Extremely bulky secondary phosphinoamines as substituents for sterically hindered aminosilanes.

Tobias Böttcher and Cameron Jones**

School of Chemistry, Monash University, P.O. Box 23, Melbourne, Victoria, 3800, Australia

Supporting Information

(4 pages)

Contents

1. Crystallographic Studies

Table S1: Summary of crystallographic data for compounds **1**, **2**, **2-K**, **3**, **4**, **5**, **6**, **7**, **8**, **9**, **10**, **11** and **12**.

	1	**2**	**2-K**	**3**	**4**
empirical formula	$C_{47}H_{42}NP$	$C_{43}H_{52}N_3P$	$C_{50}H_{59}KN_3P$	$C_{47}H_{60}N_3P$	$C_{42.50}H_{45}N_2P$
formula weight	651.79	641.85	772.07	697.95	614.78
crystal system	monoclinic	monoclinic	monoclinic	triclinic	triclinic
space group	$P2_1/n$	$P2_1$	$P2_1/c$	P-1	P-1
T (K)	123(2)	123(2)	100(2) K	123(2)	100(2) K
a (Å)	9.1571(6)	8.5767(6)	18.506(4)	11.2534(6)	9.931(2)
b (Å)	41.566(3)	18.5068(14)	12.825(3)	12.2272(5)	11.495(2)
c (Å)	9.5665(6)	11.4751(10)	18.632(4)	16.8486(9)	16.176(3)
α (deg)	90	90	90	70.230(4)	92.84(3)
β (deg)	102.692(6)	92.692(7)	97.72(3)	73.735(4)	107.41(3)
γ (deg)	90	90	90	76.194(4)	90.52(3)
V (Å)	3552.3(4)	1819.4(2)	4382.0(15)	2067.62(18)	1759.2(6)
Z	4	2	4	2	2
ρ (calcd) (g cm^{-3})	1.219	1.172	1.170	1.121	1.161
μ mm^{-1}	0.112	0.109	0.194	0.101	0.110
F(000)	1384	692	1656	756	658
reflections collected	17730	8742	50871	18998	12551
independent reflections	6603	5873	9538	7695	6033
R_{int}	0.0406	0.0316	0.0735	0.0314	0.0266
R1 indices [I>2σ(I)][a]	0.0482	0.0414	0.0776	0.0424	0.0625
*w*R2 indices (all data)[b]	0.0930	0.0949	0.2331	0.1030	0.1558
largest peak and hole (eA^{-3})	0.383 and -0.489	0.416 and -0.307	0.964 and -0.746	0.506 and -0.501	1.711 and -0.882
Goodness-of-fit on F^2 [c]	1.034	1.048	1.020	1.026	1.041
CCDC No.	1401422	1401423	1401424	1401425	1401426

	5	**6**	**7**	**8**	**9**
empirical formula	$C_{47}H_{41}Cl_3NPSi$	$C_{47}H_{42}Cl_2NPSi$	$C_{61}H_{55}Cl_5NPSi$	$C_{47}H_{43}NPSi_{0.50}$	$C_{47}H_{41}Cl_5NPSi_2$
formula weight	785.22	750.78	1038.37	666.34	884.21
crystal system	orthorhombic	orthorombic	triclinic	monoclinic	monoclinic
space group	$P2_12_12_1$	$P2_12_12_1$	P-1	$P2_1/c$	$P2_1/c$
T (K)	123(2)	123(2)	100(2)	100(2)	123(2)
a (Å)	10.0456(15)	9.9729(4)	12.6871(18)	21.116(4)	10.1240(8)
b (Å)	13.252(2)	13.3211(6)	13.720(3)	9.7250(19)	20.1891(15)
c (Å)	29.583(7)	29.4129(12)	16.385(2)	18.206(4)	21.6338(19)
α (deg)	90	90	72.602(15)	90	90
β (deg)	90	90	83.732(11)	97.81(3)	92.815(7)

