Electronic Supplementary Information for Dalton Transactions

Stability of phosphinidenes – Are they synthetically accessible?

Supplementary material

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Total energies (E; in a.u.) and XYZ coordinates (in Å)

H_2C=N−P (1H) (Singlet) RB3LYP/aug-cc-pVTZ

E= – 435.4235076

P	0.000000	-1.147472	0.000000
N	0.000000	0.393784	0.000000
C	0.000000	1.671348	0.000000
H	-0.936934	2.213785	0.000000
H	0.936934	2.213785	0.000000

H_2C=N−P (1H) Triplet UB3LYP/aug-cc-pVTZ

E= – 434. 4027065

P	-0.724268	-0.854818	0.000000
N	0.000000	0.631997	0.000000
C	1.223824	1.004777	0.000000
H	2.061674	0.302794	0.000000
H	1.459412	2.066841	0.000000

H_2C=N−P (1H) (Singlet) RHF/aug-cc-pVTZ

E= – 434.1937299

C	0.000036	1.648281	0.000000
N	0.000000	0.400682	0.000000
P	-0.000021	-1.138838	0.000000
H	-0.927222	2.194083	0.000000
H	0.927328	2.194037	0.000000

H_2C=N−P (1H) Singlet UHF/aug-cc-pVTZ

E= – 434.2043557

P	0.650227	0.000000	0.901620
N	-0.648464	0.000000	-0.159091
C	-0.647743	0.000000	-1.407074
H	0.255106	0.000000	-2.008294
H	-1.583974	0.000000	-1.945504

H_2C=N−P (1H) Triplet UHF/aug-cc-pVTZ

E= – 434.2229083

P	-0.746412	-0.804927	0.000000
N	0.000000	0.683848	0.000000
C	1.261410	0.884664	0.000000
H	1.990507	0.084420	0.000000
H	1.637220	1.894568	0.000000

Electronic Supplementary Information for Dalton Transactions

Geometries optimized with 6-31G basis set (in Å and degree) and singlet-triplet gaps (in kacl/mol) calculated with different functionals*

Method	^1S (C_{2v})					^3T(C_s)							E(^3T-^1S)	
	CN (Å)	NP (Å)	CH (Å)	H^1CN (deg)	H^1CH^2 (deg)	CN (Å)	NP (Å)	CH1 (Å)	CH2 (deg)	CNP (deg)	H1CN (deg)	H2CN (deg)	6-31G*	Aug-cc-pVTZ
B3LYP	1,280	1,550	1,087	120,1	119,8	1,285	1,666	1,098	1,093	132,0	123,8	119,3	12,8	13,1
B3P86	1,278	1,544	1,087	120,0	120,0	1,283	1,659	1,097	1,092	131,3	123,7	119,2	12,8	12,8
B3PW91	1,278	1,545	1,087	120,0	120,0	1,284	1,662	1,099	1,093	131,1	123,9	119,2	12,0	12,0
BLYP	1,279	1,549	1,086	120,1	119,8	1,284	1,668	1,097	1,092	131,3	123,8	119,3	11,0	11,4
BP86	1,291	1,559	1,096	120,0	120,0	1,297	1,670	1,108	1,102	133,0	123,8	119,0	17,0	17,0
BPW91	1,290	1,558	1,094	120,0	120,0	1,295	1,671	1,105	1,100	132,8	123,9	118,9	16,2	16,3
G96LYP	1,293	1,561	1,094	120,1	119,8	1,297	1,671	1,106	1,100	134,1	123,8	119,2	17,1	17,2
MPW1PW1	1,275	1,543	1,086	120,0	120,0	1,282	1,661	1,096	1,091	130,4	123,9	119,1	10,4	10,3
PBE1PBE	1,276	1,543	1,087	120,0	120,0	1,282	1,662	1,098	1,093	130,2	123,9	119,2	10,5	10,4
MPW1K	1,266	1,535	1,081	120,0	120,0	1,274	1,656	1,090	1,085	128,9	123,8	119,2	5,9	5,6

$H_2C=N-P$ (1H) B3LYP/6-311+G**

E= – 435.4068347

P	0.000000	-1.149876	0.000000
N	0.000000	0.393876	0.000000
C	0.000000	1.675720	0.000000
H	-0.939447	2.218348	0.000000
H	0.939447	2.218348	0.000000

