

# Phosphinidene generation from phosphorus heterocycles and cages – A theoretical study

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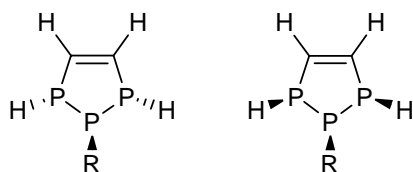
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## Supplementary material

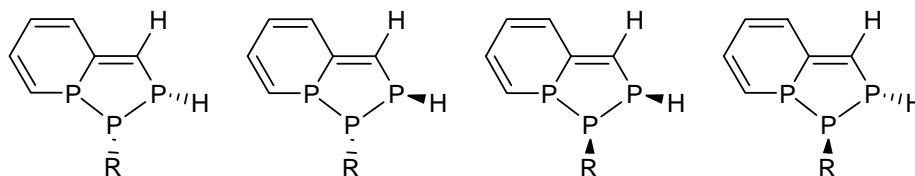
Relative energies of the isomers of complexes **1Pa-d**, **2Pa-d**, **3Pa-d**, **4Pa-d**, and **6Pa-d** at the B3LYP/6-311+G\*\*//B3LYP/6-311+G\*\* level of theory (in kcal mol<sup>-1</sup>):

### 1Pa-d

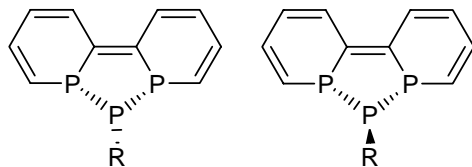


R:	Isomer 1	Isomer 2
H ( <b>a</b> )	0.0	5.5
NH <sub>2</sub> ( <b>b</b> )	0.0	1.7
N=CH <sub>2</sub> ( <b>c</b> )	0.0	4.7
N=C(SiH <sub>3</sub> ) <sub>2</sub> ( <b>d</b> )	0.0	3.7

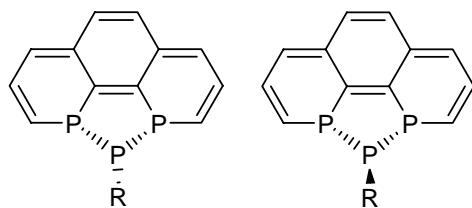
### 2Pa-d



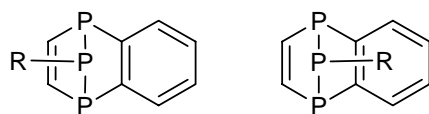
R:	Isomer 1	Isomer 2	Isomer 3	Isomer 4
H ( <b>a</b> )	2.0	0.3	1.4	0.0
NH <sub>2</sub> ( <b>b</b> )	0.0	0.3	0.8	0.6
N=CH <sub>2</sub> ( <b>c</b> )	0.4	0.3	0.0	0.2
N=C(SiH <sub>3</sub> ) <sub>2</sub> ( <b>d</b> )	1.4	2.0	0.0	0.4

**3Pa-c**

R:	Isomer 1	Isomer 2
H ( <b>a</b> )	0.3	0.0
NH <sub>2</sub> ( <b>b</b> )	0.0	0.7
N=CH <sub>2</sub> ( <b>c</b> )	0.0	0.4

**4Pa-c**

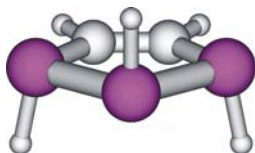
R:	Isomer 1	Isomer 2
H ( <b>a</b> )	0.7	0.0
NH <sub>2</sub> ( <b>b</b> )	0.4	0.0
N=CH <sub>2</sub> ( <b>c</b> )	0.1	0.0

**6Pa-c**

R:	Isomer 1	Isomer 2
H ( <b>a</b> )	0.5	0.0
NH <sub>2</sub> ( <b>b</b> )	1.6	0.0
N=CH <sub>2</sub> ( <b>c</b> )	1.2	0.0
N=C(SiH <sub>3</sub> ) <sub>2</sub> ( <b>d</b> )	1.3	0.0

Optimised geometries (in angströms) and total energies (in hartrees) at the B3LYP/6-311+G\*\* level of theory.

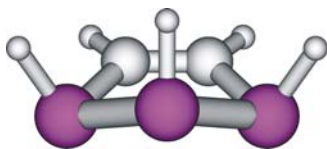
**1Pa** (isomer 1,  $C_s$ )



E=-1103.3575868

P	0.011332	-1.469839	0.000000
H	1.424485	-1.615352	0.000000
P	0.024796	0.008595	1.692470
P	0.024796	0.008595	-1.692470
C	0.024796	1.538479	0.668052
C	0.024796	1.538479	-0.668052
H	-1.376039	-0.008002	1.959948
H	-1.376039	-0.008002	-1.959948
H	0.058088	2.479678	1.213906
H	0.058088	2.479678	-1.213906

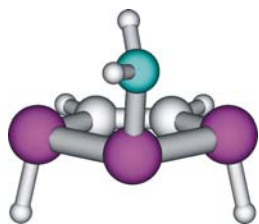
**1Pa** (isomer 2,  $C_s$ )



E=-1103.348865

P	0.677271	-1.335225	0.000000
H	1.920482	-0.636527	0.000000
P	-0.307018	-0.080414	1.617303
P	-0.307018	-0.080414	-1.617303
C	-0.307018	1.496374	0.668719
C	-0.307018	1.496374	-0.668719
H	0.861777	0.142680	2.399178
H	0.861777	0.142680	-2.399178
H	-0.454163	2.417741	1.227904
H	-0.454163	2.417741	-1.227904

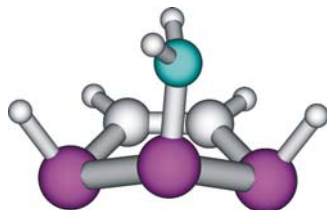
### 1Pb (isomer 1)



E=-1158.7386633

C	-1.797822	-0.603479	0.346190
P	-0.364420	-1.675492	-0.076613
P	1.130385	-0.044831	-0.563619
N	2.139169	0.008892	0.829071
C	-1.741117	0.732770	0.337821
P	-0.225719	1.687000	-0.083106
H	-0.753123	-1.964243	-1.417553
H	-0.587727	1.986554	-1.429353
H	-2.707741	-1.108522	0.665677
H	-2.606293	1.316202	0.648530
H	3.039164	-0.434715	0.714288
H	1.771483	-0.133420	1.760918

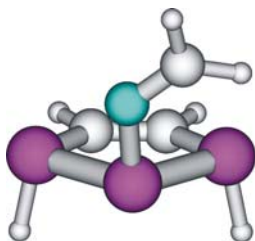
### 1Pb (isomer 2)



E=-1158.7358871

C	-1.248482	1.150895	0.604067
P	0.154087	1.617230	-0.487868
P	1.150886	-0.416104	-0.494415
N	1.768687	-0.489447	1.107291
C	-1.701267	-0.110935	0.621414
P	-0.926236	-1.378091	-0.456498
H	1.014106	2.192858	0.487936
H	-0.629647	-2.361852	0.530123
H	-1.778565	1.945733	1.123652
H	-2.606607	-0.374283	1.163023
H	2.483502	-1.185749	1.268934
H	1.153847	-0.375858	1.904128

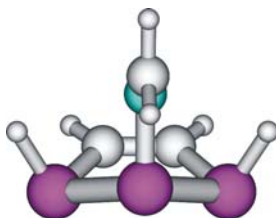
### 1Pc (isomer 1)



E=-1196.8213251

C	1.996583	-0.131616	-0.663950
C	1.622926	1.146720	-0.552223
P	0.060296	1.680947	0.257149
P	-0.669181	-0.372456	0.868752
P	1.013117	-1.554313	-0.032841
N	-1.860716	-0.763997	-0.331120
H	1.744527	-1.719214	1.180801
H	0.612274	2.039686	1.520086
H	2.910632	-0.384227	-1.198815
H	2.227839	1.934016	-0.998343
C	-2.685516	0.047668	-0.847877
H	-3.454134	-0.343682	-1.516799
H	-2.683571	1.132094	-0.680695

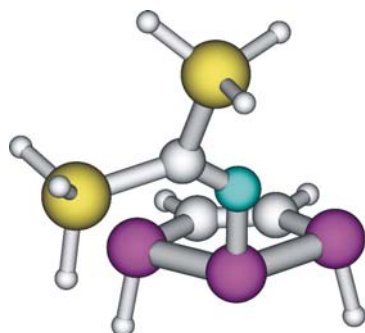
### 1Pc (isomer 2)



E=-1196.8137511

C	1.737231	-0.667660	0.819732
P	0.742569	-1.616728	-0.398153
P	-0.785573	-0.000168	-0.822867
N	-1.647372	-0.000238	0.740643
C	-2.915405	-0.000063	0.668756
C	1.737058	0.668087	0.819694
P	0.742145	1.616821	-0.398248
H	-0.081296	-2.339888	0.509360
H	-0.081901	2.339831	0.509222
H	2.418607	-1.228253	1.455658
H	2.418289	1.228896	1.455584
H	-3.494570	-0.000092	1.595052
H	-3.487939	0.000115	-0.269440

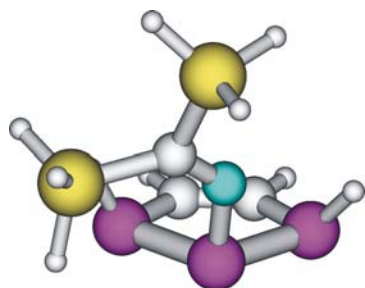
**1Pd (isomer 1)**



E=-1778.2548315

C	-1.779767	-0.207978	-0.036747
i	-3.083173	-1.451489	0.619641
i	-2.337041	1.624016	-0.247105
N	-0.663983	-0.766108	-0.339717
P	0.723160	-0.052795	-1.121319
P	1.257324	1.612433	0.307425
C	2.638264	0.762797	1.169982
C	3.018859	-0.488844	0.896289
P	2.218662	-1.549106	-0.378856
H	2.042583	2.383605	-0.597800
H	3.118272	1.319942	1.972528
H	3.812964	-0.953679	1.478072
H	3.183503	-1.310591	-1.402528
H	-3.748894	1.557933	-0.711052
H	-2.305272	2.337522	1.052711
H	-1.526788	2.349377	-1.256916
H	-2.404786	-2.567065	1.318269
H	-4.014198	-0.754679	1.549297
H	-3.877849	-1.968844	-0.525966

