Synthesis and structures of complexes demonstrating the coordinative versatility of the 2,4-diimino-3-phosphinopentane anion

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Supporting Information Package

Figure S1: Solid state structure of **5AlCl$_2$**. Ellipsoids are 50% probability, hydrogen atoms are removed for clarity and the full numbering scheme is highlighted.

Table S1: Crystal data and structure refinement for **5AlCl$_2$**.

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **5Al**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S3: Bond lengths [Å] and angles [°] for **5AlCl$_2$**.

Table S4: Anisotropic displacement parameters (Å^{2}x 10^3)for **5AlCl$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table S5: Torsion angles [°] for **5AlCl$_2$**.

Figure S2: Solid state structure of **5Li**. Ellipsoids are 50% probability, hydrogen atoms and toluene solvate are removed for clarity. Numbering scheme of core atoms is included.

Table S6: Crystal data and structure refinement for **5Li**.

Table S7: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **5Li**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S8: Bond lengths [Å] and angles [°] for **5Li**.

Table S9: Anisotropic displacement parameters (Å^{2}x 10^3)for **5Li**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Figure S3: Solid State Structure of **6Sb**. Ellipsoids are 50% probability, hydrogen atoms are removed for clarity. This highlights the complete numbering scheme and includes the *n*-pentane solvate.

Table S10: Crystal data and structure refinement for **6Sb**.

Table S11: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **6Sb**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S12: Bond lengths [Å] and angles [°] for **6Sb**.

Table S13: Anisotropic displacement parameters (Å^{2}x 10^3)for **6Sb**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

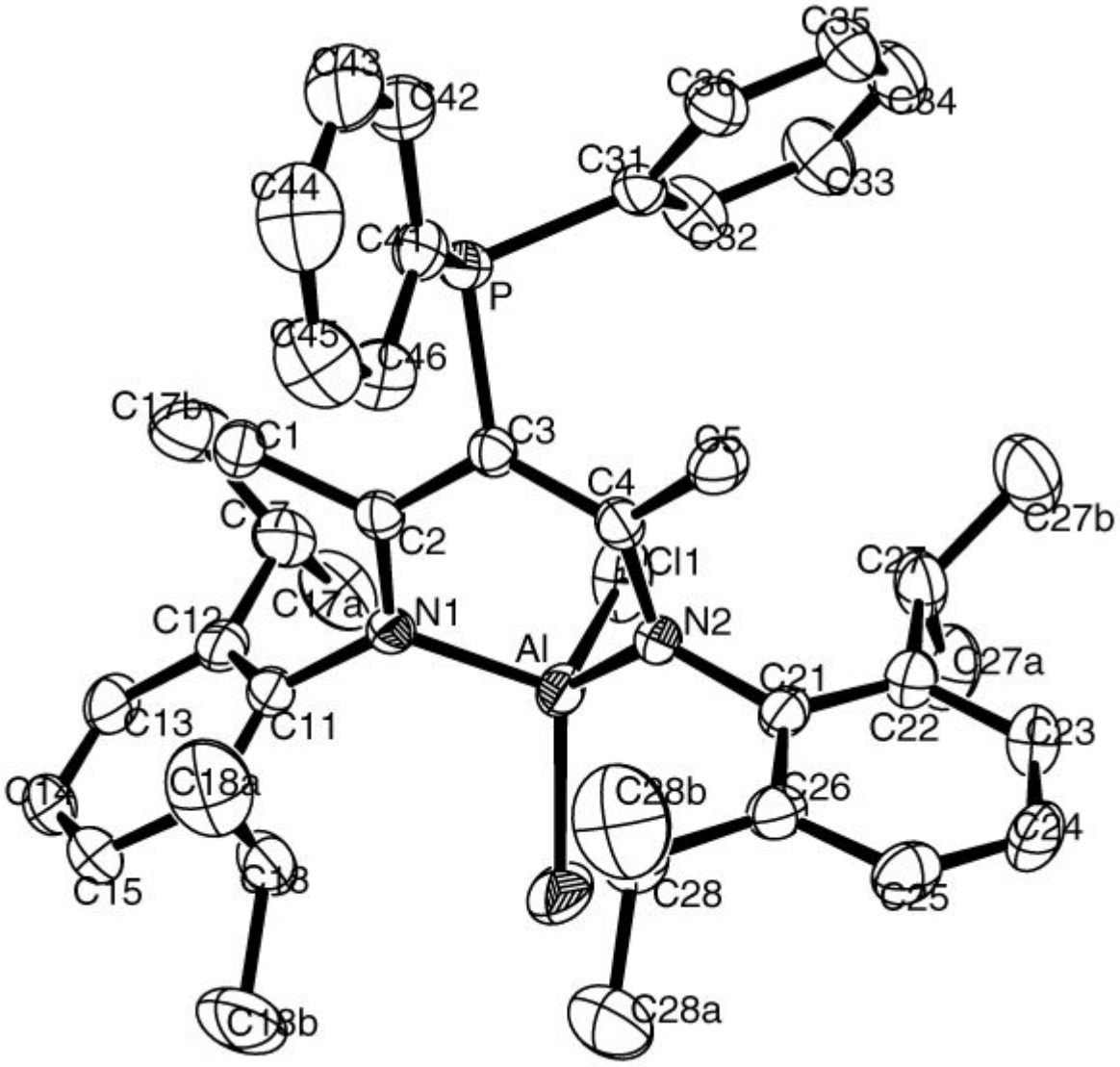

Figure S1: Solid state structure of **5AlCl$_2$**. Ellipsoids are 50% probability, hydrogen atoms are removed for clarity and the full numbering scheme is highlighted.

Table S1. Crystal data and structure refinement for **5AlCl$_2$**.

Identification code	dal0386	
Empirical formula	C41 H50 Al Cl2 N2 P	
Formula weight	699.68	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 18.3867(11) Å	α= 90°.
	b = 20.2465(12) Å	β= 90°.
	c = 21.2320(13) Å	γ = 90°.
Volume	7904.0(8) Å^3	
Z	8	
Density (calculated)	1.176 Mg/m^3	
Absorption coefficient	0.257 mm^{-1}	
F(000)	2976	
Crystal size	0.32 x 0.16 x 0.13 mm^3	
Theta range for data collection	1.78 to 26.49°.	
Index ranges	-22<=h<=23, -25<=k<=25, -26<=l<=26	
Reflections collected	48531	
Independent reflections	8131 [R(int) = 0.1194]	
Completeness to theta = 26.49°	99.4 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9674 and 0.9223	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8131 / 0 / 424	
Goodness-of-fit on F^2	1.007	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1175	
R indices (all data)	R1 = 0.1092, wR2 = 0.1380	
Largest diff. peak and hole	0.476 and -0.474 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5AlCl$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	7423(1)	1833(1)	6205(1)	53(1)
Cl(2)	7080(1)	763(1)	7468(1)	61(1)
P	4781(1)	2226(1)	5401(1)	25(1)
Al	6620(1)	1352(1)	6758(1)	29(1)
N(1)	6027(1)	858(1)	6227(1)	25(1)
N(2)	5927(1)	1960(1)	7035(1)	24(1)
C(1)	5128(2)	808(1)	5377(1)	33(1)
C(2)	5511(2)	1172(1)	5903(1)	24(1)
C(3)	5276(1)	1825(1)	6043(1)	24(1)
C(4)	5403(2)	2147(1)	6635(1)	25(1)
C(5)	4921(2)	2712(1)	6827(1)	33(1)
C(11)	6170(2)	162(1)	6092(1)	29(1)
C(12)	6621(2)	-17(1)	5592(1)	33(1)
C(13)	6730(2)	-691(2)	5479(2)	42(1)
C(14)	6407(2)	-1157(2)	5852(2)	48(1)
C(15)	5974(2)	-975(2)	6348(2)	46(1)
C(16)	5855(2)	-315(1)	6489(1)	35(1)
C(17)	6995(2)	481(2)	5165(2)	40(1)
C(17A)	7816(2)	461(2)	5264(2)	64(1)
C(17B)	6814(3)	373(2)	4469(2)	68(1)
C(18)	5378(2)	-124(2)	7046(2)	47(1)
C(18A)	4591(2)	-29(2)	6856(2)	71(1)
C(18B)	5436(3)	-614(2)	7587(2)	82(2)
C(21)	5945(2)	2288(1)	7651(1)	27(1)
C(22)	6373(2)	2853(1)	7735(1)	34(1)
C(23)	6324(2)	3181(2)	8308(2)	44(1)
C(24)	5870(2)	2963(2)	8780(2)	44(1)
C(25)	5466(2)	2403(2)	8695(1)	38(1)
C(26)	5501(2)	2046(1)	8135(1)	31(1)
C(27)	6898(2)	3118(2)	7239(2)	42(1)
C(27A)	7679(2)	2972(2)	7436(2)	60(1)