$[(H_2CNP)_2]$ (2H) B3LYP/6-311+G**

E= – 870.8692328

P	-0.511312	0.889630	0.168535
P	0.511211	-0.889483	-0.168608
N	-2.087828	0.450378	-0.316996
N	2.087712	-0.450380	0.316988
C	-2.830972	-0.476390	0.126409
C	2.831220	0.476145	-0.126280
H	-2.539985	-1.152726	0.941105
H	2.540611	1.152560	-0.941043
H	-3.818491	-0.625040	-0.313278
H	3.818704	0.624500	0.313592

$[(H_2CNP)_2]$ (3H) B3LYP/6-311+G**

E= – 870.8428218

P	-1.379508	0.000000	0.000000
P	1.379508	0.000000	0.000000
N	0.000000	1.139395	0.000000
N	0.000000	-1.139395	0.000000
C	0.000000	2.435440	0.000000
C	0.000000	-2.435440	0.000000
H	0.937087	2.979091	0.000000
H	-0.937087	2.979091	0.000000
H	0.937087	-2.979091	0.000000
H	-0.937087	-2.979091	0.000000

[$(H_2CNP)_2$] (4H) B3LYP/6-311+G**

E= – 870.8684003

P	1.678678	0.016950	-0.248156
P	-1.678680	-0.016952	-0.248157
N	0.771755	1.303495	-0.113707
N	-0.771758	-1.303492	-0.113703
C	-0.552383	1.362122	0.447548
C	0.552391	-1.362116	0.447546
H	0.995484	-2.350345	0.302893
H	0.528998	-1.161548	1.530095
H	-0.995476	2.350353	0.302915
H	-0.529005	1.161517	1.530090

[$(H_2CNP)_3$] (5H) B3LYP/6-311+G**

E= – 1306.3265534

P	-0.043385	-1.266932	0.704168
P	-0.298665	1.018122	0.765859
P	1.097402	0.013881	-0.718861
N	2.539916	0.160454	0.289530
N	-1.628848	1.231100	-0.372279
N	-1.196324	-1.952777	-0.390893
C	3.662141	0.245160	-0.297176
C	-2.287938	2.315193	-0.307673
C	-2.450045	-1.774708	-0.331385
H	4.566216	0.337661	0.307969
H	3.801085	0.231680	-1.387405
H	-2.084135	3.130551	0.400573
H	-3.119724	2.467060	-0.998883
H	-3.089779	-2.350022	-1.004269
H	-2.952102	-1.078322	0.347416

$C_2H_2C{=}N{-}P$ (6) B3LYP/6-311+G**

E= – 511.5273961

P	0.000000	0.000000	2.067357
N	0.000000	0.000000	0.485969
C	0.000000	0.000000	-0.763665
C	0.000000	0.660943	-2.048488
C	0.000000	-0.660943	-2.048488
H	0.000000	1.573469	-2.624145
H	0.000000	-1.573469	-2.624145

$(C_4H_4)C=N–P$ (7) B3LYP/6-311+G**

E= – 589.06083

P	-0.000503	-2.677169	0.000000
N	-0.000263	-1.150131	0.000000
C	0.729159	2.295702	0.000000
C	-0.729159	2.295702	0.000000
C	-1.177373	1.007549	0.000000
C	1.177373	1.007549	0.000000
C	0.000000	0.151051	0.000000
H	-2.196303	0.651009	0.000000
H	2.196303	0.651009	0.000000
H	-1.349179	3.181961	0.000000
H	1.349179	3.181361	0.000000

F_2=N−P (1F) B3LYP/6-311+G**

E= – 633.9319586

P	-0.000007	2.006193	0.000000
F	-1.093298	-1.567546	0.000000
F	1.093298	-1.567546	0.000000
N	0.000000	0.430524	0.000000
C	0.000003	-0.815130	0.000000

$(NC)_2C=N–P$ (1CN) B3LYP/6-311+G**

E= – 619.9333847

P	0.000000	2.360673	0.000000
N	0.000000	0.842665	0.000000
N	2.242840	-1.741516	0.000000
N	-2.242840	-1.741516	0.000000
C	-1.233900	-1.174448	0.000000
C	1.233900	-1.174448	0.000000
C	0.000000	-0.472359	0.000000