**1Pd (isomer 2)**

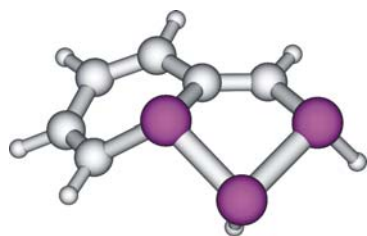


E=-1778.248869

C	0.004009	0.006867	0.073752
N	0.090299	-0.081959	1.350513

P	1.444832	-0.188869	2.425746
P	0.515182	0.766534	4.257718
C	0.682369	2.508929	3.706827
C	1.634050	2.867796	2.837338
P	2.818660	1.628783	2.184473
Si	-1.779743	-0.185469	-0.598748
Si	1.425481	0.190049	-1.210443
H	2.616082	1.851194	0.794649
H	1.809997	3.913046	2.594326
H	0.060570	3.254827	4.196481
H	-0.826278	0.535479	3.847126
H	0.991317	-0.537643	-2.430419
H	1.645001	1.615958	-1.564405
H	2.686357	-0.400843	-0.694612
H	-2.753115	0.131543	0.471257
H	-1.969953	0.726087	-1.760222
H	-1.971896	-1.581058	-1.076214

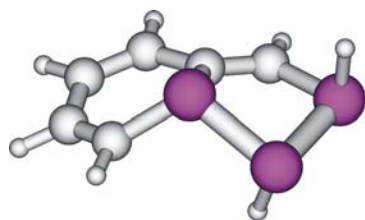
**2Pa (isomer 1)**



E=-1256.9954882

P	-1.551563	-1.371174	0.380983
H	-1.030419	-1.037394	1.668969
P	0.258361	-0.733416	-0.805781
P	-2.424892	0.678403	-0.099902
C	0.315135	0.996648	-0.161582
C	-0.859336	1.612782	0.093161
C	1.722642	-1.404977	0.024994
C	2.758592	-0.600063	0.345241
C	2.740121	0.851933	0.247172
C	1.628765	1.591871	0.015917
H	1.820782	-2.483331	0.097098
H	1.690920	2.675536	0.070337
H	3.680672	-1.052101	0.700075
H	3.674832	1.367855	0.439369
H	-2.994225	0.959960	1.174971
H	-0.906658	2.673128	0.330262

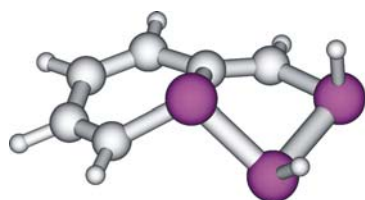
### 2Pa (isomer 2)



E=-1256.9980964

C	0.844577	1.631189	-0.062753
C	-0.323404	0.992459	0.164443
C	-1.644373	1.582380	0.000374
C	-2.753562	0.841002	-0.233301
C	-2.774684	-0.610448	-0.339047
C	-1.730839	-1.412573	-0.037455
P	-0.259223	-0.740417	0.773875
P	1.587013	-1.363349	-0.338272
P	2.445860	0.720924	-0.105047
H	1.107541	-1.112858	-1.658290
H	-1.826778	-2.490968	-0.111422
H	-1.711355	2.666140	-0.041619
H	-3.701701	-1.061511	-0.681478
H	-3.690312	1.357737	-0.414433
H	2.644582	0.549886	1.302569
H	0.866976	2.690159	-0.307250

### 2Pa (isomer 3)



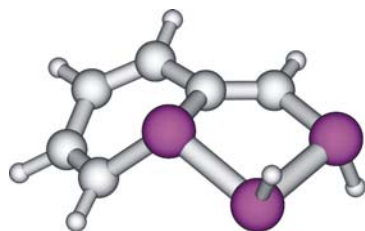
E=-1256.996439

C	-0.013138	-0.002834	0.016451
P	-0.062348	-0.162538	1.848710
P	2.188915	0.158703	2.034419
P	2.489305	-1.135826	0.219679
C	3.885990	-0.474660	-0.729493
C	3.749755	-0.101623	-2.019366
C	2.474413	0.006478	-2.709632
C	1.264906	-0.092931	-2.109768
C	1.099411	-0.323693	-0.683023
H	2.383964	-0.861133	3.010826
H	4.873645	-0.553991	-0.286265
H	0.366830	0.100317	-2.690149



H	4.639217	0.138637	-2.595009
H	2.507901	0.239118	-3.768877
H	-0.024102	-1.595686	1.912589
H	-0.893680	0.390033	-0.484251

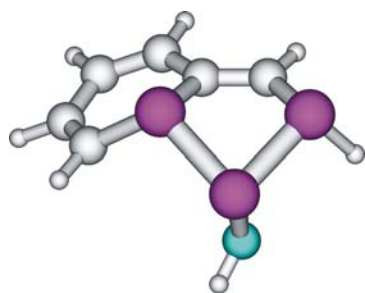
**2Pa** (isomer 4)



E=-1256.998628

C	-0.023885	0.078998	0.020762
C	-0.055350	-0.049699	1.362818
C	1.141819	-0.118425	2.196364
C	1.182789	0.416046	3.439878
C	0.059983	1.087451	4.077932
C	-1.207933	1.052254	3.613574
P	-1.649026	-0.089445	2.274196
P	-2.877297	1.001010	0.719924
P	-1.505501	0.432596	-0.990989
H	-3.740161	-0.108202	0.522675
H	-2.008212	1.548059	4.153401
H	2.055650	-0.495230	1.745532
H	0.272424	1.641017	4.988205
H	2.125982	0.411672	3.975790
H	-1.109591	1.743896	-1.392028
H	0.918610	-0.013581	-0.516429

**2Pb** (isomer 1)

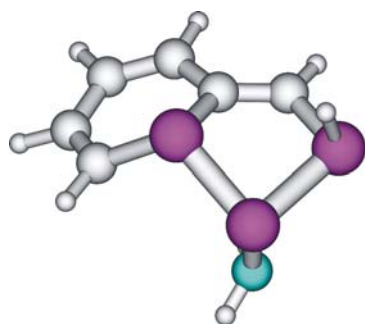


E=-1312.384445

C	0.003560	-0.036909	0.030879
C	-0.000290	-0.020690	1.386903
C	1.184226	0.061635	2.219696
C	1.163330	0.546995	3.486240

C	-0.028673	1.022784	4.165433
C	-1.288422	0.895421	3.688927
P	-1.642473	-0.086551	2.216383
P	-2.736324	1.211918	0.669488
P	-1.596881	-0.036859	-0.852724
N	-1.929577	2.715993	0.529232
H	-2.130630	1.246331	4.276911
H	2.139386	-0.182612	1.761493
H	0.117528	1.499572	5.130902
H	2.102905	0.638511	4.020788
H	-1.332154	1.008135	-1.782108
H	0.925914	-0.134265	-0.536574
H	-2.373659	3.501279	0.986247
H	-0.918427	2.755408	0.600203

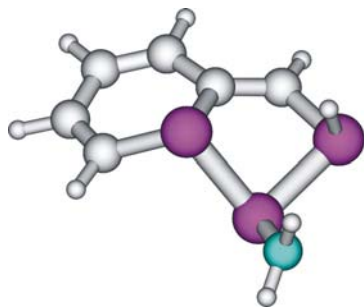
**2Pb** (isomer 2)



E=-1312.3839549

C	-0.617705	1.776351	0.212097
P	-2.266999	1.031165	-0.110363
P	-1.598911	-1.144922	-0.142467
P	0.373896	-0.442466	-1.045742
C	1.769884	-1.379845	-0.393426
C	2.833655	-0.762310	0.169649
C	2.897020	0.659657	0.457292
C	1.854605	1.519162	0.342886
C	0.524396	1.101577	-0.067215
N	-1.376197	-1.379787	1.538792
H	1.811362	-2.442153	-0.612715
H	1.979012	2.548827	0.668099
H	3.712703	-1.351140	0.416493
H	3.840109	1.041365	0.834734
H	-2.249261	1.059406	-1.543385
H	-0.591391	2.745542	0.703097
H	-1.268049	-2.338836	1.837611
H	-0.792010	-0.748703	2.075412

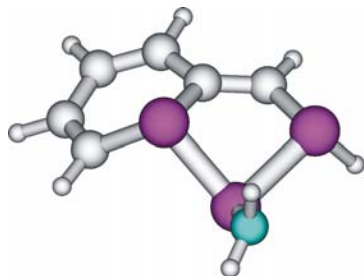
### 2Pb (isomer 3)



E=-1312.383204

C	0.103510	-0.017248	-0.074696
C	0.031581	-0.024942	1.283052
C	1.191971	0.097329	2.146280
C	1.129247	0.494621	3.439925
C	-0.096005	0.842884	4.132666
C	-1.333519	0.687749	3.611858
P	-1.636559	-0.168688	2.046916
P	-2.493501	1.294355	0.496006
N	-4.106189	0.827852	0.207761
P	-1.412658	0.062374	-1.094854
H	-2.204411	0.945212	4.206978
H	2.164462	-0.063226	1.687918
H	0.005798	1.247130	5.136136
H	2.056821	0.608891	3.991084
H	-2.008747	-1.182237	-0.683124
H	1.066026	0.030190	-0.576372
H	-4.833562	1.448946	0.528259
H	-4.395949	-0.141684	0.178398

### 2Pb (isomer 4)

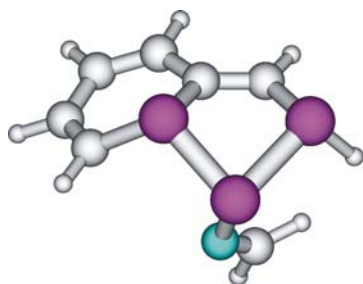


E=-1312.383524

C	0.063197	0.102758	-0.002084
P	0.086704	0.105815	1.821404
P	2.371972	-0.006971	1.929424
N	2.544853	-0.889338	3.382023
C	1.004797	-0.584206	-0.692586