C(27B)	6795(2)	3855(2)	7109(2)	64(1)
C(28)	5044(2)	1425(2)	8077(2)	41(1)
C(28A)	5274(2)	917(2)	8570(2)	70(1)
C(28B)	4237(2)	1562(2)	8126(2)	78(1)
C(31)	5041(2)	3096(1)	5477(1)	28(1)
C(32)	5775(2)	3236(2)	5423(2)	40(1)
C(33)	6027(2)	3878(2)	5460(2)	50(1)
C(34)	5543(2)	4390(2)	5534(2)	47(1)
C(35)	4815(2)	4265(2)	5578(2)	42(1)
C(36)	4556(2)	3619(1)	5548(1)	35(1)
C(41)	3818(2)	2176(1)	5617(1)	28(1)
C(42)	3296(2)	2484(2)	5243(2)	39(1)
C(43)	2565(2)	2381(2)	5350(2)	50(1)
C(44)	2347(2)	1957(2)	5815(2)	59(1)
C(45)	2846(2)	1640(2)	6180(2)	53(1)
C(46)	3580(2)	1754(2)	6086(1)	40(1)

Table S3. Bond lengths [Å] and angles [°] for **5AlCl$_2$**.

Cl(1)-Al	2.1228(12)
Cl(2)-Al	2.1007(12)
P-C(3)	1.830(3)
P-C(41)	1.831(3)
P-C(31)	1.831(3)
Al-N(1)	1.861(2)
Al-N(2)	1.867(2)
N(1)-C(2)	1.334(3)
N(1)-C(11)	1.462(3)
N(2)-C(4)	1.339(3)
N(2)-C(21)	1.467(3)
C(1)-C(2)	1.511(4)
C(2)-C(3)	1.423(4)
C(3)-C(4)	1.433(4)
C(4)-C(5)	1.503(4)
C(11)-C(12)	1.394(4)
C(11)-C(16)	1.408(4)
C(12)-C(13)	1.400(4)
C(12)-C(17)	1.521(4)
C(13)-C(14)	1.367(5)
C(14)-C(15)	1.371(5)
C(15)-C(16)	1.386(4)
C(16)-C(18)	1.522(4)
C(17)-C(17A)	1.526(5)
C(17)-C(17B)	1.530(5)
C(18)-C(18A)	1.514(5)
C(18)-C(18B)	1.521(5)
C(21)-C(22)	1.399(4)
C(21)-C(26)	1.403(4)
C(22)-C(23)	1.390(4)
C(22)-C(27)	1.525(4)
C(23)-C(24)	1.376(5)
C(24)-C(25)	1.368(4)
C(25)-C(26)	1.393(4)

C(26)-C(28)	1.516(4)
C(27)-C(27A)	1.525(5)
C(27)-C(27B)	1.529(4)
C(28)-C(28B)	1.513(5)
C(28)-C(28A)	1.527(5)
C(31)-C(32)	1.383(4)
C(31)-C(36)	1.394(4)
C(32)-C(33)	1.383(4)
C(33)-C(34)	1.374(5)
C(34)-C(35)	1.365(5)
C(35)-C(36)	1.393(4)
C(41)-C(46)	1.384(4)
C(41)-C(42)	1.393(4)
C(42)-C(43)	1.378(4)
C(43)-C(44)	1.369(5)
C(44)-C(45)	1.361(5)
C(45)-C(46)	1.383(4)

C(3)-P-C(41)	105.68(12)
C(3)-P-C(31)	103.36(12)
C(41)-P-C(31)	106.50(13)
N(1)-Al-N(2)	98.32(10)
N(1)-Al-Cl(2)	111.43(8)
N(2)-Al-Cl(2)	115.08(8)
N(1)-Al-Cl(1)	108.61(8)
N(2)-Al-Cl(1)	110.26(8)
Cl(2)-Al-Cl(1)	112.21(6)
C(2)-N(1)-C(11)	119.2(2)
C(2)-N(1)-Al	118.22(18)
C(11)-N(1)-Al	122.09(17)
C(4)-N(2)-C(21)	117.0(2)
C(4)-N(2)-Al	118.60(18)
C(21)-N(2)-Al	124.23(17)
N(1)-C(2)-C(3)	123.5(2)
N(1)-C(2)-C(1)	118.7(2)
C(3)-C(2)-C(1)	117.8(2)

C(2)-C(3)-C(4)	123.9(2)
C(2)-C(3)-P	114.02(19)
C(4)-C(3)-P	122.1(2)
N(2)-C(4)-C(3)	122.9(2)
N(2)-C(4)-C(5)	117.8(2)
C(3)-C(4)-C(5)	119.2(2)
C(12)-C(11)-C(16)	121.5(3)
C(12)-C(11)-N(1)	120.5(3)
C(16)-C(11)-N(1)	118.0(2)
C(11)-C(12)-C(13)	118.0(3)
C(11)-C(12)-C(17)	123.4(3)
C(13)-C(12)-C(17)	118.7(3)
C(14)-C(13)-C(12)	120.8(3)
C(13)-C(14)-C(15)	120.7(3)
C(14)-C(15)-C(16)	121.2(3)
C(15)-C(16)-C(11)	117.8(3)
C(15)-C(16)-C(18)	120.3(3)
C(11)-C(16)-C(18)	121.9(3)
C(12)-C(17)-C(17A)	110.3(3)
C(12)-C(17)-C(17B)	112.5(3)
C(17A)-C(17)-C(17B)	110.1(3)
C(18A)-C(18)-C(18B)	110.5(3)
C(18A)-C(18)-C(16)	112.0(3)
C(18B)-C(18)-C(16)	112.4(3)
C(22)-C(21)-C(26)	121.3(3)
C(22)-C(21)-N(2)	119.8(2)
C(26)-C(21)-N(2)	118.8(2)
C(23)-C(22)-C(21)	117.7(3)
C(23)-C(22)-C(27)	118.6(3)
C(21)-C(22)-C(27)	123.7(3)
C(24)-C(23)-C(22)	121.7(3)
C(25)-C(24)-C(23)	119.9(3)
C(24)-C(25)-C(26)	121.3(3)
C(25)-C(26)-C(21)	118.1(3)
C(25)-C(26)-C(28)	118.4(3)
C(21)-C(26)-C(28)	123.5(3)

C(22)-C(27)-C(27A)	109.8(3)
C(22)-C(27)-C(27B)	113.0(3)
C(27A)-C(27)-C(27B)	110.7(3)
C(28B)-C(28)-C(26)	112.7(3)
C(28B)-C(28)-C(28A)	110.2(3)
C(26)-C(28)-C(28A)	110.5(3)
C(32)-C(31)-C(36)	118.5(3)
C(32)-C(31)-P	116.4(2)
C(36)-C(31)-P	125.0(2)
C(31)-C(32)-C(33)	121.0(3)
C(34)-C(33)-C(32)	119.9(3)
C(35)-C(34)-C(33)	120.2(3)
C(34)-C(35)-C(36)	120.4(3)
C(35)-C(36)-C(31)	120.0(3)
C(46)-C(41)-C(42)	117.9(3)
C(46)-C(41)-P	121.3(2)
C(42)-C(41)-P	120.0(2)
C(43)-C(42)-C(41)	120.7(3)
C(44)-C(43)-C(42)	119.9(3)
C(45)-C(44)-C(43)	120.6(3)
C(44)-C(45)-C(46)	119.8(3)
C(45)-C(46)-C(41)	121.0(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for **5AlCl$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	37(1)	59(1)	63(1)	-20(1)	15(1)	-13(1)
Cl(2)	85(1)	48(1)	49(1)	-5(1)	-36(1)	20(1)
P	28(1)	26(1)	23(1)	1(1)	0(1)	4(1)
Al	30(1)	29(1)	28(1)	-5(1)	-6(1)	5(1)
N(1)	30(1)	22(1)	23(1)	0(1)	-2(1)	4(1)
N(2)	29(1)	23(1)	21(1)	-1(1)	0(1)	1(1)
C(1)	35(2)	28(2)	35(2)	-4(1)	-8(1)	1(1)
C(2)	28(2)	23(1)	22(1)	1(1)	4(1)	-3(1)
C(3)	27(2)	22(1)	23(1)	0(1)	2(1)	-1(1)
C(4)	29(2)	21(1)	26(2)	0(1)	2(1)	-2(1)
C(5)	37(2)	35(2)	26(2)	-3(1)	-1(1)	8(1)
C(11)	34(2)	23(2)	30(2)	-2(1)	-8(1)	4(1)
C(12)	37(2)	30(2)	33(2)	-3(1)	-9(1)	9(1)
C(13)	56(2)	33(2)	38(2)	-13(2)	-9(2)	16(2)
C(14)	75(3)	21(2)	49(2)	-6(2)	-15(2)	10(2)
C(15)	69(2)	24(2)	43(2)	3(1)	-11(2)	-3(2)
C(16)	50(2)	23(2)	33(2)	-1(1)	-7(1)	-3(1)
C(17)	47(2)	34(2)	38(2)	-2(1)	8(2)	15(2)
C(17A)	52(2)	51(2)	88(3)	1(2)	21(2)	14(2)
C(17B)	106(4)	59(2)	38(2)	3(2)	10(2)	27(2)
C(18)	74(3)	29(2)	39(2)	1(2)	7(2)	-10(2)
C(18A)	74(3)	68(3)	70(3)	-5(2)	26(2)	-11(2)
C(18B)	148(5)	50(2)	47(2)	17(2)	20(3)	-7(3)
C(21)	30(2)	28(2)	23(1)	-3(1)	-3(1)	5(1)
C(22)	40(2)	31(2)	30(2)	-5(1)	-2(1)	2(1)
C(23)	54(2)	35(2)	41(2)	-11(2)	-4(2)	-3(2)
C(24)	58(2)	44(2)	29(2)	-13(2)	-3(2)	6(2)
C(25)	42(2)	45(2)	27(2)	-2(1)	5(1)	10(2)
C(26)	33(2)	33(2)	26(2)	0(1)	-2(1)	5(1)
C(27)	49(2)	32(2)	43(2)	-6(2)	5(2)	-11(2)
C(27A)	51(2)	67(3)	62(2)	-11(2)	8(2)	-19(2)