$(H_3Si)_2C=N–P$ (1SiH_3) B3LYP/6-311+G**

E= – 1016.8628334

P	0.000000	0.000000	2.498228
Si	0.000000	1.669631	-1.200424
Si	0.000000	-1.669631	-1.200424
N	0.000000	0.000000	0.960344
C	0.000000	0.000000	-0.333242
H	-1.301587	-2.365538	-1.009155
H	0.232562	-1.452609	-2.648914
H	1.073129	-2.529490	-0.634187
H	1.301587	2.365538	-1.009155
H	-0.232562	1.452609	-2.648914
H	-1.073129	2.529490	-0.634187

$(Me_3Si)_2C=N–P$ (1SiMe_3) B3LYP/6-311+G**

E= – 1252.9017139

P	0.000448	3.163262	-0.000022
Si	-1.694848	-0.540242	0.001262
Si	1.694728	-0.540202	-0.001260
N	0.000208	1.617699	-0.000287
C	-2.099248	-1.157310	-1.739135
C	-1.656841	-2.008091	1.191457
C	0.000007	0.329998	-0.000557
C	2.101085	-1.150534	1.741024
C	3.007619	0.689607	-0.563014
C	1.654807	-2.013267	-1.185439
C	-3.008124	0.692667	0.555885
H	-3.085917	-1.632670	-1.759067
H	-2.111907	-0.330390	-2.454953
H	-1.368633	-1.891012	-2.089872
H	-3.987660	0.205744	0.598538
H	-2.790072	1.093975	1.549642
H	-3.089432	1.536695	-0.134411
H	-2.627141	-2.515637	1.187908
H	-0.901450	-2.748748	0.915287
H	-1.452994	-1.685792	2.216263
H	2.625338	-2.520367	-1.181596
H	0.900300	-2.753067	-0.904624
H	1.448858	-1.695452	-2.211224
H	3.987176	0.202536	-0.603526
H	2.789022	1.085548	-1.558801
H	3.089240	1.537346	0.122676
H	3.087922	-1.625494	1.762053
H	2.114054	-0.320740	2.453507
H	1.370960	-1.883049	2.095303

($C_4H_3P^2$)C=N–P (7P$^{\alpha}$) B3LYP/6-311+G**

E= – 891.7269965

P	-0.622036	-1.546453	0.000000
P	2.752742	0.824378	0.000000
N	1.264893	0.498266	0.000000
C	0.000000	0.189467	0.000000
C	-1.076703	1.139845	0.000000
C	-2.299489	0.517801	0.000000
C	-2.218090	-0.910546	0.000000
H	-0.909591	2.209045	0.000000
H	-3.240180	1.055482	0.000000
H	-3.099369	-1.540657	0.000000

($C_4H_3P^3$)C=N–P (7P$^{\beta}$) B3LYP/6-311+G**

E= – 891.7237836

P	0.299809	-2.403670	0.000000
P	-1.230744	2.750700	0.000000
N	-0.561004	1.383643	0.000000
C	0.000000	0.197292	0.000000
C	1.438481	-0.001284	0.000000
C	1.760420	-1.320645	0.000000
C	-0.733405	-1.036639	0.000000
H	2.134484	0.828548	0.000000
H	-1.814376	-1.061246	0.000000
H	2.777965	-1.690607	0.000000

($C_4H_3N^2$)C=N–P (7N$^{\alpha}$) B3LYP/6-311+G**

E= – 605.1135225

P	-0.282456	-2.629870	0.000000
N	1.265879	0.763534	0.000000
N	-0.159595	-1.114312	0.000000
C	0.000000	0.181982	0.000000
C	-1.045064	1.180119	0.000000
C	-0.385572	2.377692	0.000000
C	1.026565	2.057142	0.000000
H	-2.106936	0.986679	0.000000
H	-0.819989	3.366931	0.000000
H	1.844210	2.768277	0.000000

$(C_4H_3N^3)C{=}N{-}P\ (7N^{\beta})$ B3LYP/6-311+G**

E= – 605.1078032

P	-0.613591	-2.593748	0.000000
N	-0.292787	-1.105036	0.000000
N	1.290333	2.037088	0.000000
C	0.000000	0.163951	0.000000
C	-0.894843	1.299451	0.000000
C	-0.070421	2.386629	0.000000
C	1.344814	0.735961	0.000000
H	-1.973022	1.263843	0.000000
H	2.269375	0.172302	0.000000
H	-0.352611	3.429754	0.000000

