

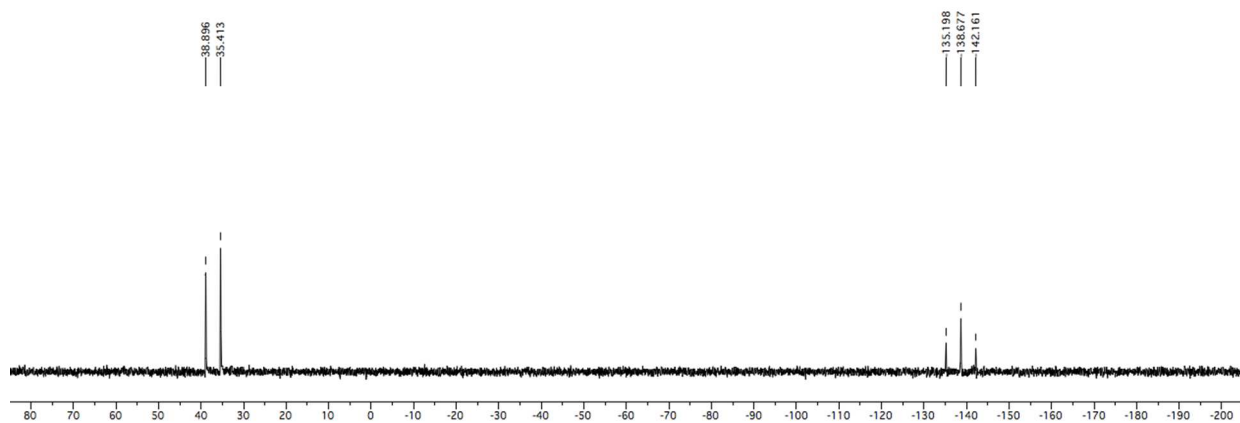
Supplementary Information

Low Valent Chemistry: An Alternative Approach to Phosphorus-Containing Oligomers

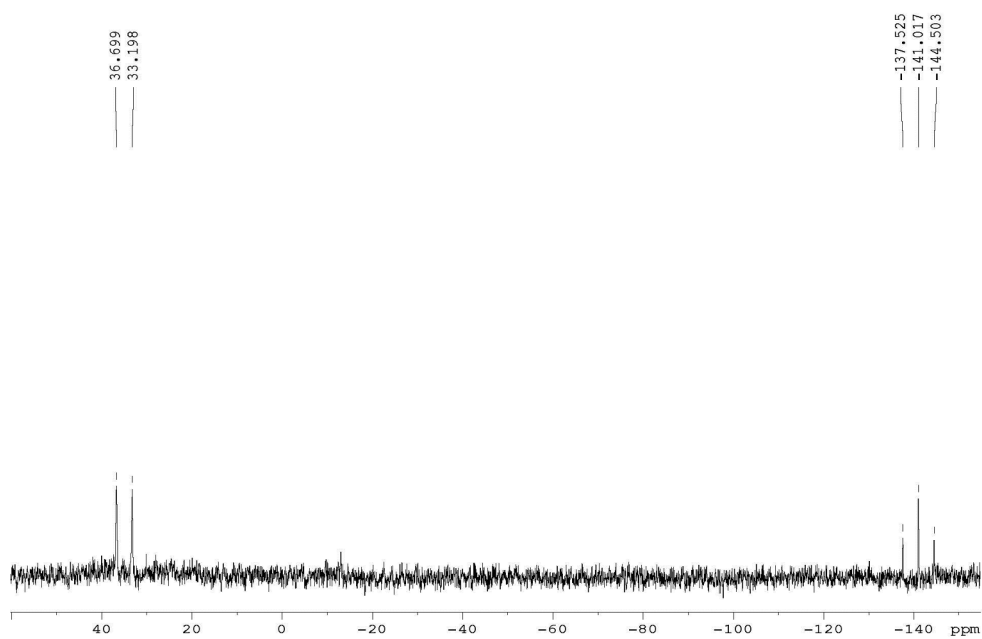
*Stephanie C. Kosnik, Gregory J. Farrar, Erin L. Norton, Benjamin F. T. Cooper, Bobby
D. Ellis and Charles L. B. Macdonald**

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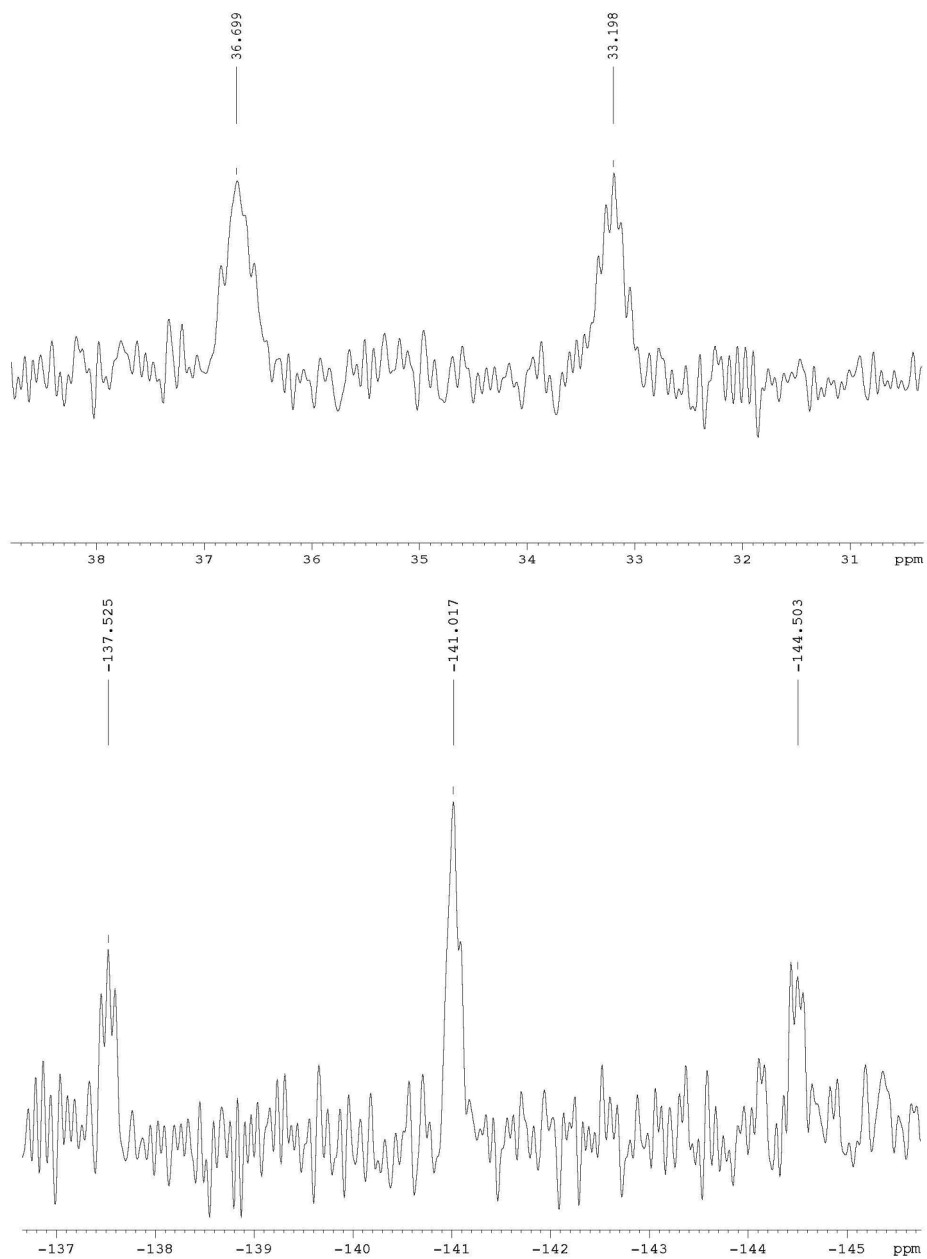
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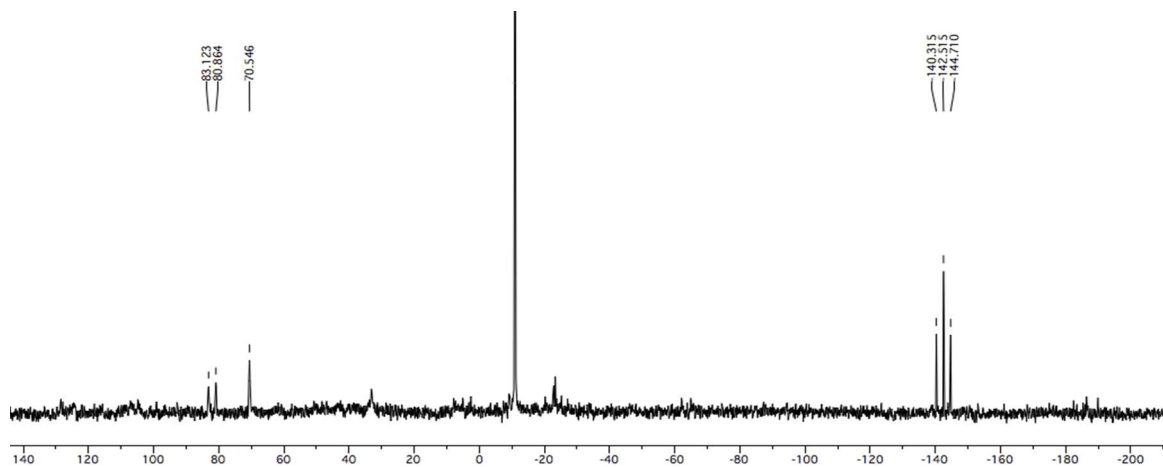
S-1. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 1.



