.217379	3.106302
H	2.532025	0.584967	1.874644

**6e** *B3LYP/6-311+G\*\**: -591.345455 *ccsd(T)/cc-PVDZ//B3LYP/6-311+G\*\** : -590.039385  
*NIMAG=1*

C	-0.571150	0.351322	-2.637627
C	-0.610687	0.308890	-1.222467
C	0.722213	0.275846	-0.741282
P	0.671778	-0.426093	0.937610
N	1.601000	0.356150	1.935664
C	-1.666109	0.118486	-0.227190
C	-1.190645	-0.325749	0.952573
H	0.891315	0.329338	-2.216874
H	-0.182277	-0.537724	-3.126078
H	-1.325798	0.865051	-3.236046
H	0.813312	-1.845860	0.819167
H	-2.719453	0.200367	-0.476018
H	-1.809524	-0.697115	1.761197
H	1.282988	1.207578	-0.767763
H	1.664036	0.003929	2.884570

**7a** *B3LYP/6-31+G\*//B3LYP/3-21G\** : -1072.053085  
*NIMAG=1*

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.388460
C	1.124550	0.000000	2.240803
P	0.635060	0.265430	3.953567
C	-1.109213	-0.008559	3.503853
C	-1.254930	-0.044880	2.166163
C	2.129909	-2.752540	0.747327
C	1.026778	-3.708752	0.631271
C	-0.359973	-3.211109	0.773368
P	-1.482985	-4.710688	0.662276
C	-0.074509	-5.741575	0.177823
C	1.123079	-5.075822	0.321978
H	3.116770	-3.215594	0.702565
H	0.917507	0.108289	-0.564223
H	2.036393	-1.996331	-0.052525
H	-0.929182	0.052157	-0.553983
H	2.025286	-2.133573	1.666053
H	-0.566589	-2.409843	0.020817
H	2.129374	0.182671	1.883980
H	-0.490436	-2.677414	1.723476
H	0.933456	-0.977974	4.594499
H	-2.086283	-4.513277	-0.614631
H	-0.157224	-6.783333	-0.103841
H	-1.923926	-0.023184	4.216265
H	-2.216972	-0.089395	1.664470
H	2.084381	-5.559627	0.178818



**7b** B3LYP/6-31+G\*\*/B3LYP/3-21G\* : -1868.466095

NIMAG=1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.376739
C	1.135322	0.000000	2.229441
P	0.627251	0.265491	3.937619
S	1.201109	1.940481	4.817129
C	-1.267010	-0.024389	2.158680
C	-1.133879	0.069215	3.492988
C	0.353144	-3.257323	2.082459
C	1.402627	-3.725091	1.150814
C	2.002461	-2.746790	0.242209
P	-0.051359	-4.715902	3.170019
C	1.161520	-5.770106	2.328839
C	1.803912	-5.071915	1.333616
S	0.030399	-4.538804	5.125464
H	2.771733	-3.162378	-0.414580
H	0.918033	0.109205	-0.568315
H	1.223091	-2.224503	-0.354596
H	-0.930731	-0.012196	-0.560040
H	2.425915	-1.918926	0.850462
H	-0.531346	-2.858347	1.562142
H	2.140102	0.221301	1.888314
H	0.733145	-2.380860	2.661287
H	0.950807	-0.883844	4.696915
H	-1.307592	-5.148834	2.674412
H	1.402583	-6.779569	2.641543
H	-1.944650	0.097535	4.212418
H	-2.225326	-0.084353	1.646261
H	2.599495	-5.505326	0.730545