$[((H_3Si)_2CNP)_2]\ (2SiH_3)$ B3LYP/6-311+G**

E= – 2033.7404062

P	-0.369949	-0.532587	-0.834874
P	0.369972	0.532528	0.835030
Si	-3.175081	1.855289	-0.126764
Si	3.175121	-1.855286	0.126690
Si	-4.593559	-1.111605	0.238558
Si	4.593495	1.111662	-0.238665
N	-1.978722	-0.730835	-0.430263
N	1.978734	0.730803	0.430382
C	-3.031181	-0.066214	-0.126567
C	3.031185	0.066215	0.126581
H	4.563465	-2.159479	0.561534
H	2.199547	-2.437600	1.079222
H	2.978595	-2.420123	-1.231180
H	5.473212	1.098871	0.960168
H	5.337391	0.490127	-1.366392
H	4.199593	2.498882	-0.575526
H	-4.563381	2.159481	-0.561749
H	-2.978676	2.420176	1.231103
H	-2.199413	2.437555	-1.079229
H	-5.337443	-0.490111	1.366315
H	-5.473254	-1.098657	-0.960290
H	-4.199750	-2.498876	0.575310

[$(H_3Si)_2CNP)_2$] (3SiH_3) B3LYP/6-311+G**

E= – 2033.7289184

P	0.000033	-1.377020	-0.000039
P	-0.000032	1.377019	-0.000040
Si	3.411748	1.630551	0.087431
Si	3.411726	-1.630554	-0.087371
Si	-3.411726	1.630553	-0.087371
Si	-3.411749	-1.630550	0.087431
N	1.141439	0.000007	-0.000038
N	-1.141439	-0.000007	-0.000038
C	2.461973	0.000010	-0.000048
C	-2.461972	-0.000010	-0.000048
H	3.684433	-1.998918	-1.501123
H	4.704527	-1.450511	0.618873
H	2.619432	-2.707568	0.560033
H	4.704148	1.450893	-0.619633
H	2.619020	2.707806	-0.559032
H	3.685294	1.998267	1.501191
H	-4.704143	-1.450895	-0.619646
H	-2.619016	-2.707808	-0.559020
H	-3.685309	-1.998259	1.501190
H	-3.684450	1.998907	-1.501122
H	-4.704520	1.450515	0.618889
H	-2.619424	2.707571	0.560017

[$(H_3Si)_2CNP)_2$] (4SiH_3) B3LYP/6-311+G**

E= – 2033.7458411

P	-0.649482	-0.406638	1.583933
P	0.649482	-0.406638	-1.583933
Si	-2.288399	1.739766	-0.068251
Si	2.288398	1.739767	0.068251
Si	-3.143097	-1.247184	-0.090353
Si	3.143098	-1.247183	0.090353
N	0.884391	-0.344566	1.223125
N	-0.884391	-0.344566	-1.223125
C	-1.621383	-0.052901	-0.013335
C	1.621383	-0.052901	0.013335
H	-4.004823	-1.057785	1.107263
H	-3.919435	-0.954713	-1.316926
H	-2.641918	-2.642921	-0.114067
H	-3.066356	1.985363	1.173258
H	-1.158610	2.694856	-0.149767
H	-3.167889	1.907973	-1.250793
H	3.167885	1.907975	1.250796
H	3.066359	1.985362	-1.173256
H	1.158609	2.694856	0.149762