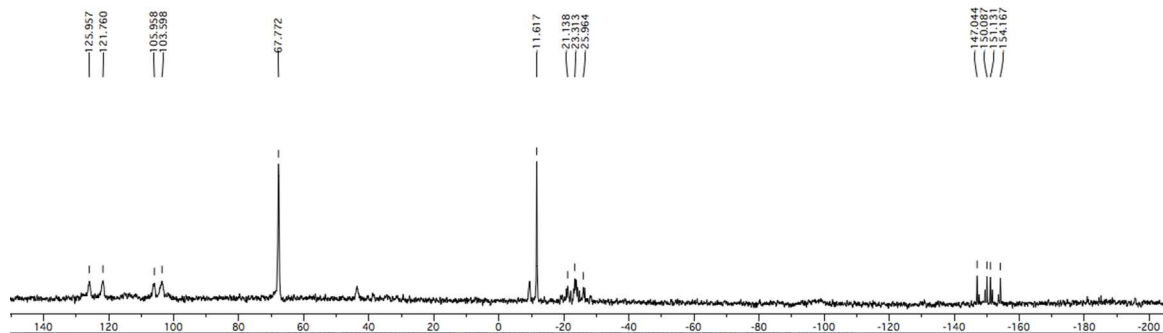
S-2 ^{31}P NMR spectrum of compound 1 obtained at 121.45 MHz.



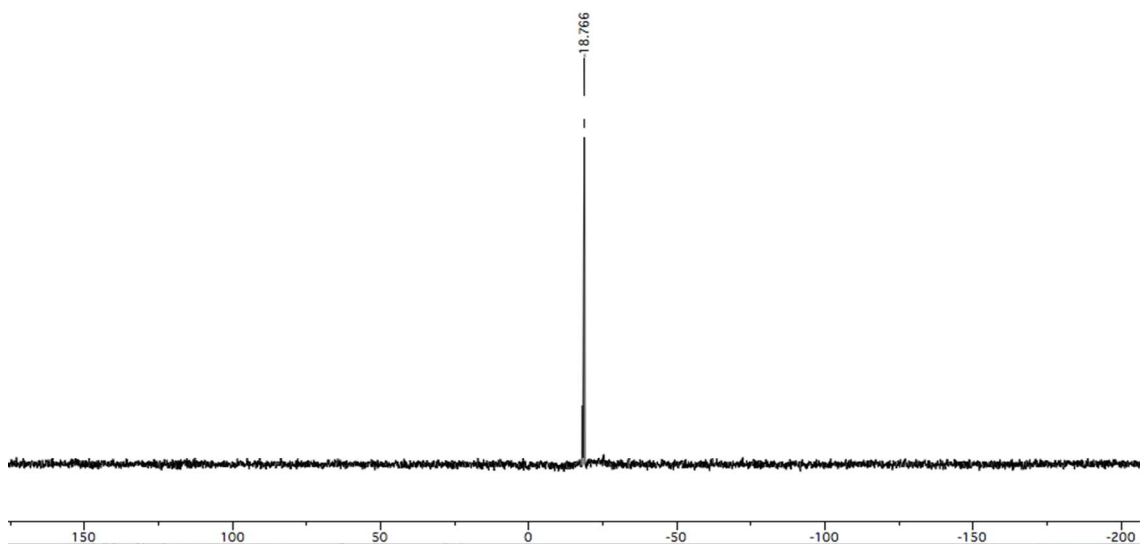
S-3. Enlarged pieces of ^{31}P NMR spectrum of compound 1 on a 300 MHz (^{31}P = 121. MHz) spectrometer



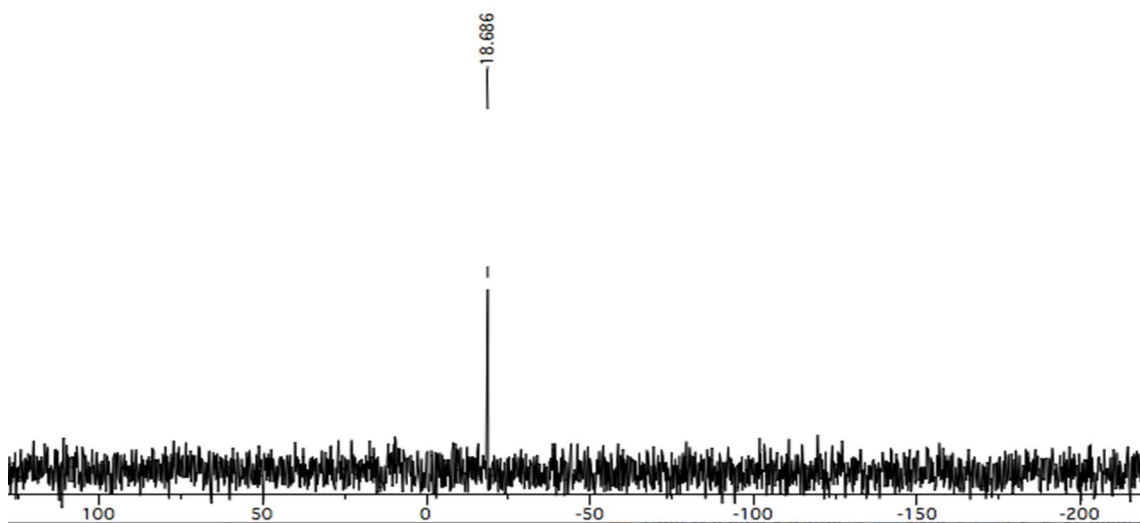
S-4 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of a reaction mixture containing compound 2.



