

Supporting Information

C – H Bond Activations by Monoanionic PNP-Supported Scandium Dialkyl Complexes

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1. Spectroscopic Characterization

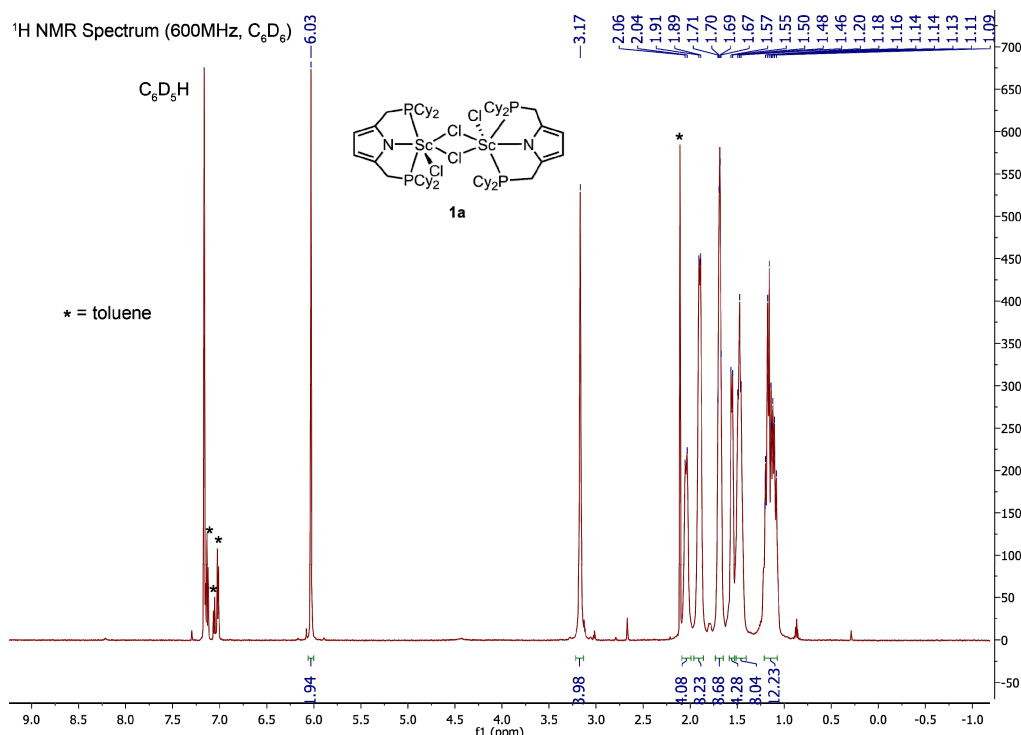


Figure S1. [(PNP-Cy)ScCl₂]₂ ¹H NMR Spectrum.

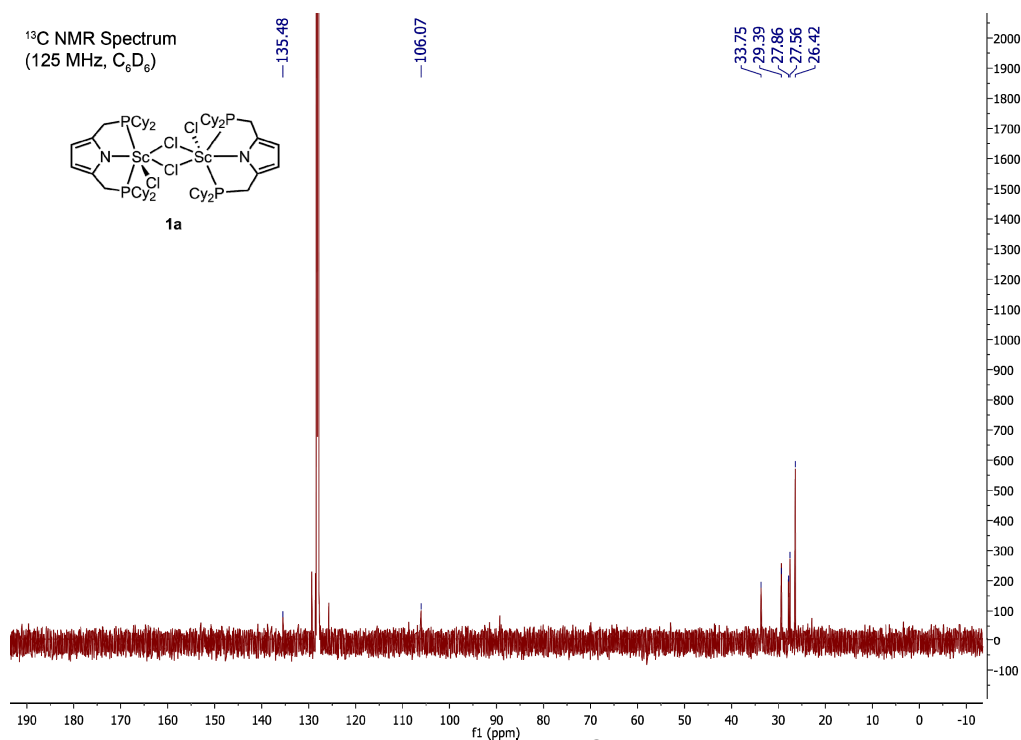


Figure S2. [(PNP-Cy)ScCl₂]₂ ¹³C NMR Spectrum.

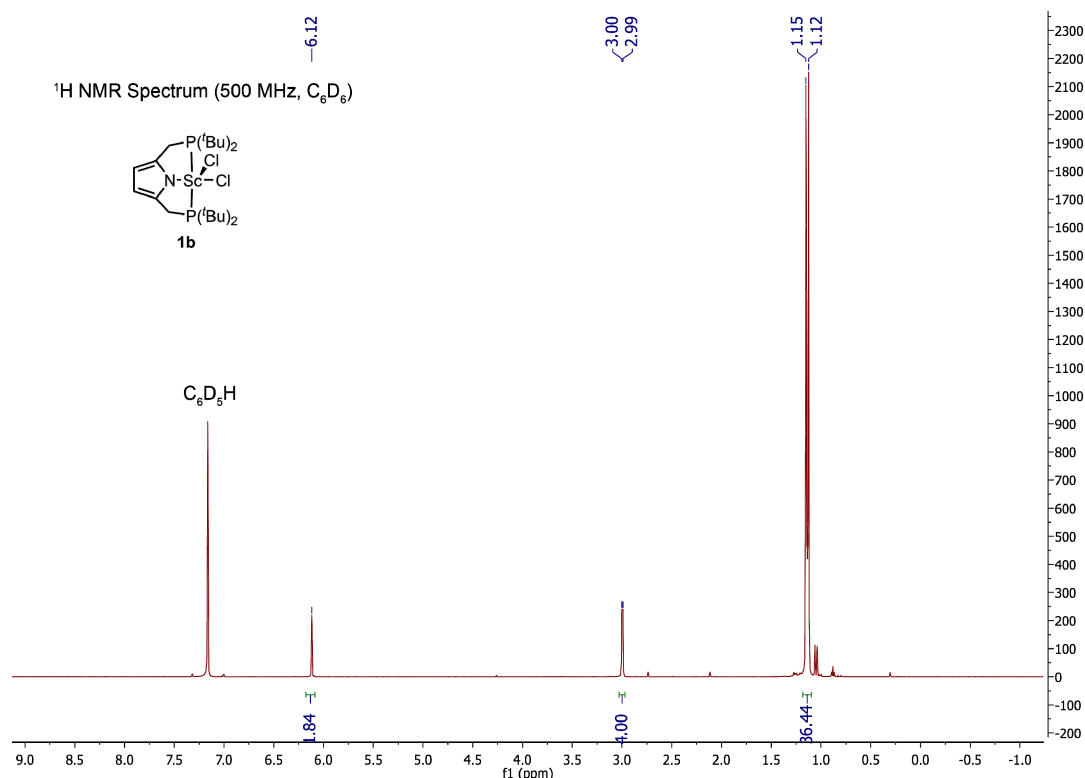


Figure S3. (PNP-*t*Bu)ScCl₂ ¹H NMR Spectrum.

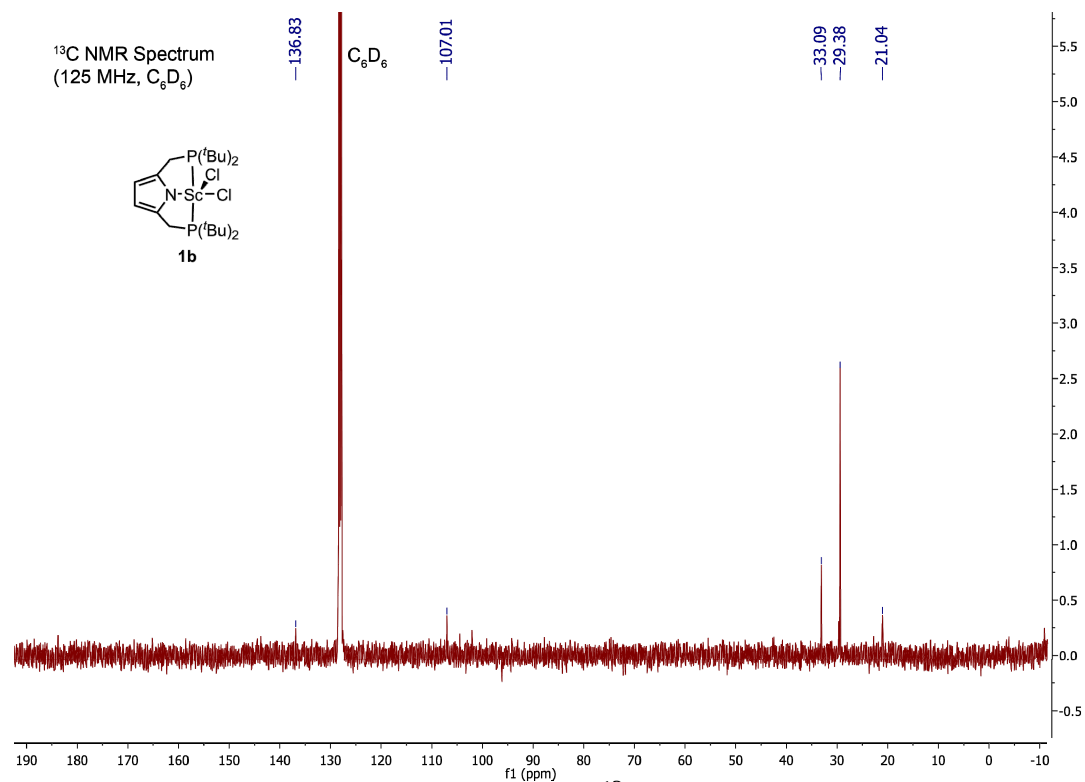


Figure S4. (PNP-*t*Bu)ScCl₂ ¹³C NMR Spectrum.

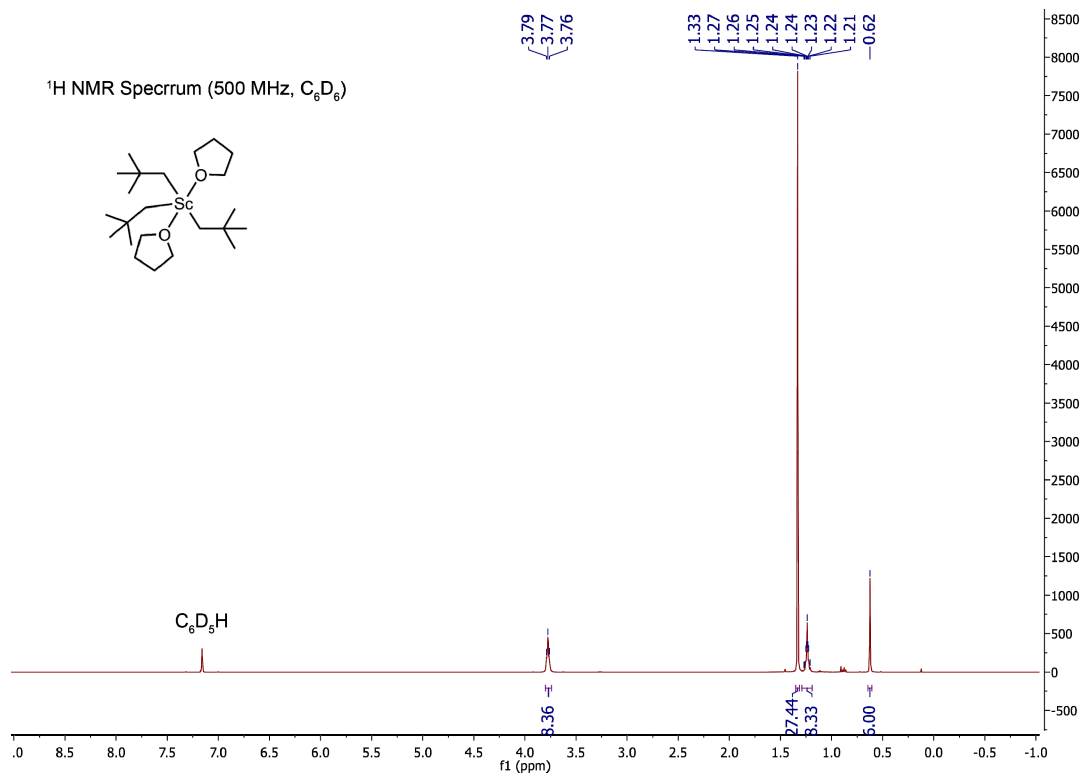


Figure S5. ScNp₃(THF)₃ ¹H NMR Spectrum.