H	3.919438	-0.954710	1.316924
H	2.641920	-2.642921	0.114070
H	4.004822	-1.057786	-1.107265

[$(H_3Si)_2CNP)_3$] (5SiH_3) B3LYP/6-311+G**

E= – 3050.6306722

P	-1.229758	-0.239498	0.437102
P	0.050993	-1.821769	-0.519612
P	-0.043352	0.237437	-1.447670
Si	3.482942	-1.745193	-1.351477
Si	-5.370187	-0.903084	-0.976048
Si	3.290706	2.787742	-0.000147
Si	0.063319	3.389281	0.055208
Si	3.690007	-1.862589	1.949988
Si	-4.209270	0.423723	1.820284
N	-2.723012	-0.645696	-0.422900
N	1.357898	-1.756353	0.635271
N	1.413623	0.987934	-0.830140
C	-3.871944	-0.392747	0.099174
C	2.613731	-1.763225	0.361309
C	1.507268	2.172220	-0.336605
H	4.532274	-0.698596	-1.342059
H	4.151298	-3.068404	-1.491460
H	2.543968	-1.548178	-2.479416
H	5.131510	-1.940914	1.589073
H	3.461090	-0.644986	2.766930
H	3.310269	-3.070499	2.722134
H	0.626083	4.762050	-0.017002
H	-1.036209	3.242668	-0.929693
H	-0.438526	3.142410	1.429184
H	3.309535	3.531492	1.287469
H	4.228818	1.643998	0.048561
H	3.678565	3.728103	-1.084845
H	-6.210119	-1.862330	-0.209004
H	-6.196942	0.303034	-1.252543
H	-4.900166	-1.513940	-2.239818
H	-5.683053	0.506816	1.981713
H	-3.640497	-0.404284	2.912863
H	-3.635262	1.792019	1.872425

$H_3Si-P-N-C-SiH_3$ ($8SiH_3$) B3LYP/6-311+G**

E= – 1016.8600574

P	-1.398508	-1.147449	0.000011
Si	-2.397347	0.885090	0.000001
Si	3.069003	0.311000	0.000009
N	0.173994	-0.524610	-0.000016
C	1.304198	-0.200901	-0.000034
H	-2.063483	1.700318	-1.201136
H	-3.856371	0.600489	0.000107
H	-2.063313	1.700400	1.201034
H	3.062795	1.789983	-0.001177
H	3.725571	-0.222520	1.215251
H	3.726104	-0.224523	-1.214064

$(H_3Si)_2P-N-C$ ($9SiH_3$) B3LYP/6-311+G**

E= – 1016.8695868

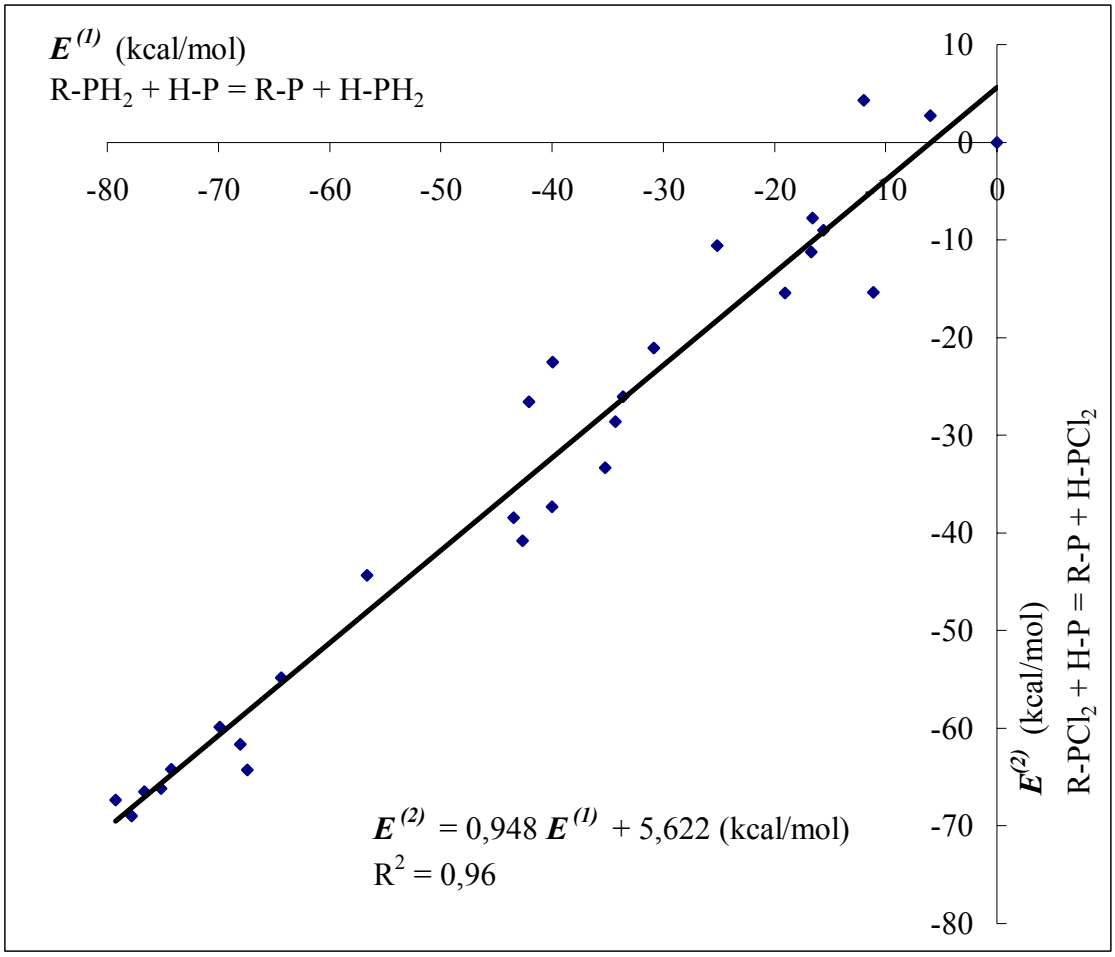
P	0.000001	0.157996	-0.842986
Si	-1.753994	-0.851155	0.235198
Si	1.753793	-0.851528	0.235182
N	0.000142	1.652401	0.043568
C	0.000425	2.724513	0.532951
H	1.583582	-0.859098	1.708264
H	1.794070	-2.240601	-0.287306
H	2.987275	-0.124115	-0.142600
H	-1.794566	-2.240227	-0.287266
H	-1.583780	-0.858735	1.708280
H	-2.987326	-0.123489	-0.142587