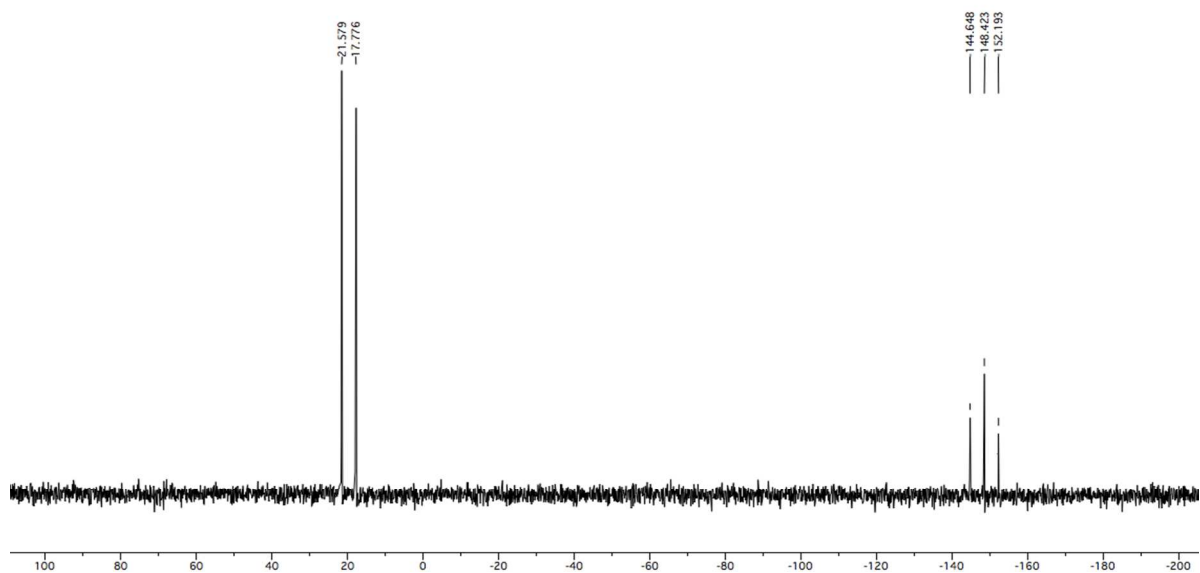
S-5 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 3.



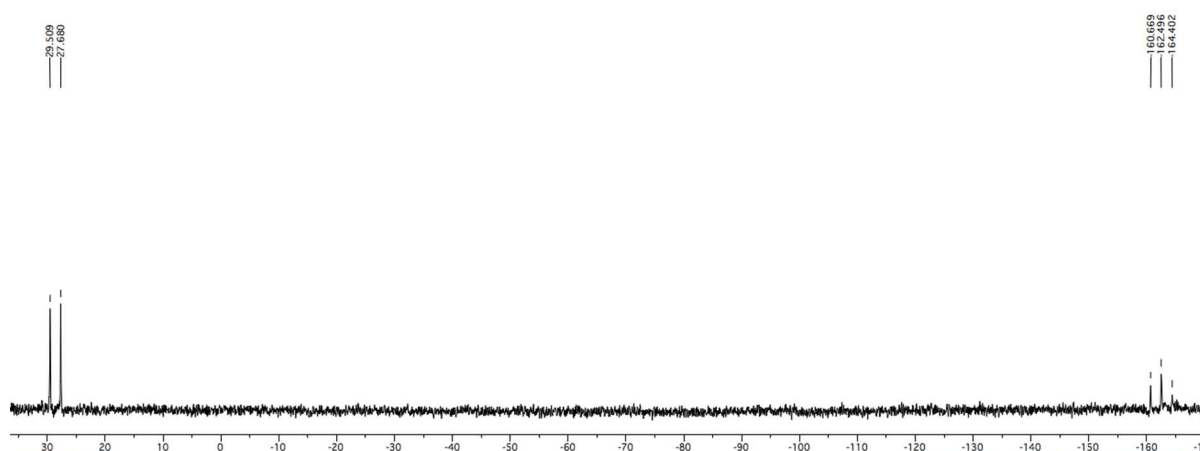
S-6 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 4.



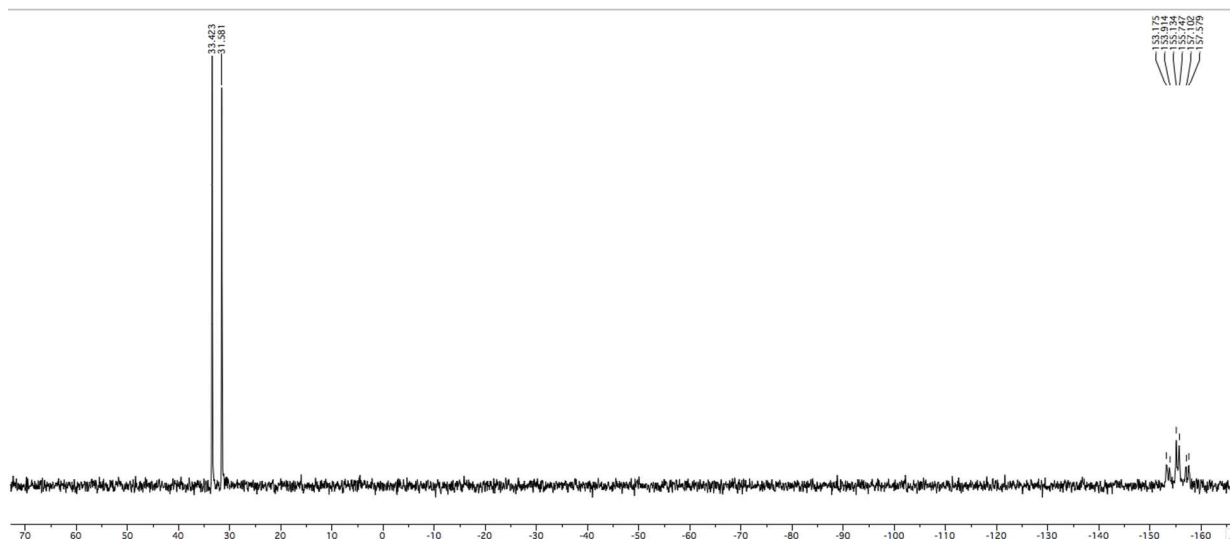
S-7 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 5.



