Supporting Information

N-Heterocyclic Carbenes Versus Transition Metals for Stabilizing Phosphinyl Radicals.

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Contents:

General Considerations:

All manipulations were performed under an atmosphere of dry argon using standard Schlenk techniques. Solvents were dried by standard methods and distilled under argon. ^{1}H, ^{31}P, and ^{13}C NMR spectra were recorded on Varian Inova 400, 500 and Bruker 300 spectrometers at 25 °C. EPR spectra were recorded on Bruker EMX spectrometer at 298 K and 100 K. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, sept = septet, m = multiplet, br = broad signal. Melting points were measured with a Büchi melting point apparatus system. NHC **1**[i] and vanadium nitride anion **7**[ii] were prepared following literature procedures while all other starting materials were purchased from commercial sources.

Compound 2: Elemental bromine (1.26 g, 7.87 mmol) was added at -78°C to a slurry of NHC **1** (3.07 g, 7.87 mmol) in 60 mL of hexane. The mixture was stirred at room temperature overnight. The precipitate was filtered via cannula and washed with 40 mL of ether. 40 mL of THF is then added to the resulting yellow solid and ammoniac gas was bubbled through the suspension at room temperature during 30 minutes. The mixture was then quenched with 20 mL of an aqueous solution of NH_4OH (14.87 M), stirred at room temperature during 30 minutes and 100 mL of ether was then added to the mixture. The organic phase was washed with brine and dried over $MgSO_4$. After filtration, the volatiles were removed under vacuum to afford **2** as a white powder. Yield 87% (2.77 g, 6.83 mmol). Mp: 190 ^{o}C. ^{1}H NMR (C_6D_6, 400 MHz): δ 1.21 (d, *J* = 6.8 Hz, 12 H), 1.29 (d, *J* = 6.8 Hz, 12 H), 3.19 (sept, *J* = 6.8 Hz, 4 H), 3.25 (s, 4 H), 7.07 (d, *J* = 8 Hz, 4 H), 7.17 (t, *J* = 8 Hz, 2 H), N*H* was not observed. ^{13}C NMR (C_6D_6, 100 MHz): δ 24.5, 25.2, 29.4, 48.8, 124.8, 129.3, 135.8, 149.6, 160.1.

Salt 3 (Cl⁻): ^{n}BuLi (2.5 M in hexane, 2.45 mL, 6.13 mmol) was added at -78°C to a solution of **2** (2.37 g, 5.84 mmol) in 40 mL of ether. The mixture was warmed up at room temperature and then stirred during 3 hours. Then the solution was cooled down at -78°C and PCl_3 (0.4 g, 2.92 mmol) was added. The mixture was then allowed to stir at room temperature overnight.

The white precipitate was filtered via cannula and 20 mL of CH_2Cl_2 was added. After filtration of LiCl, all the volatiles were removed under vaccum and the yellowish residue was washed with 25 mL of ether. The residue was dried under vacuum to afford **3 (Cl^-)** as a white powder. At the stage the product contains some impurities which cannot be separated. Yield 50 % (1.29 g, 1.48 mmol). $^{31}P\{^1H\}$ NMR (CD_3CN, 161 MHz): δ 276.3. ^1H NMR (CD_3CN, 400 MHz): δ 0.78 (d, J = 7.2 Hz, 24 H), 1.43 (d, J = 7.2 Hz, 24 H), 2.79 (sept, J = 7.2 Hz, 8 H), 3.92 (s, 8 H), 7.09 (d, J = 7.6 Hz, 8 H), 7.37 (t, J = 7.6 Hz, 4 H). ^{13}C NMR (CD_3CN, 100 MHz): δ 25.0 (d, J_{PC} = 3 Hz), 25.5, 30.0, 50.4, 126.1, 131.9, 132.3, 148.9, 159.6 (d, J_{PC} = 17 Hz, $C_{carbene}$).