P	2.231906	-1.577580	0.261050
C	3.674604	-1.363284	-0.816572
C	3.544700	-1.103949	-2.135619
C	2.284361	-0.802542	-2.792688
C	1.121656	-0.563699	-2.139710
H	4.648261	-1.608172	-0.403566
H	0.249465	-0.246440	-2.705824
H	4.431244	-1.122970	-2.763696
H	2.301732	-0.706062	-3.873062
H	-0.088330	1.509122	2.008284
H	-0.728559	0.638300	-0.520546
H	3.451667	-0.850130	3.823188
H	2.071218	-1.772109	3.532283

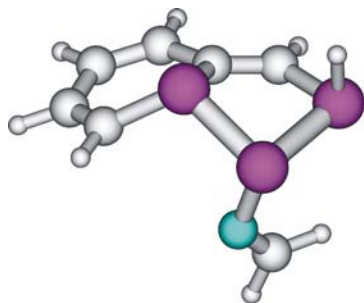
### 2Pc (isomer 1)



E=-1350.463413

C	-0.025152	0.112066	-0.032297
C	-0.010466	0.067308	1.321215
C	1.184232	0.116593	2.143063
C	1.173309	0.506815	3.440706
C	-0.015470	0.922048	4.167804
C	-1.278329	0.828014	3.699643
P	-1.637240	-0.071970	2.174730
P	-2.788886	1.257808	0.741538
N	-2.025913	2.770795	1.034335
C	-1.248848	3.426440	0.278876
P	-1.639681	0.101807	-0.889980
H	-2.116917	1.150135	4.307195
H	2.136085	-0.076273	1.654958
H	0.140915	1.337682	5.159390
H	2.118777	0.574318	3.968214
H	-1.411993	1.167222	-1.809876
H	0.893746	0.069557	-0.611791
H	-0.914881	3.087167	-0.709623
H	-0.880138	4.397687	0.614469

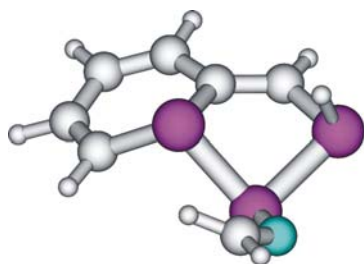
### 2Pc (isomer 2)



E=-1350.4635627

C	-0.446716	1.821382	0.408283
P	-2.098359	1.273479	-0.180270
P	-1.502873	-0.886160	-0.713607
N	-1.233367	-1.684058	0.788514
C	-1.745456	-1.381194	1.908399
C	0.680758	1.141219	0.095738
P	0.569359	-0.151637	-1.199828
C	1.834165	-1.306579	-0.629481
C	2.870697	-0.877775	0.121926
C	2.974518	0.453019	0.698727
C	1.986339	1.379710	0.690355
H	1.826110	-2.311247	-1.037582
H	2.125297	2.308388	1.237286
H	3.690257	-1.562118	0.321806
H	3.896309	0.688678	1.220394
H	-1.998950	1.619863	-1.565733
H	-0.416162	2.662353	1.096174
H	-2.409073	-0.523170	2.074675
H	-1.527952	-2.008267	2.775256

### 2Pc (isomer 3)

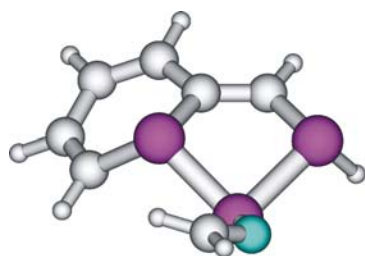


E=-1350.4640895

C	0.323555	2.051515	-0.080281
P	-1.501922	1.896275	-0.042331
P	-1.345545	-0.195531	0.863864
N	-2.801938	-0.832679	0.240260
C	-2.960272	-1.857428	-0.488629

C	1.121064	0.964684	-0.242615
P	0.320864	-0.647581	-0.642931
C	1.529087	-1.782111	0.085428
C	2.815926	-1.431216	0.299282
C	3.331664	-0.084891	0.137556
C	2.567109	1.004898	-0.110768
H	1.226267	-2.818249	0.200719
H	3.034368	1.985953	-0.131727
H	3.524775	-2.194519	0.607864
H	4.398997	0.053413	0.274455
H	-1.692654	1.416585	-1.381601
H	0.758351	3.028387	0.112339
H	-2.135271	-2.461887	-0.887870
H	-3.971030	-2.171083	-0.754887

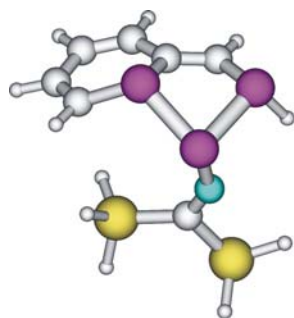
### 2Pc (isomer 4)



E=-1350.4637742

C	0.350041	2.026274	-0.146603
C	1.123748	0.933288	-0.332818
C	2.578334	0.964445	-0.334887
C	3.339202	-0.097796	0.020683
C	2.804842	-1.382983	0.441959
C	1.506987	-1.738931	0.336117
P	0.323019	-0.709897	-0.575972
P	-1.415664	-0.216820	0.827087
N	-2.822886	-0.823439	0.048768
C	-2.911647	-1.875743	-0.651672
P	-1.468319	1.908058	-0.020585
H	1.184162	-2.727007	0.648540
H	3.057385	1.919924	-0.532129
H	3.511270	-2.092520	0.863804
H	4.416192	0.025709	0.059808
H	-1.593021	2.624425	1.207584
H	0.799177	3.015671	-0.091941
H	-2.057974	-2.505008	-0.935428
H	-3.891574	-2.188558	-1.016230

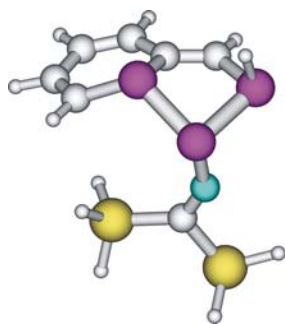
## 2Pd (isomer 1)



E=-1931.896079

P	-0.266419	1.273011	-1.300226
P	1.856393	0.353370	-0.919286
C	1.821954	0.496026	0.910756
C	1.208980	1.595879	1.422873
P	0.416965	2.771124	0.286972
C	1.998196	-1.425186	-1.126311
C	2.455783	-2.225519	-0.133200
C	2.702426	-1.794443	1.225880
C	2.417442	-0.556108	1.705170
H	1.867629	-1.822507	-2.127342
H	2.663276	-3.267392	-0.361617
H	3.103258	-2.533208	1.911536
H	2.560982	-0.355305	2.764021
N	-1.600381	0.652297	-0.484241
C	-2.194195	-0.428512	-0.141574
Si	-1.547687	-2.218562	-0.401666
H	-0.650618	-2.617509	0.709246
H	-0.849166	-2.323883	-1.705726
H	-2.738596	-3.108747	-0.401960
Si	-3.923531	-0.190448	0.645635
H	-4.065119	-1.106281	1.809916
H	-4.086245	1.219115	1.071769
H	-4.967196	-0.552138	-0.350598
H	-0.831115	2.921447	0.953090
H	1.226142	1.816196	2.487006

## 2Pd (isomer 2)

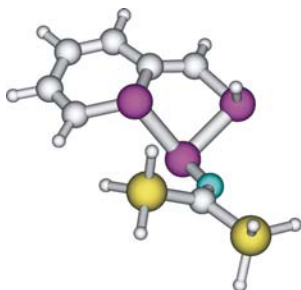


E=-1931.8951992

C	0.108364	-0.120323	-0.017276
C	0.067310	-0.055877	1.338545
C	1.233477	-0.098063	2.199402
C	1.223185	0.272157	3.505016
C	0.059846	0.753814	4.220238
C	-1.188410	0.816381	3.698274
P	-1.585426	0.066996	2.115481
P	-2.581064	1.385386	0.496737
N	-1.915913	2.891874	0.144638
C	-1.439724	3.959784	0.659929
Si	-1.035127	4.273061	2.513521
P	-1.381205	0.188995	-1.035150
Si	-1.166775	5.398827	-0.576726
H	-2.015419	1.165031	4.307589
H	0.214039	1.080161	5.244903
H	2.159466	0.247732	4.052753
H	2.179135	-0.367390	1.735964
H	0.291064	3.711196	2.864107
H	-2.094222	3.695658	3.376891
H	-0.998895	5.747611	2.697479
H	0.168352	6.007601	-0.328806
H	-1.259803	4.890767	-1.964201
H	-2.196730	6.444751	-0.334932
H	-2.134961	-0.973297	-0.666447
H	1.048522	-0.265632	-0.542139



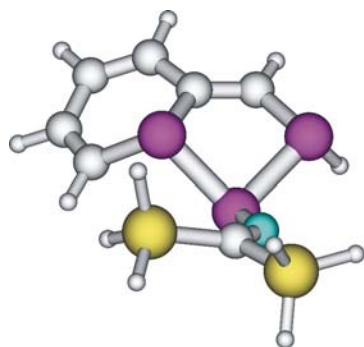
## 2Pd (isomer 3)



E=-1931.898382

C	-0.066312	-0.153769	-0.011053
P	-0.091187	-0.361615	1.804054
P	2.184428	-0.118703	1.909305
N	2.421166	-0.953514	3.349272
C	3.144495	-1.900940	3.822059
Si	2.963707	-2.182869	5.708397
C	0.995375	-0.557543	-0.759152
P	2.327216	-1.521074	0.071725
C	3.732750	-1.066736	-0.970123
C	3.589336	-0.602232	-2.231392
C	2.316475	-0.261212	-2.833811
C	1.136371	-0.241778	-2.169179
Si	4.400314	-2.996212	2.864465
H	4.719305	-1.328096	-0.601343
H	4.474848	-0.475778	-2.848090
H	2.328258	0.042675	-3.875236
H	0.244702	0.107615	-2.683276
H	4.935888	-2.287755	1.675207
H	3.779893	-4.281208	2.459019
H	5.516342	-3.285667	3.802667
H	4.073528	-1.485628	6.411556
H	1.655823	-1.662259	6.168153
H	3.078059	-3.637811	5.999968
H	-0.030932	-1.794913	1.848828
H	-0.880183	0.399720	-0.471396