γ (deg)	90	90	80.682(15)	90	90
V (Å)	3938.4(12)	3907.5(3)	2680.1(8)	3704.0(13)	4416.5(6)
Z	4	4	2	4	4
ρ (calcd) (g cm^{-3})	1.324	1.276	1.287	1.195	1.330
μ mm^{-1}	0.339	0.273	0.363	0.124	0.453
F(000)	1640	1576	1084	1414	1832
reflections collected	13854	14488	18171	32355	22407
independent reflections	7047	6782	9836	8787	8219
R_{int}	0.1607	0.0403	0.1050	0.0568	0.0557
R1 indices [I>2σ(I)][a]	0.1039	0.0520	0.0798	0.0594	0.0577
*w*R2 indices (all data)[b]	0.2826	0.1279	0.2279	0.1449	0.1466
largest peak and hole (eA^{-3})	0.897 and -0.776	1.316 and -0.985	0.654 and -0.667	0.375 and -0.353	1.049 and -0.441
Goodness-of-fit on F^2 [c]	1.029	1.041	0.940	1.150	1.021
CCDC No.	1401427	1401428	1401429	1401430	1401431

	10	**11**	**12**
empirical formula	$C_{47}H_{46}NPSi_2$	$C_{54}H_{49}Cl_9NPSi_5$	$C_{101}H_{90}Cl_8N_2P_2Si_5$
formula weight	712.00	1202.41	1817.74
crystal system	monoclinic	triclinic	monoclinic
space group	$P2_1/c$	P-1	$P2_1/n$
T (K)	100(2)	100(2)	100(2)
a (Å)	13.977(3)	10.470(2)	17.441(4)
b (Å)	9.827(2)	16.168(3)	23.780(5)
c (Å)	29.607(6)	18.415(4)	23.866(5)
α (deg)	90	108.85(3)	90
β (deg)	102.56(3)	90.82(3)	93.20(3)
γ (deg)	90	99.88(3)	90
V (Å)	3969.3(14)	2898.3(10)	9883(3)
Z	4	2	4
ρ (calcd) (g cm^{-3})	1.191	1.378	1.222
μ mm^{-1}	0.163	0.603	0.366
F(000)	1512	1236	3784
reflections collected	29006	18549	39379
independent reflections	7305	9364	10481
R_{int}	0.0775	0.0458	0.1434
R1 indices [I>2σ(I)][a]	0.0488	0.0478	0.1007
*w*R2 indices (all data)[b]	0.1310	0.1311	0.3063
largest peak and hole (eA^{-3})	0.338 and -0.735	0.809 and -0.436	0.759 and -0.324
Goodness-of-fit on F^2 [c]	1.047	1.029	1.051

CCDC No.	1401432	1401433	1401434

[a]$R1 = \Sigma||F_0| - |F_c||/\Sigma |F_0|$. [b]$wR2 = [\Sigma\{w(F_0^2 - F_e^2)^2\}/ \Sigma w(F_0^2)^2]^{1/2}$, $w = 1/[\sigma^2F_0^2 + (aP)^2 + bP]$ (a and b are constants suggested by the refinement program; $P = [\max(F_0^2,0) + 2F_e^2]/3$). [c]$GOF = [\Sigma w(F_0^2 - F_e^2)^2/(N_{obs} - N_{params})]^{1/2}$.

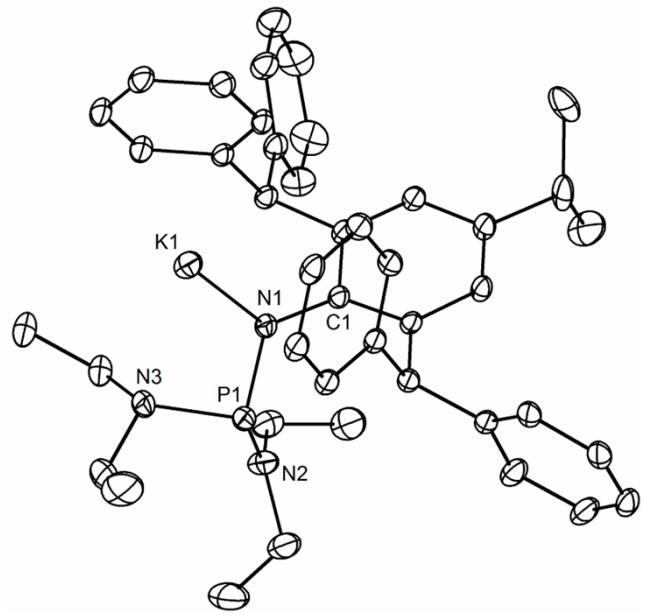

Fig. S1. Molecular structure **2-K**. (25% displacement ellipsoids are shown; C–H hydrogen atoms omitted). See main text for structural parameters.