Salt 3 (TfO^-): 20 mL of CH_2Cl_2 was added at room temperature to a mixture of **3 (Cl^-)** (1.27 g, 1.45 mmol) and AgOTf (0.37 g, 1.45 mmol). The mixture was then stirred at room temperature in the dark during two hours. During the course of the reaction a precipitate appeared which was removed by filtration. Evaporation of the volatiles under vacuum gave a yellow residue which was washed two times with 20 mL of ether. The solid was dried under vacuum to afford **3 (TfO^-)** as a white powder. Yield 83% (1.19 g, 1.20 mmol). Mp: 374°C (decomposition). $^{31}P\{^1H\}$ NMR ($CDCl_3$, 161 MHz): δ 277.0. ^1H NMR ($CDCl_3$, 400 MHz): δ 0.72 (d, J = 6.8 Hz, 24 H), 1.15 (d, J = 6.8 Hz, 24 H), 2.67 (sept, J = 6.8 Hz, 8 H), 3.93 (s, 8 H), 6.99 (d, J = 8.0 Hz, 8 H), 7.30 (t, J = 8.0 Hz, 4 H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ 24.0, 24.6, 29.0, 49.3, 121.1 (q, J_{CF} = 319 Hz, CF_3), 124.6, 130.5, 130.7, 147.3, 158.2 (d, J_{PC} = 17 Hz, $C_{carbene}$).

Radical 4: 15 mL of THF was added at room temperature to a mixture of salt **4** (1.08 g, 1.09 mmol) and KC_8 (0.16 g, 1.15 mmol). The mixture was then allowed to stir at room temperature during three hours. The solvent was removed under vacuum and the product

extracted with 20 mL of benzene. After evaporation of the solvent the radical **4** was obtained as a fine red microcrystalline powder. Yield 72% (0.66 g, 0.79 mmol). Mp: 208°C-211°C.

Compound 5: ^{n}BuLi (2.5 M in hexane, 1.20 mL, 3.01 mmol) was added at -78°C to a solution of **2** (1.16 g, 2.86 mmol) in 25 mL of THF. The mixture was then stirred at room temperature during 3 hours. The solution was cooled down at -78°C and PCl_3 (0.41 g, 3.01 mmol) was then added. The mixture was stirred at room temperature overnight and all the volatiles were removed under vacuum. Benzene was then added to the residue and LiCl was filtered via cannula. After evaporation of the solvent the yellow residue was washed two times with 20 mL of pentane. The remaining solid was dried under vacuum to afford **5** as a white powder. Yield 57% (0.82 g, 1.62 mmol). Mp: 271 ^{o}C. $^{31}P\{^{1}H\}$ NMR (C_6D_6, 161 MHz): δ 183.7. ^{1}H NMR (C_6D_6, 400 MHz): δ 1.18 (d, J = 6.8 Hz, 12 H), 1.47 (d, J = 6.8 Hz, 12 H), 3.14 (sept, J = 6.8 Hz, 4 H), 3.33 (s, 4 H), 7.07 (d, J = 8.0 Hz, 4 H), 7.19 (t, J = 8.0 Hz, 2 H). ^{13}C NMR (C_6D_6, 100 MHz): δ 24.6, 25.5, 29.6, 49.0, 125.1, 130.6, 133.6, 148.5, 155.9 (d, J_{PC} = 17 Hz, $C_{carbene}$).

Compound 7: 30 mL of THF was added at - 78°C to a mixture of **5** (0.76 g, 1.50 mmol) and the vanadium nitride anion **6** (0.99 g, 1.50 mmol). The mixture was then stirred at room temperature during six hours. All the volatiles were removed under vacuum and 25 mL of benzene was then added to the dark red residue. After removal of NaCl by filtration, the solvent was removed under vacuum. The dark red residue was then washed with 10 mL of acetonitrile and dried under vacuum to afford **7** as dark red powder. Yield 73 % (1.34 g, 1.19 mmol). Mp: 128°C-131°C. $^{31}P\{^{1}H\}$ NMR (C_6D_6, 161 MHz): δ 185.5 (bs). ^{1}H NMR (C_6D_6, 400 MHz): δ 0.90 (s, 27 H), 1.24 (d, J = 6.8 Hz, 6 H), 1.26 (d, J = 6.8 Hz, 6H), 1.65 (d, J = 6.8 Hz, 6H), 1.69 (d, J = 6.8 Hz, 6H), 2.10 (s, 18H), 3.37 (sept, J = 6.8 Hz, 2 H), 3.37-3.45 (m, 2 H), 3.46-3.52 (m, 2H), 3.54 (sept, J = 6.8 Hz, 2 H), 4.44 (d, J = 13.2 Hz, 3 H), 4.54 (d, J

= 13.2 Hz, 3 H), 6.37 (s, 6 H), 6.53 (s, 3 H), 7.18 (d, *J* = 7.6 Hz, 4 H), 7.26 (t, *J* = 7.6 Hz, 2 H). ^{13}C NMR (C_6D_6, 100 MHz): δ 21.9, 25.1, 25.4, 25.9, 26.1, 29.4, 29.6, 29.9, 36.4, 50.1, 77.7, 122.7, 124.9, 125.3, 125.8, 129.9, 135.9, 137.5, 148.3, 148.5, 157.9 (d, J_{PC} = 23 Hz, $C_{carbene}$), 158.3.