C(27B)	92(3)	40(2)	59(3)	0(2)	17(2)	-13(2)
C(28)	47(2)	44(2)	33(2)	0(2)	11(2)	-8(2)
C(28A)	103(4)	48(2)	59(3)	14(2)	7(2)	-11(2)
C(28B)	48(3)	85(3)	102(4)	-3(3)	13(2)	-20(2)
C(31)	34(2)	26(2)	24(2)	2(1)	2(1)	1(1)
C(32)	38(2)	32(2)	51(2)	4(2)	13(2)	3(1)
C(33)	40(2)	41(2)	69(3)	7(2)	11(2)	-10(2)
C(34)	58(2)	29(2)	54(2)	4(2)	4(2)	-10(2)
C(35)	53(2)	27(2)	46(2)	0(1)	-2(2)	7(2)
C(36)	35(2)	31(2)	40(2)	2(1)	-3(1)	4(1)
C(41)	27(2)	29(2)	28(2)	-4(1)	2(1)	1(1)
C(42)	37(2)	37(2)	42(2)	-1(1)	-7(1)	4(2)
C(43)	31(2)	52(2)	68(3)	-8(2)	-10(2)	6(2)
C(44)	31(2)	65(3)	79(3)	-12(2)	14(2)	-6(2)
C(45)	47(2)	53(2)	57(2)	4(2)	21(2)	-6(2)
C(46)	38(2)	43(2)	38(2)	1(2)	5(1)	0(2)

Table S5. Torsion angles [°] for **5AlCl$_2$**.

N(2)-Al-N(1)-C(2)	35.9(2)
Cl(2)-Al-N(1)-C(2)	157.07(18)
Cl(1)-Al-N(1)-C(2)	-78.8(2)
N(2)-Al-N(1)-C(11)	-152.5(2)
Cl(2)-Al-N(1)-C(11)	-31.3(2)
Cl(1)-Al-N(1)-C(11)	92.8(2)
N(1)-Al-N(2)-C(4)	-33.6(2)
Cl(2)-Al-N(2)-C(4)	-152.08(18)
Cl(1)-Al-N(2)-C(4)	79.8(2)
N(1)-Al-N(2)-C(21)	151.1(2)
Cl(2)-Al-N(2)-C(21)	32.7(2)
Cl(1)-Al-N(2)-C(21)	-95.5(2)
C(11)-N(1)-C(2)-C(3)	172.9(2)
Al-N(1)-C(2)-C(3)	-15.2(3)
C(11)-N(1)-C(2)-C(1)	-3.9(4)
Al-N(1)-C(2)-C(1)	167.95(19)
N(1)-C(2)-C(3)-C(4)	-18.3(4)
C(1)-C(2)-C(3)-C(4)	158.6(3)
N(1)-C(2)-C(3)-P	162.4(2)
C(1)-C(2)-C(3)-P	-20.8(3)
C(41)-P-C(3)-C(2)	102.1(2)
C(31)-P-C(3)-C(2)	-146.1(2)
C(41)-P-C(3)-C(4)	-77.2(2)
C(31)-P-C(3)-C(4)	34.5(2)
C(21)-N(2)-C(4)-C(3)	-173.8(2)
Al-N(2)-C(4)-C(3)	10.6(3)
C(21)-N(2)-C(4)-C(5)	5.0(4)
Al-N(2)-C(4)-C(5)	-170.60(19)
C(2)-C(3)-C(4)-N(2)	20.9(4)
P-C(3)-C(4)-N(2)	-159.8(2)
C(2)-C(3)-C(4)-C(5)	-157.9(3)
P-C(3)-C(4)-C(5)	21.4(3)
C(2)-N(1)-C(11)-C(12)	82.9(3)
Al-N(1)-C(11)-C(12)	-88.7(3)

C(2)-N(1)-C(11)-C(16)	-98.6(3)
Al-N(1)-C(11)-C(16)	89.9(3)
C(16)-C(11)-C(12)-C(13)	2.5(4)
N(1)-C(11)-C(12)-C(13)	-179.0(3)
C(16)-C(11)-C(12)-C(17)	-177.8(3)
N(1)-C(11)-C(12)-C(17)	0.7(4)
C(11)-C(12)-C(13)-C(14)	-0.5(5)
C(17)-C(12)-C(13)-C(14)	179.8(3)
C(12)-C(13)-C(14)-C(15)	-0.5(5)
C(13)-C(14)-C(15)-C(16)	-0.5(5)
C(14)-C(15)-C(16)-C(11)	2.4(5)
C(14)-C(15)-C(16)-C(18)	-179.4(3)
C(12)-C(11)-C(16)-C(15)	-3.4(4)
N(1)-C(11)-C(16)-C(15)	178.0(3)
C(12)-C(11)-C(16)-C(18)	178.4(3)
N(1)-C(11)-C(16)-C(18)	-0.2(4)
C(11)-C(12)-C(17)-C(17A)	112.5(3)
C(13)-C(12)-C(17)-C(17A)	-67.8(4)
C(11)-C(12)-C(17)-C(17B)	-124.1(3)
C(13)-C(12)-C(17)-C(17B)	55.6(4)
C(15)-C(16)-C(18)-C(18A)	-91.9(4)
C(11)-C(16)-C(18)-C(18A)	86.3(4)
C(15)-C(16)-C(18)-C(18B)	33.3(5)
C(11)-C(16)-C(18)-C(18B)	-148.6(3)
C(4)-N(2)-C(21)-C(22)	-92.2(3)
Al-N(2)-C(21)-C(22)	83.2(3)
C(4)-N(2)-C(21)-C(26)	84.6(3)
Al-N(2)-C(21)-C(26)	-100.1(3)
C(26)-C(21)-C(22)-C(23)	-2.3(4)
N(2)-C(21)-C(22)-C(23)	174.3(3)
C(26)-C(21)-C(22)-C(27)	176.6(3)
N(2)-C(21)-C(22)-C(27)	-6.8(4)
C(21)-C(22)-C(23)-C(24)	-0.1(5)
C(27)-C(22)-C(23)-C(24)	-179.0(3)
C(22)-C(23)-C(24)-C(25)	1.4(5)
C(23)-C(24)-C(25)-C(26)	-0.3(5)