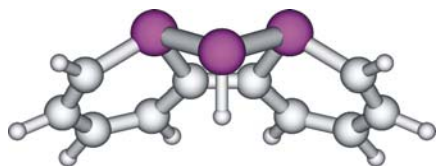
## 2Pd (isomer 4)



E=-1931.897707

C	0.020143	0.150482	-0.015552
C	-0.046516	0.014768	1.328941
C	1.119230	-0.217509	2.168058
C	1.189652	0.179143	3.460637
C	0.122539	0.875959	4.158896
C	-1.128970	1.031089	3.676402
P	-1.676132	0.169747	2.177044
P	-2.453044	1.738789	0.683734
N	-4.058521	1.354172	0.284770
C	-5.107538	0.978053	0.919240
Si	-5.282155	0.527279	2.780890
P	-1.443850	0.577642	-1.015489
Si	-6.698575	0.941739	-0.148298
H	-1.883095	1.539787	4.267564
H	0.363019	1.289360	5.134491
H	2.119339	0.030762	3.999444
H	2.001035	-0.636976	1.690701
H	-4.254359	1.209837	3.606430
H	-5.218431	-0.939896	2.986292
H	-6.628295	1.002606	3.197831
H	-7.466121	2.194878	0.083683
H	-6.339354	0.818071	-1.579451
H	-7.551888	-0.201760	0.275634
H	-0.851320	1.674912	-1.710653
H	0.962321	-0.008354	-0.535974

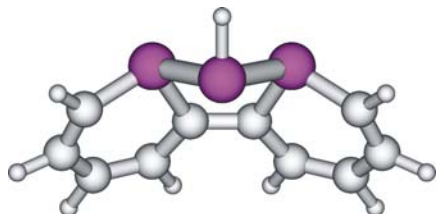
**3Pa** (isomer 1,  $C_s$ )



E=-1410.6467474

H	0.000000	-1.323590	1.714027
P	0.000001	-2.122401	0.527380
P	-1.482604	-0.893410	-0.670471
P	1.482604	-0.893410	-0.670471
C	-0.690342	0.744152	-0.381485
C	0.690343	0.744152	-0.381485
C	-2.996333	-0.695148	0.290666
C	2.996332	-0.695148	0.290667
C	-3.510315	0.531616	0.546226
C	3.510314	0.531617	0.546227
C	-2.836136	1.778046	0.266215
C	2.836136	1.778046	0.266214
C	-1.538768	1.876479	-0.141436
C	1.538768	1.876479	-0.141436
H	-3.574550	-1.588143	0.504223
H	3.574549	-1.588143	0.504225
H	-4.497506	0.598007	0.995474
H	4.497504	0.598008	0.995476
H	-3.384705	2.692300	0.464169
H	3.384705	2.692300	0.464168
H	-1.099125	2.867910	-0.200288
H	1.099125	2.867910	-0.200289

**3Pa** (isomer 2,  $C_s$ )

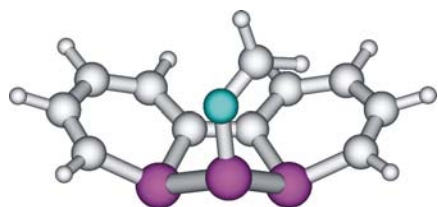


E=-1410.6471477

P	2.049462	-0.598586	0.000000
H	3.193300	0.251357	0.000000
P	0.905778	0.659498	1.519207
P	0.905778	0.659498	-1.519207
C	-0.718932	0.397252	0.689932
C	-0.718932	0.397252	-0.689932
C	0.660936	-0.348186	3.001009

C	0.660936	-0.348186	-3.001009
H	1.542346	-0.604205	3.580151
H	1.542346	-0.604205	-3.580151
C	-0.574924	-0.591327	3.494384
C	-0.574924	-0.591327	-3.494384
H	-0.666052	-1.070880	4.465175
H	-0.666052	-1.070880	-4.465175
C	-1.804044	-0.255557	2.812159
C	-1.804044	-0.255557	-2.812159
H	-2.731743	-0.432466	3.345179
H	-2.731743	-0.432466	-3.345179
C	-1.870584	0.180038	1.523601
C	-1.870584	0.180038	-1.523601
H	-2.853548	0.285478	1.074844
H	-2.853548	0.285478	-1.074844

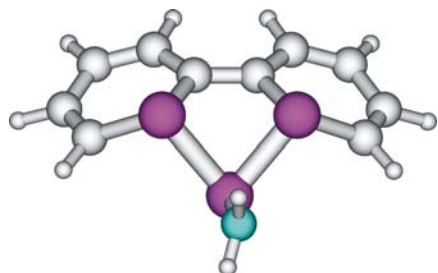
### 3Pb (isomer 1)



E=-1466.0378791

C	-3.049052	-0.582954	-0.097501
P	-1.454205	-0.668260	-0.911906
P	-0.003799	-2.089236	0.180105
N	-0.032185	-1.659654	1.810870
C	-3.566286	0.587940	0.357044
C	-2.854911	1.836623	0.388461
C	-1.533703	1.977843	0.064729
C	-0.693773	0.908103	-0.373115
C	0.700373	0.907065	-0.373633
P	1.457605	-0.669838	-0.913247
C	3.050816	-0.589257	-0.095829
C	3.570080	0.579497	0.363078
C	2.861717	1.829574	0.394408
C	1.541644	1.974503	0.067118
H	-3.660692	-1.478970	-0.111898
H	3.661500	-1.485998	-0.112471
H	-4.590658	0.594815	0.720179
H	4.593717	0.583279	0.728323
H	-3.394193	2.708484	0.741864
H	3.402120	2.699741	0.750319
H	-1.078411	2.951501	0.221881

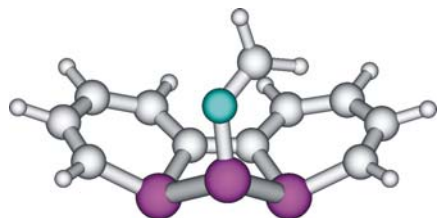
### 3Pb (isomer 2)



E=-1466.0367668

C	-3.044715	0.383746	-0.203996
P	-1.497407	0.639568	0.687943
P	-0.033532	1.754647	-0.707651
N	-0.152509	3.331804	-0.093826
C	-3.518732	-0.850481	-0.501275
C	-2.787969	-2.073032	-0.288313
C	-1.480858	-2.124997	0.099023
C	-0.673889	-0.975369	0.384455
C	0.716794	-0.956122	0.384136
P	1.494983	0.680235	0.683335
C	3.051328	0.462714	-0.200151
C	3.557899	-0.757909	-0.501907
C	2.857715	-1.998311	-0.292840
C	1.553485	-2.084638	0.097493
H	-3.665062	1.259141	-0.367251
H	3.653477	1.352350	-0.355995
H	-4.515156	-0.938636	-0.926320
H	4.557716	-0.819645	-0.923528
H	-3.296781	-3.004055	-0.512323
H	3.389880	-2.915905	-0.518344
H	-1.004210	-3.099937	0.125522
H	1.102633	-3.071733	0.125446
H	0.092917	4.099486	-0.699052
H	-0.094881	3.545946	0.894465

### 3Pc (isomer 1)

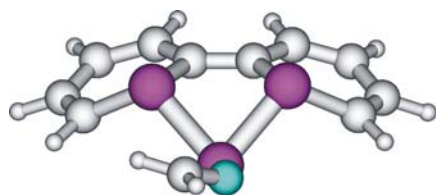


E=-1504.1163603

C	-3.091321	-0.528622	-0.23009
P	-1.508555	-0.502202	-1.07140

P	-0.030307	-2.051316	-0.21465
N	-0.204153	-1.845491	1.45702
C	-3.604450	0.580104	0.36016
C	-2.893542	1.818509	0.53800
C	-1.576531	2.001040	0.22406
C	-0.740181	0.995903	-0.35322
C	0.651025	1.006862	-0.38242
P	1.413400	-0.485509	-1.12004
C	3.028179	-0.477148	-0.33431
C	3.557061	0.653943	0.20324
C	2.835716	1.884886	0.37810
C	1.500316	2.038471	0.12742
H	-3.697121	-1.421571	-0.33895
H	3.646325	-1.360129	-0.46085
H	-4.625209	0.540953	0.73107
H	4.593979	0.637758	0.52790
H	-3.430198	2.637206	1.00422
H	3.381320	2.727100	0.78904
H	-1.118600	2.945973	0.50163
H	1.043521	2.986612	0.39581
C	0.603175	-1.425290	2.34127
H	1.629979	-1.109601	2.12931
H	0.270317	-1.372412	3.37980

### 3Pc (isomer 2)

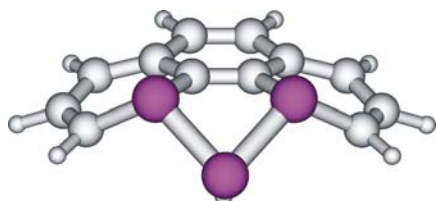


E=-1504.115755

C	-0.063858	0.135689	0.335464
C	-0.018160	-0.114939	1.665819
C	1.197524	-0.213684	2.433193
C	2.448138	-0.208001	1.889215
C	2.721216	-0.060703	0.489292
C	3.904607	-0.433869	-0.135365
C	5.042826	-0.999855	0.529954
C	6.024692	-1.713842	-0.090676
C	6.033501	-2.025443	-1.496775
C	5.145857	-1.527652	-2.391182
P	3.955722	-0.241553	-1.964087
P	1.792030	-1.058955	-2.179349
N	1.120394	-0.288120	-3.537060
C	1.678902	0.056512	-4.622333
P	1.402156	0.598919	-0.610088
H	-1.018571	0.217525	-0.173551