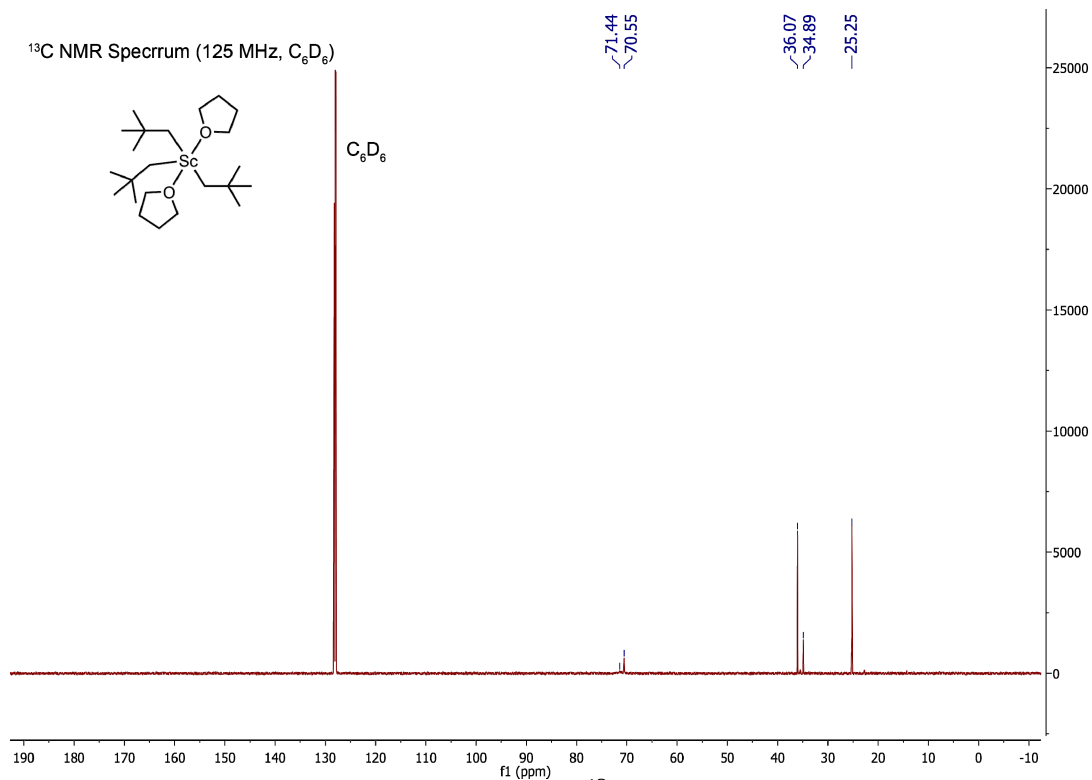


Figure S6. ScNp₃(THF)₃ ¹³C NMR Spectrum.

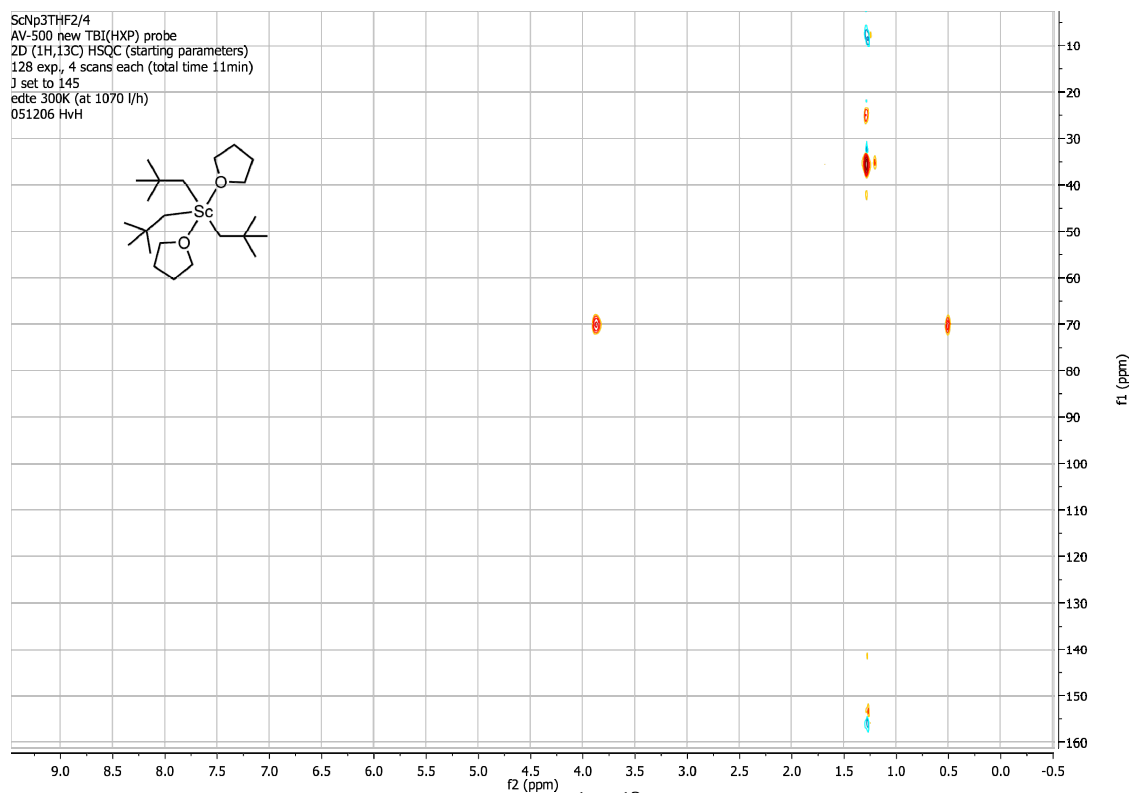


Figure S7. $\text{ScNp}_3(\text{THF})_3$ ^1H - ^{13}C HSQC Spectrum.

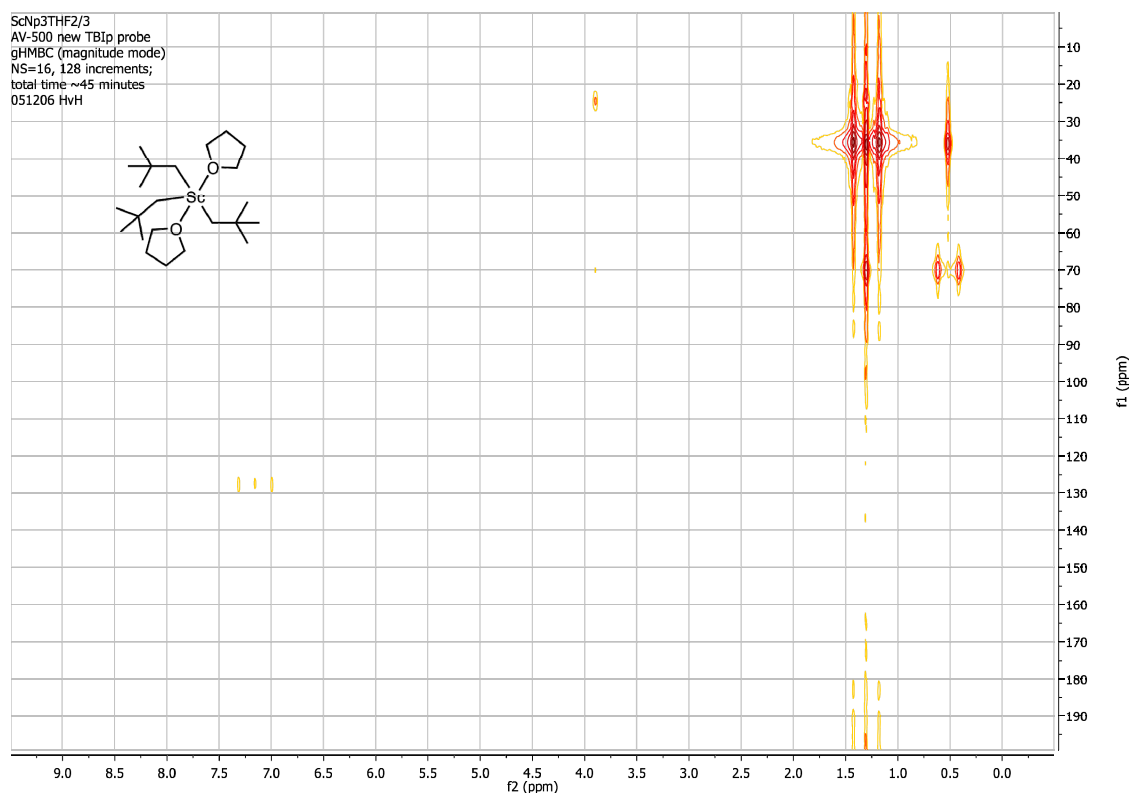


Figure S8. $\text{ScNp}_3(\text{THF})_3$ ^1H - ^{13}C HMBC Spectrum.

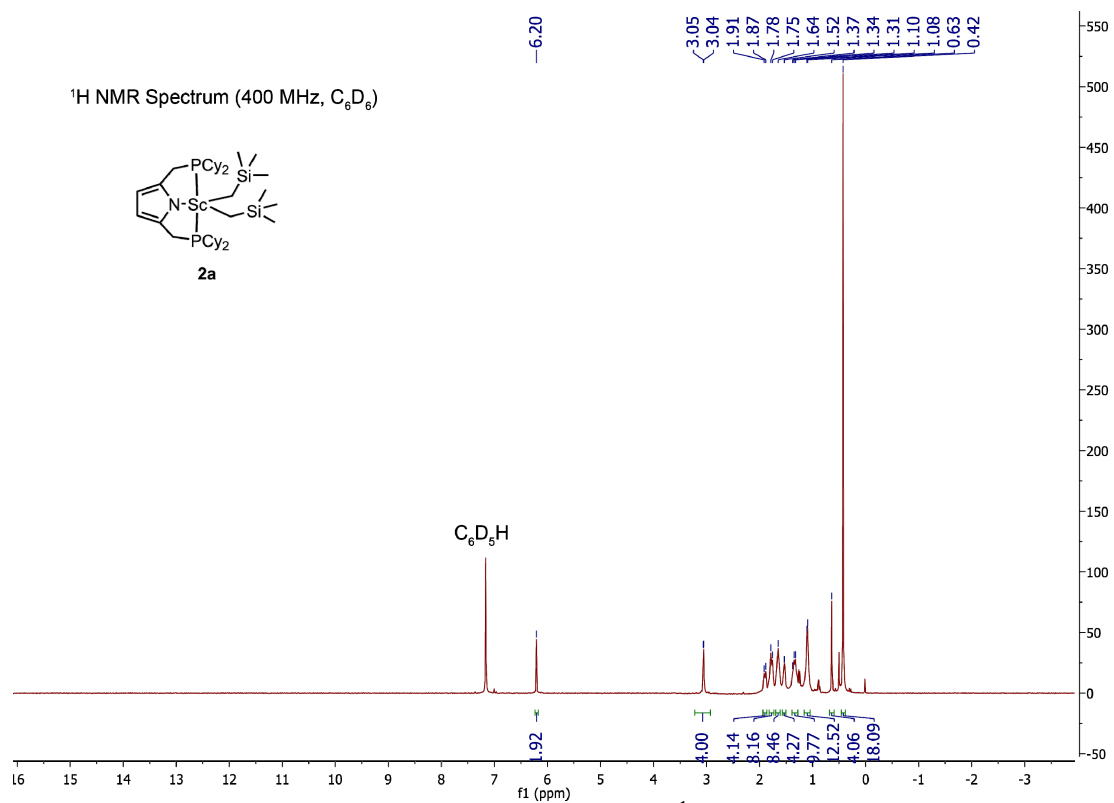


Figure S9. (PNP-Cy)Sc(CH₂SiMe₃)₂ ¹H NMR Spectrum.

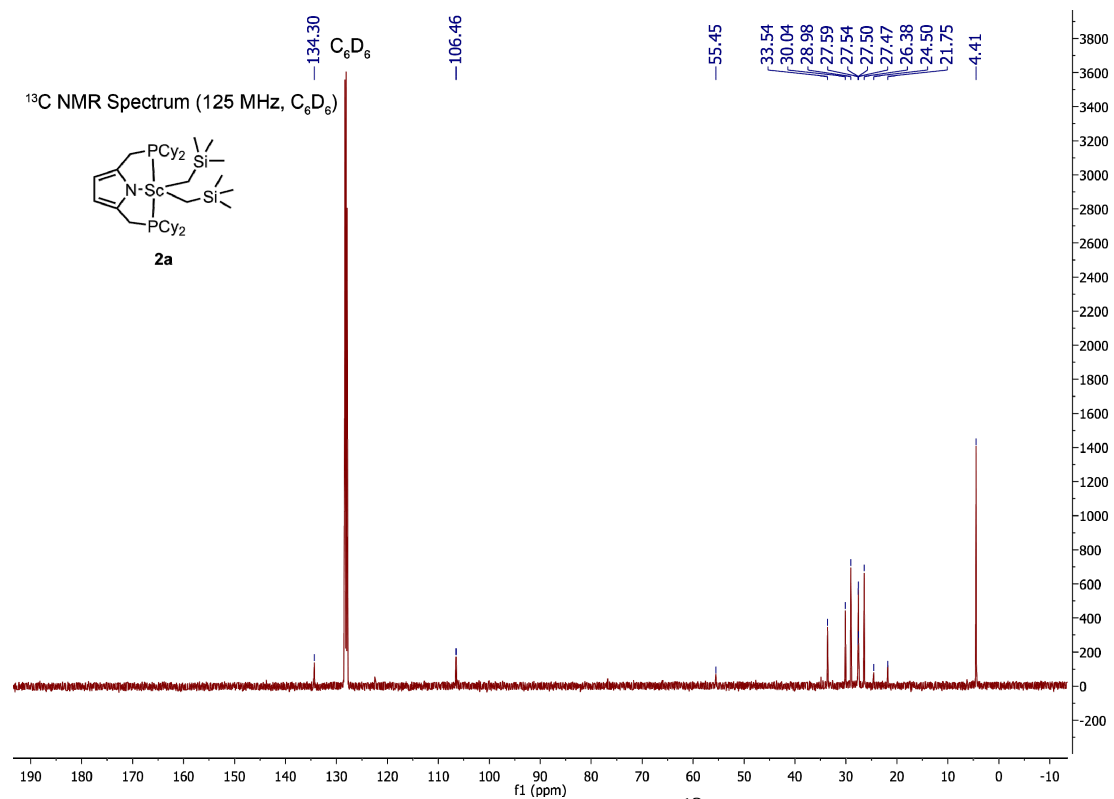


Figure S10. (PNP-Cy)Sc(CH₂SiMe₃)₂ ¹³C NMR Spectrum.