C(24)-C(25)-C(26)-C(21)	-2.1(4)
C(24)-C(25)-C(26)-C(28)	179.3(3)
C(22)-C(21)-C(26)-C(25)	3.4(4)
N(2)-C(21)-C(26)-C(25)	-173.3(2)
C(22)-C(21)-C(26)-C(28)	-178.1(3)
N(2)-C(21)-C(26)-C(28)	5.3(4)
C(23)-C(22)-C(27)-C(27A)	72.6(4)
C(21)-C(22)-C(27)-C(27A)	-106.3(3)
C(23)-C(22)-C(27)-C(27B)	-51.6(4)
C(21)-C(22)-C(27)-C(27B)	129.6(3)
C(25)-C(26)-C(28)-C(28B)	61.8(4)
C(21)-C(26)-C(28)-C(28B)	-116.7(3)
C(25)-C(26)-C(28)-C(28A)	-62.0(4)
C(21)-C(26)-C(28)-C(28A)	119.5(3)
C(3)-P-C(31)-C(32)	60.0(3)
C(41)-P-C(31)-C(32)	171.1(2)
C(3)-P-C(31)-C(36)	-123.8(2)
C(41)-P-C(31)-C(36)	-12.7(3)
C(36)-C(31)-C(32)-C(33)	2.1(5)
P-C(31)-C(32)-C(33)	178.6(3)
C(31)-C(32)-C(33)-C(34)	-1.7(5)
C(32)-C(33)-C(34)-C(35)	0.7(5)
C(33)-C(34)-C(35)-C(36)	-0.2(5)
C(34)-C(35)-C(36)-C(31)	0.6(5)
C(32)-C(31)-C(36)-C(35)	-1.5(4)
P-C(31)-C(36)-C(35)	-177.7(2)
C(3)-P-C(41)-C(46)	-15.2(3)
C(31)-P-C(41)-C(46)	-124.6(2)
C(3)-P-C(41)-C(42)	175.2(2)
C(31)-P-C(41)-C(42)	65.7(3)
C(46)-C(41)-C(42)-C(43)	1.5(5)
P-C(41)-C(42)-C(43)	171.5(2)
C(41)-C(42)-C(43)-C(44)	-1.9(5)
C(42)-C(43)-C(44)-C(45)	0.7(6)
C(43)-C(44)-C(45)-C(46)	1.0(6)
C(44)-C(45)-C(46)-C(41)	-1.4(5)

C(42)-C(41)-C(46)-C(45)	0.1(5)
P-C(41)-C(46)-C(45)	-169.7(3)

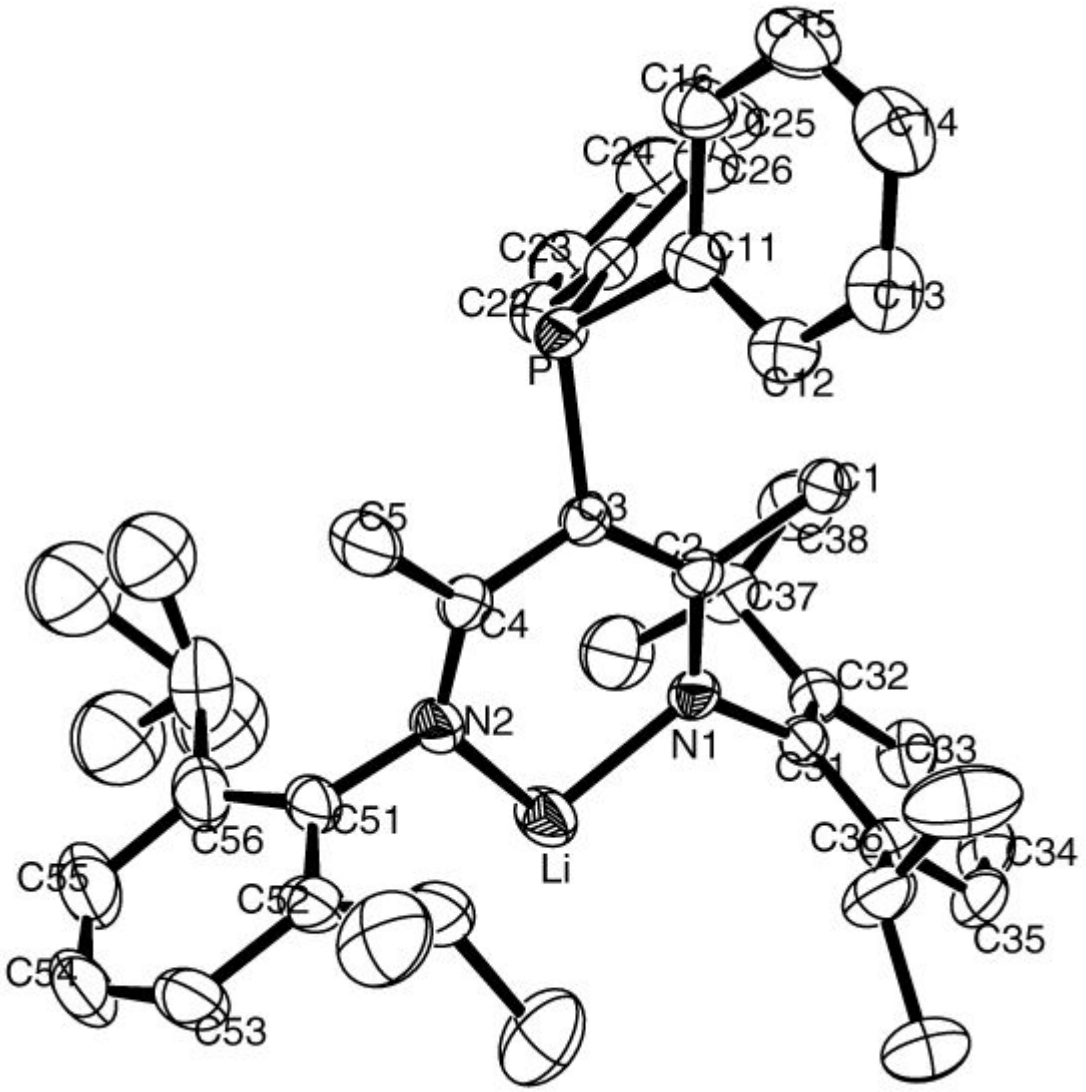

Figure S2: Solid state structure of **5Li**. Ellipsoids are 50% probability, hydrogen atoms and toluene solvate are removed for clarity. Numbering scheme of core atoms is included.

Table S6. Crystal data and structure refinement for **5Li**.

Identification code	dal0348	
Empirical formula	C48 H58 Li N2 P	
Formula weight	700.87	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1138(4) Å	α= 77.1930(10)°.
	b = 11.1175(5) Å	β= 84.7970(10)°.
	c = 19.6442(9) Å	γ = 78.2080(10)°.
Volume	2106.01(16) $Å^3$	
Z	2	
Density (calculated)	1.105 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	756	
Crystal size	0.43 x 0.27 x 0.26 mm^3	
Theta range for data collection	1.91 to 26.39°.	
Index ranges	-12<=h<=12, -11<=k<=13, -24<=l<=24	
Reflections collected	12066	
Independent reflections	8468 [R(int) = 0.0180]	
Completeness to theta = 26.39°	98.1 %	
Absorption correction	Integration	
Max. and min. transmission	0.9748 and 0.9588	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8468 / 0 / 470	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1217	
R indices (all data)	R1 = 0.0612, wR2 = 0.1312	
Largest diff. peak and hole	0.332 and -0.226 e.$Å^{-3}$	

Table S7: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5Li**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P	-60(1)	3726(1)	3262(1)	28(1)
N(1)	1218(1)	300(1)	2780(1)	27(1)
N(2)	1558(1)	2278(1)	1651(1)	32(1)
C(1)	-167(2)	825(1)	3796(1)	29(1)
C(2)	526(1)	1195(1)	3083(1)	25(1)
C(3)	369(2)	2509(1)	2759(1)	27(1)
C(4)	785(2)	2977(1)	2043(1)	31(1)
C(5)	241(2)	4346(2)	1723(1)	53(1)
C(11)	-1844(2)	3900(1)	3555(1)	32(1)
C(12)	-2752(2)	3340(2)	3301(1)	37(1)
C(13)	-4121(2)	3584(2)	3490(1)	47(1)
C(14)	-4609(2)	4392(2)	3936(1)	51(1)
C(15)	-3731(2)	4980(2)	4179(1)	49(1)
C(16)	-2366(2)	4753(2)	3988(1)	40(1)
C(21)	877(2)	3065(1)	4057(1)	30(1)
C(22)	2277(2)	2721(2)	3961(1)	39(1)
C(23)	3092(2)	2255(2)	4525(1)	49(1)
C(24)	2529(2)	2143(2)	5199(1)	51(1)
C(25)	1150(2)	2483(2)	5305(1)	48(1)
C(26)	331(2)	2946(2)	4739(1)	38(1)
C(31)	1325(2)	-997(1)	3112(1)	28(1)
C(32)	2267(2)	-1552(1)	3629(1)	31(1)
C(33)	2453(2)	-2849(2)	3877(1)	41(1)
C(34)	1750(2)	-3578(2)	3624(1)	46(1)
C(35)	822(2)	-3023(2)	3118(1)	42(1)
C(36)	591(2)	-1737(2)	2856(1)	34(1)
C(37)	3090(2)	-776(2)	3904(1)	37(1)
C(38)	3283(3)	-1191(2)	4686(1)	63(1)
C(39)	4459(2)	-784(3)	3508(1)	66(1)
C(40)	-456(2)	-1123(2)	2311(1)	47(1)
C(41)	-1799(2)	-583(3)	2642(1)	74(1)