H	5.236461	-1.783620	-3.442134
H	-0.952689	-0.253594	2.203024
H	6.809388	-2.699610	-1.849337
H	1.101287	-0.367236	3.502249
H	6.823906	-2.124945	0.516076
H	3.284765	-0.399195	2.553785
H	5.093367	-0.912217	1.610620
H	2.749083	-0.069314	-4.830049
H	1.077863	0.510845	-5.411619

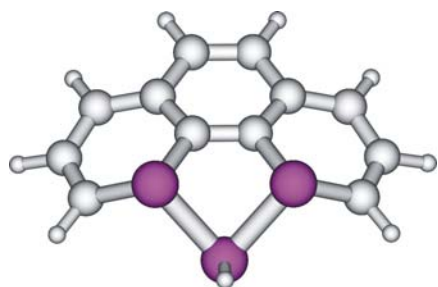
**4Pa** (isomer 1,  $C_s$ )



E=-1486.888659

P	-0.018999	0.016809	-0.053154
H	-0.159859	0.141432	1.365033
P	2.268212	-0.007279	-0.137000
P	0.283650	-2.250418	-0.137000
C	2.478051	-1.277873	1.165679
C	1.570346	-2.303847	1.165679
C	2.983947	1.399119	0.711704
C	-1.025039	-3.132215	0.711704
C	3.885117	1.233121	1.726269
C	-0.750453	-4.006437	1.726269
C	4.187627	0.004141	2.386110
C	0.506233	-4.156918	2.386110
C	3.501495	-1.180165	2.171934
C	1.598093	-3.331570	2.171934
C	3.651430	-2.323621	3.042296
C	2.751299	-3.341034	3.042296
H	2.841213	2.380819	0.273298
H	-2.016816	-3.110184	0.273298
H	4.416637	2.113820	2.077290
H	-1.559811	-4.641326	2.077290
H	4.930626	0.030007	3.176294
H	0.571109	-4.897530	3.176294
H	4.472774	-2.323205	3.751651
H	2.850982	-4.156308	3.751651

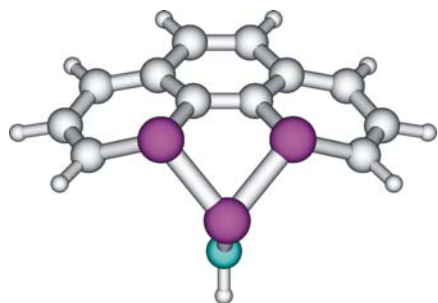
**4Pa** (isomer 2,  $C_s$ )



E=-1486.889737

P	0.004759	-0.004117	0.003123
H	0.077832	-0.067338	1.424998
P	2.285600	0.035698	-0.279295
P	0.293390	-2.266972	-0.279295
C	2.186299	-0.985334	-1.800855
C	1.289525	-2.021858	-1.800855
C	2.808548	1.587413	-1.014247
C	-1.166982	-3.007653	-1.014247
C	3.475085	1.625341	-2.205170
C	-1.108654	-3.672715	-2.205170
C	3.627305	0.529716	-3.107476
C	-0.002527	-3.665778	-3.107476
C	2.989492	-0.690032	-2.960742
C	1.112809	-2.859172	-2.960742
C	2.965272	-1.668022	-4.023010
C	2.077149	-2.694548	-4.023010
H	2.761595	2.477254	-0.395603
H	-2.054325	-3.089166	-0.395603
H	3.924089	2.568095	-2.506692
H	-1.977031	-4.252639	-2.506692
H	4.195279	0.703042	-4.015481
H	-0.092365	-4.252775	-4.015481
H	3.635844	-1.526440	-4.864410
H	2.033481	-3.378511	-4.864410

**4Pb** (isomer 1)

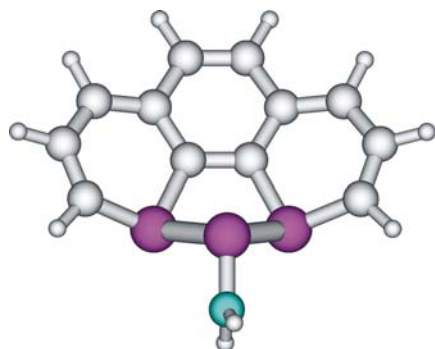




E=-1542.2812661

C	-0.679149	2.879944	0.195226
C	0.679805	2.879799	0.195270
C	1.438880	1.673891	-0.035687
C	0.691036	0.520466	-0.445733
C	-0.690807	0.520638	-0.445789
C	-1.438450	1.674183	-0.035777
C	2.798698	1.599809	0.245363
C	3.545849	0.393801	0.235475
C	3.072461	-0.840832	-0.133036
P	1.476838	-1.062269	-0.886569
P	-0.000425	-2.422875	0.318067
N	-0.000579	-1.886491	1.913029
P	-1.476904	-1.061944	-0.886734
C	-3.072489	-0.840269	-0.133115
C	-3.545643	0.394444	0.235398
C	-2.798292	1.600339	0.245240
H	-3.741081	-1.694157	-0.117266
H	3.740932	-1.694817	-0.117240
H	-4.584619	0.462258	0.547949
H	4.584861	0.461430	0.547945
H	-3.304212	2.505763	0.563602
H	3.304764	2.505142	0.563755
H	1.223642	3.790416	0.425699
H	-1.222810	3.790674	0.425624
H	-0.000815	-2.541569	2.679222
H	-0.000642	-0.910652	2.181018

**4Pb** (isomer 2)

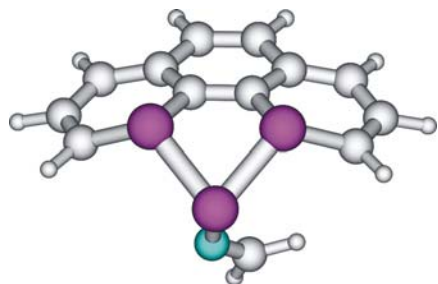


E=-1542.280699

C	-0.039113	-0.137969	-0.001412
C	-0.034857	-0.130221	1.355841
C	1.193411	-0.035693	2.106440
C	2.383821	0.271126	1.357882
C	2.379118	0.263320	-0.023452
C	1.184388	-0.052000	-0.760883
C	1.234192	-0.340268	3.459375

C	2.433527	-0.474137	4.208855
C	3.692303	-0.208794	3.741295
P	3.996360	0.577324	2.164449
P	5.050279	-0.892774	0.657183
P	3.986620	0.561953	-0.844527
C	3.673814	-0.248035	-2.408412
C	2.412017	-0.517941	-2.864549
C	1.216704	-0.372526	-2.110402
N	6.648617	-0.354241	0.613883
H	4.520483	-0.377347	-3.074458
H	4.542371	-0.326691	4.405247
H	2.305159	-0.875471	-3.885577
H	2.332833	-0.817112	5.235470
H	0.278418	-0.612191	-2.599588
H	0.298905	-0.574547	3.956952
H	-0.961839	-0.258413	1.905480
H	-0.969504	-0.272491	-0.543758
H	7.402763	-1.015829	0.700292
H	6.925281	0.619291	0.625995

**4Pc** (isomer 1)

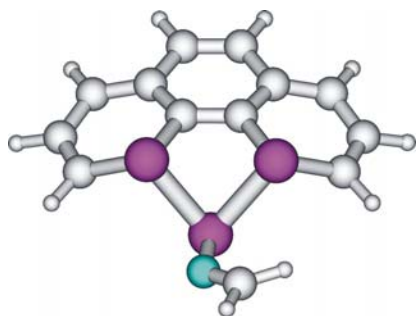


E=-1580.3598884

C	-1.352210	1.779134	-0.071027
C	-0.566869	2.938428	0.277618
C	0.790084	2.892387	0.324851
C	1.521687	1.685818	0.022008
C	0.756159	0.588533	-0.495404
C	-0.624693	0.630221	-0.528931
C	2.872243	1.557040	0.323371
C	3.592987	0.339232	0.225706
C	3.101733	-0.849999	-0.250182
P	1.516562	-0.970768	-1.043059
P	-0.043300	-2.400861	-0.000521
P	-1.450916	-0.882712	-1.111412
C	-3.061651	-0.663878	-0.386900
C	-3.513619	0.564895	0.030199
C	-2.726145	1.737971	0.142730
N	0.091117	-2.013530	1.621450
C	-0.691888	-1.523746	2.492652
H	-3.756823	-1.494130	-0.452738

H	3.748993	-1.718913	-0.291089
H	-4.561543	0.650073	0.305723
H	4.627781	0.357108	0.558197
H	-3.213608	2.640727	0.495715
H	3.391214	2.420766	0.725122
H	1.352653	3.764161	0.643475
H	-1.090948	3.846812	0.557026
H	-0.321553	-1.348437	3.504208
H	-1.736094	-1.264572	2.288926

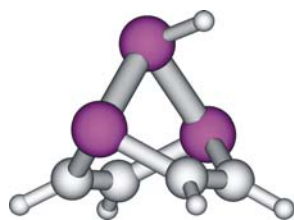
#### 4Pc (isomer 2)



E=-1580.3597356

C	1.011731	-0.342810	-0.366049
C	0.450865	0.918361	-0.356907
C	1.249145	2.085652	-0.082704
C	2.677450	1.892024	-0.022894
C	3.226476	0.651030	-0.021369
C	2.410195	-0.536484	-0.086070
P	-1.358551	1.019724	-0.616102
P	-1.681133	-0.807601	0.829287
P	-0.127703	-1.746503	-0.660919
C	0.799770	-3.049061	0.141967
C	2.143704	-2.957646	0.379758
C	2.931342	-1.785001	0.219207
C	0.678792	3.311075	0.227894
C	-0.715779	3.524106	0.397394
C	-1.689403	2.589980	0.171505
N	-3.072938	-1.595855	0.294129
C	-4.147950	-1.138167	-0.200976
H	-2.730037	2.861389	0.315620
H	0.293468	-3.997939	0.282911
H	-1.022629	4.509589	0.737890
H	2.661039	-3.849724	0.723518
H	1.344258	4.141988	0.437472
H	3.992149	-1.855643	0.434918
H	4.299306	0.528886	0.087344
H	3.308152	2.768591	0.084279
H	-4.952845	-1.826378	-0.462853
H	-4.329523	-0.072435	-0.388542