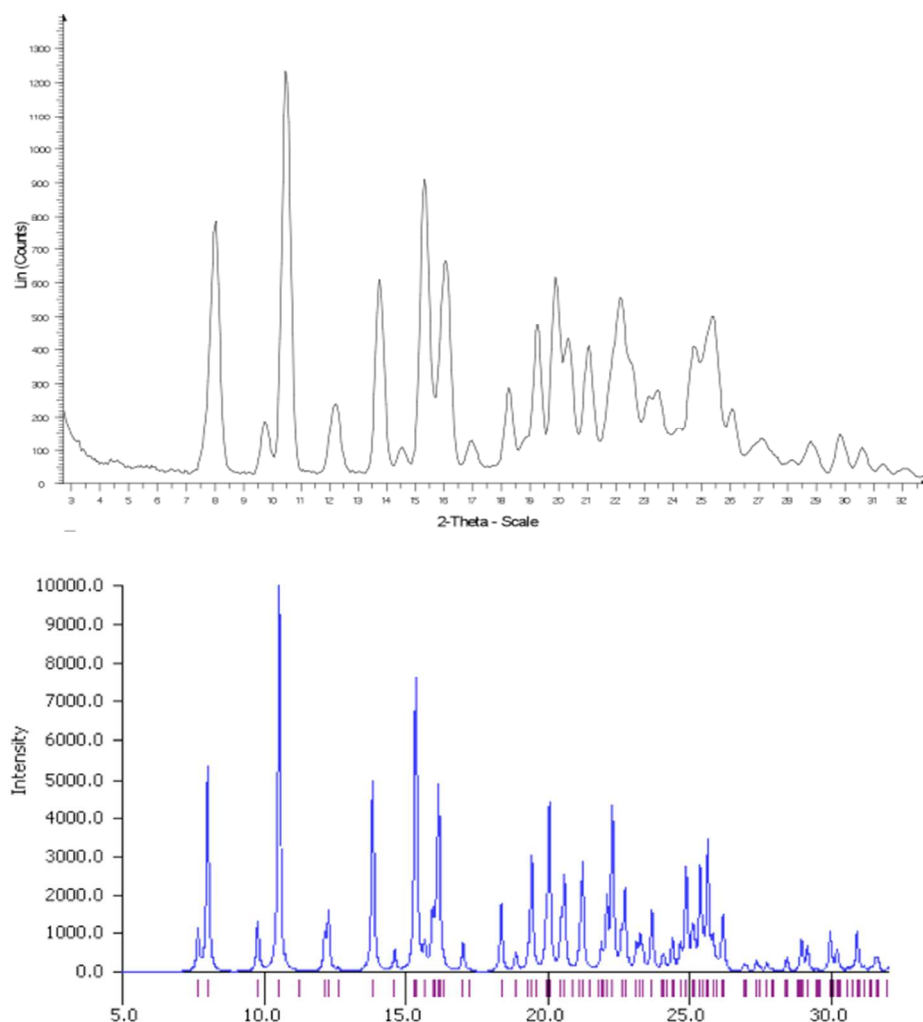
S-8 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound 6.



S-9 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound $1\cdot\text{CuBr}$



S-10 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound $1\bullet\text{AgBr}$



S-11. Powder XRD pattern of compound 6. The simulated pattern, (above) and the experimental, (below).

Table S. 1. Crystal data and structure refinement for the polymorph of compound 6.

Empirical formula	$C_{58}H_{46}P_6 \cdot 0.81(C_4H_8O)$
Formula weight	989.25
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	$a = 12.6149(11)$ Å $\alpha = 86.0290(10)^\circ$.
	$b = 13.2909(12)$ Å $\beta = 74.7350(10)^\circ$.

	c = 17.6210(16) Å γ = 83.9100(10)°.
Volume	2831.4(4) Å ³
Z	2
Density (calculated)	1.160 Mg/m ³
Absorption coefficient	0.228 mm ⁻¹
F(000)	1037
Crystal size	0.20 x 0.10 x 0.05 mm ³
Theta range for data collection	1.199 to 26.437°.
Index ranges	-15<=h<=15, -16<=k<=16, -22<=l<=22
Reflections collected	30110
Independent reflections	11528 [R(int) = 0.0875]
Completeness to theta = 25.242°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.989 and 0.848
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11528 / 0 / 593
Goodness-of-fit on F ²	1.070
Final R indices [I>2sigma(I)]	R1 = 0.1055, wR2 = 0.2217
R indices (all data)	R1 = 0.1481, wR2 = 0.2427
Extinction coefficient	n/a
Largest diff. peak and hole	1.250 and -0.739 e.Å ⁻³

$R_1 = \Sigma(|F_o| - |F_c|) / \Sigma F_o$, $wR2 = [\Sigma(\mathbf{w}(F_o^2 - F_c^2)^2) / \Sigma(\mathbf{w}F_o^4)]^{1/2}$, $GOF = [\Sigma(\mathbf{w}(F_o^2 - F_c^2)^2) / (No. of reflns. - No. of params.)]^{1/2}$.

Computational Investigations

Calculations were performed with the Gaussian 09 suite of programs¹ using Compute Canada's Shared Hierarchical Academic Research Computing Network (SharcNet). Unless indicated otherwise, model complexes were fully optimized with no symmetry constraints using the PBE1PBE density functional theory (DFT) method²⁻⁴ in conjunction with the 6-311G(d,p) basis sets for all atoms.⁵ For the models containing ⁱPr substituents, the GD3 dispersion correction was employed.⁶ Frequency calculations were also performed at the same level of theory in order to confirm that the optimized structures were minima on the potential energy hypersurface and to determine thermochemical information. Geometry optimizations were started using models in which the relevant phosphorus, nitrogen and carbon atoms were placed at the positions found experimentally using X-ray crystallography and the hydrogen atoms were placed in geometrically appropriate positions using Gaussview.⁷ Details of the calculated results, including Cartesian coordinates for all models are presented in the following sections; any readers interested in further information regarding these calculations is encouraged to contact the principal investigator (cmacd@uwindsor.ca).