C(42)	-679(3)	-1994(2)	1845(1)	64(1)
C(51)	1975(2)	2790(2)	950(1)	38(1)
C(52)	1172(2)	2846(2)	392(1)	42(1)
C(53)	1751(3)	3143(2)	-287(1)	57(1)
C(54)	3040(3)	3395(2)	-403(1)	68(1)
C(55)	3786(2)	3389(2)	146(1)	63(1)
C(56)	3277(2)	3094(2)	832(1)	50(1)
C(57)	-255(2)	2583(2)	515(1)	46(1)
C(58)	-292(3)	1251(2)	458(1)	67(1)
C(59)	-1246(3)	3495(2)	13(1)	67(1)
C(60)	4095(2)	3139(2)	1436(1)	65(1)
C(61A)	3718(6)	4307(5)	1655(3)	77(1)
C(62A)	5655(6)	2847(6)	1218(3)	95(2)
C(61B)	4477(8)	4467(7)	1376(4)	90(2)
C(62B)	5310(8)	2181(7)	1641(4)	96(2)
Li	2254(3)	521(3)	1921(1)	41(1)
C(10S)	5412(4)	-3141(3)	2387(1)	102(1)
C(11S)	4667(3)	-2138(2)	1837(1)	60(1)
C(12S)	3414(3)	-2183(2)	1657(2)	77(1)
C(13S)	2761(3)	-1283(3)	1136(2)	83(1)
C(14S)	3347(3)	-317(2)	781(1)	67(1)
C(15S)	4574(3)	-238(2)	957(2)	78(1)
C(16S)	5235(3)	-1139(3)	1482(2)	82(1)

Table S8. Bond lengths [Å] and angles [°] for **5Li**.

P-C(3)	1.8084(15)
P-C(11)	1.8282(17)
P-C(21)	1.8309(16)
N(1)-C(2)	1.3180(18)
N(1)-C(31)	1.4322(18)
N(1)-Li	1.899(3)
N(2)-C(4)	1.310(2)
N(2)-C(51)	1.4299(19)
N(2)-Li	1.908(3)
C(1)-C(2)	1.518(2)
C(2)-C(3)	1.442(2)
C(3)-C(4)	1.442(2)
C(4)-C(5)	1.520(2)
C(11)-C(12)	1.391(2)
C(11)-C(16)	1.405(2)
C(12)-C(13)	1.388(2)
C(13)-C(14)	1.381(3)
C(14)-C(15)	1.376(3)
C(15)-C(16)	1.384(3)
C(21)-C(26)	1.391(2)
C(21)-C(22)	1.396(2)
C(22)-C(23)	1.383(3)
C(23)-C(24)	1.382(3)
C(24)-C(25)	1.378(3)
C(25)-C(26)	1.388(2)
C(31)-C(32)	1.406(2)
C(31)-C(36)	1.408(2)
C(31)-Li	2.776(3)
C(32)-C(33)	1.395(2)
C(32)-C(37)	1.520(2)
C(33)-C(34)	1.374(3)
C(34)-C(35)	1.382(3)
C(35)-C(36)	1.387(2)
C(36)-C(40)	1.522(2)

C(37)-C(38)	1.521(3)
C(37)-C(39)	1.525(3)
C(40)-C(41)	1.519(3)
C(40)-C(42)	1.532(3)
C(51)-C(52)	1.406(3)
C(51)-C(56)	1.412(3)
C(51)-Li	2.784(3)
C(52)-C(53)	1.404(2)
C(52)-C(57)	1.517(3)
C(53)-C(54)	1.378(3)
C(54)-C(55)	1.369(4)
C(55)-C(56)	1.393(3)
C(56)-C(60)	1.521(3)
C(57)-C(58)	1.518(3)
C(57)-C(59)	1.525(3)
C(60)-C(61A)	1.426(5)
C(60)-C(62B)	1.474(8)
C(60)-C(61B)	1.578(7)
C(60)-C(62A)	1.583(6)
Li-C(14S)	2.674(4)
Li-C(13S)	2.732(4)
C(10S)-C(11S)	1.500(3)
C(11S)-C(12S)	1.359(4)
C(11S)-C(16S)	1.377(4)
C(12S)-C(13S)	1.372(4)
C(13S)-C(14S)	1.359(4)
C(14S)-C(15S)	1.342(4)
C(15S)-C(16S)	1.380(4)

C(3)-P-C(11)	109.94(7)
C(3)-P-C(21)	103.90(7)
C(11)-P-C(21)	105.20(7)
C(2)-N(1)-C(31)	121.10(12)
C(2)-N(1)-Li	126.66(13)
C(31)-N(1)-Li	112.14(12)
C(4)-N(2)-C(51)	121.77(13)

C(4)-N(2)-Li	125.95(13)
C(51)-N(2)-Li	112.28(13)
N(1)-C(2)-C(3)	122.71(13)
N(1)-C(2)-C(1)	118.69(12)
C(3)-C(2)-C(1)	118.57(12)
C(2)-C(3)-C(4)	124.09(13)
C(2)-C(3)-P	122.01(10)
C(4)-C(3)-P	112.85(10)
N(2)-C(4)-C(3)	123.69(13)
N(2)-C(4)-C(5)	118.66(14)
C(3)-C(4)-C(5)	117.60(14)
C(12)-C(11)-C(16)	117.73(15)
C(12)-C(11)-P	122.77(12)
C(16)-C(11)-P	119.02(13)
C(13)-C(12)-C(11)	120.93(16)
C(14)-C(13)-C(12)	120.49(18)
C(15)-C(14)-C(13)	119.42(18)
C(14)-C(15)-C(16)	120.61(18)
C(15)-C(16)-C(11)	120.75(17)
C(26)-C(21)-C(22)	117.83(15)
C(26)-C(21)-P	125.96(12)
C(22)-C(21)-P	116.10(12)
C(23)-C(22)-C(21)	121.11(16)
C(24)-C(23)-C(22)	120.15(18)
C(25)-C(24)-C(23)	119.64(17)
C(24)-C(25)-C(26)	120.23(17)
C(25)-C(26)-C(21)	121.02(16)
C(32)-C(31)-C(36)	120.60(14)
C(32)-C(31)-N(1)	120.18(13)
C(36)-C(31)-N(1)	118.80(13)
C(32)-C(31)-Li	116.25(12)
C(36)-C(31)-Li	104.33(12)
N(1)-C(31)-Li	39.32(8)
C(33)-C(32)-C(31)	118.15(15)
C(33)-C(32)-C(37)	120.30(15)
C(31)-C(32)-C(37)	121.54(13)

C(34)-C(33)-C(32)	121.57(17)
C(33)-C(34)-C(35)	119.80(15)
C(34)-C(35)-C(36)	121.07(16)
C(35)-C(36)-C(31)	118.81(16)
C(35)-C(36)-C(40)	121.00(15)
C(31)-C(36)-C(40)	120.18(14)
C(32)-C(37)-C(38)	113.32(15)
C(32)-C(37)-C(39)	110.87(15)
C(38)-C(37)-C(39)	110.11(17)
C(41)-C(40)-C(36)	111.80(16)
C(41)-C(40)-C(42)	109.85(18)
C(36)-C(40)-C(42)	113.68(17)
C(52)-C(51)-C(56)	121.41(16)
C(52)-C(51)-N(2)	120.35(16)
C(56)-C(51)-N(2)	117.84(16)
C(52)-C(51)-Li	113.88(13)
C(56)-C(51)-Li	106.07(13)
N(2)-C(51)-Li	39.35(9)
C(53)-C(52)-C(51)	117.13(19)
C(53)-C(52)-C(57)	121.16(18)
C(51)-C(52)-C(57)	121.70(15)
C(54)-C(53)-C(52)	121.6(2)
C(55)-C(54)-C(53)	120.50(19)
C(54)-C(55)-C(56)	120.9(2)
C(55)-C(56)-C(51)	118.4(2)
C(55)-C(56)-C(60)	120.4(2)
C(51)-C(56)-C(60)	121.24(17)
C(52)-C(57)-C(58)	111.44(17)
C(52)-C(57)-C(59)	112.86(16)
C(58)-C(57)-C(59)	108.81(17)
C(61A)-C(60)-C(62B)	125.5(4)
C(61A)-C(60)-C(56)	112.0(3)
C(62B)-C(60)-C(56)	121.2(4)
C(61A)-C(60)-C(61B)	35.4(3)
C(62B)-C(60)-C(61B)	107.5(4)
C(56)-C(60)-C(61B)	112.8(3)