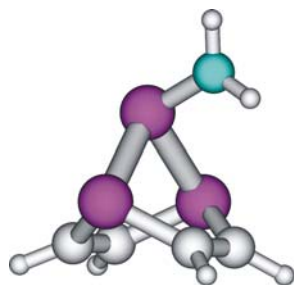
### 5Pa ( $C_s$ )



E=-1179.554597

H	-1.420656	-1.234957	-1.453393
P	-1.242764	-1.080318	-0.047093
P	1.024171	-1.174999	-0.024099
P	-1.021027	1.177732	-0.024099
C	1.231704	0.188649	-1.289122
C	0.358233	1.193462	-1.289122
C	0.963278	-0.046274	1.474138
C	0.088239	0.960344	1.474138
H	2.083494	0.141278	-1.961799
H	0.429869	2.043556	-1.961799
H	1.651933	-0.231230	2.293074
H	0.000925	1.668037	2.293074

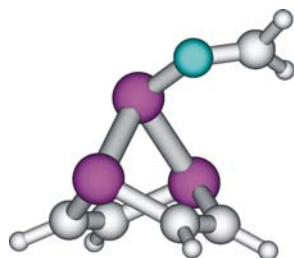
### 5Pb



E=-1234.9453599

C	0.397494	0.668562	1.647985
P	0.261532	1.575115	0.027864
P	-1.101411	-0.021045	-0.915245
N	-2.483146	-0.007571	0.060564
C	0.430418	-0.666307	1.644154
P	0.337307	-1.572217	0.021833
C	1.677127	-0.634335	-0.855655
C	1.646430	0.705360	-0.851340
H	0.493601	1.254632	2.558384
H	0.553301	-1.250942	2.552290
H	2.379008	1.305311	-1.383494
H	2.435231	-1.196148	-1.393793
H	-3.385836	-0.171535	-0.355558
H	-2.463515	-0.055792	1.070592

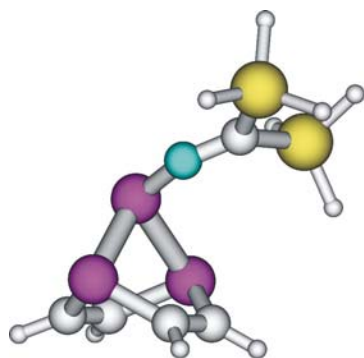
### 5Pc



E=-1273.023816

C	-1.630831	-0.544332	-0.758744
C	-1.640564	-0.564194	0.574474
P	-0.027333	-0.540519	1.504337
C	0.803380	-1.924905	0.575542
C	0.800559	-1.908101	-0.762354
P	-0.000360	-0.477649	-1.652225
P	1.010759	0.817358	-0.063829
N	0.131401	2.268741	-0.218276
C	-0.553345	2.877990	0.656315
H	1.274856	-2.684059	-1.356119
H	1.287588	-2.711202	1.147353
H	-2.538466	-0.592877	-1.354156
H	-2.558916	-0.633501	1.151427
H	-1.003740	3.840839	0.407961
H	-0.728865	2.500868	1.672578

### 5Pd

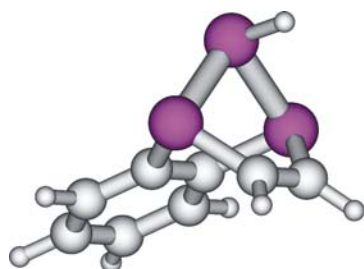


E=-1854.4582427

C	1.526328	-0.767430	1.668245
C	1.356109	0.555557	1.680844
P	1.453467	1.513588	0.092071
P	0.488728	-0.219357	-1.151954
N	-1.026500	-0.653492	-0.573589
C	-2.114484	-0.095201	-0.187630
i	-3.579352	-1.277041	0.152027

P	1.844731	-1.627138	0.052110
C	3.229884	-0.527323	-0.522652
C	3.054039	0.800570	-0.523292
i	-2.371331	1.803281	0.004021
H	4.137938	-0.993522	-0.893683
H	3.806984	1.486128	-0.901588
H	1.513033	-1.369942	2.572419
H	1.189222	1.114847	2.597670
H	-1.819096	2.500132	-1.184765
H	-3.831314	2.056224	0.107488
H	-1.706790	2.304384	1.233310
H	-4.178070	-0.944873	1.473542
H	-4.626509	-1.069555	-0.884534
H	-3.105480	-2.680153	0.134092

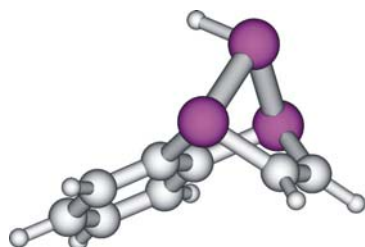
**6Pa** (isomer 1,  $C_s$ )



E=-1333.2526551

P	-1.456193	-1.694378	0.000000
H	-1.047038	-3.059617	0.000000
P	0.013573	-0.964264	1.561909
P	0.013573	-0.964264	-1.561909
C	-0.004474	0.700028	0.703988
C	-0.004474	0.700028	-0.703988
C	-0.012600	1.906416	1.399314
C	-0.012600	1.906416	-1.399314
C	-0.018299	3.115053	0.695561
C	-0.018299	3.115053	-0.695561
C	1.519806	-1.612058	0.666296
C	1.519806	-1.612058	-0.666296
H	-0.018826	1.910555	2.483907
H	-0.018826	1.910555	-2.483907
H	-0.025519	4.053639	1.238431
H	-0.025519	4.053639	-1.238431
H	2.379123	-1.919235	1.256524
H	2.379123	-1.919235	-1.256524

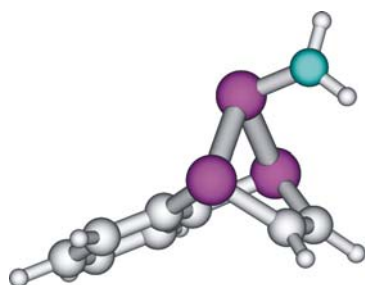
**6Pa** (isomer 2,  $C_s$ )



E=-1333.2534982

P	-1.286019	-1.956324	0.000000
H	-2.356899	-1.014807	0.000000
P	-0.002285	-0.934353	1.563145
P	-0.002285	-0.934353	-1.563145
C	-0.016365	0.722052	0.702848
C	-0.016365	0.722052	-0.702848
C	-0.021271	1.927334	1.398740
C	-0.021271	1.927334	-1.398740
C	-0.032407	3.137698	0.695083
C	-0.032407	3.137698	-0.695083
C	1.499309	-1.599880	0.667694
C	1.499309	-1.599880	-0.667694
H	2.350098	-1.936084	1.253575
H	2.350098	-1.936084	-1.253575
H	-0.022727	1.932066	2.483547
H	-0.022727	1.932066	-2.483547
H	-0.045090	4.075929	1.238472
H	-0.045090	4.075929	-1.238472

**6Pb** (isomer 1)

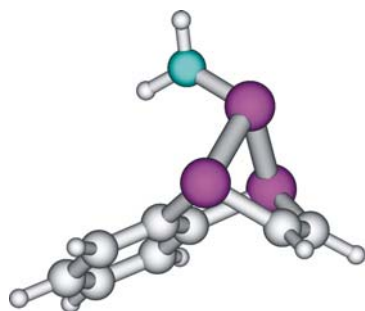


E=-1388.6402241

C	3.365709	0.677273	-0.278280
C	3.356075	-0.716371	-0.258748
C	2.154099	-1.407459	-0.102976
C	0.958161	-0.702769	0.047271
C	0.967972	0.706573	0.030349
C	2.174005	1.389501	-0.140331
P	-0.685977	-1.560073	0.215727

P	-1.519091	-0.008835	-1.236135
N	-3.191833	-0.085822	-0.927579
P	-0.663672	1.587567	0.186611
C	-1.241315	0.700316	1.718479
C	-1.253797	-0.635399	1.731431
H	2.184073	2.473852	-0.163243
H	2.148463	-2.492094	-0.098420
H	4.301372	1.211480	-0.401060
H	4.284101	-1.266869	-0.366370
H	-1.509969	1.292858	2.589593
H	-1.529796	-1.208048	2.613430
H	-3.815909	0.215354	-1.660422
H	-3.573867	0.024348	0.003322

**6Pb (isomer 2)**

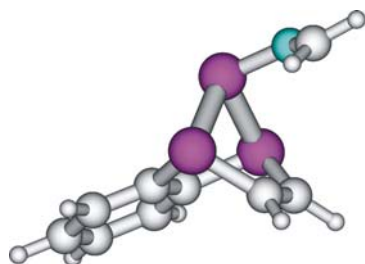


E=-1388.6427661

C	3.217547	0.654396	0.249181
C	2.018061	1.373202	0.251908
C	0.812841	0.720889	-0.007941
C	0.808808	-0.659918	-0.278139
C	2.009067	-1.369991	-0.286725
C	3.213155	-0.711092	-0.019336
P	-0.830008	-1.477824	-0.609532
C	-1.428804	-0.297740	-1.907166
C	-1.426388	1.018319	-1.648373
P	-0.817750	1.615609	-0.003567
P	-1.951049	-0.176549	0.904525
N	-1.174244	-0.541506	2.370282
H	-1.801084	-0.700211	-2.845345
H	-1.799835	1.746805	-2.363045
H	2.009661	-2.434335	-0.496489
H	2.026198	2.438126	0.458680
H	4.143536	-1.268077	-0.018212
H	4.151442	1.163854	0.459337
H	-0.172014	-0.479629	2.495451
H	-1.701813	-0.462940	3.225807