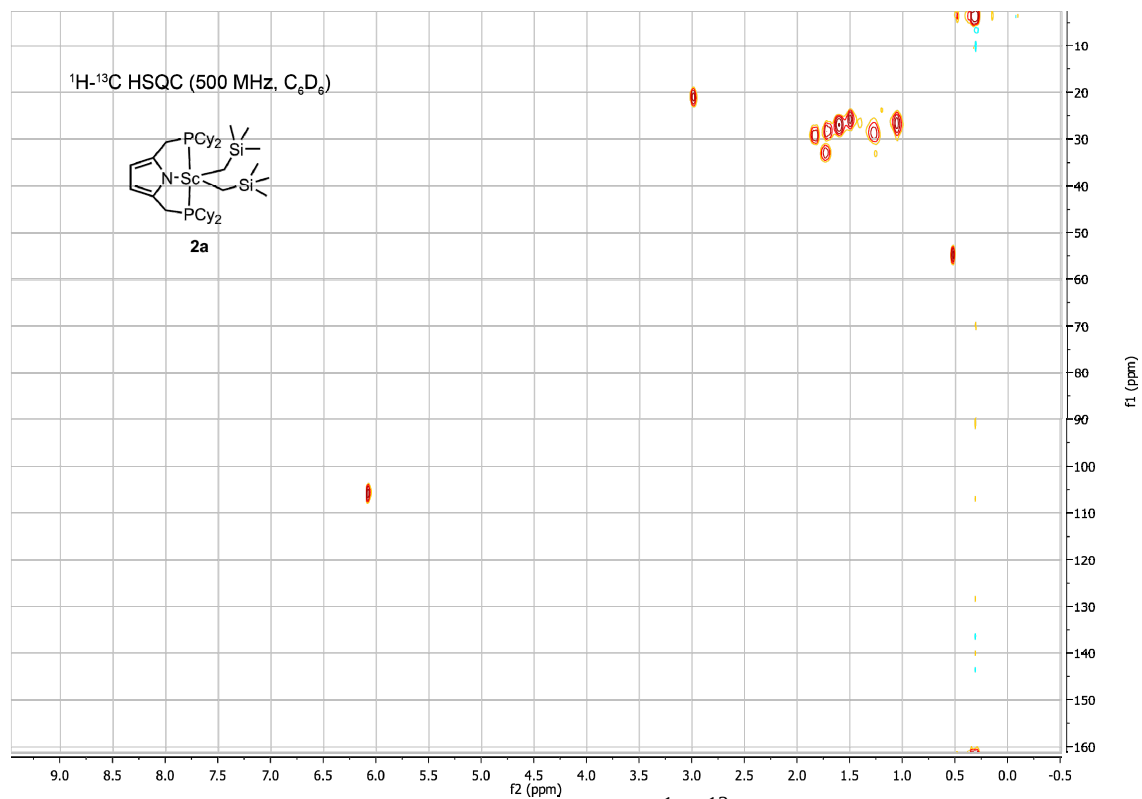


Figure S11. (PNP-Cy)Sc(CH₂SiMe₃)₂ ^1H - ^{13}C HSQC Spectrum.

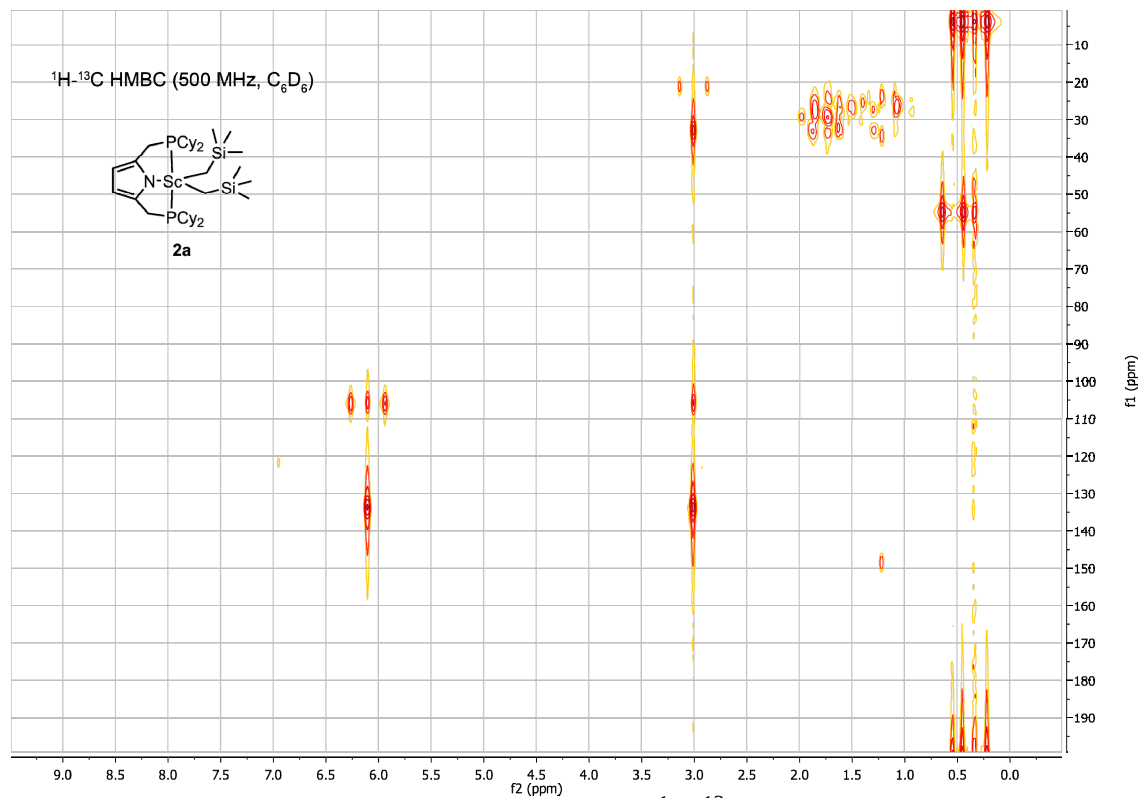


Figure S12. (PNP-Cy)Sc(CH₂SiMe₃)₂ ^1H - ^{13}C HMBC Spectrum.

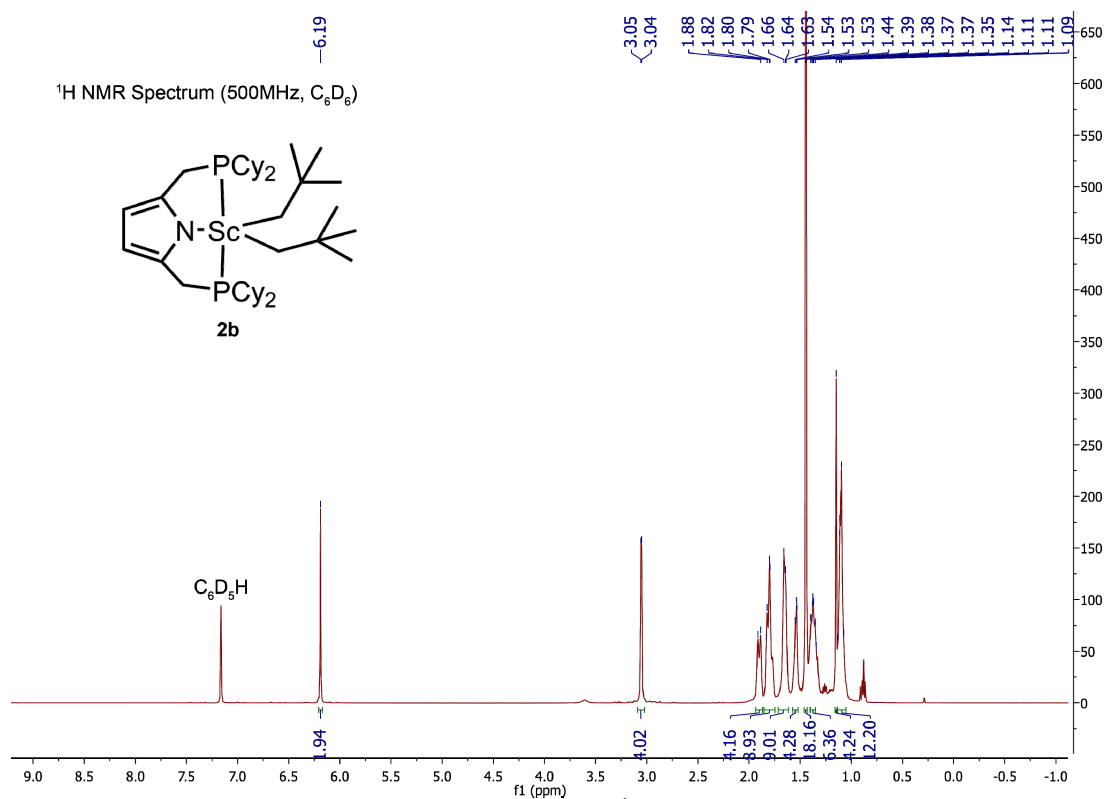


Figure S13. (PNP-Cy)ScNp₂ ¹H NMR Spectrum.

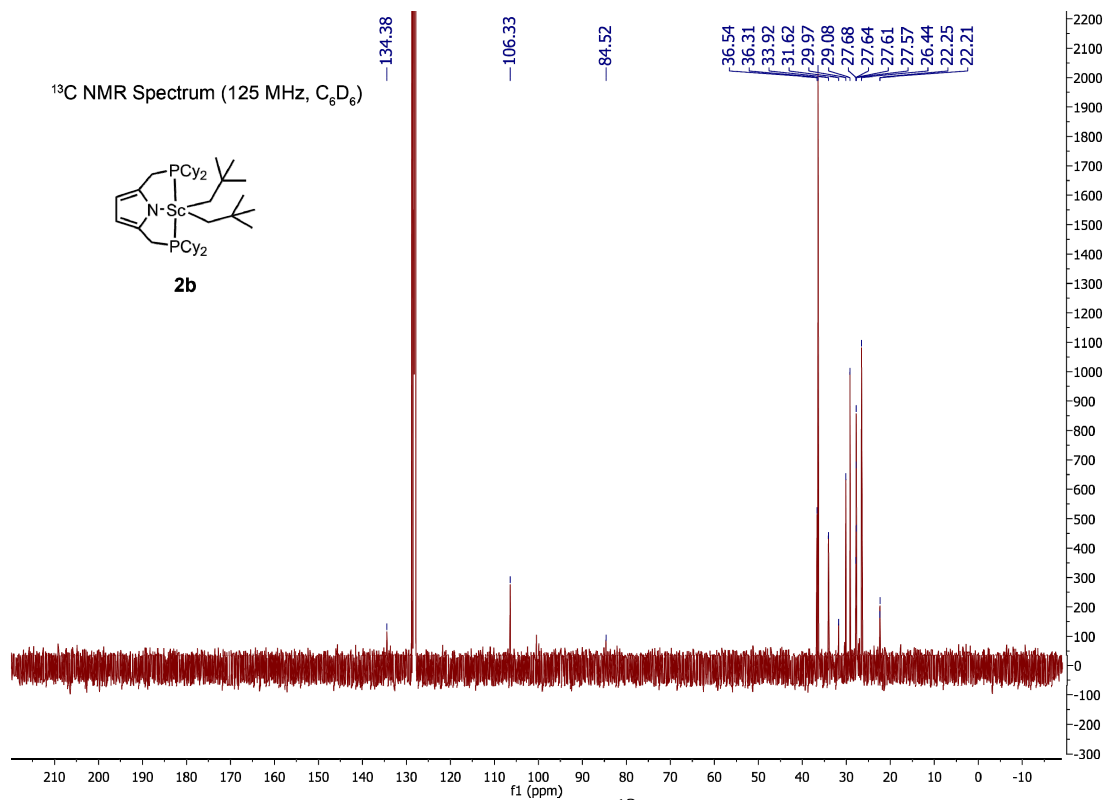
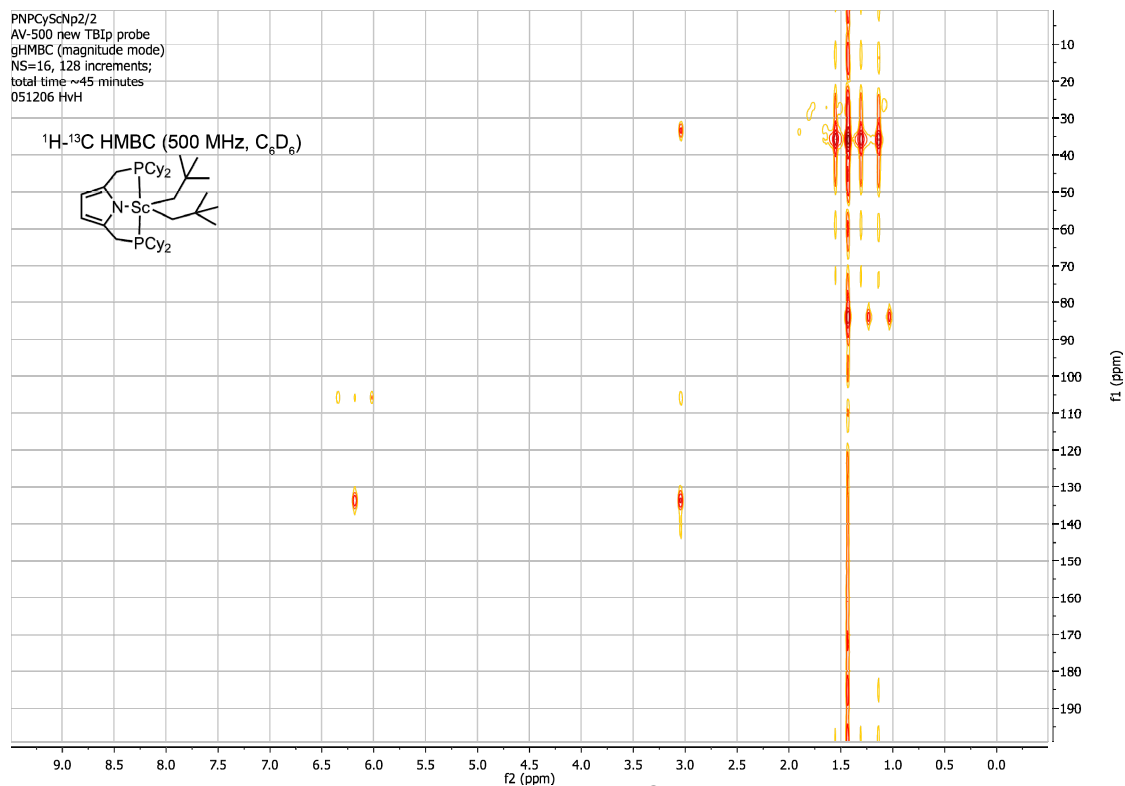
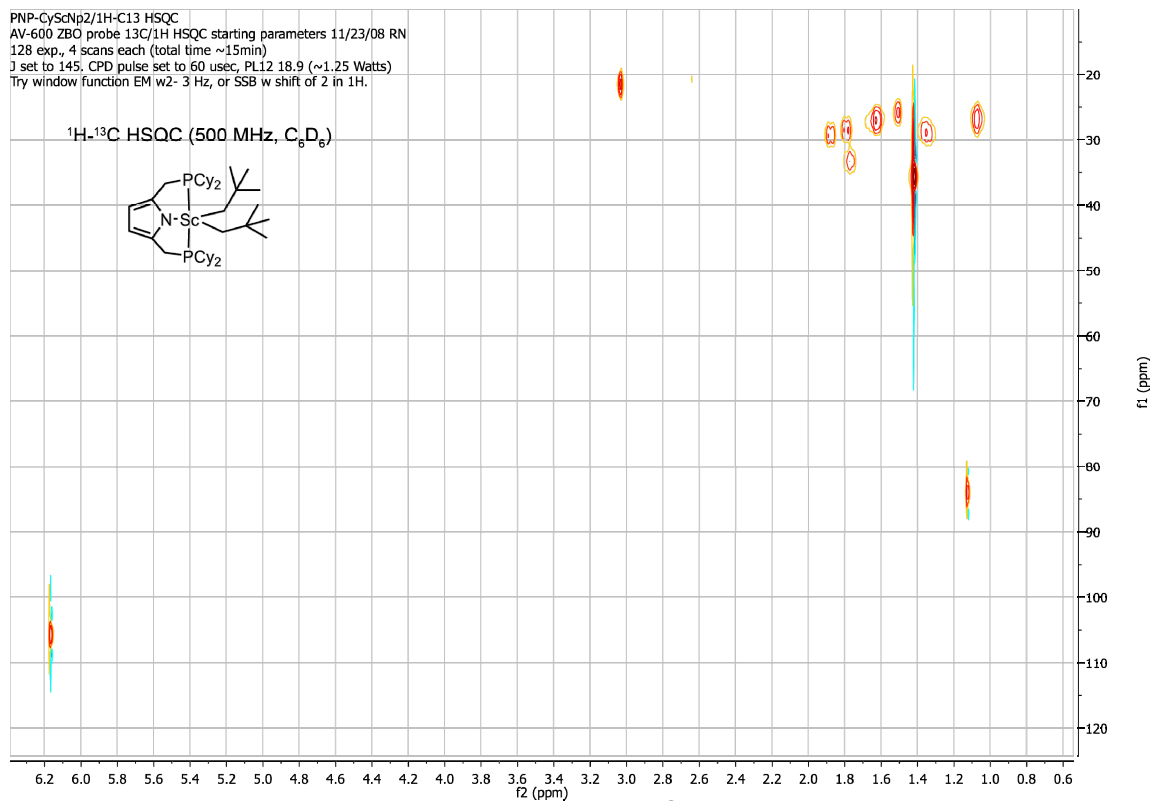