C(61A)-C(60)-C(62A)	111.9(4)
C(62B)-C(60)-C(62A)	40.7(3)
C(56)-C(60)-C(62A)	109.1(3)
C(61B)-C(60)-C(62A)	79.3(4)
N(1)-Li-N(2)	94.99(13)
N(1)-Li-C(14S)	150.22(16)
N(2)-Li-C(14S)	108.35(13)
N(1)-Li-C(13S)	121.15(15)
N(2)-Li-C(13S)	129.68(15)
C(14S)-Li-C(13S)	29.08(9)
N(1)-Li-C(31)	28.54(6)
N(2)-Li-C(31)	123.20(13)
C(14S)-Li-C(31)	123.79(12)
C(13S)-Li-C(31)	95.44(12)
N(1)-Li-C(51)	123.02(14)
N(2)-Li-C(51)	28.37(6)
C(14S)-Li-C(51)	80.41(10)
C(13S)-Li-C(51)	104.83(12)
C(31)-Li-C(51)	150.35(12)
C(12S)-C(11S)-C(16S)	116.9(2)
C(12S)-C(11S)-C(10S)	121.8(3)
C(16S)-C(11S)-C(10S)	121.3(3)
C(11S)-C(12S)-C(13S)	121.3(2)
C(14S)-C(13S)-C(12S)	121.0(3)
C(14S)-C(13S)-Li	73.09(17)
C(12S)-C(13S)-Li	93.6(2)
C(15S)-C(14S)-C(13S)	118.9(2)
C(15S)-C(14S)-Li	89.52(19)
C(13S)-C(14S)-Li	77.82(18)
C(14S)-C(15S)-C(16S)	120.4(2)
C(11S)-C(16S)-C(15S)	121.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2$x 10^3)for **5Li**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P	37(1)	21(1)	27(1)	-5(1)	1(1)	-6(1)
N(1)	35(1)	21(1)	25(1)	-3(1)	-3(1)	-5(1)
N(2)	44(1)	27(1)	24(1)	-3(1)	3(1)	-7(1)
C(1)	35(1)	23(1)	27(1)	-3(1)	1(1)	-5(1)
C(2)	29(1)	24(1)	23(1)	-5(1)	-4(1)	-7(1)
C(3)	33(1)	21(1)	25(1)	-5(1)	0(1)	-5(1)
C(4)	41(1)	23(1)	28(1)	-3(1)	-1(1)	-6(1)
C(5)	88(2)	27(1)	33(1)	0(1)	11(1)	1(1)
C(11)	38(1)	24(1)	29(1)	-1(1)	-2(1)	1(1)
C(12)	39(1)	34(1)	35(1)	-7(1)	-6(1)	-1(1)
C(13)	37(1)	47(1)	53(1)	-2(1)	-10(1)	-4(1)
C(14)	35(1)	49(1)	56(1)	-1(1)	2(1)	9(1)
C(15)	52(1)	38(1)	49(1)	-9(1)	5(1)	11(1)
C(16)	45(1)	32(1)	39(1)	-9(1)	-1(1)	2(1)
C(21)	35(1)	24(1)	33(1)	-8(1)	-1(1)	-10(1)
C(22)	37(1)	42(1)	42(1)	-11(1)	1(1)	-13(1)
C(23)	35(1)	56(1)	59(1)	-12(1)	-10(1)	-11(1)
C(24)	54(1)	55(1)	49(1)	-11(1)	-22(1)	-8(1)
C(25)	59(1)	52(1)	33(1)	-10(1)	-7(1)	-7(1)
C(26)	39(1)	40(1)	34(1)	-10(1)	-1(1)	-6(1)
C(31)	33(1)	22(1)	27(1)	-5(1)	5(1)	-5(1)
C(32)	31(1)	25(1)	34(1)	-4(1)	2(1)	-2(1)
C(33)	38(1)	28(1)	49(1)	1(1)	-3(1)	2(1)
C(34)	48(1)	20(1)	64(1)	-4(1)	6(1)	-3(1)
C(35)	48(1)	28(1)	54(1)	-14(1)	7(1)	-14(1)
C(36)	42(1)	29(1)	34(1)	-10(1)	3(1)	-9(1)
C(37)	37(1)	33(1)	39(1)	-4(1)	-9(1)	-1(1)
C(38)	88(2)	59(1)	46(1)	-6(1)	-21(1)	-16(1)
C(39)	45(1)	88(2)	76(2)	-30(1)	0(1)	-24(1)
C(40)	64(1)	40(1)	45(1)	-12(1)	-15(1)	-17(1)
C(41)	64(1)	80(2)	88(2)	-45(1)	-39(1)	14(1)

C(42)	77(2)	71(2)	58(1)	-31(1)	-11(1)	-25(1)
C(51)	55(1)	25(1)	29(1)	-3(1)	8(1)	-5(1)
C(52)	68(1)	27(1)	28(1)	-6(1)	3(1)	-5(1)
C(53)	98(2)	41(1)	28(1)	-8(1)	6(1)	-10(1)
C(54)	98(2)	56(1)	43(1)	-9(1)	35(1)	-18(1)
C(55)	68(1)	57(1)	57(1)	-3(1)	26(1)	-14(1)
C(56)	56(1)	37(1)	49(1)	-1(1)	14(1)	-9(1)
C(57)	67(1)	40(1)	31(1)	-6(1)	-6(1)	-9(1)
C(58)	78(2)	39(1)	81(2)	1(1)	-22(1)	-12(1)
C(59)	84(2)	42(1)	69(1)	0(1)	-21(1)	-2(1)
C(60)	55(1)	69(2)	64(1)	8(1)	-2(1)	-24(1)
Li	54(2)	31(1)	32(1)	-4(1)	7(1)	-1(1)
C(10S)	163(3)	72(2)	57(2)	-4(1)	-19(2)	6(2)
C(11S)	86(2)	48(1)	41(1)	-13(1)	5(1)	-2(1)
C(12S)	66(2)	54(1)	102(2)	-10(1)	25(2)	-13(1)
C(13S)	58(2)	67(2)	119(2)	-19(2)	-7(2)	-1(1)
C(14S)	76(2)	54(1)	59(1)	-12(1)	1(1)	12(1)
C(15S)	86(2)	53(1)	86(2)	2(1)	8(2)	-19(1)
C(16S)	84(2)	66(2)	99(2)	-8(2)	-27(2)	-24(1)