Radical 8: 15 mL of THF was added at room temperature to a mixture of **7** (1.23 g, 1.11 mmol) and KC_8 (0.16g, 1.17 mmol). The mixture was then stirred at room temperature during three hours and the solvent was removed under vacuum. 25 mL of benzene was then added to the dark red residue and KCl and graphite were removed via filtration. All the volatiles were removed under vacuum to afford the radical **8** as a dark red powder. Yield 85 % (1.01 g, 0.94 mmol). Mp: 98°C-102°C.

Computational Details

Full Reference 23:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, J. A., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Gaussian 03, Revision E.01, Wallingford CT, 2004.

Cartesian Coordinates of the Calculated Stationary Points of I, I-H, 4, 4-H, 8, 8-H, PH_3 and PH_2

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209
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I-H:

210
Energy (RI-BP86/def2-SVP) = -5710.465181176 a.u.

C	-5.789122	2.373341	-1.500128
C	-5.542222	1.995534	-0.161982
C	-6.648473	1.800266	0.702392
C	-7.966291	1.993675	0.252642
C	-8.178238	2.373854	-1.092119
C	-7.101907	2.564066	-1.980025
N	-4.213217	1.822287	0.309419
C	-3.814939	2.604770	1.492200
C	-3.725397	4.163008	1.357295
C	-5.120172	4.822632	1.285201
C	-9.135318	1.827429	1.198583
C	-7.334199	2.971335	-3.418230
V	-3.050686	0.366863	-0.095181
N	-3.228391	-0.470245	-1.802932
C	-4.237967	-1.460729	-1.992406
C	-3.903429	-2.818490	-2.238438
C	-4.894654	-3.797402	-2.422002

C	-6.251776	-3.408437	-2.367809
C	-6.620725	-2.070876	-2.133139
C	-5.605257	-1.110992	-1.938270
C	-4.525013	-5.244997	-2.660711
C	-8.075107	-1.654999	-2.147089
N	-3.130732	-0.846798	1.376602
C	-1.930542	-1.385428	2.035370
C	-1.817978	-2.939188	2.171816
C	-1.962191	-3.603403	0.791356
C	-4.339876	-0.871204	2.132532
C	-4.402207	-0.290231	3.426708
C	-5.583002	-0.320837	4.186820
C	-6.726999	-0.943887	3.636609
C	-6.702267	-1.522447	2.354184
C	-5.501792	-1.479613	1.612038
C	-7.933585	-2.179714	1.773011
C	-5.636349	0.285500	5.572129
C	-0.411278	-3.225950	2.740819
C	-2.866767	-3.522420	3.142639
N	-1.467147	0.905655	-0.101097
P	-0.202261	2.007901	0.242620
N	1.284713	1.172792	0.296189
V	2.944476	0.953271	0.321944
N	3.809879	2.602700	-0.064483
C	5.074545	3.026156	0.427543
C	6.213333	3.030569	-0.416051
C	7.462967	3.472858	0.051885
C	7.573742	3.903772	1.393628
C	6.464856	3.899117	2.261411
C	5.220311	3.458654	1.763688
C	8.661704	3.512800	-0.870208
C	6.589435	4.362226	3.695994
C	-2.902128	4.564350	0.120226
C	-3.012302	4.662339	2.633983
N	3.255066	-0.206315	-1.164732
C	4.472986	-0.019036	-1.882123
C	5.705617	-0.431447	-1.332445
C	6.917118	-0.259623	-2.037166
C	6.880859	0.333613	-3.312612
C	5.664314	0.762659	-3.891911
C	4.474148	0.583008	-3.168187
C	8.225094	-0.706010	-1.424269
C	5.653356	1.385602	-5.270832
N	3.282031	0.139905	2.014434
C	4.471393	-0.626057	2.202993
C	4.417590	-2.031859	2.394837
C	5.584551	-2.792562	2.577253
C	6.833102	-2.130533	2.578274
C	6.923709	-0.737892	2.399625
C	5.736850	-0.000272	2.203413
C	5.516864	-4.293699	2.753269
C	8.258988	-0.030934	2.473897
C	2.182937	-0.927731	-1.866772
C	2.342588	-2.475960	-2.022864
C	2.586723	-3.124373	-0.649011
C	1.013303	-2.995638	-2.612371
C	3.486462	-2.854910	-2.987783
C	2.218075	-0.086920	3.013793
C	2.167449	0.922260	4.205488
C	1.782143	2.325843	3.703956
C	3.519698	0.977774	4.942688
C	1.078524	0.412205	5.174183
C	3.283508	3.306599	-1.245752
C	2.895423	4.817289	-1.092792
C	4.141042	5.731027	-1.058223
C	2.055768	5.053029	0.176321
C	2.062528	5.177968	-2.343091
C	-2.154356	-0.457765	-2.815232