Figure S14. (PNP-Cy)ScNp₂ ¹³C NMR Spectrum:



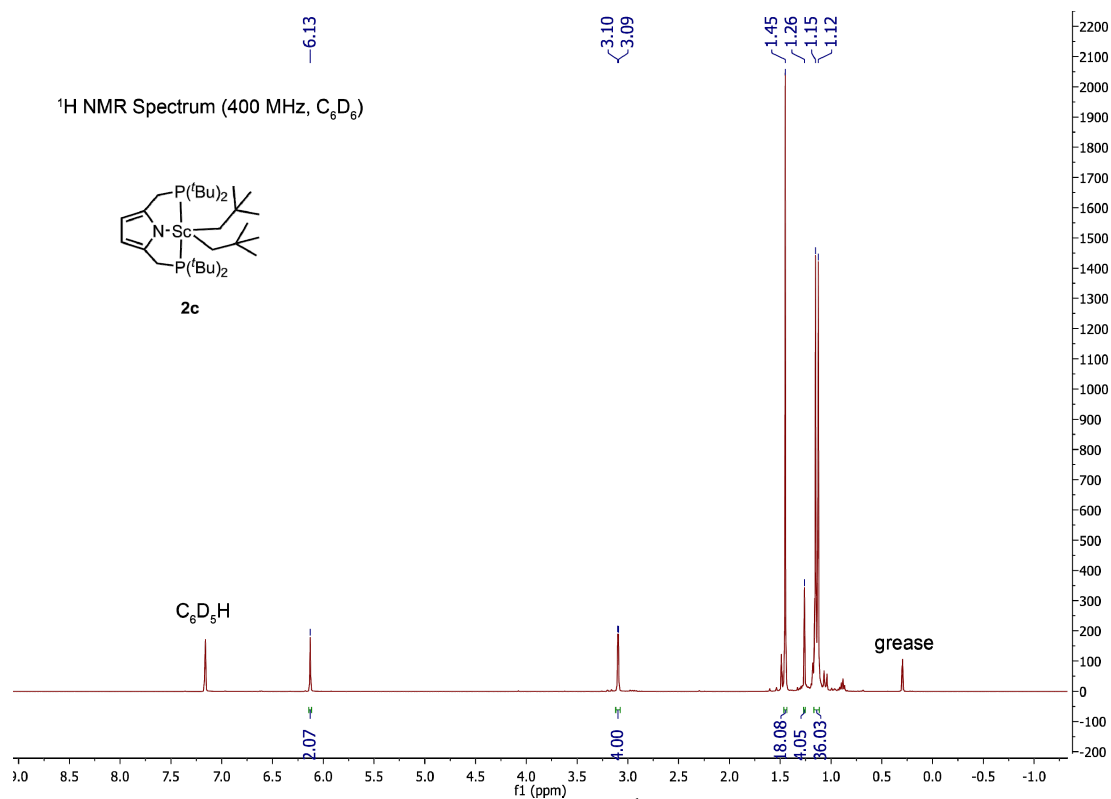


Figure S17. (PNP-*t*Bu)ScNp₂ ¹H NMR Spectrum.

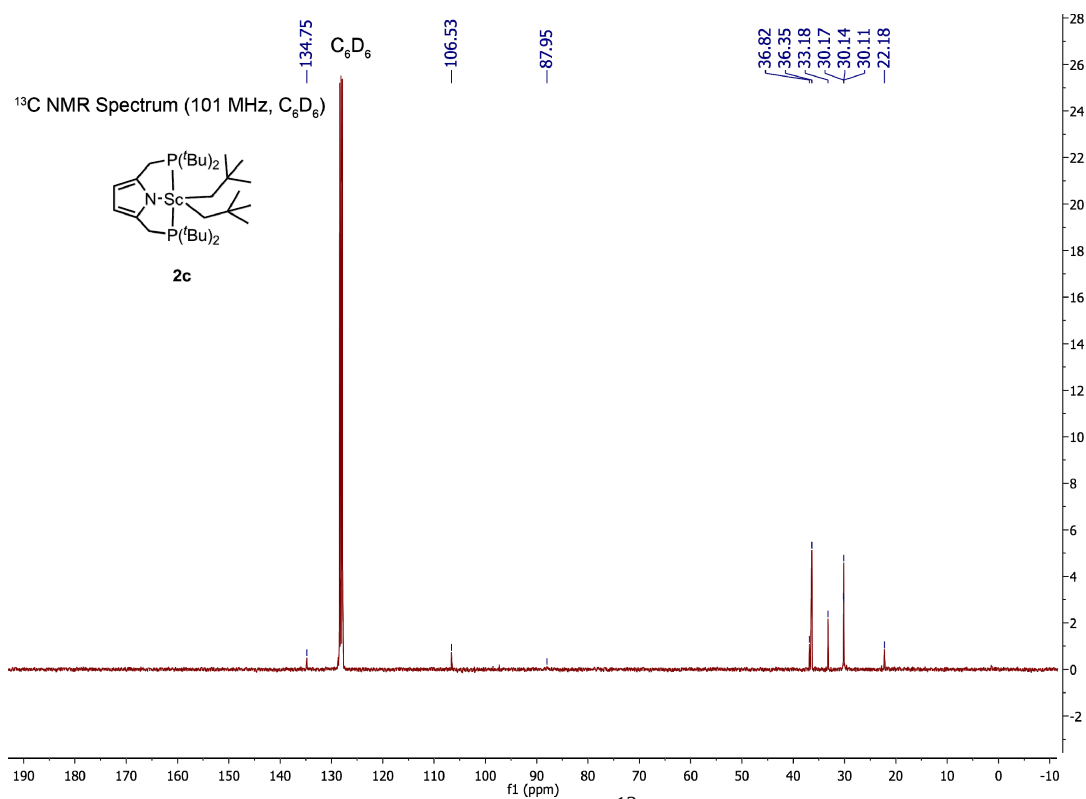


Figure S18. (PNP-*t*Bu)ScNp₂ ¹³C NMR Spectrum

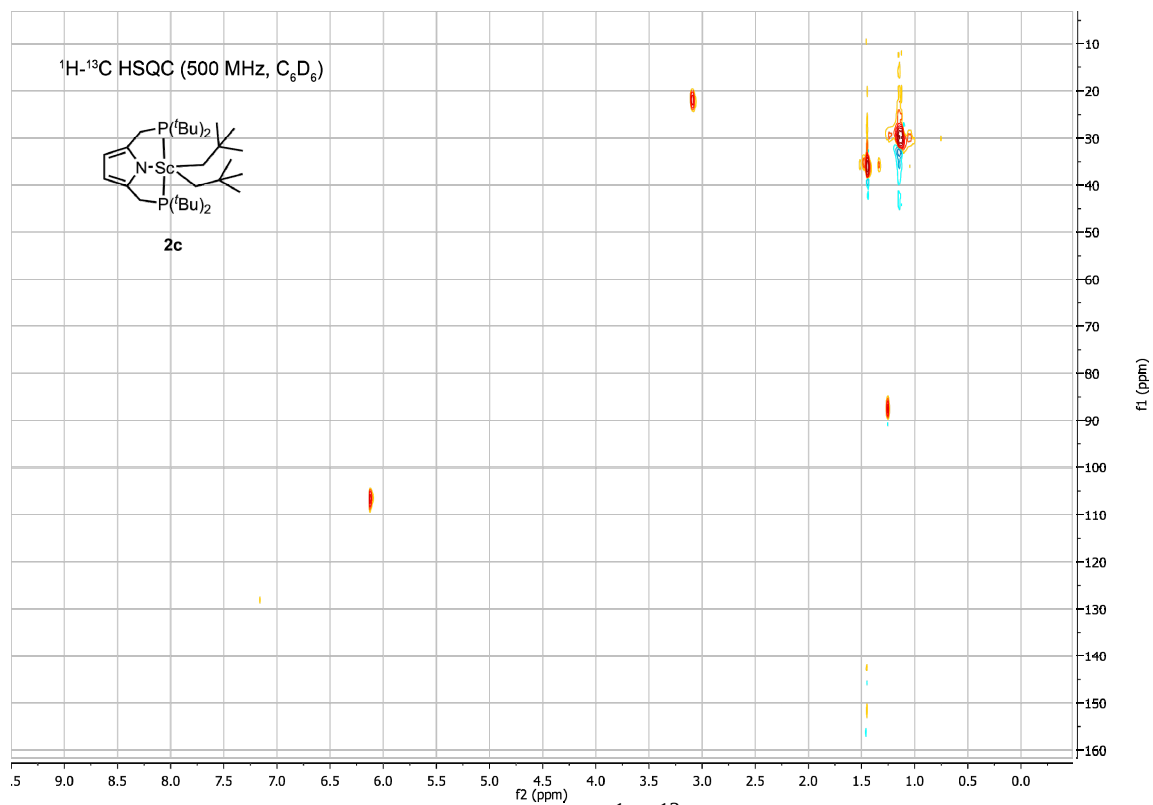


Figure S19. (PNP-*t*Bu)ScNp₂ ^1H - ^{13}C HSQC Spectrum.

2. X-Ray Crystallography

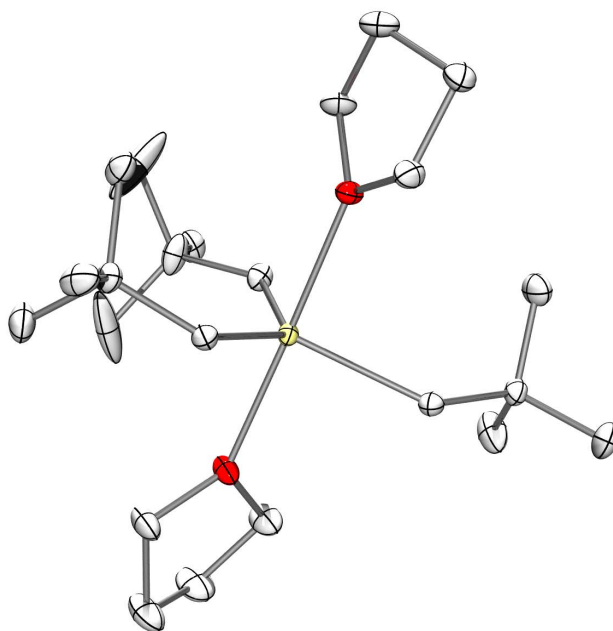


Figure S20. Crystal structure of ScNp₃(THF)₂.

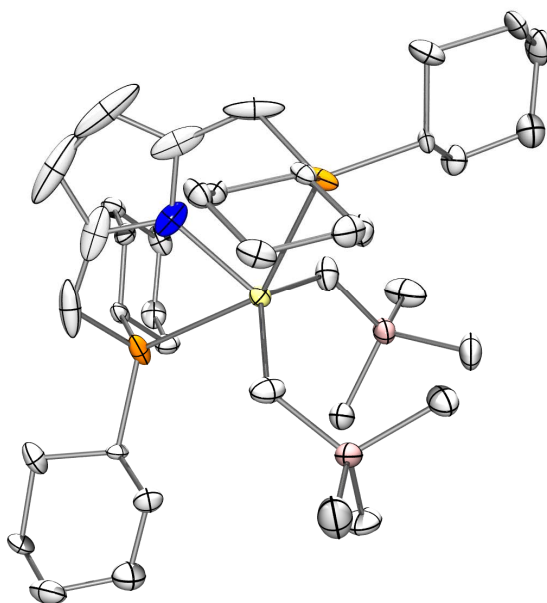


Figure S21. Crystal structure of (PNP-Cy)Sc(CH₂SiMe₃)₂ (**2a**) (Trigonal bipyramidal structure, phosphine occupy axial positions, and pyrrole and alkyl groups occupy equatorial positions).