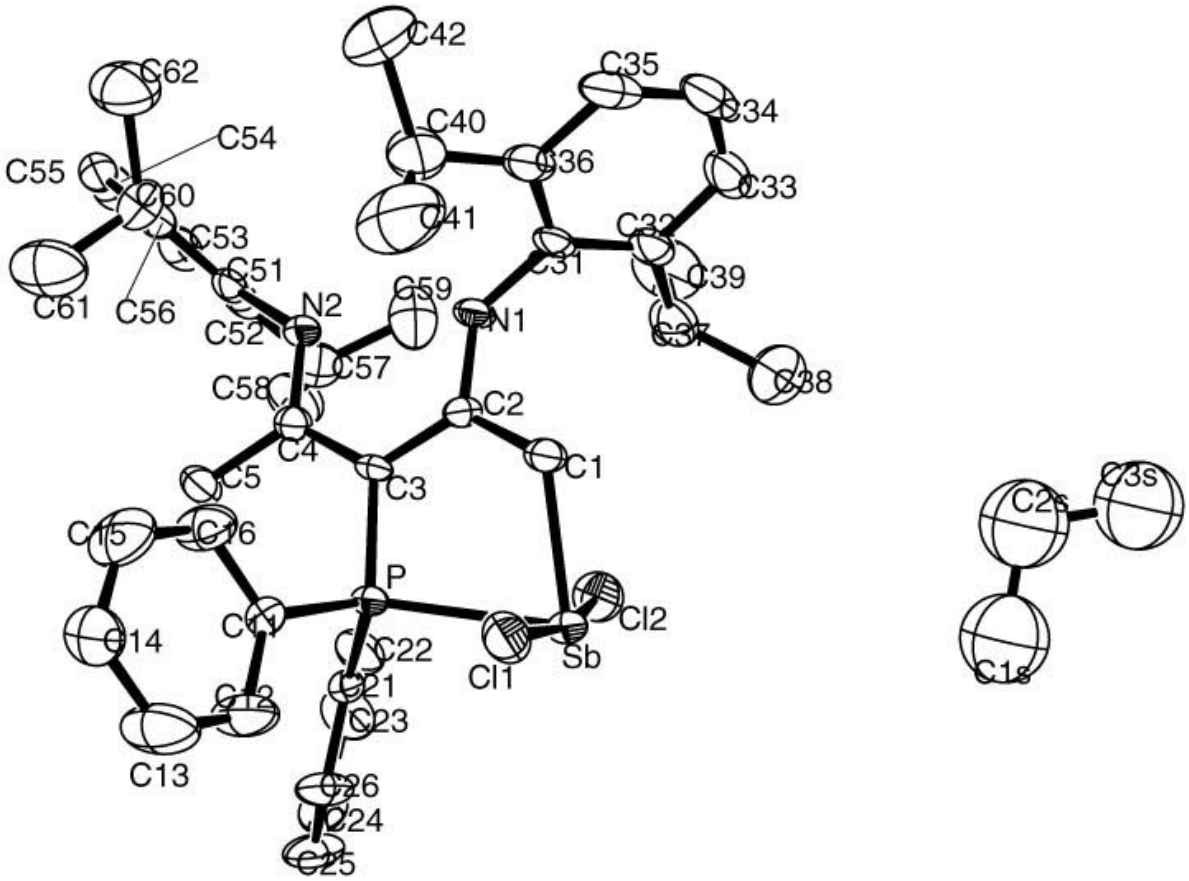

Figure S3: Solid State Structure of **6Sb**. Ellipsoids are 50% probability, hydrogen atoms are removed for clarity. This highlights the complete numbering scheme and includes the *n*-pentane solvate.

Table S10. Crystal data and structure refinement for **6Sb**.

Identification code	dal0343	
Empirical formula	C43.50 H56 Cl2 N2 P Sb	
Formula weight	830.52	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 34.699(3) Å	α= 90°.
	b = 11.3045(9) Å	β= 96.0247(15)°.
	c = 20.9953(15) Å	γ = 90°.
Volume	8190.0(11) $Å^3$	
Z	8	
Density (calculated)	1.347 Mg/m^3	
Absorption coefficient	0.875 mm^{-1}	
F(000)	3448	
Crystal size	0.78 x 0.14 x 0.11 mm^3	
Theta range for data collection	1.90 to 26.38°.	
Index ranges	-43<=h<=42, -14<=k<=11, -26<=l<=25	
Reflections collected	21380	
Independent reflections	8350 [R(int) = 0.0606]	
Completeness to theta = 26.38°	99.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9099 and 0.5484	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8350 / 6 / 435	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1386	
R indices (all data)	R1 = 0.0882, wR2 = 0.1525	
Largest diff. peak and hole	1.856 and -1.251 $e.Å^{-3}$	

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6Sb**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sb	576(1)	405(1)	326(1)	30(1)
Cl(1)	137(1)	-1554(1)	332(1)	41(1)
Cl(2)	1052(1)	2057(1)	214(1)	47(1)
P	1180(1)	-969(1)	458(1)	22(1)
N(1)	1142(1)	-183(4)	-1383(2)	26(1)
N(2)	1824(1)	-1047(4)	-1027(2)	26(1)
C(1)	649(1)	-87(5)	-655(2)	30(1)
C(2)	1057(1)	-350(4)	-782(2)	23(1)
C(3)	1341(1)	-818(4)	-317(2)	23(1)
C(4)	1720(1)	-1206(4)	-458(2)	24(1)
C(5)	1995(2)	-1778(5)	56(2)	36(1)
C(11)	1108(1)	-2530(4)	615(2)	26(1)
C(12)	969(2)	-2910(6)	1167(3)	60(2)
C(13)	912(3)	-4098(7)	1277(3)	77(3)
C(14)	995(2)	-4925(6)	819(3)	56(2)
C(15)	1110(2)	-4539(6)	273(3)	64(2)
C(16)	1174(2)	-3355(6)	161(3)	48(2)
C(21)	1520(1)	-322(4)	1081(2)	25(1)
C(22)	1802(2)	455(5)	928(3)	40(1)
C(23)	2047(2)	988(6)	1402(3)	48(2)
C(24)	2016(2)	761(6)	2026(3)	47(2)
C(25)	1727(2)	41(7)	2196(3)	50(2)
C(26)	1480(2)	-505(6)	1721(2)	41(1)
C(31)	874(1)	150(5)	-1917(2)	27(1)
C(32)	776(2)	1342(5)	-2015(2)	34(1)
C(33)	514(2)	1610(6)	-2547(3)	46(2)
C(34)	362(2)	745(7)	-2962(3)	47(2)
C(35)	467(2)	-403(7)	-2863(2)	46(2)
C(36)	727(2)	-746(6)	-2342(2)	39(1)
C(37)	950(2)	2324(5)	-1587(3)	47(2)
C(38)	643(3)	3195(7)	-1401(4)	78(2)

C(39)	1268(2)	2954(7)	-1910(4)	74(2)
C(40)	853(2)	-2020(6)	-2251(3)	61(2)
C(41)	597(4)	-2693(8)	-1855(5)	121(4)
C(42)	893(3)	-2660(8)	-2875(4)	88(3)
C(51)	2197(1)	-1377(5)	-1202(2)	28(1)
C(52)	2500(2)	-542(5)	-1112(2)	35(1)
C(53)	2850(2)	-828(6)	-1347(3)	42(2)
C(54)	2896(2)	-1867(6)	-1656(3)	48(2)
C(55)	2601(2)	-2671(6)	-1732(3)	44(2)
C(56)	2242(2)	-2452(5)	-1515(2)	34(1)
C(57)	2447(2)	628(6)	-778(3)	43(1)
C(58)	2822(2)	1204(7)	-486(3)	60(2)
C(59)	2227(2)	1489(6)	-1224(4)	58(2)
C(60)	1919(2)	-3353(5)	-1598(3)	46(2)
C(61)	1972(3)	-4329(7)	-1103(4)	76(2)
C(62)	1868(3)	-3891(7)	-2273(3)	77(2)
C(1S)	36(4)	5650(2)	-87(2)	142(3)
C(2S)	55(4)	5762(9)	-814(3)	142(3)
C(3S)	-199(6)	6805(17)	-1079(7)	142(3)

Table S12. Bond lengths [Å] and angles [°] for **6Sb**.

Sb-C(1)	2.174(5)
Sb-Cl(2)	2.5212(16)
Sb-P	2.6011(13)
Sb-Cl(1)	2.6885(16)
P-C(3)	1.783(4)
P-C(11)	1.817(5)
P-C(21)	1.821(5)
N(1)-C(2)	1.339(5)
N(1)-C(31)	1.432(6)
N(2)-C(4)	1.297(6)
N(2)-C(51)	1.431(6)
C(1)-C(2)	1.496(6)
C(2)-C(3)	1.414(6)
C(3)-C(4)	1.446(6)
C(4)-C(5)	1.510(7)
C(11)-C(16)	1.370(7)
C(11)-C(12)	1.372(7)
C(12)-C(13)	1.380(9)
C(13)-C(14)	1.394(10)
C(14)-C(15)	1.325(9)
C(15)-C(16)	1.382(9)
C(21)-C(22)	1.378(7)
C(21)-C(26)	1.379(7)
C(22)-C(23)	1.379(8)
C(23)-C(24)	1.350(8)
C(24)-C(25)	1.370(9)
C(25)-C(26)	1.389(8)
C(31)-C(32)	1.400(8)
C(31)-C(36)	1.409(8)
C(32)-C(33)	1.398(8)
C(32)-C(37)	1.513(8)
C(33)-C(34)	1.378(9)
C(34)-C(35)	1.357(9)
C(35)-C(36)	1.398(8)

C(36)-C(40)	1.512(9)
C(37)-C(39)	1.530(9)
C(37)-C(38)	1.533(9)
C(40)-C(41)	1.487(12)
C(40)-C(42)	1.517(9)
C(51)-C(56)	1.399(7)
C(51)-C(52)	1.411(8)
C(52)-C(53)	1.397(7)
C(52)-C(57)	1.516(8)
C(53)-C(54)	1.360(9)
C(54)-C(55)	1.367(9)
C(55)-C(56)	1.391(7)
C(56)-C(60)	1.512(8)
C(57)-C(59)	1.503(9)
C(57)-C(58)	1.523(8)
C(60)-C(61)	1.514(10)
C(60)-C(62)	1.536(9)
C(1S)-C(2S)	1.5389(10)
C(1S)-C(1S)#1	1.5401(10)
C(2S)-C(3S)	1.5397(10)