Isodesmic reaction energies (in kcal/mol) at different levels of theory

	R-PCl_2 + H-P → R-P + H-PCl_2			**R-PH_2 + H-P → R-P + H-PH_2**		
	B3LYP/ 3-21G(*)	**B3LYP/ 6-311+G****	**MP2/ 6-31G*// B3LYP/ 6-311+G****	**B3LYP/ 3-21G(*)**	**B3LYP/ 6-311+G****	**MP2/ 6-31G*// B3LYP/ 6-311+G****
H-P	0,0	0,0	0,0	0,0	0,0	0,0
F-P	3,9	1,4	4,3	-14,5	-11,3	-12,0
Cl-P	-10,9	-10,0	-9,0	-17,5	-15,5	-15,6
Br-P	-13,4	-12,6	-11,3	-20,0	-17,0	-16,7
HO-P	-12,0	-11,1	-10,6	-28,7	-23,6	-25,1
HS-P	-31,8	-29,4	-28,6	-37,1	-34,1	-34,3
H_2N-P	-27,7	-26,3	-26,6	-45,0	-40,2	-42,1
F_2N-P	-45,1	-44,4	-38,4	-50,7	-46,4	-43,4
(C_4H_4N)-P	-23,6	-23,2	-21,0	-33,0	-30,8	-30,8
H_2P-P	-36,0	-33,6	-37,3	-39,0	-36,0	-40,0
F_2P-P	-42,8	-33,8	-40,8	-44,9	-33,5	-42,6
CH_2=P-P	-34,1	-31,2	-33,3	-35,6	-32,2	-35,2
F_2B-P	-16,4	-18,0	-15,4	-11,9	-12,6	-11,1
H_3C-P	1,3	0,4	2,7	-6,9	-7,3	-6,0
Ph-P	-11,4	-11,5	-7,8	-18,6	-18,2	-16,6
HC≡CP	-22,2	-22,4	-15,4	-25,0	-24,3	-19,1
H_2C=N-P	-52,0	-46,9	-44,3	-65,7	-58,0	-56,6
F_2C=N-P	-34,5	-31,7	-26,1	-44,3	-37,8	-33,6
$(NC)_2C$=N-P	-66,7	-63,9	-64,2	-71,0	-64,9	-67,4
$(H_3Si)_2C$=N-P	-66,4	-61,7	-66,5	-79,8	-71,5	-76,7
(C_3H_2)=N-P	-32,9	-26,1	-22,5	-51,8	-40,1	-39,9
(C_5H_4)=N-P	-62,2	-58,2	-59,8	-74,6	-67,6	-69,9
($C_4H_3P^2$)=N-P	-69,5	-64,8	-69,0	-80,6	-72,9	-77,8
($C_4H_3P^3$)=N-P	-66,2	-62,0	-66,2	-77,7	-70,5	-75,2
($C_4H_3N^2$)=N-P	-64,4	-60,3	-61,6	-71,5	-65,1	-68,0
($C_4H_3N^3$)=N-P	-67,0	-62,3	-64,2	-78,4	-71,6	-74,2