C	-2.340743	0.534675	-4.008163
C	-2.244943	1.989148	-3.512531
C	-3.690019	0.306328	-4.716817
C	-1.189737	0.260397	-5.000162
H	3.443025	-2.541459	2.380259
H	4.471494	-4.652968	2.817641
H	6.045600	-4.616729	3.674359
H	6.001752	-4.821424	1.904598
H	7.754286	-2.717440	2.731459
H	8.254711	0.910771	1.890168
H	9.084099	-0.672525	2.104749
H	8.505115	0.239886	3.523936
H	5.788224	1.089758	2.077729
H	2.332245	-1.104665	3.447276
H	1.238374	-0.058654	2.500288
H	1.335167	-0.586573	5.586044
H	0.094451	0.327043	4.667078
H	0.955869	1.107527	6.030461
H	1.782104	3.060032	4.536707
H	0.773091	2.330839	3.242670
H	2.493062	2.681751	2.931922
H	3.835648	-0.027473	5.291212
H	3.452266	1.639793	5.831706
H	4.321686	1.368853	4.286225
H	6.116307	2.666664	-1.449899
H	8.804221	4.531232	-1.292979
H	8.541108	2.816849	-1.723436
H	9.598775	3.252146	-0.337781
H	8.549888	4.252266	1.769819
H	5.910748	5.215509	3.905354
H	7.621608	4.685659	3.933517
H	6.314139	3.554963	4.406690
H	4.336246	3.455359	2.417941
H	2.376092	2.755429	-1.571713
H	4.005216	3.220104	-2.092611
H	1.126452	4.583056	-2.395052
H	2.633590	4.992420	-3.277523
H	1.779248	6.250760	-2.332271
H	4.787643	5.566981	-1.945539
H	4.759071	5.563913	-0.155732
H	3.831106	6.797688	-1.060859
H	1.755475	6.119043	0.251296
H	2.626420	4.794936	1.089753
H	1.128017	4.444860	0.181835
H	5.708531	-0.919591	-0.347189
H	9.024898	-0.796256	-2.185620
H	8.121090	-1.683632	-0.912036
H	8.572525	0.019508	-0.658144
H	7.819906	0.456035	-3.877898
H	6.377623	2.223308	-5.346079
H	4.652078	1.776863	-5.537072
H	5.940640	0.644932	-6.047592
H	3.520799	0.913650	-3.607749
H	2.033751	-0.502065	-2.888760
H	1.247866	-0.739316	-1.304861
H	3.357765	-2.370074	-3.977886
H	3.502073	-3.953653	-3.150056
H	4.478592	-2.558894	-2.597042
H	3.527219	-2.754513	-0.195684
H	2.655410	-4.228788	-0.738684
H	1.761288	-2.892543	0.056385
H	0.157481	-2.773396	-1.941411
H	1.052392	-4.094938	-2.759507
H	0.797683	-2.533056	-3.598613
H	-2.845674	-3.118637	-2.265268
H	-3.428260	-5.384407	-2.721256
H	-4.968598	-5.624331	-3.605218
H	-4.903022	-5.897667	-1.845482