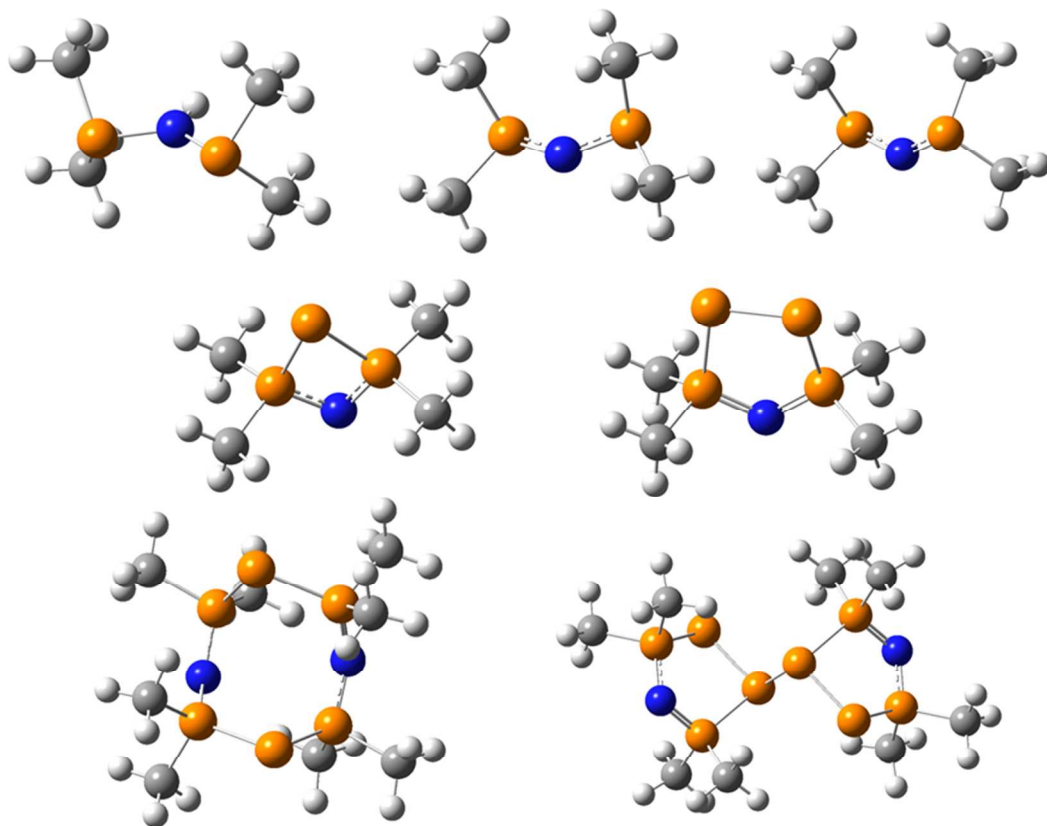


Figure S-10. Gaussview depictions of the optimized geometries for the model compounds bearing Me substituents. Legend: P: orange; N: blue; C: grey; H: white.

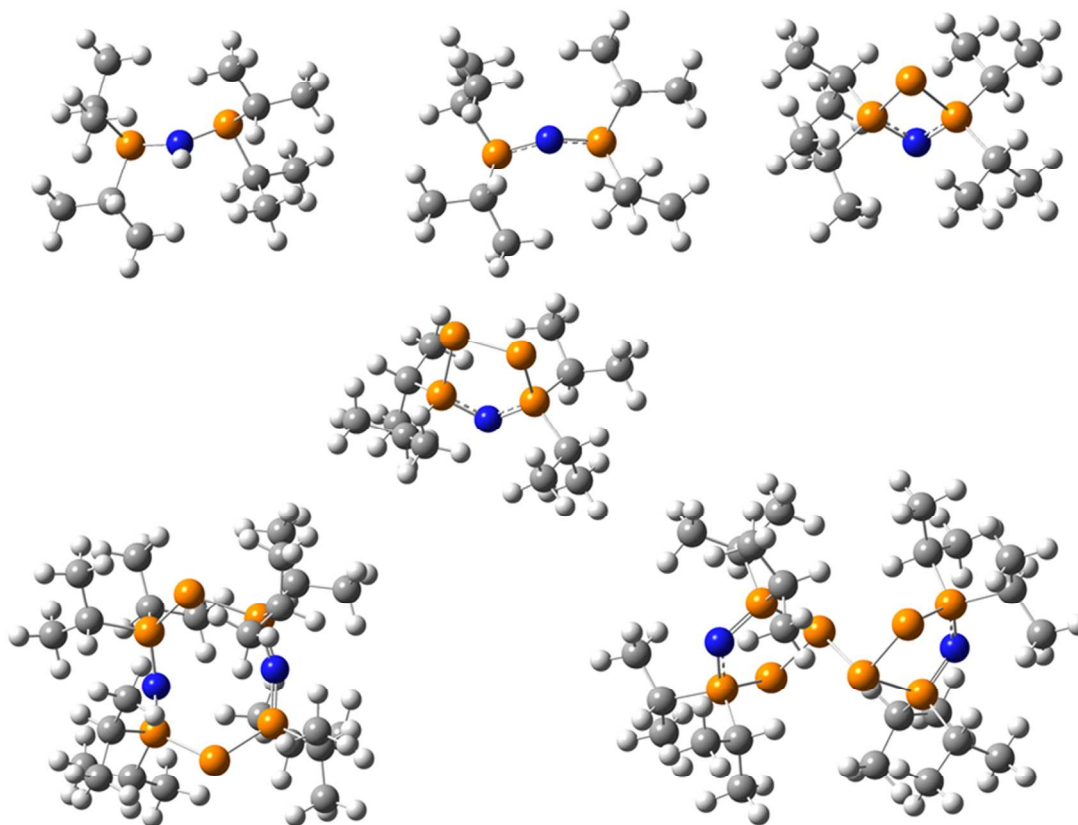


Figure S-11. Gaussview depictions of the optimized geometries for the model compounds bearing ^iPr substituents. Legend: P: orange; N: blue; C: grey; H: white.

Summary of data for Me models:

$\text{HN}(\text{PMe}_2)_2$

1\1\GINC-SAW51\FOpt\RPBE1PBE\6-311G(d,p)\C4H13N1P2\CMACD\28-May-2014\0

\#\ PBE1PBE/6-311G(d,p) scf=tight opt freq pop=(full,nboread) test\Op

timization of $(\text{PMe}_2)_2\text{NH}$ \0,1\ P,1.4720269988,0.9277167061,-0.3502822509

\N,0.0003184478,0.1157490849,0.0010828853\ P,-1.471011669,0.9290397393,

0.3509730252\ C,1.983964591,0.0776039996,-1.9079007185\ H,1.3084726125,0

.3688659255,-2.715397963\ C,2.6322186076,0.0769479916,0.8077177133\ H,2.

3945266318,0.3678769706,1.8334026302\ C,-2.6310946402,0.0796075547,-0.8

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141066857,-1.8136666388\H,-2.3920407707,0.3702863246,-1.8335994258\H,-
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N(PMe₂)₂ radical (cisoid)

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2014\0\# UPBE1PBE/6-311G(d,p) scf=tight opt freq pop=(full,nboread) test

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8119131725,0.600268207\H,8.2185119367,9.4442896925,0.1744729312\H,8.63
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N(PMe₂)₂ radical (transoid)

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32066938\H,-1.3749702305,2.3618527417,0.6321933981\C,-2.7445285652,-1.
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,2.6012784218,-0.3205425377\H,-3.7943471217,-0.9159704428,0.3374633627
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61,1.1429334973\H,-1.391018107,1.0029593006,1.7858492413\H,1.974909445
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H atom

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[(N(PMe₂)₂)P] 4-membered ring zwitterion

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[(N(PMe₂)₂)P₂] 5-membered ring radical

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201
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5905142106,12.463262057,3.8509551626\H,10.7178857333,13.4235717682,3.
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[(N(PMe₂)₂)P]₂ 8-membered ring zwitterion

1\1\GINC-SAW20\FOpt\RPBE1PBE\6-311G(d,p)\C8H24N2P6\CMACD\22-May-
2014\0

\\# PBE1PBE/6-311G(d,p) scf=tight opt freq pop=(full,nboread) test\\Op

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[(N(PMe₂)₂)P₂]₂ bridged two ring zwitterion

1\1\GINC-SAW20\FOpt\RPBE1PBE\6-311G(d,p)\C8H24N2P8\CMACD\22-May-
 2014\0

\# PBE1PBE/6-311G(d,p) scf=tight opt freq pop=(full,nboread) test\Op

timization of [PP(PMe₂)₂N]₂ P-P dimer zwitterion\0,1\P,7.1023154919,9

.3333422953,3.6526404713\P,7.4846995858,10.5937125065,1.8635459195\N,8

.1612735765,11.9859761466,2.3084377234\P,8.8464465939,12.0146355589,3.