$(Me_3Si)_2C$=N-P	-64,2	-61,8	-67,3	-81,7	-74,5	-79,3

Correlation between the isodesmic reactions (MP2/6-31G//B3LYP/6-311+G** in kcal/mol)*

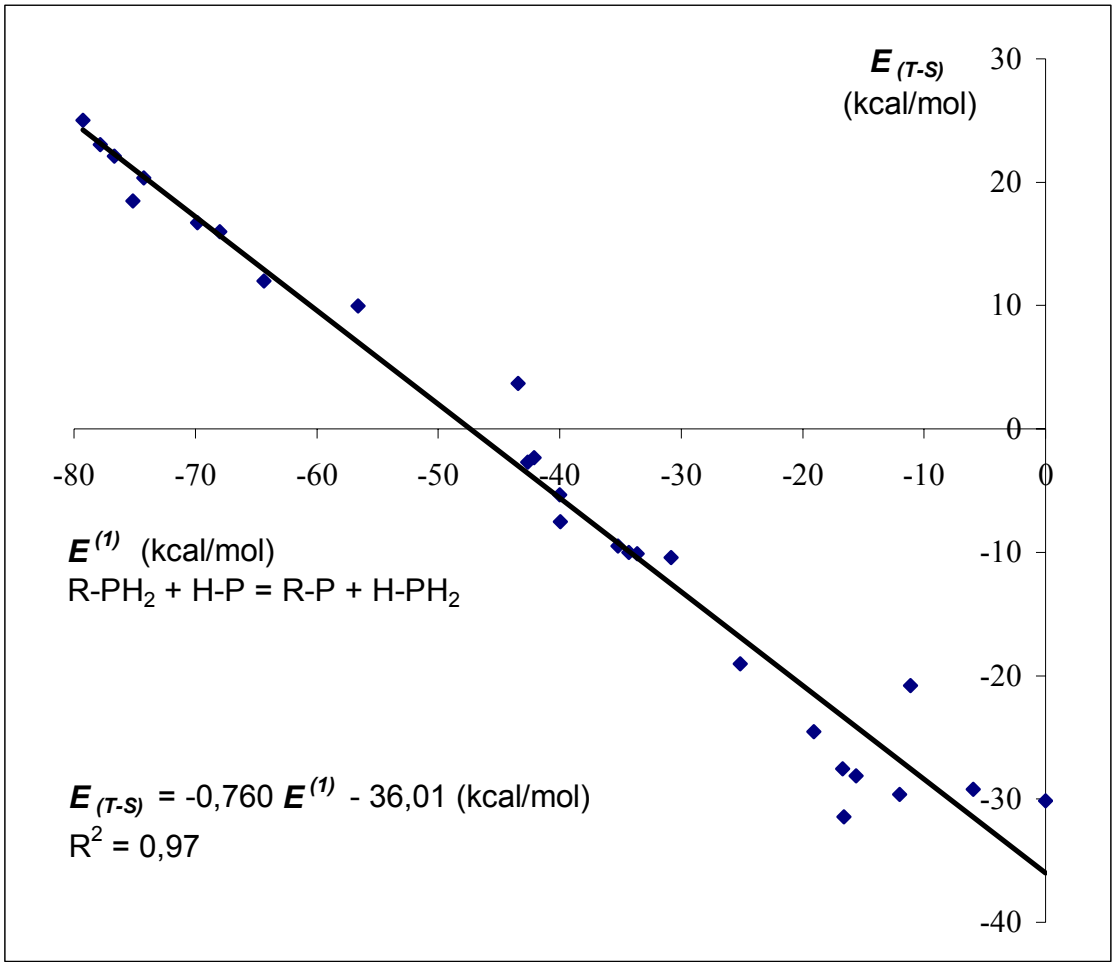


Singlet triplet splitting (in kcal/mol) at different levels of theory

	$E_{(T-S)}$			RHF → UHF instability (at B3LYP/ 6-311+G**)
	3-21G*	**6-311+G****	**CCSD(T)/ aug-cc-pVDZ// B3LYP/6-311+G****	
H-P	-33,8	-32,0	-30,1	+
F-P	-30,3	-30,6	-29,6	+
Cl-P	-29,3	-28,6	-28,1	+
Br-P	-27,9	-27,7	-27,6	+
HO-P	-17,0	-18,7	-19,1	+
HS-P	-7,4	-8,4	-10,0	+
H_2N-P	0,9	-1,3	-2,3	+
F_2N-P	12,7	10,4	3,7	-
(C_4H_4N)-P	-9,4	-9,5	-10,4	+
H_2P-P	-0,6	-1,9	-5,3	-
F_2P-P	10,3	-0,2	-2,7	-
CH_2=P-P	-7,3	-8,5	-9,5	-
F_2B-P	-20,6	-19,4	-20,8	+
H_3C-P	-30,9	-28,8	-29,2	+
Ph-P	-23,4	-22,3	-31,4	+
HC≡CP	-25,1	-23,5	-24,6	+
H_2C=N-P	17,2	13,5	10,0	-
F_2C=N-P	-2,8	-5,1	-10,1	-
$(NC)_2C$=N-P	21,9	19,3	19,0	-
$(H_3Si)_2C$=N-P	27,8	24,1	22,1	-
(C_3H_2)=N-P	1,1	-3,2	-7,5	-
(C_5H_4)=N-P	22,3	18,9	16,7	-
($C_4H_3P^2$)=N-P	26,0	22,3	23,0	-
($C_4H_3P^3$)=N-P	22,5	19,1	18,5	-
($C_4H_3N^2$)=N-P	22,1	18,4	16,0	-
($C_4H_3N^3$)=N-P	25,4	21,6	20,3	-

$(Me_3Si)_2C$=N-P	27,4	24,7	25,4	-

Correlation between the isodesmic reaction energies (in kcal/mol) and the singlet-triplet splitting values (in kcal/mol)