H	-7.036815	-4.167876	-2.521085
H	-8.232946	-0.704578	-1.600504
H	-8.727859	-2.431854	-1.700226
H	-8.431004	-1.496033	-3.188428
H	-5.876553	-0.059220	-1.774204
H	-2.043537	-1.475673	-3.248653
H	-1.200041	-0.210641	-2.312134
H	-1.245391	-0.768818	-5.413107
H	-0.198986	0.376604	-4.512417
H	-1.228320	0.967856	-5.854504
H	-2.422809	2.706917	-4.340530
H	-1.242713	2.202923	-3.086457
H	-2.988801	2.188878	-2.715943
H	-3.797953	-0.744216	-5.057585
H	-3.778795	0.963445	-5.607508
H	-4.542332	0.526122	-4.044363
H	-6.469217	1.478587	1.739110
H	-9.439622	2.806194	1.629652
H	-8.880898	1.161355	2.046316
H	-10.025224	1.412004	0.683941
H	-9.208367	2.527422	-1.454050
H	-6.805958	3.917047	-3.661080
H	-8.410376	3.120642	-3.632684
H	-6.951562	2.202937	-4.122627
H	-4.931019	2.530067	-2.169738
H	-2.813696	2.238583	1.803588
H	-4.497074	2.372136	2.344249
H	-1.986209	4.246475	2.712526
H	-3.570029	4.371546	3.549565
H	-2.929928	5.768982	2.631244
H	-5.755698	4.520588	2.143544
H	-5.662299	4.560489	0.356810
H	-5.018480	5.928337	1.314347
H	-2.837321	5.669249	0.034887
H	-3.356893	4.173810	-0.811496
H	-1.866114	4.172200	0.186303
H	-5.452664	-1.950117	0.619287
H	-8.696021	-2.382297	2.550852
H	-7.684846	-3.138155	1.274193
H	-8.403389	-1.532112	1.002507
H	-7.655495	-0.986938	4.230240
H	-6.469848	1.012515	5.666984
H	-4.696049	0.812186	5.826834
H	-5.804084	-0.494491	6.345242
H	-3.505408	0.192861	3.843617
H	-1.825722	-0.950438	3.058795
H	-1.057519	-1.035656	1.451279
H	-2.814465	-3.032519	4.137119
H	-2.687619	-4.608469	3.291741
H	-3.899642	-3.401351	2.764168
H	-2.954819	-3.390849	0.348195
H	-1.844571	-4.704647	0.867581
H	-1.192716	-3.228970	0.083900
H	0.384498	-2.844335	2.067611
H	-0.253498	-4.317265	2.866734
H	-0.270056	-2.749960	3.734013
H	-0.085495	2.579786	-1.089974

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137
Energy (RI-BP86/def2-SVP) = -2771.687384481 a.u.

P	56.1962328	12.6401255	4.9418447
N	55.0494978	11.4135442	5.2196998
N	57.6015733	11.6711060	4.9592074
C	53.7626626	11.3919056	5.0973678

C	58.8477930	11.9917004	5.0942798
N	52.9890641	10.2766924	5.4713803
N	52.8559789	12.3411941	4.5844607
N	59.4587409	13.1856651	5.5259431
N	59.8903817	11.0997258	4.8007201
C	51.6205737	10.3851708	4.9732957
C	53.5370159	9.0008473	5.8259968
C	51.4697719	11.8986540	4.7507796
C	53.1284125	13.7245707	4.3240779
C	60.9034442	13.0080901	5.7023022
C	58.8104561	14.2603773	6.2221881
C	61.2018197	11.7332304	4.8927443
C	59.7180281	9.8520164	4.1166752
H	50.8869186	9.9866699	5.7038628
H	51.4883017	9.8157161	4.0212785
C	53.4341019	8.5730395	7.1792702
C	54.1120320	8.1625929	4.8303055
H	50.8593474	12.1401288	3.8562888
H	50.9907602	12.3960218	5.6272754
C	53.1562231	14.6618075	5.3967073
C	53.2766894	14.1479201	2.9723036
H	61.1612962	12.8796637	6.7798916
H	61.4646398	13.8905345	5.3312036
C	58.4729963	14.1200329	7.5993674
C	58.6120392	15.4916622	5.5357004
H	61.6122883	11.9739898	3.8829804
H	61.9375386	11.0730161	5.3981896
C	59.6417433	8.6566748	4.8842697
C	59.6852725	9.8206390	2.6948045
C	53.9180923	7.2937965	7.5178093
C	52.8239650	9.4645459	8.2586658
C	54.5892256	6.8957012	5.2220155
C	54.2262040	8.5884413	3.3680967
C	53.3638127	16.0208830	5.0883455
C	52.9479307	14.2444001	6.8521447
C	53.4770068	15.5185662	2.7182247
C	53.2331630	13.1580257	1.8110301
C	57.9182678	15.2313962	8.2640579
C	58.6906011	12.8167638	8.3686330
C	58.0569727	16.5726316	6.2480344
C	58.9803742	15.6596252	4.0636157
C	59.5398275	7.4294031	4.1996159
C	59.6195384	8.6939380	6.4095964
C	59.5874355	8.5674402	2.0574256
C	59.7274614	11.0949216	1.8519743
H	53.8473473	6.9460541	8.5606210
C	54.4924935	6.4598743	6.5499810
H	52.5198993	10.4059880	7.7561636
C	53.8603674	9.8360326	9.3380415
C	51.5640086	8.8329477	8.8850731
H	55.0448617	6.2353255	4.4676527
H	53.7513910	9.5857118	3.2716834
C	55.6993645	8.7495263	2.9446410
C	53.4679867	7.6252567	2.4306599
H	53.3982242	16.7598660	5.9040054
C	53.5232693	16.4492443	3.7645255
H	52.8748697	13.1377976	6.8757818
C	54.1439539	14.6359803	7.7406597
C	51.6273752	14.8124429	7.4157484
H	53.6016409	15.8637541	1.6798247
H	53.0595094	12.1560931	2.2547871
C	52.0686716	13.4550141	0.8444757
C	54.5825834	13.1031071	1.0682019
H	57.6431643	15.1425877	9.3267537
C	57.7126041	16.4477571	7.5997372
H	59.1548212	12.0878831	7.6739307
C	59.6593009	13.0092861	9.5544035
C	57.3558461	12.1993942	8.8325573