7c B3LYP/6-31+G\*\*/B3LYP/3-21G\* : -1222.527912

NIMAG=1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.387261
C	1.295676	0.000000	2.155537
C	1.169489	0.052184	3.490562
P	-0.588190	0.108056	3.964285
O	-1.149842	-0.892747	4.935290
C	-1.105908	0.107253	2.247173
C	0.210553	3.024457	0.505116
C	-1.127070	3.627926	0.424599
C	-2.303939	2.824712	0.796902
P	1.387894	4.281211	-0.153824
C	0.065295	5.481436	-0.449492
C	-1.149534	4.963934	-0.083811
O	2.601579	4.659910	0.643185
H	-3.218690	3.415239	0.895884
H	-0.926859	-0.060436	-0.559730
H	-2.466864	2.035003	0.042610
H	0.923559	-0.143904	-0.551726
H	-2.085098	2.245762	1.724224
H	0.225223	2.007788	-0.015157
H	-2.128203	-0.012222	1.915804
H	0.454944	2.722724	1.536942
H	-0.732138	1.456172	4.391799
H	1.649871	3.799856	-1.463814
H	0.201881	6.461919	-0.885191
H	1.996693	0.060409	4.187851
H	2.239796	-0.040706	1.623145
H	-2.084383	5.505388	-0.179485

**7d** B3LYP/6-31+G\*\*/B3LYP/3-21G\* : -1150.550884

NIMAG=1

C	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.668474
C	1.658530	0.000000	2.514303
C	1.606478	1.036248	3.580901
C	0.392835	1.762669	3.630134
C	-0.592006	1.345887	2.759690
C	2.840116	1.317896	4.311991
C	5.083288	-1.024070	4.159190
C	4.810716	-0.970355	2.819278
C	4.876799	0.160711	1.943676
P	4.717658	-0.371207	0.222298
C	5.958153	-0.337297	-0.908798
C	4.317865	-2.180362	2.082315
C	4.190361	-2.034861	0.753539
H	2.742853	2.108558	5.060165
H	5.527119	-0.184822	4.681804
H	3.273628	0.395352	4.759611
H	4.947269	-1.942037	4.721508
H	3.622505	1.573407	3.557243
H	1.939224	-0.991819	2.896213
H	5.407292	1.065366	2.217615
H	2.491640	0.244887	1.814513
H	3.631198	0.318887	-0.347579
H	-0.731233	-1.117583	2.115764
H	-1.542981	1.848718	2.635614
H	3.876543	-2.804174	0.061507
H	4.118088	-3.100200	2.622047
H	0.277325	2.603147	4.307482
H	0.616243	0.705664	-0.546430
H	6.009585	0.470707	-1.630077
H	-0.812548	-0.476241	-0.536229
H	6.845026	-0.944178	-0.765196

7e B3LYP/6-31+G\*\*/B3LYP/3-21G\* : -1182.694567

NIMAG=1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.388041
C	1.111038	0.000000	2.246284
P	0.614826	-0.088423	3.959247
N	1.276798	1.027217	4.828253
C	-1.290503	-0.108010	2.153657
C	-1.162455	-0.166071	3.488786
C	0.058465	-3.033047	0.543756
P	-0.993825	-4.440863	-0.075106
N	-2.110561	-5.154570	0.739443
C	0.444561	-5.501823	-0.321788
C	1.602269	-4.842950	-0.009931
C	1.449599	-3.499165	0.453949
C	2.541232	-2.570796	0.790153
H	3.515600	-3.058126	0.883512
H	0.918007	0.137316	-0.560513
H	2.604869	-1.780802	0.021344
H	-0.932239	0.069731	-0.551280
H	2.274394	-1.999402	1.711166
H	-0.065751	-2.037184	-0.001593
H	2.116445	0.236095	1.928888
H	-0.187775	-2.728478	1.575372
H	0.780846	-1.459239	4.349162
H	-1.252014	-3.958418	-1.399361
H	0.395506	-6.511944	-0.703765
H	-1.990677	-0.252076	4.181171
H	-2.233264	-0.130666	1.616085
H	2.585981	-5.290228	-0.100875
H	-2.995620	-4.718243	1.003968
H	1.102035	1.124746	5.832140