7910338618\P,8.8624825229,10.0597994646,4.7179485348\P,5.2881692893,10
 .5200739834,4.392056591\P,4.9057212543,9.2595053119,6.1810160971\N,4.2
 284345233,7.867623719,5.7360712679\P,3.5438334216,7.8390355346,4.25323
 23786\P,3.5280222094,9.7939571958,3.326533315\C,8.5698828278,9.5887857
 482,0.8106073499\H,9.4129593391,9.2417413346,1.4112480628\C,6.03170594
 34,10.9535339626,0.8517483071\H,5.3594361002,11.6075103261,1.406650337
 2\C,10.5695015098,12.5698124399,3.6550767689\H,10.5999463244,13.570747
 9568,3.2181206511\C,8.0237506876,13.3326115595,4.7357474754\H,6.984242
 6807,13.0364767588,4.8890249712\C,6.3589576034,8.8990645554,7.19226831
 63\H,6.8916150389,9.8135445037,7.4553836739\C,3.821155351,10.264532601
 7,7.2344705627\H,2.977928446,10.6117906733,6.6341706016\C,1.8207685335
 ,7.2837480186,4.388524947\H,1.790196886,6.2828198129,4.8254836149\C,4.
 3668610168,6.5211816307,3.3086182512\H,5.4064121282,6.8173224481,3.155
 6539211\H,3.8824297368,6.3848370227,2.3389850994\H,4.3336436701,5.5875
 664163,3.8771343897\H,1.3529253082,7.2675898665,3.4012674652\H,1.28020
 23411,7.9806548895,5.029611444\H,3.4513206735,9.6366327401,8.048998525
 6\H,4.3583310922,11.1244147039,7.6407102988\H,6.0150529421,8.383145993
 8,8.0927786053\H,7.0308205675,8.2449435495,6.6370580932\H,5.4994501521
 ,10.0388638184,0.5885384894\H,6.3757699417,11.4694881911,-0.0486838882
 \H,8.0330282045,8.728754803,0.4042536872\H,8.9398772865,10.2166877585,
 -0.0038461677\H,11.1097324646,11.872891421,3.0137198631\H,11.037797036
 2,12.5859072904,4.6421183206\H,8.0567986068,14.2661632284,4.1671179241
 \H,8.5084594805,13.4690553894,5.7052266073\\Version=EM64L-G09RevD.01\S
 tate=1-A\HF=-3158.3629235\RMSD=3.089e-09\RMSF=5.447e-06\Dipole=0.00042
 64,-0.0003767,-0.0002814\Quadrupole=-5.9500878,-1.1294755,7.0795633,11
 .3209385,-5.6324892,5.8062899\PG=C01 [X(C8H24N2P8)]\\@

Summary of data for ⁱPr models:

HN(PⁱPr₂)₂

1\1\GINC-SAW51\FOpt\RPBE1PBE\6-311G(d,p)\C12H29N1P2\CMACD\28-May-2014\

0\# PBE1PBE/6-311G(d,p) scf=tight EmpiricalDispersion=GD3 opt freq po

p=(full,nboread) test\Optimization of (PiPr2)2NH\0,1\N,-0.1239228125

,0.1210970766,0.169774067\P,-1.6095832022,-0.1511048352,-0.6514067833\

P,1.4029461964,0.1691583806,-0.6287181526\C,-2.5769763366,1.4025669016

, -0.2500087434\H,-3.5929729149,1.1904758707,-0.6088508509\C,-2.6320477

802,1.7708542469,1.2272338795\H,-3.1880839724,2.7035508841,1.372283517

7\H,-1.6240934054,1.9318090816,1.6253989619\H,-3.1186404627,1.00162638

08,1.8336520941\C,-2.0090745854,2.5460788282,-1.0879709237\H,-2.585165

8817,3.464406257,-0.9314284592\H,-2.0264220122,2.3094441126,-2.1553760

482\H,-0.9706690136,2.7519804399,-0.8119405183\C,-2.3901261214,-1.3881

299219,0.5102860377\H,-2.2777020343,-1.009468654,1.5359318081\C,-3.876

5339464,-1.5564730649,0.2081416434\H,-4.3049409279,-2.3466032005,0.833

6353456\H,-4.0354069707,-1.8426791168,-0.8375389988\H,-4.4450230131,-0

.6422528237,0.397047286\C,-1.6546102354,-2.7209052638,0.4053287378\H,-

2.0858578756,-3.4527996306,1.0968135024\H,-0.5939988338,-2.6164657549,

0.6464534479\H,-1.7309170652,-3.1307241683,-0.6073740148\C,2.306983284

2,1.2501676798,0.5987362942\H,2.1648275691,0.8223845268,1.6014186831\C

,3.8021188986,1.3041062484,0.2961249853\H,4.2928110561,2.0326780858,0.

9501589504\H,3.984516025,1.6144831261,-0.7383959512\H,4.2955609115,0.3

424415452,0.4505587931\C,1.7051268825,2.6530156651,0.5811525844\H,2.22

74777719,3.2996591693,1.2945183843\H,0.6457555674,2.6428257578,0.84593

76471\H,1.7984715264,3.1061448815,-0.4116207378\C,2.0644820198,-1.5519

473513,-0.2712575654\H,1.2310155567,-2.1574979857,-0.653378056\C,2.266

8330501,-1.8966388716,1.1977216427\H,2.4761713,-2.9652310889,1.3203523
 546\H,1.3786849703,-1.6696649663,1.7967378268\H,3.1110701698,-1.348865
 2498,1.6277981209\C,3.2868815038,-1.8910397685,-1.1220179665\H,3.51082
 89019,-2.9612471145,-1.0561270274\H,4.1806207829,-1.3529884189,-0.7949
 694042\H,3.1191685254,-1.6464910358,-2.1747341554\H,-0.1300404963,0.10
 43026596,1.1845865014\\Version=EM64L-G09RevD.01\State=1-A\HF=-1211.497
 7082\RMSD=2.297e-09\RMSF=6.999e-06\Dipole=-0.0350545,-0.1028624,0.9993
 205\Quadrupole=3.0173017,0.5609355,-3.5782372,-0.265712,0.0108368,0.19
 77339\PG=C01 [X(C12H29N1P2)]\\@