H	57.8907818	17.5313002	5.7321602
H	59.3790898	14.6812548	3.7244675
C	57.7416590	15.9767084	3.2025364
C	60.0885669	16.7146550	3.8674063
H	59.4752030	6.4929569	4.7747451
C	59.5188439	7.3811481	2.7994137
H	59.9600535	9.7082141	6.7056978
C	60.5754710	7.6719633	7.0526578
C	58.1754133	8.5287991	6.9298341
H	59.5597923	8.5202231	0.9573458
H	59.8500370	11.9506624	2.5464402
C	58.3945933	11.3169025	1.1089147
C	60.9247028	11.1091557	0.8796433
H	54.8671630	5.4634641	6.8322113
H	54.2118624	8.9399966	9.8916915
H	53.4208504	10.5345309	10.0805677
H	54.7467748	10.3244111	8.8876760
H	50.8036275	8.5851701	8.1163071
H	51.0975842	9.5263620	9.6158607
H	51.8038397	7.8938828	9.4269695
H	56.2225104	9.4761124	3.5970266
H	55.7637315	9.1101920	1.8969272
H	56.2450865	7.7843771	2.9965810
H	53.5059626	7.9910300	1.3833585
H	52.4013234	7.5217591	2.7187279
H	53.9143138	6.6088402	2.4399799
H	53.6820698	17.5167873	3.5461432
H	55.0920731	14.2314896	7.3337132
H	54.0082561	14.2440803	8.7700297
H	54.2528549	15.7380696	7.8166165
H	51.6477735	15.9219374	7.4486736
H	51.4551862	14.4515829	8.4512284
H	50.7528244	14.5170273	6.8004541
H	52.1922208	14.4389428	0.3449717
H	51.0916716	13.4708616	1.3698579
H	52.0149655	12.6843380	0.0474351
H	54.5651525	12.3225901	0.2794138
H	55.4090209	12.8708014	1.7698562
H	54.8164426	14.0706399	0.5759936
H	57.2815761	17.3045208	8.1407991
H	60.6307129	13.4347450	9.2285008
H	59.8607875	12.0399491	10.0558212
H	59.2373228	13.6953803	10.3181569
H	56.8293942	12.8635238	9.5495763
H	57.5332153	11.2300115	9.3423714
H	56.6812985	12.0163218	7.9727233
H	56.9556788	15.2063904	3.3355781
H	58.0145345	16.0164980	2.1272772
H	57.2993704	16.9593705	3.4702958
H	59.7473024	17.7264376	4.1720731
H	60.3886023	16.7741179	2.8003479
H	60.9937837	16.4775549	4.4634265
H	59.4444105	6.4116788	2.2823010
H	60.2570646	6.6259308	6.8601422
H	60.5973811	7.8040142	8.1542754
H	61.6128147	7.7812597	6.6747314
H	57.5051332	9.2978374	6.4975551
H	58.1454760	8.6160190	8.0363420
H	57.7654854	7.5329890	6.6600033
H	58.1919668	10.4991317	0.3858951
H	58.4175848	12.2695612	0.5398703
H	57.5498959	11.3610135	1.8237220
H	61.8881714	10.9709122	1.4119162
H	60.9718376	12.0722258	0.3299573
H	60.8458490	10.3011544	0.1226046