C(1)-Sb-Cl(2)	87.64(15)
C(1)-Sb-P	77.00(13)
Cl(2)-Sb-P	85.60(5)
C(1)-Sb-Cl(1)	85.23(15)
Cl(2)-Sb-Cl(1)	171.11(5)
P-Sb-Cl(1)	87.63(4)
C(3)-P-C(11)	108.7(2)
C(3)-P-C(21)	112.2(2)
C(11)-P-C(21)	110.5(2)
C(3)-P-Sb	99.85(16)
C(11)-P-Sb	118.30(16)
C(21)-P-Sb	106.89(16)
C(2)-N(1)-C(31)	125.8(4)
C(4)-N(2)-C(51)	123.1(4)
C(2)-C(1)-Sb	115.2(3)

N(1)-C(2)-C(3)	119.7(4)
N(1)-C(2)-C(1)	116.5(4)
C(3)-C(2)-C(1)	123.7(4)
C(2)-C(3)-C(4)	123.8(4)
C(2)-C(3)-P	113.8(3)
C(4)-C(3)-P	122.3(3)
N(2)-C(4)-C(3)	119.5(4)
N(2)-C(4)-C(5)	120.2(4)
C(3)-C(4)-C(5)	120.3(4)
C(16)-C(11)-C(12)	118.3(5)
C(16)-C(11)-P	119.9(4)
C(12)-C(11)-P	121.7(4)
C(11)-C(12)-C(13)	121.1(6)
C(12)-C(13)-C(14)	119.5(6)
C(15)-C(14)-C(13)	118.6(6)
C(14)-C(15)-C(16)	122.3(6)
C(11)-C(16)-C(15)	119.9(6)
C(22)-C(21)-C(26)	118.0(5)
C(22)-C(21)-P	120.6(4)
C(26)-C(21)-P	121.1(4)
C(21)-C(22)-C(23)	120.6(5)
C(24)-C(23)-C(22)	120.8(6)
C(23)-C(24)-C(25)	120.1(5)
C(24)-C(25)-C(26)	119.3(5)
C(21)-C(26)-C(25)	121.1(5)
C(32)-C(31)-C(36)	122.2(5)
C(32)-C(31)-N(1)	119.7(5)
C(36)-C(31)-N(1)	118.1(5)
C(33)-C(32)-C(31)	117.0(5)
C(33)-C(32)-C(37)	120.1(6)
C(31)-C(32)-C(37)	122.9(5)
C(34)-C(33)-C(32)	121.7(6)
C(35)-C(34)-C(33)	120.2(5)
C(34)-C(35)-C(36)	121.7(6)
C(35)-C(36)-C(31)	117.2(6)
C(35)-C(36)-C(40)	121.2(6)

C(31)-C(36)-C(40)	121.6(5)
C(32)-C(37)-C(39)	109.9(5)
C(32)-C(37)-C(38)	112.2(6)
C(39)-C(37)-C(38)	111.6(6)
C(41)-C(40)-C(36)	112.1(7)
C(41)-C(40)-C(42)	110.7(7)
C(36)-C(40)-C(42)	113.3(6)
C(56)-C(51)-C(52)	121.7(5)
C(56)-C(51)-N(2)	119.8(5)
C(52)-C(51)-N(2)	118.2(5)
C(53)-C(52)-C(51)	117.5(5)
C(53)-C(52)-C(57)	121.0(5)
C(51)-C(52)-C(57)	121.4(5)
C(54)-C(53)-C(52)	121.2(6)
C(53)-C(54)-C(55)	120.4(5)
C(54)-C(55)-C(56)	122.0(6)
C(55)-C(56)-C(51)	117.2(5)
C(55)-C(56)-C(60)	121.4(5)
C(51)-C(56)-C(60)	121.4(4)
C(59)-C(57)-C(52)	110.8(5)
C(59)-C(57)-C(58)	109.3(5)
C(52)-C(57)-C(58)	114.8(5)
C(56)-C(60)-C(61)	112.1(6)
C(56)-C(60)-C(62)	112.6(5)
C(61)-C(60)-C(62)	109.8(6)
C(2S)-C(1S)-C(1S)#1	109.82(9)
C(1S)-C(2S)-C(3S)	109.88(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **6Sb**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sb	33(1)	39(1)	19(1)	-1(1)	6(1)	10(1)
Cl(1)	37(1)	47(1)	38(1)	10(1)	5(1)	7(1)
Cl(2)	65(1)	33(1)	44(1)	-2(1)	4(1)	-1(1)
P	25(1)	28(1)	15(1)	1(1)	4(1)	3(1)
N(1)	26(2)	40(3)	14(2)	2(2)	4(2)	2(2)
N(2)	28(2)	32(2)	18(2)	1(2)	6(2)	6(2)
C(1)	26(3)	45(3)	18(2)	0(2)	2(2)	7(2)
C(2)	28(2)	25(3)	17(2)	-2(2)	5(2)	1(2)
C(3)	27(2)	29(3)	11(2)	3(2)	4(2)	3(2)
C(4)	27(2)	24(3)	22(2)	0(2)	2(2)	-1(2)
C(5)	32(3)	52(4)	25(3)	11(2)	4(2)	13(3)
C(11)	26(2)	28(3)	25(2)	-1(2)	6(2)	3(2)
C(12)	113(6)	36(4)	35(3)	-2(3)	30(4)	-10(4)
C(13)	147(8)	45(4)	44(4)	2(3)	33(5)	-20(5)
C(14)	87(5)	29(3)	52(4)	2(3)	10(4)	-9(3)
C(15)	99(6)	37(4)	60(4)	-18(3)	22(4)	-9(4)
C(16)	66(4)	41(4)	39(3)	-11(3)	14(3)	-10(3)
C(21)	28(2)	27(3)	20(2)	-2(2)	2(2)	5(2)
C(22)	50(3)	34(3)	33(3)	6(3)	-2(2)	-9(3)
C(23)	59(4)	37(4)	44(3)	-2(3)	-11(3)	-17(3)
C(24)	39(3)	56(4)	41(3)	-22(3)	-10(3)	6(3)
C(25)	42(3)	87(5)	22(3)	-18(3)	3(2)	3(3)
C(26)	33(3)	68(4)	22(2)	-4(3)	9(2)	-5(3)
C(31)	25(2)	44(3)	14(2)	8(2)	6(2)	5(2)
C(32)	32(3)	50(4)	22(2)	10(2)	8(2)	5(3)
C(33)	39(3)	67(5)	34(3)	21(3)	9(3)	14(3)
C(34)	32(3)	85(5)	23(3)	15(3)	1(2)	4(3)
C(35)	35(3)	81(5)	21(3)	-5(3)	2(2)	-5(3)
C(36)	37(3)	58(4)	21(2)	-1(2)	3(2)	3(3)
C(37)	65(4)	36(4)	39(3)	11(3)	3(3)	3(3)
C(38)	107(7)	61(5)	66(5)	-9(4)	6(5)	24(5)

C(39)	86(6)	65(5)	68(5)	8(4)	-1(4)	-28(4)
C(40)	80(5)	51(4)	45(4)	-17(3)	-17(3)	5(4)
C(41)	237(14)	49(5)	88(7)	2(5)	65(8)	6(7)
C(42)	117(7)	78(6)	69(5)	-36(5)	8(5)	17(5)
C(51)	27(3)	38(3)	20(2)	10(2)	7(2)	9(2)
C(52)	36(3)	44(3)	27(3)	17(2)	5(2)	5(3)
C(53)	28(3)	63(4)	38(3)	18(3)	12(2)	9(3)
C(54)	38(3)	68(5)	42(3)	23(3)	21(3)	19(3)
C(55)	54(4)	53(4)	28(3)	8(3)	12(3)	28(3)
C(56)	39(3)	42(3)	22(2)	8(2)	7(2)	13(3)
C(57)	39(3)	49(4)	41(3)	2(3)	9(3)	-7(3)
C(58)	61(4)	64(5)	50(4)	3(3)	-14(3)	-12(4)
C(59)	48(4)	45(4)	78(5)	-5(4)	-14(3)	-4(3)
C(60)	53(4)	38(4)	48(3)	-8(3)	9(3)	9(3)
C(61)	108(7)	67(5)	56(4)	2(4)	21(4)	-26(5)
C(62)	122(7)	58(5)	50(4)	-10(4)	-1(4)	-11(5)