N(PiPr₂)₂ radical

1\1\GINC-SAW4\FOpt\UPBE1PBE\6-311G(d,p)\C12H28N1P2(2)\CMACD\23-May-
 201

4\0\# UPBE1PBE/6-311G(d,p) scf=tight EmpiricalDispersion=GD3 opt freq

pop=(full,nboread) test\\Optimization of (PiPr₂)₂N radical\\0,2\N,0.2

661987268,0.4889502869,-0.1773908831\P,1.8403774604,0.0973321779,-0.04
 65793539\P,-0.8819267073,1.630828785,-0.0149663966\C,2.1294003101,-1.0
 748857671,-1.4704053343\H,3.1373028044,-1.4757376616,-1.3071329215\C,1
 .1240734233,-2.2198420316,-1.5192635377\H,1.3107206233,-2.8623477145,-
 2.3869521554\H,0.1067951584,-1.8251231096,-1.5993162417\H,1.1701978608
 ,-2.8490286884,-0.625448173\C,2.1432652031,-0.2733982945,-2.7687623056
 \H,2.3212870856,-0.9323479549,-3.6251346406\H,2.923848179,0.4924924705
 ,-2.7594303514\H,1.1861698539,0.2310889461,-2.9256824494\C,1.998064357
 ,-1.0143472876,1.4558285589\H,1.1830014258,-1.745660495,1.3966304942\C
 ,3.3374692725,-1.7464906859,1.44532182\H,3.4638256352,-2.3081340349,2.
 3768554687\H,4.1739172225,-1.0425856911,1.3704684816\H,3.4183728783,-2
 .45818663,0.6202635833\C,1.8349048104,-0.1967964957,2.7310316435\H,1.9
 169480774,-0.843839815,3.6109393198\H,0.8618018563,0.2950371585,2.7725

805906\H,2.6089636366,0.5740049343,2.806417248\C,-2.2622443855,0.96335
 36777,-1.0888302216\H,-2.4763265808,-0.0491611409,-0.725897091\C,-3.52
 38395427,1.8141759639,-0.9843287292\H,-4.2635427329,1.4737788718,-1.71
 64709655\H,-3.3138100989,2.8687243962,-1.1926320872\H,-3.989332105,1.7
 499104057,0.0009583626\C,-1.779183463,0.8717449738,-2.530917716\H,-2.5
 681917,0.4554511929,-3.1664145843\H,-0.9009020384,0.2301874301,-2.6121
 847508\H,-1.5177455223,1.8600098477,-2.9242341859\C,-1.5065266619,1.49
 91555676,1.7482300376\H,-0.557811499,1.5767859111,2.2933423676\C,-2.14
 35547124,0.1548461276,2.0760412417\H,-2.3248518828,0.0624858712,3.1529
 814849\H,-1.4972430296,-0.6717180241,1.7669748809\H,-3.1083852497,0.03
 71691443,1.5722378288\C,-2.362266629,2.686650002,2.182323155\H,-2.5036
 046537,2.6680653476,3.2683289645\H,-3.3553804417,2.6718922988,1.727787
 9392\H,-1.8904476646,3.6380722734,1.9211145243\\Version=EM64L-G09RevD.
 01\State=2-A\HF=-1210.8516174\S2=0.757915\S2-1=0.\S2A=0.750042\RMSD=2.
 962e-09\RMSF=5.661e-06\Dipole=-0.3222882,-0.5871315,0.3140634\Quadrupo
 le=1.3209864,-2.3198759,0.9988895,-3.1352563,0.3373627,0.746884\PG=C01
 [X(C12H28N1P2)]\@

[(N(PⁱPr₂)₂)P] 4-membered ring zwitterion

1\1\GINC-SAW67\FOpt\RPBE1PBE\6-311G(d,p)\C12H28N1P3\CMACD\24-May-
 2014\

0\# PBE1PBE/6-311G(d,p) scf=tight EmpiricalDispersion=GD3 opt freq po

p=(full,nboread) test\\Optimization of P(PiPr₂)₂N zwitterion\\0,1\P,-0

.0581929869,0.0913221843,0.0731635273\P,2.3743086619,0.0396745626,0.09
 74167697\P,1.1975063162,1.8587293104,0.0662537244\N,1.1358678491,-1.04
 87312541,0.1871447645\C,-1.3228008635,-0.0124942544,1.4243039852\C,-1.
 0140461193,-0.1947504043,-1.4771828963\H,-0.2566194702,-0.0056834053,-
 2.2451923013\C,3.5576519543,-0.1311177353,1.503641822\C,3.4035371398,-

0.2461000704,-1.4063735953\H,-2.1287720984,-0.6339317435,1.012783493\H
 ,4.2350133852,0.7278863525,1.4125604515\H,3.8814230826,-1.2194677571,-
 1.2410975641\C,2.5228414406,-0.351512752,-2.6436837676\H,1.7867099298,
 -1.1502702533,-2.5289990526\H,1.9963986001,0.590959579,-2.8250095075\H
 ,3.1381833709,-0.5721466978,-3.5214256254\C,4.4703226311,0.8352584102,
 -1.5514145335\H,5.1675650604,0.8539891219,-0.7091156234\H,5.0558278761
 ,0.6659767929,-2.4602246108\H,4.0062482208,1.823949636,-1.6349564604\C
 ,2.8110015863,-0.0320111344,2.8271783273\H,2.1565255609,-0.8973981472,
 2.9542571557\H,3.5236438724,-0.0137299725,3.657289693\H,2.2009335656,0
 .873550848,2.8726659213\C,4.3530568756,-1.4333278812,1.4174246804\H,5.
 0376251903,-1.4555506956,0.5663092576\H,4.9523109279,-1.5597422702,2.3
 244669174\H,3.6784866599,-2.2922734658,1.3424490823\C,-1.4567993402,-1
 .6523827483,-1.5719357651\H,-2.2497149814,-1.8822658988,-0.8522995954\
 H,-1.8551311683,-1.8571973274,-2.5708986232\H,-0.6186781245,-2.3285634
 062,-1.3857871416\C,-2.1600913676,0.7887127013,-1.6756419913\H,-2.5941
 116809,0.6586142007,-2.6719942601\H,-2.9615823007,0.6249755807,-0.9488
 362606\H,-1.8227894554,1.8263882489,-1.5941718956\C,-1.8777774902,1.37
 01871245,1.7603041022\H,-2.3114636146,1.8755062028,0.8941805391\H,-2.6
 591370174,1.2821897761,2.5219814451\H,-1.0839062219,2.0101303269,2.156
 2873583\C,-0.7506597518,-0.6997200908,2.6563782059\H,-0.2621445029,-1.
 6418085757,2.3998553983\H,-0.0131982104,-0.0582140855,3.1439141348\H,-
 1.5512186813,-0.8969842423,3.3765243048\\Version=EM64L-G09RevD.01\Stat
 e=1-A\HF=-1552.1293326\RMSD=7.440e-09\RMSF=4.998e-06\Dipole=0.0400009,
 -0.5400822,-0.1055436\Quadrupole=9.0280555,-9.7936252,0.7655698,-0.634
 2016,0.155572,0.5426193\PG=C01 [X(C12H28N1P3)]\\@