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138
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C     58.654954    15.495389     5.423836
C     58.849964    14.273266     6.126720
C     58.475723    14.140300     7.495232
C     57.877599    15.246949     8.130336
C     57.668663    16.452564     7.447321
C     58.057314    16.573017     6.107367
N     59.499414    13.188977     5.446814
C     58.865943    11.979063     5.089701
N     59.897527    11.046152     4.873366
C     61.218389    11.665534     4.927949
C     60.939779    12.999394     5.643717
C     59.711516     9.796865     4.194567
C     59.635917     8.605376     4.968021
C     59.522201     7.374751     4.291252
C     59.486184     7.319736     2.891594
C     59.552748     8.502075     2.143225
C     59.665590     9.758140     2.772674
C     59.623007     8.654241     6.493111
C     60.544196     7.605180     7.142409
C     59.713615    11.025969     1.919530
C     58.371469    11.269010     1.199915
N     57.621511    11.686450     4.962081
P     56.187991    12.597233     4.747944
N     55.043885    11.434430     5.317943
C     53.775870    11.380141     5.102504
N     52.998703    10.256853     5.440151
C     51.653626    10.343723     4.878634
C     51.496889    11.851115     4.620711
N     52.884515    12.315091     4.533759
C     53.549534     8.986544     5.811656
C     53.434653     8.567882     7.166535
C     53.923475     7.294448     7.519583
C     54.511320     6.456132     6.563566
C     54.618605     6.882262     5.233304
C     54.139524     8.144326     4.828464
C     53.141105    13.718758     4.380045
C     53.124543    14.578411     5.517502
C     53.337502    15.956810     5.312569
C     53.529502    16.479549     4.027764
C     53.509897    15.626816     2.915850
C     53.316667    14.240427     3.065765
C     52.812132     9.465826     8.233038
C     53.854524     9.890548     9.286981
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C     55.749137     8.729168     2.961834
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C     53.959209    14.410647     7.924971
C     53.291297    13.337595     1.834984
C     52.072661    13.638752     0.937649
C     58.706370    12.854249     8.290401
C     59.638794    13.095550     9.496626
C     59.067277    15.655548     3.962500
C     57.847574    15.913939     3.055700
C     51.578673     8.816089     8.891915
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H	59.755338	17.751432	4.059077
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 C   -3.9419130   -2.5420849   -0.6123236
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 C   -3.2223365   -2.1031077    3.0194601
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 C    6.3413932   -0.0330685    0.2617216
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C	-1.1630806	-1.2786706	-2.6224519
C	-0.4822921	-2.6532984	-2.9220936
C	-1.5066589	-3.7658988	-3.2250922
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C	0.4009835	-3.0744548	-1.7342946
C	-1.7760581	2.1093637	-3.6650822
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H	2.8495982	5.4807628	1.9264986
H	4.1886099	-4.6254038	2.1730317
H	4.4827945	-5.9494820	0.0833406
H	5.0500885	-4.8048021	-2.0583241
H	4.4236984	1.5144003	-2.1720738
H	4.2535204	4.0955521	-3.8675506
H	5.0292647	2.5560622	-4.3373711
H	5.7066560	3.5314339	-2.9905348
H	1.9487201	1.3426124	-2.4653464
H	2.8152893	1.2845185	-4.0373305
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H	4.4942436	-0.8547009	2.3195897
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H	3.4030206	-2.2302389	-3.3719435
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H	-3.6925095	0.3355143	3.1397577
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H	0.3511473	-5.3579846	2.6178987
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H	-3.8799996	-4.0447755	5.4384140
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H	-0.3528947	-0.5411171	-2.4643890