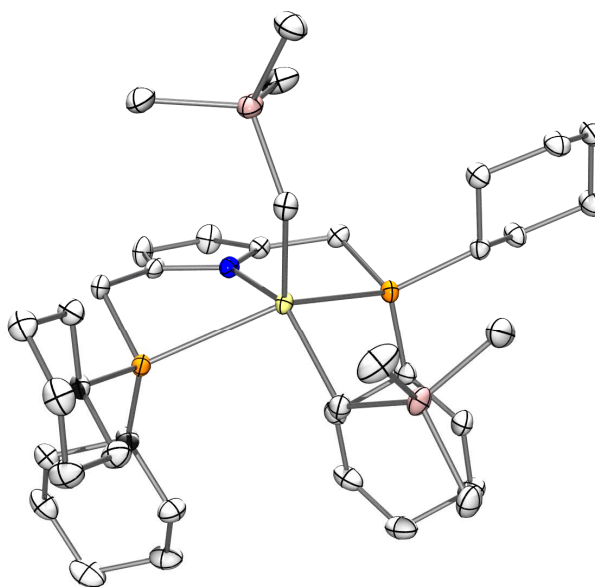


Figure S22. Crystal structure of (PNP-Cy)Sc(CH₂SiMe₃)₂ (**2a**) (Square pyramidal structure, phosphines, pyrrole, and one alkyl group from basal plane, remaining alkyl group is in the apical position).

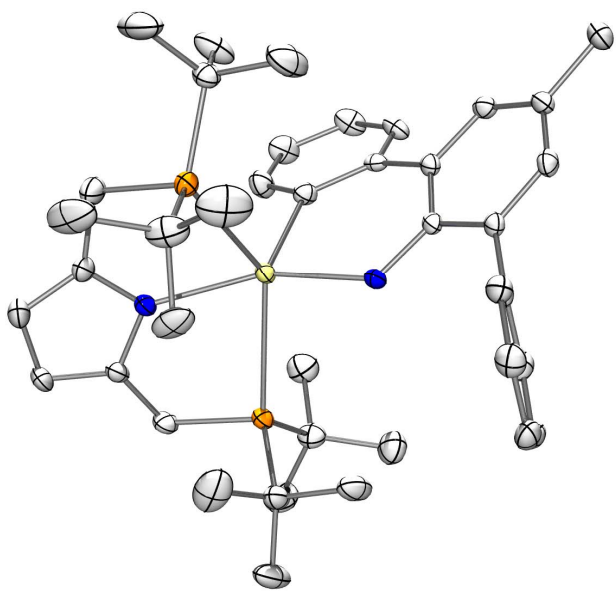


Figure S23. Crystal structure of (PNP-tBu)ScNHAr (**4**).

3. X-ray Data Tables

Table S1. Crystal data and structure refinement for ScNp₃(THF)₂.

Empirical formula	C ₂₃ H ₄₉ O ₂ Sc	
Formula weight	402.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 10.0932(5) Å	α = 90°.
	b = 17.2222(8) Å	β = 93.760(2)°.
	c = 14.5726(6) Å	γ = 90°.
Volume	2527.7(2) Å ³	
Z	4	
Density (calculated)	1.058 Mg/m ³	
Absorption coefficient	0.304 mm ⁻¹	
F(000)	896	
Crystal size	0.10 x 0.10 x 0.05 mm ³	
Theta range for data collection	1.833 to 25.400°.	
Index ranges	-12 ≤ h ≤ 12, -20 ≤ k ≤ 20, -17 ≤ l ≤ 17	
Reflections collected	36715	
Independent reflections	4637 [R(int) = 0.0455]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7452 and 0.6739	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4637 / 0 / 244	
Goodness-of-fit on F ²	1.057	
Final R indices [I > 2σ(I)]	R1 = 0.0358, wR2 = 0.0838	
R indices (all data)	R1 = 0.0466, wR2 = 0.0899	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.274 and -0.282 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{ScNp}_3(\text{THF})_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	4277(2)	907(1)	2994(1)	14(1)
C(2)	5605(2)	-953(1)	3938(1)	15(1)
C(3)	8895(2)	-11(1)	1822(1)	25(1)
C(4)	6279(2)	-1757(1)	4010(1)	17(1)
C(5)	6305(2)	-2129(1)	3056(1)	21(1)
C(6)	7456(2)	273(1)	1901(1)	17(1)
C(7)	2831(2)	-1136(1)	1032(1)	24(1)
C(8)	3366(2)	-905(1)	1984(1)	19(1)
C(9)	3564(2)	1141(1)	1326(1)	23(1)
C(10)	5149(2)	-957(1)	1002(1)	20(1)
C(11)	4048(2)	-1498(1)	644(1)	24(1)
C(12)	3807(2)	1520(1)	2272(1)	16(1)
C(13)	5555(2)	-2319(1)	4628(1)	23(1)
C(14)	9643(2)	484(1)	1161(1)	22(1)
C(15)	7734(2)	428(1)	4913(1)	24(1)
C(16)	7432(2)	1512(1)	3918(1)	24(1)
C(17)	2510(2)	1908(1)	2522(1)	29(1)
C(18)	7712(2)	-1664(1)	4415(1)	26(1)
C(19)	4867(2)	2149(1)	2203(1)	29(1)
C(20)	8553(2)	1685(1)	4617(1)	32(1)
C(21)	8278(2)	1149(1)	5397(1)	32(1)
C(22)	9649(2)	32(2)	2761(2)	62(1)
C(23)	8875(3)	-845(1)	1450(3)	72(1)
O(1)	4732(1)	-660(1)	1876(1)	15(1)
O(2)	7148(1)	687(1)	4023(1)	18(1)
Sc(1)	5931(1)	28(1)	2941(1)	11(1)

Table S3. Bond lengths [Å] and angles [°] for ScNp₃(THF)₂.

C(1)-C(12)	1.544(2)
C(1)-Sc(1)	2.2575(16)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(4)	1.543(2)
C(2)-Sc(1)	2.2678(16)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(14)	1.522(2)
C(3)-C(22)	1.524(3)
C(3)-C(23)	1.536(3)
C(3)-C(6)	1.544(2)
C(4)-C(5)	1.532(2)
C(4)-C(18)	1.535(2)
C(4)-C(13)	1.537(2)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-Sc(1)	2.2700(17)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.509(2)
C(7)-C(11)	1.519(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-O(1)	1.460(2)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(12)	1.530(2)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-O(1)	1.4590(19)
C(10)-C(11)	1.516(2)

C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(19)	1.530(2)
C(12)-C(17)	1.535(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-O(2)	1.459(2)
C(15)-C(21)	1.514(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-O(2)	1.460(2)
C(16)-C(20)	1.501(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.504(3)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800

C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
O(1)-Sc(1)	2.2426(11)
O(2)-Sc(1)	2.2429(11)
C(12)-C(1)-Sc(1)	129.06(11)
C(12)-C(1)-H(1A)	105.0
Sc(1)-C(1)-H(1A)	105.0
C(12)-C(1)-H(1B)	105.0
Sc(1)-C(1)-H(1B)	105.0
H(1A)-C(1)-H(1B)	105.9
C(4)-C(2)-Sc(1)	129.07(11)
C(4)-C(2)-H(2A)	105.0
Sc(1)-C(2)-H(2A)	105.0
C(4)-C(2)-H(2B)	105.0
Sc(1)-C(2)-H(2B)	105.0
H(2A)-C(2)-H(2B)	105.9
C(14)-C(3)-C(22)	107.57(17)
C(14)-C(3)-C(23)	107.21(17)
C(22)-C(3)-C(23)	110.9(2)
C(14)-C(3)-C(6)	112.21(15)
C(22)-C(3)-C(6)	109.55(16)
C(23)-C(3)-C(6)	109.42(17)
C(5)-C(4)-C(18)	108.72(15)
C(5)-C(4)-C(13)	107.78(14)
C(18)-C(4)-C(13)	108.21(14)
C(5)-C(4)-C(2)	110.34(13)
C(18)-C(4)-C(2)	109.40(14)
C(13)-C(4)-C(2)	112.29(14)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5

H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-Sc(1)	132.34(12)
C(3)-C(6)-H(6A)	104.2
Sc(1)-C(6)-H(6A)	104.2
C(3)-C(6)-H(6B)	104.2
Sc(1)-C(6)-H(6B)	104.2
H(6A)-C(6)-H(6B)	105.5
C(8)-C(7)-C(11)	101.56(14)
C(8)-C(7)-H(7A)	111.5
C(11)-C(7)-H(7A)	111.5
C(8)-C(7)-H(7B)	111.5
C(11)-C(7)-H(7B)	111.5
H(7A)-C(7)-H(7B)	109.3
O(1)-C(8)-C(7)	105.13(13)
O(1)-C(8)-H(8A)	110.7
C(7)-C(8)-H(8A)	110.7
O(1)-C(8)-H(8B)	110.7
C(7)-C(8)-H(8B)	110.7
H(8A)-C(8)-H(8B)	108.8
C(12)-C(9)-H(9A)	109.5
C(12)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(12)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(1)-C(10)-C(11)	105.63(14)
O(1)-C(10)-H(10A)	110.6
C(11)-C(10)-H(10A)	110.6
O(1)-C(10)-H(10B)	110.6
C(11)-C(10)-H(10B)	110.6
H(10A)-C(10)-H(10B)	108.7
C(10)-C(11)-C(7)	102.22(14)
C(10)-C(11)-H(11A)	111.3
C(7)-C(11)-H(11A)	111.3
C(10)-C(11)-H(11B)	111.3
C(7)-C(11)-H(11B)	111.3

H(11A)-C(11)-H(11B)	109.2
C(9)-C(12)-C(19)	108.32(15)
C(9)-C(12)-C(17)	108.10(14)
C(19)-C(12)-C(17)	108.58(15)
C(9)-C(12)-C(1)	110.23(14)
C(19)-C(12)-C(1)	110.12(14)
C(17)-C(12)-C(1)	111.41(14)
C(4)-C(13)-H(13A)	109.5
C(4)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(4)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(3)-C(14)-H(14A)	109.5
C(3)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(3)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(2)-C(15)-C(21)	106.07(14)
O(2)-C(15)-H(15A)	110.5
C(21)-C(15)-H(15A)	110.5
O(2)-C(15)-H(15B)	110.5
C(21)-C(15)-H(15B)	110.5
H(15A)-C(15)-H(15B)	108.7
O(2)-C(16)-C(20)	105.49(15)
O(2)-C(16)-H(16A)	110.6
C(20)-C(16)-H(16A)	110.6
O(2)-C(16)-H(16B)	110.6
C(20)-C(16)-H(16B)	110.6
H(16A)-C(16)-H(16B)	108.8
C(12)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5

H(17B)-C(17)-H(17C)	109.5
C(4)-C(18)-H(18A)	109.5
C(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(12)-C(19)-H(19A)	109.5
C(12)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(12)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-C(21)	102.84(16)
C(16)-C(20)-H(20A)	111.2
C(21)-C(20)-H(20A)	111.2
C(16)-C(20)-H(20B)	111.2
C(21)-C(20)-H(20B)	111.2
H(20A)-C(20)-H(20B)	109.1
C(20)-C(21)-C(15)	103.35(15)
C(20)-C(21)-H(21A)	111.1
C(15)-C(21)-H(21A)	111.1
C(20)-C(21)-H(21B)	111.1
C(15)-C(21)-H(21B)	111.1
H(21A)-C(21)-H(21B)	109.1
C(3)-C(22)-H(22A)	109.5
C(3)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(3)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(3)-C(23)-H(23A)	109.5
C(3)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(3)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5

H(23B)-C(23)-H(23C)	109.5
C(10)-O(1)-C(8)	108.71(12)
C(10)-O(1)-Sc(1)	128.02(10)
C(8)-O(1)-Sc(1)	123.24(9)
C(15)-O(2)-C(16)	108.63(13)
C(15)-O(2)-Sc(1)	129.92(10)
C(16)-O(2)-Sc(1)	121.41(10)
O(1)-Sc(1)-O(2)	178.46(4)
O(1)-Sc(1)-C(1)	90.69(5)
O(2)-Sc(1)-C(1)	90.50(5)
O(1)-Sc(1)-C(2)	87.42(5)
O(2)-Sc(1)-C(2)	91.26(5)
C(1)-Sc(1)-C(2)	109.82(6)
O(1)-Sc(1)-C(6)	89.71(5)
O(2)-Sc(1)-C(6)	90.65(5)
C(1)-Sc(1)-C(6)	115.70(6)
C(2)-Sc(1)-C(6)	134.43(6)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{ScNp}_3(\text{THF})_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	13(1)	16(1)	-2(1)	0(1)	0(1)
C(2)	16(1)	13(1)	16(1)	0(1)	-1(1)	0(1)
C(3)	16(1)	24(1)	36(1)	10(1)	10(1)	5(1)
C(4)	21(1)	12(1)	16(1)	3(1)	1(1)	1(1)
C(5)	27(1)	17(1)	20(1)	3(1)	4(1)	6(1)
C(6)	14(1)	16(1)	21(1)	0(1)	2(1)	-1(1)
C(7)	21(1)	21(1)	28(1)	-4(1)	-6(1)	-2(1)
C(8)	13(1)	20(1)	24(1)	-6(1)	1(1)	-3(1)
C(9)	28(1)	21(1)	19(1)	3(1)	-3(1)	2(1)
C(10)	26(1)	22(1)	14(1)	-6(1)	4(1)	-3(1)
C(11)	30(1)	21(1)	20(1)	-7(1)	1(1)	-5(1)
C(12)	16(1)	12(1)	20(1)	0(1)	-2(1)	2(1)
C(13)	38(1)	13(1)	19(1)	2(1)	4(1)	0(1)
C(14)	16(1)	29(1)	22(1)	3(1)	5(1)	-1(1)
C(15)	28(1)	22(1)	20(1)	4(1)	-10(1)	-3(1)
C(16)	31(1)	16(1)	26(1)	2(1)	-5(1)	-6(1)
C(17)	28(1)	25(1)	34(1)	-2(1)	-3(1)	13(1)
C(18)	23(1)	21(1)	34(1)	4(1)	-7(1)	5(1)
C(19)	29(1)	18(1)	39(1)	10(1)	-9(1)	-4(1)
C(20)	35(1)	25(1)	33(1)	-2(1)	-7(1)	-12(1)
C(21)	34(1)	31(1)	28(1)	2(1)	-13(1)	-9(1)
C(22)	18(1)	132(3)	38(1)	48(2)	9(1)	23(1)
C(23)	40(1)	21(1)	160(3)	4(2)	60(2)	6(1)
O(1)	14(1)	16(1)	14(1)	-4(1)	1(1)	-2(1)
O(2)	20(1)	14(1)	18(1)	3(1)	-6(1)	-3(1)
Sc(1)	10(1)	10(1)	13(1)	0(1)	0(1)	0(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $\text{ScNp}_3(\text{THF})_2$.

	x	y	z	U(eq)
H(1A)	3476	598	3103	17
H(1B)	4486	1204	3567	17
H(2A)	5763	-720	4557	18
H(2B)	4641	-1065	3867	18
H(5A)	6820	-1801	2661	32
H(5B)	5395	-2181	2784	32
H(5C)	6716	-2644	3113	32
H(6A)	6998	133	1302	20
H(6B)	7529	846	1895	20
H(7A)	2517	-679	667	28
H(7B)	2098	-1516	1055	28
H(8A)	2840	-473	2223	23
H(8B)	3342	-1350	2413	23
H(9A)	3256	1534	875	35
H(9B)	2887	735	1358	35
H(9C)	4392	910	1140	35
H(10A)	5999	-1242	1094	24
H(10B)	5263	-527	565	24
H(11A)	4196	-2034	876	28
H(11B)	3968	-1507	-36	28
H(13A)	4637	-2387	4379	35
H(13B)	5559	-2105	5251	35
H(13C)	6009	-2822	4646	35
H(14A)	9700	1019	1388	33
H(14B)	9171	476	552	33
H(14C)	10540	275	1118	33
H(15A)	8455	50	4829	29
H(15B)	7054	179	5274	29
H(16A)	6643	1829	4035	29
H(16B)	7696	1624	3289	29

H(17A)	2645	2157	3125	43
H(17B)	1811	1514	2543	43
H(17C)	2246	2299	2057	43
H(18A)	8148	-2173	4447	39
H(18B)	7707	-1443	5034	39
H(18C)	8197	-1317	4022	39
H(19A)	5692	1912	2020	44
H(19B)	5028	2403	2801	44
H(19C)	4560	2535	1742	44
H(20A)	8538	2235	4814	38
H(20B)	9423	1570	4371	38
H(21A)	7618	1378	5792	38
H(21B)	9101	1032	5778	38
H(22A)	10568	-137	2707	94
H(22B)	9221	-308	3193	94
H(22C)	9643	568	2987	94
H(23A)	8387	-859	846	107
H(23B)	8439	-1186	1876	107
H(23C)	9788	-1023	1390	107

Table S6. Crystal data and structure refinement for (PNP-*t*Bu)ScCl₂.