*Bond lengths (PN and CN in Å), electron densities (ρ in a. u.) and ellipticities (ε) at the critical points and Wiberg indices for the PN and CN bonds in the R'$_2$C=N–P phosphinidenes (B3LYP/6-311+G**)*

	PN bond				CN bond			
	PN	**ρ**	**ε**	**Wiberg index**	**CN**	**ρ**	**ε**	**Wiberg index**
H_2P-NH_2	1,723	0,158	0,008	0,910				
HP=NH (*E*)	1,587	0,202	0,238	1,843				
HP=NH (*Z*)	1,576	0,204	0,247	1,831				
P≡N	1,489	0,239	0,000	2,778				
H_2C=N-P	1,546	0,190	0,072	1,688	1,286	0,337	0,343	1,533
F_2C=N-P	1,576	0,178	0,200	1,401	1,246	0,385	0,790	1,571
$(NC)_2C$=N-P	1,518	0,202	0,077	1,809	1,315	0,322	0,519	1,298
$(H_3Si)_2C$=N-P	1,538	0,193	0,038	1,771	1,294	0,325	0,177	1,459
(C_3H_2)=N-P	1,581	0,175	0,108	1,450	1,250	0,370	0,290	1,556
(C_5H_4)=N-P	1,527	0,199	0,041	1,801	1,301	0,326	0,208	1,356
$(Me_3Si)_2C$=N-P	1,546	0,189	0,033	1,736	1,288	0,329	0,129	1,497
$(C_4H_3P^2)$=N-P	1,523	0,200	0,032	1,826	1,302	0,324	0,143	1,358
$(C_4H_3P^3)$=N-P	1,522	0,201	0,033	1,829	1,312	0,319	0,182	1,303
$(C_4H_3N^2)$=N-P	1,521	0,202	0,045	1,822	1,306	0,326	0,269	1,317
$(C_4H_3N^3)$=N-P	1,523	0,200	0,042	1,823	1,302	0,325	0,198	1,340