H	-1.7001151	-0.9609038	-3.5453353
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H	1.1683675	-2.3075836	-1.5022037
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H	-2.1829135	-3.4845335	-4.0586554
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C	-6.449223	2.575509	1.379942
C	-6.176128	1.648505	0.358181
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C	-7.294397	0.868144	-0.294491
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C	-0.829892	-4.922532	1.834699
C	-2.013038	-4.520602	2.485457
C	-2.414352	-3.175740	2.402331
C	1.198319	-4.440373	0.393102
C	-2.825147	-5.517872	3.283907
C	3.520292	0.547793	-4.086008
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H	2.509785	4.524169	2.744914
H	1.656746	3.767530	1.355834
H	3.902402	0.150005	2.605661
H	4.343996	-1.484025	5.197475
H	4.281984	0.296688	5.056538
H	5.622900	-0.621170	4.293094
H	1.897791	-1.609634	4.161055
H	1.588645	-0.788709	2.598684
H	1.903395	0.178105	4.079759
H	5.521976	-1.841450	-1.358994
H	6.943020	-4.577134	-1.033307
H	7.616913	-2.997431	-0.536715
H	7.301158	-3.337127	-2.270185
H	4.888100	-3.460754	-3.151446
H	3.506994	-3.153118	-2.045970
H	4.433870	-4.681316	-1.924045
H	-3.768019	-1.026401	2.839607
H	-3.515060	0.552248	2.116009
H	-4.185261	0.068550	5.005725
H	-3.949570	1.651768	4.198250
H	-3.021734	1.250375	5.681815
H	-0.794703	1.719217	4.456512
H	-1.739811	2.167105	2.999542
H	-0.462935	0.919152	2.882841
H	-1.162692	-0.478317	5.608088
H	-0.788220	-1.369202	4.098953
H	-2.317545	-1.689895	4.970303
H	0.152408	-1.911495	0.519818
H	-0.508262	-5.975806	1.888876
H	-3.342513	-2.880761	2.910650
H	1.944636	-3.625533	0.324778
H	0.960628	-4.756816	-0.645707
H	1.675432	-5.303788	0.897051
H	-3.842318	-5.138556	3.505947
H	-2.338086	-5.745694	4.257092
H	-2.930139	-6.482323	2.745616
H	-0.648038	0.129610	-2.652798
H	-2.099362	-0.004880	-3.658864
H	0.369487	-2.185477	-5.310929
H	0.693219	-0.622750	-4.497173
H	-0.767957	-0.816591	-5.517939
H	-0.503792	-2.882685	-1.680982
H	0.857574	-1.865676	-2.230484
H	0.511687	-3.420796	-3.061742
H	-2.702425	-2.334089	-4.731826
H	-2.567712	-3.230662	-3.189410
H	-1.510022	-3.662596	-4.567121
H	-3.442661	-2.509428	-0.063331
H	-7.188557	-2.769845	-2.231678
H	-4.089895	-0.079360	-3.598723
H	-6.967745	-3.849830	-0.028548
H	-5.494574	-3.602207	0.970582

```
H     -5.487282    -4.798398    -0.348731
H     -7.579477    -0.557470    -3.839190
H     -6.837388    -1.810924    -4.864851
H     -6.127569    -0.167609    -4.814154
H     -0.543319     2.903229    -0.024503
H     -1.766780     3.902395     0.777498
H     -1.662040     3.742236    -3.561776
H     -2.259936     2.309345    -2.660874
H     -0.519586     2.733078    -2.619176
H     -3.281040     5.303725    -2.389939
H     -3.438565     5.288007    -0.603645
H     -3.998694     3.887030    -1.562494
H      0.279324     4.773096    -1.293231
H     -0.910193     5.832100    -0.465344
H     -0.824820     5.809111    -2.254049
H     -4.629705     0.793324    -0.905048
H     -7.487370     2.709123     1.726417
H     -3.297714     3.740443     1.993544
H     -7.616534     1.354054    -1.241118
H     -8.184883     0.808008     0.362311
H     -6.976952    -0.161032    -0.554443
H     -4.818462     4.747322     3.524002
H     -6.368901     3.904980     3.842932
H     -6.300422     5.214801     2.636601
H      1.365872     1.153762    -1.941112
```

PH_3:

```
4
Energy (RI-BP86/def2-SVP) = -343.0756533945 a.u.
 P    -0.1059128    0.1834483   -0.0748910
 H     0.0712448   -0.1234021    1.3216502
 H     1.2698233   -0.1233952   -0.3733760
 H    -0.5280475   -1.1613956   -0.3733785
```

PH_2:

```
3
Energy (RI-BP86/def2-SVP) = -342.4387987960
 P    -0.0812174    0.0000000   -0.0574237
 H     0.1535756    0.0000000    1.3689498
 H     1.3418564    0.0000000   -0.3115213
```

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[ii] P. Agarwal, N. A. Piro, K. Meyer, P. Muller, C. C. Cummins, *Angew. Chem., Int. Ed.* 2007, **46**, 3111.