Empirical formula	C ₂₂ H ₄₂ Cl ₂ N ₁ P ₂ Sc	
Formula weight	498.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2(1)	
Unit cell dimensions	a = 12.1315(5) Å	α = 90°.
	b = 27.9260(12) Å	β = 90°.
	c = 15.9238(6) Å	γ = 90°.
Volume	5394.7(4) Å ³	
Z	8	
Density (calculated)	1.227 Mg/m ³	
Absorption coefficient	0.598 mm ⁻¹	
F(000)	2128	
Crystal size	0.10 x 0.10 x 0.03 mm ³	
Theta range for data collection	1.46 to 25.37°.	
Index ranges	-14 ≤ h ≤ 14, -33 ≤ k ≤ 33, -19 ≤ l ≤ 19	
Reflections collected	97035	
Independent reflections	9837 [R(int) = 0.0510]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9823 and 0.9426	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9837 / 1 / 539	
Goodness-of-fit on F ²	1.045	
Final R indices [I > 2σ(I)]	R ₁ = 0.0358, wR ₂ = 0.0720	
R indices (all data)	R ₁ = 0.0427, wR ₂ = 0.0752	
Absolute structure parameter	0.00(2)	
Largest diff. peak and hole	0.739 and -0.761 e.Å ⁻³	

Table S7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-*t*Bu)ScCl₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(23)	4113(3)	8047(1)	7512(2)	24(1)
C(24)	4056(3)	7800(1)	6779(2)	21(1)
C(25)	5023(3)	7911(1)	6323(2)	23(1)
C(26)	5639(2)	8214(1)	6796(2)	16(1)
C(28)	6762(2)	8413(1)	6632(2)	20(1)
C(29)	3693(3)	7951(1)	9969(3)	43(1)
C(30)	4668(5)	7629(2)	9735(7)	177(5)
C(31)	2694(3)	7633(1)	10020(2)	39(1)
C(32)	3863(6)	8187(2)	10804(3)	110(3)
C(33)	2495(3)	8847(1)	9219(3)	41(1)
C(34)	2721(3)	9182(2)	9957(4)	80(2)
C(35)	2511(4)	9142(2)	8409(4)	136(3)
C(36)	1361(3)	8617(2)	9315(3)	45(1)
C(37)	8410(2)	9122(1)	7201(2)	23(1)
C(38)	8977(3)	8674(1)	7557(2)	31(1)
C(39)	8924(3)	9232(1)	6339(2)	26(1)
C(40)	8604(3)	9535(1)	7824(2)	37(1)
C(41)	6163(3)	9432(1)	6412(2)	25(1)
C(42)	6378(3)	9341(1)	5470(2)	36(1)
C(43)	6481(3)	9945(1)	6646(2)	35(1)
C(44)	4914(3)	9368(1)	6569(2)	29(1)
N(2)	5100(2)	8307(1)	7556(2)	22(1)
C(22)	4109(4)	5212(2)	6867(3)	83(2)
C(1)	-801(2)	5751(1)	8776(2)	20(1)
C(2)	-654(3)	5436(1)	9423(2)	25(1)
C(3)	398(3)	5226(1)	9314(2)	25(1)
C(4)	847(2)	5420(1)	8605(2)	19(1)
C(5)	-1789(2)	6048(1)	8562(2)	24(1)
C(6)	1905(3)	5293(1)	8164(2)	26(1)
C(7)	-1007(3)	7016(1)	9036(2)	27(1)
C(8)	-1917(3)	7025(1)	9700(2)	45(1)

C(9)	-767(3)	7528(1)	8734(2)	29(1)
C(10)	52(3)	6818(1)	9432(2)	44(1)
C(11)	-2470(2)	6874(1)	7447(2)	19(1)
C(12)	-3000(3)	6461(1)	6950(2)	28(1)
C(13)	-1932(3)	7218(1)	6818(2)	25(1)
C(14)	-3380(3)	7132(1)	7943(2)	31(1)
C(15)	3433(3)	6117(1)	8353(2)	24(1)
C(16)	2761(4)	6241(2)	9122(3)	72(2)
C(17)	3847(4)	6580(2)	7982(3)	58(1)
C(18)	4399(4)	5815(2)	8612(4)	102(2)
C(19)	3203(3)	5565(1)	6662(2)	25(1)
C(20)	3666(5)	5973(2)	6155(2)	70(2)
C(21)	2345(3)	5314(2)	6120(3)	69(2)
N(1)	124(2)	5756(1)	8259(1)	18(1)
P(1)	-1327(1)	6621(1)	8107(1)	17(1)
P(2)	2457(1)	5816(1)	7595(1)	18(1)
Cl(1)	1284(1)	7045(1)	7167(1)	49(1)
Cl(2)	-248(1)	6048(1)	6010(1)	47(1)
Sc(1)	482(1)	6274(1)	7303(1)	19(1)
P(3)	3663(1)	8409(1)	9109(1)	23(1)
P(4)	6887(1)	9002(1)	7138(1)	17(1)
Cl(3)	5478(1)	9569(1)	8998(1)	27(1)
Cl(4)	7032(1)	8399(1)	9345(1)	27(1)
Sc(2)	5674(1)	8769(1)	8531(1)	18(1)
C(27)	3150(8)	8132(5)	8103(6)	28(2)
C(27A)	3497(16)	7942(5)	8300(8)	27(4)

Table S8. Bond lengths [Å] and angles [°] for (PNP-*t*Bu)ScCl₂.

C(23)-C(24)	1.356(4)
C(23)-N(2)	1.402(4)
C(23)-C(27A)	1.490(10)
C(23)-C(27)	1.519(8)
C(24)-C(25)	1.413(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.357(4)
C(25)-H(25)	0.9500
C(26)-N(2)	1.400(4)
C(26)-C(28)	1.495(4)
C(28)-P(4)	1.837(3)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(32)	1.498(6)
C(29)-C(31)	1.504(5)
C(29)-C(30)	1.531(6)
C(29)-P(3)	1.875(4)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(36)	1.526(5)
C(33)-C(34)	1.528(6)
C(33)-C(35)	1.530(6)
C(33)-P(3)	1.879(4)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800

C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.537(4)
C(37)-C(40)	1.538(4)
C(37)-C(39)	1.539(4)
C(37)-P(4)	1.881(3)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(43)	1.528(4)
C(41)-C(42)	1.544(4)
C(41)-C(44)	1.546(5)
C(41)-P(4)	1.886(3)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
N(2)-Sc(2)	2.135(2)
C(22)-C(19)	1.512(5)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800

C(1)-C(2)	1.366(4)
C(1)-N(1)	1.393(4)
C(1)-C(5)	1.497(4)
C(2)-C(3)	1.415(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.366(4)
C(3)-H(3)	0.9500
C(4)-N(1)	1.397(4)
C(4)-C(6)	1.506(4)
C(5)-P(1)	1.844(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-P(2)	1.843(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.529(5)
C(7)-C(10)	1.534(5)
C(7)-C(9)	1.536(4)
C(7)-P(1)	1.885(3)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(13)	1.533(4)
C(11)-C(14)	1.537(4)
C(11)-C(12)	1.541(4)
C(11)-P(1)	1.878(3)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800

C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(18)	1.502(5)
C(15)-C(17)	1.507(5)
C(15)-C(16)	1.511(5)
C(15)-P(2)	1.890(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.506(5)
C(19)-C(21)	1.523(5)
C(19)-P(2)	1.875(3)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
N(1)-Sc(1)	2.145(2)
P(1)-Sc(1)	2.7198(9)
P(2)-Sc(1)	2.7557(9)
Cl(1)-Sc(1)	2.3717(10)
Cl(2)-Sc(1)	2.3287(11)
P(3)-C(27A)	1.846(9)
P(3)-C(27)	1.885(7)
P(3)-Sc(2)	2.7948(9)
P(4)-Sc(2)	2.7400(9)

Cl(3)-Sc(2)	2.3658(9)
Cl(4)-Sc(2)	2.3373(10)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(27A)-H(27C)	0.9900
C(27A)-H(27D)	0.9900
C(24)-C(23)-N(2)	110.5(3)
C(24)-C(23)-C(27A)	126.8(5)
N(2)-C(23)-C(27A)	119.2(6)
C(24)-C(23)-C(27)	125.0(4)
N(2)-C(23)-C(27)	123.0(4)
C(27A)-C(23)-C(27)	28.7(4)
C(23)-C(24)-C(25)	106.8(3)
C(23)-C(24)-H(24)	126.6
C(25)-C(24)-H(24)	126.6
C(26)-C(25)-C(24)	107.9(3)
C(26)-C(25)-H(25)	126.0
C(24)-C(25)-H(25)	126.0
C(25)-C(26)-N(2)	109.8(3)
C(25)-C(26)-C(28)	129.5(3)
N(2)-C(26)-C(28)	120.5(2)
C(26)-C(28)-P(4)	109.3(2)
C(26)-C(28)-H(28A)	109.8
P(4)-C(28)-H(28A)	109.8
C(26)-C(28)-H(28B)	109.8
P(4)-C(28)-H(28B)	109.8
H(28A)-C(28)-H(28B)	108.3
C(32)-C(29)-C(31)	108.8(4)
C(32)-C(29)-C(30)	111.7(6)
C(31)-C(29)-C(30)	106.8(4)
C(32)-C(29)-P(3)	110.5(3)
C(31)-C(29)-P(3)	115.2(3)
C(30)-C(29)-P(3)	103.7(4)
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5

H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(29)-C(31)-H(31A)	109.5
C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(29)-C(32)-H(32A)	109.5
C(29)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(29)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(36)-C(33)-C(34)	110.0(4)
C(36)-C(33)-C(35)	108.8(3)
C(34)-C(33)-C(35)	108.4(4)
C(36)-C(33)-P(3)	114.5(3)
C(34)-C(33)-P(3)	109.6(3)
C(35)-C(33)-P(3)	105.3(3)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5

H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(40)	107.7(3)
C(38)-C(37)-C(39)	108.0(3)
C(40)-C(37)-C(39)	111.4(2)
C(38)-C(37)-P(4)	108.3(2)
C(40)-C(37)-P(4)	108.6(2)
C(39)-C(37)-P(4)	112.7(2)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(43)-C(41)-C(42)	110.4(3)
C(43)-C(41)-C(44)	108.4(3)
C(42)-C(41)-C(44)	107.7(3)
C(43)-C(41)-P(4)	109.3(2)
C(42)-C(41)-P(4)	114.3(2)
C(44)-C(41)-P(4)	106.5(2)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5

H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(41)-C(44)-H(44A)	109.5
C(41)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(41)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(26)-N(2)-C(23)	105.0(2)
C(26)-N(2)-Sc(2)	126.05(19)
C(23)-N(2)-Sc(2)	128.93(19)
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(2)-C(1)-N(1)	110.3(3)
C(2)-C(1)-C(5)	129.3(3)
N(1)-C(1)-C(5)	120.3(2)
C(1)-C(2)-C(3)	107.0(3)
C(1)-C(2)-H(2)	126.5
C(3)-C(2)-H(2)	126.5
C(4)-C(3)-C(2)	107.2(3)
C(4)-C(3)-H(3)	126.4
C(2)-C(3)-H(3)	126.4
C(3)-C(4)-N(1)	110.0(3)
C(3)-C(4)-C(6)	129.2(3)

N(1)-C(4)-C(6)	120.6(3)
C(1)-C(5)-P(1)	109.1(2)
C(1)-C(5)-H(5A)	109.9
P(1)-C(5)-H(5A)	109.9
C(1)-C(5)-H(5B)	109.9
P(1)-C(5)-H(5B)	109.9
H(5A)-C(5)-H(5B)	108.3
C(4)-C(6)-P(2)	110.6(2)
C(4)-C(6)-H(6A)	109.5
P(2)-C(6)-H(6A)	109.5
C(4)-C(6)-H(6B)	109.5
P(2)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1
C(8)-C(7)-C(10)	109.1(3)
C(8)-C(7)-C(9)	109.8(3)
C(10)-C(7)-C(9)	107.8(3)
C(8)-C(7)-P(1)	113.8(2)
C(10)-C(7)-P(1)	106.5(2)
C(9)-C(7)-P(1)	109.7(2)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5

H(10B)-C(10)-H(10C)	109.5
C(13)-C(11)-C(14)	110.4(2)
C(13)-C(11)-C(12)	108.2(2)
C(14)-C(11)-C(12)	108.4(2)
C(13)-C(11)-P(1)	106.67(19)
C(14)-C(11)-P(1)	114.8(2)
C(12)-C(11)-P(1)	108.3(2)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(18)-C(15)-C(17)	109.2(4)
C(18)-C(15)-C(16)	109.1(4)
C(17)-C(15)-C(16)	107.6(3)
C(18)-C(15)-P(2)	114.5(2)
C(17)-C(15)-P(2)	109.9(2)
C(16)-C(15)-P(2)	106.3(2)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5