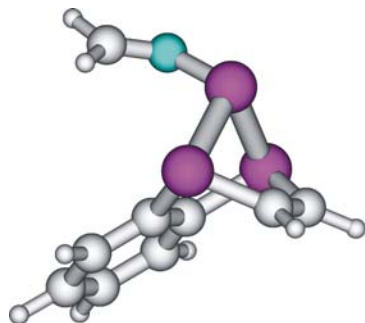
**6Pc (isomer 1)**



E=-1426.719649

C	-0.002045	0.002134	0.012380
C	0.013051	0.022527	1.408254
C	1.224449	0.022422	2.096083
C	2.430676	-0.000895	1.394052
C	2.424264	-0.033798	-0.001112
C	1.198979	-0.029819	-0.696707
P	3.997028	-0.063218	-1.002013
C	3.539182	-1.510460	-2.080426
C	2.377720	-1.496790	-2.736866
P	1.252090	-0.025327	-2.562601
P	2.948108	1.478755	-2.362555
N	3.632303	1.388204	-3.928620
C	4.817370	1.062730	-4.237290
H	2.039600	-2.332105	-3.344514
H	4.214673	-2.361614	-2.110811
H	-0.946836	0.013662	-0.520117
H	3.372228	0.004432	1.932302
H	-0.922219	0.041139	1.956556
H	1.232754	0.040066	3.180218
H	5.130956	1.119837	-5.281421
H	5.571808	0.722316	-3.515671

**6Pc (isomer 2)**

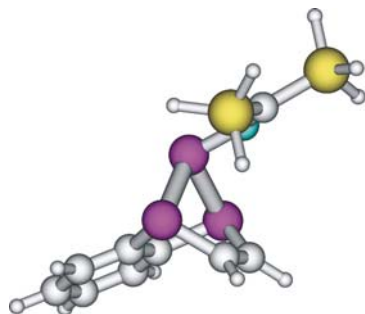


E=-1426.7215332

C	-0.874752	-0.429586	-0.642118
C	-2.073471	-0.406984	-1.352307

C	-3.254927	-0.014132	-0.715536
C	-3.236883	0.348334	0.627408
C	-2.037089	0.323332	1.345553
C	-0.854981	-0.059926	0.713894
P	0.770004	-0.111454	1.619055
P	1.992064	0.527363	-0.236723
N	1.380193	2.013763	-0.818874
C	0.885006	2.971582	-0.153108
P	0.728327	-0.943304	-1.430859
C	1.214129	-2.200779	-0.148047
C	1.248501	-1.843270	1.142404
H	1.478803	-3.201915	-0.477057
H	1.548885	-2.533213	1.926214
H	-2.091142	-0.688600	-2.399712
H	-2.028572	0.604468	2.393370
H	-4.184818	0.010093	-1.272658
H	-4.153112	0.653975	1.120271
H	0.603865	3.890884	-0.670400
H	0.715622	2.947470	0.931150

**6Pd** (isomer 1)

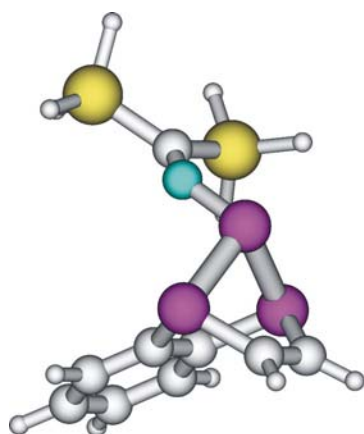


E=-2008.1535020

C	-0.040081	0.001475	0.049015
C	0.004066	-0.034983	1.443227
C	1.235233	-0.056540	2.101382
C	2.429863	-0.024252	1.354436
C	2.376083	0.023568	-0.039154
C	1.141209	0.028568	-0.689573
P	1.362682	-0.095597	3.958647
P	3.032326	1.494927	3.694931
N	4.124875	1.476787	4.991229
C	4.035617	1.449647	6.271112
Si	2.410178	1.276810	7.289598
P	4.043319	0.014177	2.287447
C	3.695749	-1.467230	3.357415
C	2.565082	-1.510077	4.064671
Si	5.688739	1.670251	7.208199
H	-0.917250	-0.049857	2.015296
H	3.293505	0.057203	-0.616706

H	-0.997904	0.008169	-0.459195
H	1.103228	0.056354	-1.772844
H	2.292349	-2.366058	4.676654
H	4.411655	-2.284949	3.349407
H	1.362277	2.159204	6.718311
H	1.936272	-0.130018	7.297390
H	2.712361	1.689253	8.684409
H	5.803807	0.613956	8.250773
H	6.820454	1.585241	6.256702
H	5.689308	2.988375	7.898926

**6Pd** (isomer 2)

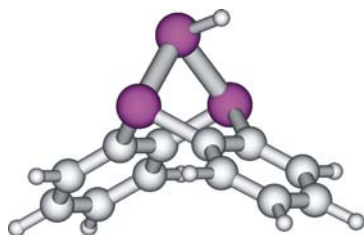


E=-2008.1556394

C	1.733653	2.968843	0.997541
C	1.961366	3.079412	-0.370541
C	1.889137	1.947086	-1.187724
C	1.582818	0.706224	-0.631842
C	1.350246	0.594396	0.749991
C	1.430497	1.725485	1.560859
P	1.475993	-0.833903	-1.665364
C	2.608702	-1.877530	-0.628402
C	2.373498	-1.997624	0.685859
P	0.950730	-1.082461	1.446797
P	-0.226151	-1.745564	-0.446356
N	-1.481995	-0.672798	-0.809106
C	-2.451308	-0.117082	-0.178384
Si	-3.689249	0.852113	-1.267960
Si	-2.776213	-0.248531	1.714833
H	2.066611	2.037275	-2.254036
H	1.254490	1.644398	2.628197
H	2.191955	4.044826	-0.806993
H	1.787804	3.847715	1.630338
H	3.424240	-2.402694	-1.117884
H	2.982579	-2.629435	1.326710
H	-2.576370	-1.652133	2.155985
H	-1.870929	0.651410	2.471749

H	-4.182444	0.162454	1.961165
H	-3.938330	2.186414	-0.657494
H	-3.143651	1.000688	-2.636768
H	-4.985772	0.122195	-1.303745

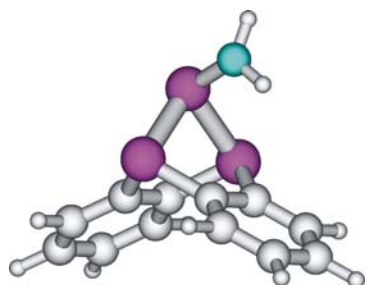
**7Pa (C<sub>s</sub>)**



E=-1486.9509287

P	2.461080	-0.200472	0.000000
H	2.514211	-1.624583	0.000000
P	0.827504	0.011654	1.554390
P	0.827504	0.011654	-1.554390
C	-0.032545	1.417507	0.684786
C	-0.032545	1.417507	-0.684786
C	-0.681783	2.438230	1.374384
C	-0.681783	2.438230	-1.374384
C	-1.316037	3.465004	0.666056
C	-1.316037	3.465004	-0.666056
H	-0.692097	2.443361	2.459154
H	-0.692097	2.443361	-2.459154
H	-1.810716	4.265135	1.205363
H	-1.810716	4.265135	-1.205363
C	-0.108161	-1.352169	0.688051
C	-0.108161	-1.352169	-0.688051
C	-0.813658	-2.335667	1.378228
C	-0.813658	-2.335667	-1.378228
H	-0.821340	-2.340303	2.462841
H	-0.821340	-2.340303	-2.462841
C	-1.506794	-3.322401	0.671270
C	-1.506794	-3.322401	-0.671270
H	-2.049751	-4.090193	1.211111
H	-2.049751	-4.090193	-1.211111

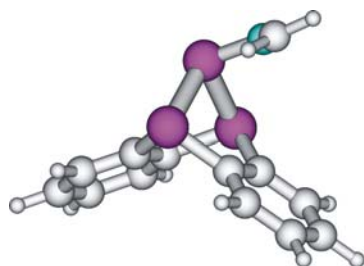
## 7Pb



E=-1542.3377406

C	2.237475	-1.131307	1.409376
C	1.279503	-0.404242	0.703673
C	1.275083	-0.431586	-0.704641
C	2.231190	-1.185117	-1.385374
C	3.193011	-1.906867	-0.671561
C	3.195942	-1.880424	0.719718
P	-0.020389	0.618985	1.558571
P	-0.004484	2.246796	-0.034439
N	1.610637	2.793034	0.047034
P	-0.027520	0.557046	-1.592600
C	-1.496793	-0.150338	-0.706295
C	-2.599562	-0.673279	-1.385559
C	-3.685752	-1.178743	-0.671062
C	-3.679612	-1.156275	0.722532
C	-2.587814	-0.626422	1.410489
C	-1.492079	-0.124727	0.704710
H	2.243339	-1.112977	2.494015
H	2.231030	-1.210712	-2.469924
H	3.945026	-2.436622	1.272322
H	3.939375	-2.484407	-1.205689
H	-2.589940	-0.603561	2.494937
H	-2.609999	-0.687787	-2.470085
H	-4.525697	-1.549534	1.275127
H	-4.536746	-1.589423	-1.203116
H	2.392081	2.157875	-0.060465
H	1.799419	3.719472	-0.305397