[(N(PⁱPr₂)₂)P₂] 5-membered ring radical

1\1\GINC-SAW191\FOpt\UPBE1PBE\6-311G(d,p)\C12H28N1P4(2)\CMACD\23-May-2

014\0\# UPBE1PBE/6-311G(d,p) scf=tight EmpiricalDispersion=GD3 opt fr
eq pop=(full,nboread) test\Optimization of P2(PiPr2)2N radical\0,2\P
,2.3756000134,-2.1984428378,-0.1599702804\P,0.3306014949,-2.0837179929
,0.4615781353\P,0.0360434302,0.0332991633,-0.0169420131\P,2.8099168855
, -0.0569803775,-0.0079781557\N,1.4506180818,0.831015654,-0.0769794237\
C,-0.8660601199,0.1851530705,-1.6269504889\H,-0.7467598427,1.24381551,
-1.8907716769\C,-0.2063977265,-0.6746703786,-2.6988952227\H,-0.6284116
885,-0.4311434133,-3.6789617769\H,-0.3805232798,-1.7357399457,-2.50151
13888\H,0.8702354589,-0.5207334177,-2.742649427\C,-2.3475857388,-0.165
8179748,-1.5061454995\H,-2.4744480444,-1.1856700645,-1.1274476502\H,-2
.812036852,-0.126302583,-2.4962300866\H,-2.90157993,0.514993474,-0.856
163375\C,-1.0612725944,0.8730045257,1.2039148155\H,-2.0013463301,0.309
4882194,1.1847469509\C,-0.4800591105,0.8122754023,2.6092449485\H,-1.18
10253141,1.2625414757,3.3187145823\H,0.4552787967,1.3763812271,2.65559
97489\H,-0.2883426661,-0.216242439,2.9250622911\C,-1.3063910229,2.3215
080908,0.7806181415\H,-0.3560323722,2.858380573,0.713054061\H,-1.93024
00883,2.8227922658,1.5271666422\H,-1.8134626872,2.4043014542,-0.183463
4535\C,3.9534929798,0.5136351521,-1.3370249853\H,4.854974812,-0.100331
3832,-1.227378685\C,3.3627081285,0.2774549459,-2.7196291468\H,4.088036
9157,0.5677727431,-3.4858256428\H,2.4659041053,0.8876284151,-2.8561771
239\H,3.1028454118,-0.7724683601,-2.8760459778\C,4.2944138161,1.990689
1906,-1.1381261418\H,3.3813282373,2.5922350599,-1.1578859328\H,4.94581
19543,2.3307398245,-1.9492043068\H,4.8105976179,2.1862418295,-0.195391
6849\C,3.7280712152,0.2792826502,1.5645800519\H,3.6792152394,1.3712701
374,1.6634389317\C,3.0191186537,-0.362416654,2.7516467204\H,3.46091565
2,-0.0004190512,3.6853045253\H,3.1228242433,-1.4502279056,2.7191181127

\H,1.95502614,-0.133826972,2.7659774599\C,5.1829782484,-0.1816834104,1
 .5060779816\H,5.241287089,-1.2533729267,1.2877108668\H,5.653909815,-0.
 0222169758,2.4809301372\H,5.7769017021,0.3546999399,0.7628216919\\Vers
 ion=EM64L-G09RevD.01\State=2-A\HF=-1893.3835028\S2=0.75444\S2-1=0.\S2A
 =0.750013\RMSD=4.312e-09\RMSF=3.718e-06\Dipole=0.0561874,1.7116947,-0.
 1313658\Quadrupole=8.6373147,-10.9284207,2.291106,-0.5829934,0.8045959
 ,0.994426\PG=C01 [X(C12H28N1P4)]\\@

[(N(PⁱPr₂)₂)P]₂ 8-membered ring zwitterion

1\1\GINC-SAW37\FOpt\RPBE1PBE\6-311G(d,p)\C24H56N2P6\CMACD\24-May-2014\

0\\# PBE1PBE/6-311G(d,p) scf=tight EmpiricalDispersion=GD3 opt freq po
 p=(full,nboread) test\\Optimization of [P(PiPr₂)₂N]₂ 8-membered zwitte
 rion Me start\\0,1\C,3.5581255296,-1.1286091288,1.0271550476\P,2.15827
 76909,-0.5423157469,-0.0361936596\C,3.0081759853,0.0107575444,-1.60098
 91697\N,1.4863960731,0.6664616041,0.7957971674\P,1.0725828751,-2.28773
 57699,-0.7018445918\P,0.74305745,2.062916156,0.4630651112\P,-0.8057021
 677,-2.2129303773,0.3241024092\C,1.9228292722,3.180495292,-0.460273087
 5\C,0.5290752655,2.8505296763,2.1258070688\P,-0.9863980401,2.157761962
 3,-0.7943714175\C,-1.6892620119,-3.6521091082,-0.4574787375\C,-0.72001
 60813,-2.7162885654,2.1120393469\N,-1.7354485614,-0.9190063325,0.31967
 75001\P,-2.2401325403,0.4762400198,-0.2611201211\C,-3.53845876,0.93323
 32689,0.9916321471\C,-3.1007341342,0.1958027209,-1.8832791826\H,2.2698
 085538,2.5079095969,-1.2493598944\H,1.5417940792,2.8374427974,2.546474
 0634\H,3.5455743554,0.9188151329,-1.2997692825\H,4.0103039573,-1.93503
 86868,0.4381479135\H,0.0832922696,-3.4599305442,2.1581599303\H,-2.6312
 075536,-3.678310694,0.1036508151\H,-3.7025811935,-0.6976955272,-1.6724
 023224\H,-2.976159164,0.7511511657,1.9158572743\C,4.0207422815,-1.0095

992372,-2.1189201628\H,3.5414079285,-1.975288452,-2.3076210684\H,4.433
7640897,-0.6576652724,-3.0698808557\H,4.8563323388,-1.1668007227,-1.43
31735228\C,1.995558154,0.3523261743,-2.6932524361\H,1.5588794072,-0.56
4995651,-3.0951909539\H,1.1636303163,0.9658868521,-2.3354502435\H,2.49
78092682,0.8849041992,-3.5083008997\C,4.5794200561,-0.0259987839,1.283
2066415\H,4.1186262364,0.7785483031,1.8628890399\H,5.4179395014,-0.421
5702543,1.8653659744\H,4.9878031756,0.4025333054,0.3640704466\C,3.0616
768373,-1.7203787062,2.3376776344\H,2.6106644892,-0.9466338633,2.96404
94245\H,2.3242093887,-2.5070555348,2.161006933\H,3.9012178672,-2.15593
52172,2.8888049794\C,3.1233519584,3.5480629768,0.4077450095\H,3.543926
3275,2.6738281454,0.9090964924\H,3.908415513,3.9885325462,-0.215295466
\H,2.860035507,4.2872112752,1.1698727473\C,1.3234714313,4.3981320254,-
1.1598503945\H,2.1059531511,4.8891799656,-1.7489437353\H,0.5177791072,
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