H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-C(22)	109.7(4)
C(20)-C(19)-C(21)	107.4(3)
C(22)-C(19)-C(21)	108.7(4)
C(20)-C(19)-P(2)	108.8(2)
C(22)-C(19)-P(2)	115.0(2)
C(21)-C(19)-P(2)	106.9(2)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(1)-N(1)-C(4)	105.4(2)
C(1)-N(1)-Sc(1)	126.18(19)
C(4)-N(1)-Sc(1)	127.29(19)
C(5)-P(1)-C(11)	108.80(14)
C(5)-P(1)-C(7)	105.15(14)

C(11)-P(1)-C(7)	111.80(14)
C(5)-P(1)-Sc(1)	96.94(10)
C(11)-P(1)-Sc(1)	117.80(9)
C(7)-P(1)-Sc(1)	114.32(11)
C(6)-P(2)-C(19)	105.60(15)
C(6)-P(2)-C(15)	105.49(15)
C(19)-P(2)-C(15)	111.71(14)
C(6)-P(2)-Sc(1)	97.79(10)
C(19)-P(2)-Sc(1)	117.31(10)
C(15)-P(2)-Sc(1)	116.48(10)
N(1)-Sc(1)-Cl(2)	111.62(7)
N(1)-Sc(1)-Cl(1)	139.44(7)
Cl(2)-Sc(1)-Cl(1)	108.73(5)
N(1)-Sc(1)-P(1)	75.09(7)
Cl(2)-Sc(1)-P(1)	101.88(3)
Cl(1)-Sc(1)-P(1)	92.90(3)
N(1)-Sc(1)-P(2)	75.08(7)
Cl(2)-Sc(1)-P(2)	110.76(4)
Cl(1)-Sc(1)-P(2)	94.61(3)
P(1)-Sc(1)-P(2)	141.94(3)
C(27A)-P(3)-C(29)	91.7(5)
C(27A)-P(3)-C(33)	116.3(7)
C(29)-P(3)-C(33)	113.02(17)
C(27A)-P(3)-C(27)	23.1(3)
C(29)-P(3)-C(27)	110.4(5)
C(33)-P(3)-C(27)	95.6(5)
C(27A)-P(3)-Sc(2)	96.9(4)
C(29)-P(3)-Sc(2)	117.94(12)
C(33)-P(3)-Sc(2)	117.06(11)
C(27)-P(3)-Sc(2)	99.0(2)
C(28)-P(4)-C(37)	105.33(14)
C(28)-P(4)-C(41)	105.32(14)
C(37)-P(4)-C(41)	112.10(14)
C(28)-P(4)-Sc(2)	95.64(10)
C(37)-P(4)-Sc(2)	121.77(10)
C(41)-P(4)-Sc(2)	113.44(10)

N(2)-Sc(2)-Cl(4)	111.47(8)
N(2)-Sc(2)-Cl(3)	139.98(8)
Cl(4)-Sc(2)-Cl(3)	108.32(3)
N(2)-Sc(2)-P(4)	74.32(7)
Cl(4)-Sc(2)-P(4)	100.11(3)
Cl(3)-Sc(2)-P(4)	94.85(3)
N(2)-Sc(2)-P(3)	74.78(7)
Cl(4)-Sc(2)-P(3)	105.89(3)
Cl(3)-Sc(2)-P(3)	98.50(3)
P(4)-Sc(2)-P(3)	145.15(3)
C(23)-C(27)-P(3)	109.7(5)
C(23)-C(27)-H(27A)	109.7
P(3)-C(27)-H(27A)	109.7
C(23)-C(27)-H(27B)	109.7
P(3)-C(27)-H(27B)	109.7
H(27A)-C(27)-H(27B)	108.2
C(23)-C(27A)-P(3)	113.2(6)
C(23)-C(27A)-H(27C)	108.9
P(3)-C(27A)-H(27C)	108.9
C(23)-C(27A)-H(27D)	108.9
P(3)-C(27A)-H(27D)	108.9
H(27C)-C(27A)-H(27D)	107.8

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-*t*Bu)ScCl₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(23)	30(2)	22(2)	21(2)	-4(1)	3(1)	-13(1)
C(24)	24(2)	23(2)	17(1)	-3(1)	-2(1)	-9(1)
C(25)	26(2)	27(2)	16(1)	-9(1)	-1(1)	-1(1)
C(26)	20(2)	13(1)	17(1)	-1(1)	2(1)	2(1)
C(28)	24(2)	16(2)	20(1)	-4(1)	2(1)	0(1)
C(29)	26(2)	28(2)	75(3)	17(2)	3(2)	-4(2)
C(30)	60(4)	69(4)	403(14)	138(6)	108(6)	39(3)
C(31)	44(2)	36(2)	36(2)	0(2)	20(2)	-12(2)
C(32)	178(6)	96(4)	56(3)	52(3)	-80(4)	-103(4)
C(33)	20(2)	43(2)	59(2)	25(2)	-5(2)	-1(2)
C(34)	34(3)	39(2)	166(6)	-51(3)	13(3)	3(2)
C(35)	29(2)	195(7)	184(7)	172(6)	-8(3)	-12(3)
C(36)	28(2)	57(3)	49(2)	18(2)	3(2)	-9(2)
C(37)	22(2)	23(2)	25(2)	-2(1)	3(1)	-6(1)
C(38)	19(2)	39(2)	34(2)	10(2)	-1(1)	-4(1)
C(39)	23(2)	25(2)	29(2)	0(1)	9(1)	-5(1)
C(40)	35(2)	41(2)	33(2)	-12(2)	6(2)	-16(2)
C(41)	26(2)	22(2)	26(2)	2(1)	6(1)	10(1)
C(42)	35(2)	49(2)	24(2)	7(2)	1(2)	20(2)
C(43)	37(2)	18(2)	50(2)	7(2)	14(2)	7(2)
C(44)	31(2)	29(2)	26(2)	0(1)	3(1)	12(2)
N(2)	29(1)	21(1)	16(1)	-5(1)	5(1)	-9(1)
C(22)	87(4)	119(4)	43(3)	6(3)	14(2)	84(4)
C(1)	22(2)	18(2)	19(1)	2(1)	2(1)	-7(1)
C(2)	32(2)	23(2)	21(2)	3(1)	1(1)	-10(2)
C(3)	36(2)	18(2)	21(2)	5(1)	-12(1)	-7(1)
C(4)	24(2)	11(1)	23(2)	1(1)	-9(1)	-6(1)
C(5)	24(2)	21(2)	25(2)	2(1)	6(1)	-6(1)
C(6)	27(2)	17(2)	34(2)	4(1)	-5(2)	1(1)
C(7)	40(2)	24(2)	16(1)	-2(1)	-5(1)	-3(2)
C(8)	69(3)	46(2)	20(2)	-6(2)	8(2)	-8(2)

C(9)	37(2)	24(2)	24(2)	-3(1)	-4(1)	-2(2)
C(10)	63(3)	25(2)	43(2)	1(2)	-34(2)	-2(2)
C(11)	15(1)	23(2)	20(2)	-1(1)	-3(1)	1(1)
C(12)	24(2)	32(2)	28(2)	-3(1)	-6(1)	-4(2)
C(13)	25(2)	26(2)	23(2)	5(1)	-6(1)	0(1)
C(14)	20(2)	34(2)	40(2)	-3(2)	3(2)	5(2)
C(15)	22(2)	20(2)	29(2)	-3(1)	-7(1)	1(1)
C(16)	55(3)	130(4)	31(2)	-36(3)	6(2)	-50(3)
C(17)	74(3)	53(3)	47(2)	5(2)	-14(2)	-38(2)
C(18)	86(4)	50(3)	169(6)	-45(3)	-101(4)	34(3)
C(19)	19(2)	30(2)	26(2)	-2(1)	-2(1)	9(1)
C(20)	135(5)	44(3)	32(2)	-4(2)	31(3)	-19(3)
C(21)	36(2)	104(4)	67(3)	-64(3)	10(2)	-15(2)
N(1)	22(1)	15(1)	16(1)	2(1)	-2(1)	-1(1)
P(1)	16(1)	18(1)	17(1)	1(1)	0(1)	-1(1)
P(2)	18(1)	15(1)	22(1)	1(1)	-2(1)	2(1)
Cl(1)	27(1)	25(1)	95(1)	28(1)	19(1)	2(1)
Cl(2)	63(1)	62(1)	17(1)	-5(1)	-3(1)	29(1)
Sc(1)	17(1)	20(1)	21(1)	9(1)	3(1)	2(1)
P(3)	28(1)	24(1)	17(1)	-7(1)	9(1)	-10(1)
P(4)	20(1)	14(1)	16(1)	-2(1)	3(1)	-1(1)
Cl(3)	35(1)	20(1)	26(1)	-8(1)	5(1)	-4(1)
Cl(4)	35(1)	28(1)	18(1)	-2(1)	-3(1)	-3(1)
Sc(2)	24(1)	18(1)	13(1)	-5(1)	3(1)	-7(1)
C(27)	31(4)	32(6)	20(4)	-6(4)	4(3)	-16(4)
C(27A)	50(9)	13(6)	18(5)	-4(4)	9(5)	-17(5)

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-*t*Bu)ScCl₂.

	x	y	z	U(eq)
H(24)	3478	7593	6606	26
H(25)	5209	7793	5781	27
H(28A)	6882	8445	6020	24
H(28B)	7329	8193	6859	24
H(30A)	4546	7307	9959	266
H(30B)	5347	7762	9972	266
H(30C)	4734	7613	9122	266
H(31A)	2824	7379	10433	58
H(31B)	2553	7490	9469	58
H(31C)	2054	7824	10192	58
H(32A)	3240	8400	10923	165
H(32B)	4546	8374	10792	165
H(32C)	3913	7942	11243	165
H(34A)	2192	9447	9947	120
H(34B)	3472	9310	9912	120
H(34C)	2645	9005	10485	120
H(35A)	2472	8927	7924	205
H(35B)	3194	9329	8383	205
H(35C)	1877	9360	8403	205
H(36A)	789	8861	9240	67
H(36B)	1296	8476	9876	67
H(36C)	1270	8366	8890	67
H(38A)	8973	8420	7132	46
H(38B)	8579	8564	8057	46
H(38C)	9739	8751	7708	46
H(39A)	8631	9535	6126	38
H(39B)	8741	8974	5945	38
H(39C)	9726	9255	6396	38
H(40A)	9396	9598	7870	55
H(40B)	8312	9446	8376	55

H(40C)	8228	9823	7623	55
H(42A)	5996	9584	5135	54
H(42B)	6104	9023	5317	54
H(42C)	7172	9358	5359	54
H(43A)	7272	9991	6554	52
H(43B)	6308	10002	7239	52
H(43C)	6066	10170	6296	52
H(44A)	4749	9434	7160	43
H(44B)	4699	9039	6432	43
H(44C)	4501	9592	6213	43
H(22A)	4397	5074	6346	124
H(22B)	3813	4956	7223	124
H(22C)	4704	5377	7166	124
H(2)	-1162	5369	9862	30
H(3)	731	4994	9668	30
H(5A)	-2230	6109	9074	28
H(5B)	-2258	5875	8153	28
H(6A)	1768	5029	7763	31
H(6B)	2453	5181	8580	31
H(8A)	-1682	7222	10176	68
H(8B)	-2063	6698	9895	68
H(8C)	-2591	7159	9456	68
H(9A)	-1446	7672	8517	43
H(9B)	-211	7519	8288	43
H(9C)	-490	7719	9205	43
H(10A)	649	6826	9017	65
H(10B)	-71	6487	9613	65
H(10C)	255	7014	9918	65
H(12A)	-3516	6592	6535	42
H(12B)	-3398	6250	7337	42
H(12C)	-2424	6278	6661	42
H(13A)	-1397	7043	6474	37
H(13B)	-1554	7475	7124	37
H(13C)	-2500	7357	6455	37
H(14A)	-3075	7420	8207	47
H(14B)	-3669	6918	8378	47

H(14C)	-3978	7223	7561	47
H(16A)	2394	5952	9332	108
H(16B)	2206	6482	8974	108
H(16C)	3248	6370	9558	108
H(17A)	4257	6759	8409	87
H(17B)	3220	6771	7788	87
H(17C)	4333	6510	7506	87
H(18A)	4843	5737	8117	153
H(18B)	4134	5519	8873	153
H(18C)	4852	5993	9016	153
H(20A)	4256	6130	6474	105
H(20B)	3081	6206	6037	105
H(20C)	3964	5850	5625	105
H(21A)	1753	5540	5981	104
H(21B)	2037	5042	6428	104
H(21C)	2692	5201	5601	104
H(27A)	2778	7825	8226	33
H(27B)	2608	8348	7833	33
H(27C)	3756	7632	8530	32
H(27D)	2704	7908	8165	32

Table S11. Crystal data and structure refinement for (PNP-*t*Bu)ScNp₂.