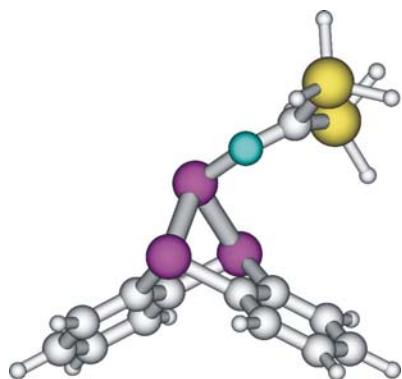
## 7Pc



E=-1580.4173272

C	1.954590	-1.461424	1.437856
C	1.102578	-0.644625	0.695851
C	1.060418	-0.767673	-0.705129
C	1.872500	-1.701659	-1.345425
C	2.730097	-2.512933	-0.595950
C	2.770673	-2.393594	0.789470
P	-0.009967	0.608168	1.503314
P	0.135989	2.101734	-0.245005
N	1.789588	2.471571	-0.511866
P	-0.105934	0.331999	-1.645503
C	-1.637694	-0.101764	-0.679742
C	-2.811034	-0.529517	-1.302498
C	-3.941069	-0.822807	-0.537605
C	-3.904746	-0.682843	0.848005
C	-2.737301	-0.251934	1.479757
C	-1.599542	0.036036	0.723933
H	1.987539	-1.374188	2.518784
H	1.844804	-1.797186	-2.425611
H	3.438294	-3.020781	1.369799
H	3.367093	-3.232390	-1.098290
H	-2.713943	-0.141021	2.558404
H	-2.846002	-0.630718	-2.381835
H	-4.785342	-0.908080	1.439283
H	-4.849953	-1.156851	-1.025549
C	2.712989	2.533297	0.353982
H	3.709374	2.856028	0.045620
H	2.584951	2.284305	1.415339

## 7Pd

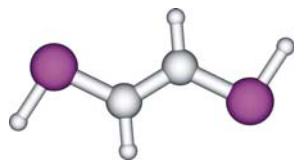


E=-2161.8511191

C	-3.659954	-0.462309	-1.365018
C	-2.402248	-0.357113	-0.768907
C	-2.238579	-0.713592	0.586607
C	-3.334204	-1.172664	1.320578
C	-4.588778	-1.266261	0.717210
C	-4.751478	-0.910879	-0.620231
P	-0.542647	-0.564034	1.332369
P	0.248248	-1.446584	-0.650980
N	1.845759	-0.926532	-0.942094
C	2.924947	-0.923685	-0.246736
i	4.499344	-0.400841	-1.199789
P	-0.901478	0.199902	-1.715851
C	-0.384436	1.535722	-0.532828
C	-0.224822	1.194875	0.822818
C	0.149588	2.171368	1.744375
C	0.372829	3.484733	1.319634
C	0.216363	3.821092	-0.021176
C	-0.165504	2.847421	-0.949362
i	3.100004	-1.461225	1.594582
H	-3.789095	-0.196374	-2.408598
H	-0.285410	3.114024	-1.993993
H	-5.727598	-0.985312	-1.086495
H	0.394914	4.838570	-0.350745
H	-5.438117	-1.617770	1.292376
H	0.672802	4.239469	2.038063
H	-3.210191	-1.454484	2.360552
H	0.271406	1.914240	2.791194
H	4.535226	-1.762956	1.833283
H	2.681379	-0.370685	2.510240
H	2.282915	-2.674984	1.845677
H	5.264767	0.578581	-0.380714
H	5.366659	-1.592904	-1.404620
H	4.124985	0.193712	-2.503508

## P-ligands

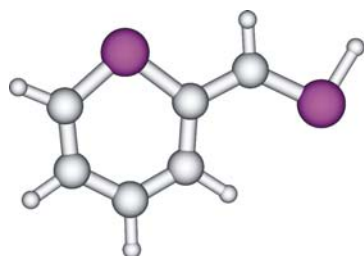
### 1P (isomer 2)



E=-761.3394349

C	-0.336534	0.632195	0.000000
C	0.336534	-0.632195	0.000000
H	-1.425131	0.593890	0.000000
H	1.425131	-0.593890	0.000000
P	0.336534	2.191573	0.000000
P	-0.336534	-2.191573	0.000000
H	1.709807	1.788849	0.000000
H	-1.709807	-1.788849	0.000000

### 2P

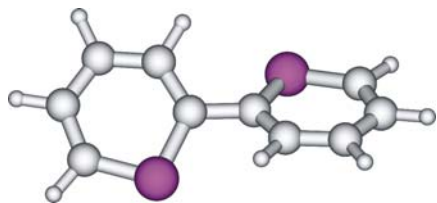


E=-915.0229376

C	0.000000	0.286712	0.000000
P	-1.758307	0.130170	0.000000
C	-1.947331	-1.600828	0.000000
C	-0.909440	-2.521046	0.000000
C	0.439185	-2.144761	0.000000
C	0.861985	-0.824055	0.000000
C	0.508575	1.654887	0.000000
P	2.135855	2.139870	0.000000
H	1.871544	3.541153	0.000000
H	-0.263537	2.420624	0.000000
H	1.933111	-0.639243	0.000000
H	1.192651	-2.924871	0.000000
H	-1.146909	-3.581019	0.000000
H	-2.967914	-1.972696	0.000000



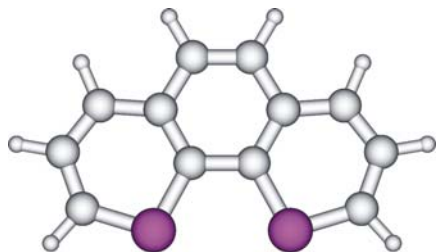
### 3P ( $C_2$ )



E=-1068.708966

C	-0.022971	0.743119	0.095826
C	0.022971	-0.743119	0.095826
P	-1.483566	1.516566	-0.526697
P	1.483566	-1.516566	-0.526697
C	-1.080797	3.197670	-0.333516
C	1.080797	-3.197670	-0.333516
C	0.117805	3.692921	0.165261
C	-0.117805	-3.692921	0.165261
C	1.154210	2.862442	0.589058
C	-1.154210	-2.862442	0.589058
C	1.080797	1.471412	0.553363
C	-1.080797	-1.471412	0.553363
H	1.935142	0.913197	0.926584
H	-1.935142	-0.913197	0.926584
H	2.060410	3.316558	0.974925
H	-2.060410	-3.316558	0.974925
H	0.257264	4.768241	0.229536
H	-0.257264	-4.768241	0.229536
H	-1.840210	3.907057	-0.650550
H	1.840210	-3.907057	-0.650550

### 4P ( $C_s$ )

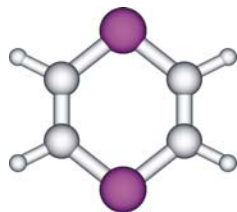


E=-1144.9508053

C	0.000000	0.730222	-0.112897
C	0.000000	-0.730222	-0.112897
C	0.000000	1.427291	1.128925
C	0.000000	-1.427291	1.128925

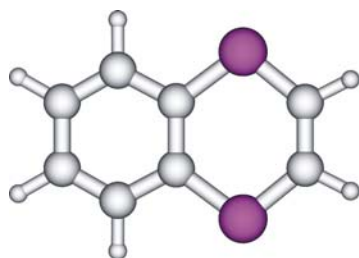
C	0.000000	0.677331	2.352178
C	0.000000	-0.677331	2.352178
P	0.000000	1.590096	-1.680878
P	0.000000	-1.590096	-1.680878
C	0.000000	3.235839	-1.178609
C	0.000000	-3.235839	-1.178609
C	0.000000	3.696534	0.144769
C	0.000000	-3.696534	0.144769
C	0.000000	2.841678	1.224074
C	0.000000	-2.841678	1.224074
H	0.000000	3.970984	-1.978383
H	0.000000	-3.970984	-1.978383
H	0.000000	4.766839	0.328902
H	0.000000	-4.766839	0.328902
H	0.000000	3.265942	2.223085
H	0.000000	-3.265942	2.223085
H	0.000000	1.224839	3.288934
H	0.000000	-1.224839	3.288934

**5P** ( $D_{2h}$ )



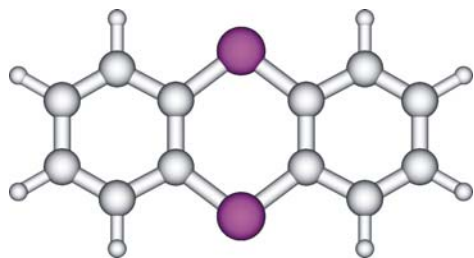
$E = -837.5962367$

P	0.000000	0.000000	1.786323
P	0.000000	0.000000	-1.786323
C	0.000000	1.361945	0.692862
C	0.000000	-1.361945	0.692862
C	0.000000	1.361945	-0.692862
C	0.000000	-1.361945	-0.692862
H	0.000000	2.331120	1.188908
H	0.000000	-2.331120	1.188908
H	0.000000	2.331120	-1.188908
H	0.000000	-2.331120	-1.188908

**6P** ( $C_{2v}$ )

E=-991.2740414

P	0.000000	1.786326	-1.074682
P	0.000000	-1.786326	-1.074682
C	0.000000	0.714787	0.357667
C	0.000000	0.701597	-2.407384
C	0.000000	-0.714787	0.357667
C	0.000000	-0.701597	-2.407384
C	0.000000	1.390697	1.607045
H	0.000000	1.193188	-3.378604
C	0.000000	-1.390697	1.607045
H	0.000000	-1.193188	-3.378604
C	0.000000	0.703968	2.800847
C	0.000000	-0.703968	2.800847
H	0.000000	2.476339	1.610188
H	0.000000	-2.476339	1.610188
H	0.000000	1.246284	3.739587
H	0.000000	-1.246284	3.739587

**7P** ( $D_{2h}$ )

E=-1144.9446989

P	0.000000	0.000000	1.781997
P	0.000000	0.000000	-1.781997
C	0.000000	1.403549	0.718789
C	0.000000	-1.403549	0.718789
C	0.000000	1.403549	-0.718789
C	0.000000	-1.403549	-0.718789
C	0.000000	2.663863	1.394145
C	0.000000	-2.663863	1.394145
C	0.000000	2.663863	-1.394145

C	0.000000	-2.663863	-1.394145
C	0.000000	3.850226	0.708384
C	0.000000	3.850226	-0.708384
C	0.000000	-3.850226	0.708384
C	0.000000	-3.850226	-0.708384
H	0.000000	-2.667348	2.479617
H	0.000000	2.667348	2.479617
H	0.000000	-2.667348	-2.479617
H	0.000000	2.667348	-2.479617
H	0.000000	-4.790337	1.248196
H	0.000000	-4.790337	-1.248196
H	0.000000	4.790337	1.248196
H	0.000000	4.790337	-1.248196