Empirical formula	C ₃₂ H ₆₄ N ₂ P ₂ Sc	
Formula weight	569.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.2218(5) Å	α = 90°.
	b = 11.6604(4) Å	β = 108.445(2)°.
	c = 21.0181(8) Å	γ = 90°.
Volume	3538.9(2) Å ³	
Z	4	
Density (calculated)	1.069 Mg/m ³	
Absorption coefficient	0.317 mm ⁻¹	
F(000)	1256	
Crystal size	0.10 x 0.09 x 0.08 mm ³	
Theta range for data collection	1.41 to 25.40°.	
Index ranges	-18 ≤ h ≤ 18, -13 ≤ k ≤ 14, -25 ≤ l ≤ 25	
Reflections collected	47510	
Independent reflections	6499 [R(int) = 0.0331]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9751 and 0.9690	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6499 / 0 / 368	
Goodness-of-fit on F ²	1.038	
Final R indices [I > 2σ(I)]	R1 = 0.0468, wR2 = 0.1191	
R indices (all data)	R1 = 0.0548, wR2 = 0.1252	
Largest diff. peak and hole	1.528 and -0.622 e.Å ⁻³	

Table S12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-*t*Bu)ScNp₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4201(2)	4605(3)	1697(2)	45(1)
C(2)	4933(2)	3776(3)	1647(2)	36(1)
C(3)	4708(3)	3203(4)	982(2)	63(1)
C(4)	4948(3)	2790(3)	2169(2)	51(1)
C(5)	5917(2)	4245(4)	1890(2)	67(1)
C(6)	1910(2)	3003(2)	979(1)	38(1)
C(7)	1724(2)	1724(2)	1000(2)	36(1)
C(11)	1083(2)	6296(2)	417(1)	17(1)
C(12)	1275(2)	6638(2)	1135(1)	16(1)
C(13)	955(2)	7560(2)	1405(1)	23(1)
C(14)	1408(2)	7519(2)	2108(1)	23(1)
C(15)	1980(2)	6580(2)	2229(1)	16(1)
C(16)	2636(2)	6129(2)	2876(1)	18(1)
C(17)	1912(2)	5347(2)	-573(1)	18(1)
C(18)	1070(2)	4551(2)	-710(1)	21(1)
C(19)	2738(2)	4626(2)	-619(1)	28(1)
C(20)	1668(2)	6257(2)	-1124(1)	29(1)
C(21)	2857(2)	7297(2)	407(1)	18(1)
C(22)	3665(2)	7178(2)	120(1)	28(1)
C(23)	2236(2)	8307(2)	72(1)	30(1)
C(24)	3279(2)	7585(2)	1157(1)	24(1)
C(25)	1438(2)	4194(2)	2962(1)	20(1)
C(26)	705(2)	4324(3)	2268(1)	33(1)
C(28)	1170(2)	4990(3)	3450(1)	30(1)
C(27)	1417(2)	2950(2)	3181(2)	33(1)
C(29)	3579(2)	4082(2)	3617(1)	22(1)
C(30)	3425(2)	4314(3)	4295(1)	37(1)
C(31)	3758(2)	2797(2)	3553(2)	31(1)
C(32)	4451(2)	4739(2)	3617(1)	27(1)
N(1)	1908(1)	6016(2)	1635(1)	14(1)
P(1)	2204(1)	5893(1)	314(1)	12(1)

P(2)	2597(1)	4545(1)	2856(1)	15(1)
Sc(1)	2668(1)	4502(1)	1499(1)	15(1)
C(8)	1730(9)	1373(8)	1746(6)	43(3)
C(9)	2769(9)	1096(9)	1071(7)	37(3)
C(10)	1010(13)	1174(13)	578(8)	62(2)
C(8A)	949(8)	1556(6)	1326(5)	92(4)
C(9A)	2506(6)	1092(6)	1374(5)	74(3)
C(10A)	1256(6)	1244(6)	279(4)	62(2)

Table S13. Bond lengths [Å] and angles [°] for (PNP-*t*Bu)ScNp₂.

C(1)-C(2)	1.503(4)
C(1)-Sc(1)	2.240(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.489(5)
C(2)-C(5)	1.524(5)
C(2)-C(4)	1.585(4)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.522(4)
C(6)-Sc(1)	2.187(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(10)	1.331(16)
C(7)-C(9A)	1.408(8)
C(7)-C(8A)	1.553(7)
C(7)-C(10A)	1.560(7)
C(7)-C(8)	1.617(10)
C(7)-C(9)	1.715(12)
C(11)-C(12)	1.499(3)
C(11)-P(1)	1.847(2)
C(11)-H(15A)	0.9900
C(11)-H(15B)	0.9900
C(12)-C(13)	1.375(3)
C(12)-N(1)	1.385(3)
C(13)-C(14)	1.419(3)
C(13)-H(17)	0.9500

C(14)-C(15)	1.372(3)
C(14)-H(18)	0.9500
C(15)-N(1)	1.385(3)
C(15)-C(16)	1.505(3)
C(16)-P(2)	1.848(2)
C(16)-H(20A)	0.9900
C(16)-H(20B)	0.9900
C(17)-C(20)	1.526(3)
C(17)-C(18)	1.535(3)
C(17)-C(19)	1.542(3)
C(17)-P(1)	1.886(2)
C(18)-H(22A)	0.9800
C(18)-H(22B)	0.9800
C(18)-H(22C)	0.9800
C(19)-H(23A)	0.9800
C(19)-H(23B)	0.9800
C(19)-H(23C)	0.9800
C(20)-H(24A)	0.9800
C(20)-H(24B)	0.9800
C(20)-H(24C)	0.9800
C(21)-C(23)	1.534(3)
C(21)-C(22)	1.538(3)
C(21)-C(24)	1.539(3)
C(21)-P(1)	1.894(2)
C(22)-H(26A)	0.9800
C(22)-H(26B)	0.9800
C(22)-H(26C)	0.9800
C(23)-H(27A)	0.9800
C(23)-H(27B)	0.9800
C(23)-H(27C)	0.9800
C(24)-H(28A)	0.9800
C(24)-H(28B)	0.9800
C(24)-H(28C)	0.9800
C(25)-C(27)	1.526(4)
C(25)-C(28)	1.531(3)
C(25)-C(26)	1.538(3)

C(25)-P(2)	1.891(2)
C(26)-H(30A)	0.9800
C(26)-H(30B)	0.9800
C(26)-H(30C)	0.9800
C(28)-H(31A)	0.9800
C(28)-H(31B)	0.9800
C(28)-H(31C)	0.9800
C(27)-H(32A)	0.9800
C(27)-H(32B)	0.9800
C(27)-H(32C)	0.9800
C(29)-C(32)	1.532(4)
C(29)-C(31)	1.537(4)
C(29)-C(30)	1.541(3)
C(29)-P(2)	1.889(2)
C(30)-H(34A)	0.9800
C(30)-H(34B)	0.9800
C(30)-H(34C)	0.9800
C(31)-H(35A)	0.9800
C(31)-H(35B)	0.9800
C(31)-H(35C)	0.9800
C(32)-H(36A)	0.9800
C(32)-H(36B)	0.9800
C(32)-H(36C)	0.9800
N(1)-Sc(1)	2.1783(19)
P(1)-Sc(1)	2.8667(7)
P(2)-Sc(1)	2.8887(7)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(8A)-H(8A1)	0.9800

C(8A)-H(8A2)	0.9800
C(8A)-H(8A3)	0.9800
C(9A)-H(9A1)	0.9800
C(9A)-H(9A2)	0.9800
C(9A)-H(9A3)	0.9800
C(10A)-H(10D)	0.9800
C(10A)-H(10E)	0.9800
C(10A)-H(10F)	0.9800

C(2)-C(1)-Sc(1)	134.7(3)
C(2)-C(1)-H(1A)	103.5
Sc(1)-C(1)-H(1A)	103.5
C(2)-C(1)-H(1B)	103.5
Sc(1)-C(1)-H(1B)	103.5
H(1A)-C(1)-H(1B)	105.3
C(3)-C(2)-C(1)	113.5(3)
C(3)-C(2)-C(5)	112.7(3)
C(1)-C(2)-C(5)	114.7(3)
C(3)-C(2)-C(4)	105.9(3)
C(1)-C(2)-C(4)	105.5(3)
C(5)-C(2)-C(4)	103.3(3)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5

C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-Sc(1)	147.4(2)
C(7)-C(6)-H(6A)	99.9
Sc(1)-C(6)-H(6A)	99.9
C(7)-C(6)-H(6B)	99.9
Sc(1)-C(6)-H(6B)	99.9
H(6A)-C(6)-H(6B)	104.2
C(10)-C(7)-C(9A)	119.2(8)
C(10)-C(7)-C(6)	125.0(7)
C(9A)-C(7)-C(6)	113.4(4)
C(10)-C(7)-C(8A)	70.1(8)
C(9A)-C(7)-C(8A)	108.3(6)
C(6)-C(7)-C(8A)	108.1(3)
C(10)-C(7)-C(10A)	32.2(8)
C(9A)-C(7)-C(10A)	113.5(5)
C(6)-C(7)-C(10A)	110.8(4)
C(8A)-C(7)-C(10A)	101.9(5)
C(10)-C(7)-C(8)	106.1(9)
C(9A)-C(7)-C(8)	65.4(6)
C(6)-C(7)-C(8)	109.4(4)
C(8A)-C(7)-C(8)	46.6(5)
C(10A)-C(7)-C(8)	135.4(5)
C(10)-C(7)-C(9)	113.0(8)
C(9A)-C(7)-C(9)	29.7(5)
C(6)-C(7)-C(9)	104.2(4)
C(8A)-C(7)-C(9)	136.2(5)
C(10A)-C(7)-C(9)	93.2(5)
C(8)-C(7)-C(9)	95.0(6)
C(12)-C(11)-P(1)	106.96(15)
C(12)-C(11)-H(15A)	110.3
P(1)-C(11)-H(15A)	110.3
C(12)-C(11)-H(15B)	110.3
P(1)-C(11)-H(15B)	110.3
H(15A)-C(11)-H(15B)	108.6

C(13)-C(12)-N(1)	110.4(2)
C(13)-C(12)-C(11)	130.0(2)
N(1)-C(12)-C(11)	119.4(2)
C(12)-C(13)-C(14)	106.5(2)
C(12)-C(13)-H(17)	126.7
C(14)-C(13)-H(17)	126.7
C(15)-C(14)-C(13)	106.9(2)
C(15)-C(14)-H(18)	126.5
C(13)-C(14)-H(18)	126.5
C(14)-C(15)-N(1)	110.3(2)
C(14)-C(15)-C(16)	130.3(2)
N(1)-C(15)-C(16)	119.4(2)
C(15)-C(16)-P(2)	108.75(16)
C(15)-C(16)-H(20A)	109.9
P(2)-C(16)-H(20A)	109.9
C(15)-C(16)-H(20B)	109.9
P(2)-C(16)-H(20B)	109.9
H(20A)-C(16)-H(20B)	108.3
C(20)-C(17)-C(18)	106.90(19)
C(20)-C(17)-C(19)	109.8(2)
C(18)-C(17)-C(19)	107.9(2)
C(20)-C(17)-P(1)	116.15(17)
C(18)-C(17)-P(1)	108.10(15)
C(19)-C(17)-P(1)	107.71(16)
C(17)-C(18)-H(22A)	109.5
C(17)-C(18)-H(22B)	109.5
H(22A)-C(18)-H(22B)	109.5
C(17)-C(18)-H(22C)	109.5
H(22A)-C(18)-H(22C)	109.5
H(22B)-C(18)-H(22C)	109.5
C(17)-C(19)-H(23A)	109.5
C(17)-C(19)-H(23B)	109.5
H(23A)-C(19)-H(23B)	109.5
C(17)-C(19)-H(23C)	109.5
H(23A)-C(19)-H(23C)	109.5
H(23B)-C(19)-H(23C)	109.5

C(17)-C(20)-H(24A)	109.5
C(17)-C(20)-H(24B)	109.5
H(24A)-C(20)-H(24B)	109.5
C(17)-C(20)-H(24C)	109.5
H(24A)-C(20)-H(24C)	109.5
H(24B)-C(20)-H(24C)	109.5
C(23)-C(21)-C(22)	110.0(2)
C(23)-C(21)-C(24)	107.4(2)
C(22)-C(21)-C(24)	107.17(19)
C(23)-C(21)-P(1)	112.91(17)
C(22)-C(21)-P(1)	109.93(17)
C(24)-C(21)-P(1)	109.15(16)
C(21)-C(22)-H(26A)	109.5
C(21)-C(22)-H(26B)	109.5
H(26A)-C(22)-H(26B)	109.5
C(21)-C(22)-H(26C)	109.5
H(26A)-C(22)-H(26C)	109.5
H(26B)-C(22)-H(26C)	109.5
C(21)-C(23)-H(27A)	109.5
C(21)-C(23)-H(27B)	109.5
H(27A)-C(23)-H(27B)	109.5
C(21)-C(23)-H(27C)	109.5
H(27A)-C(23)-H(27C)	109.5
H(27B)-C(23)-H(27C)	109.5
C(21)-C(24)-H(28A)	109.5
C(21)-C(24)-H(28B)	109.5
H(28A)-C(24)-H(28B)	109.5
C(21)-C(24)-H(28C)	109.5
H(28A)-C(24)-H(28C)	109.5
H(28B)-C(24)-H(28C)	109.5
C(27)-C(25)-C(28)	109.8(2)
C(27)-C(25)-C(26)	107.6(2)
C(28)-C(25)-C(26)	107.9(2)
C(27)-C(25)-P(2)	110.56(17)
C(28)-C(25)-P(2)	113.81(17)
C(26)-C(25)-P(2)	106.95(16)

C(25)-C(26)-H(30A)	109.5
C(25)-C(26)-H(30B)	109.5
H(30A)-C(26)-H(30B)	109.5
C(25)-C(26)-H(30C)	109.5
H(30A)-C(26)-H(30C)	109.5
H(30B)-C(26)-H(30C)	109.5
C(25)-C(28)-H(31A)	109.5
C(25)-C(28)-H(31B)	109.5
H(31A)-C(28)-H(31B)	109.5
C(25)-C(28)-H(31C)	109.5
H(31A)-C(28)-H(31C)	109.5
H(31B)-C(28)-H(31C)	109.5
C(25)-C(27)-H(32A)	109.5
C(25)-C(27)-H(32B)	109.5
H(32A)-C(27)-H(32B)	109.5
C(25)-C(27)-H(32C)	109.5
H(32A)-C(27)-H(32C)	109.5
H(32B)-C(27)-H(32C)	109.5
C(32)-C(29)-C(31)	108.0(2)
C(32)-C(29)-C(30)	107.3(2)
C(31)-C(29)-C(30)	109.6(2)
C(32)-C(29)-P(2)	108.12(17)
C(31)-C(29)-P(2)	108.62(18)
C(30)-C(29)-P(2)	114.98(17)
C(29)-C(30)-H(34A)	109.5
C(29)-C(30)-H(34B)	109.5
H(34A)-C(30)-H(34B)	109.5
C(29)-C(30)-H(34C)	109.5
H(34A)-C(30)-H(34C)	109.5
H(34B)-C(30)-H(34C)	109.5
C(29)-C(31)-H(35A)	109.5
C(29)-C(31)-H(35B)	109.5
H(35A)-C(31)-H(35B)	109.5
C(29)-C(31)-H(35C)	109.5
H(35A)-C(31)-H(35C)	109.5
H(35B)-C(31)-H(35C)	109.5

C(29)-C(32)-H(36A)	109.5
C(29)-C(32)-H(36B)	109.5
H(36A)-C(32)-H(36B)	109.5
C(29)-C(32)-H(36C)	109.5
H(36A)-C(32)-H(36C)	109.5
H(36B)-C(32)-H(36C)	109.5
C(15)-N(1)-C(12)	105.80(18)
C(15)-N(1)-Sc(1)	127.52(15)
C(12)-N(1)-Sc(1)	126.64(14)
C(11)-P(1)-C(17)	105.27(10)
C(11)-P(1)-C(21)	104.03(11)
C(17)-P(1)-C(21)	110.17(10)
C(11)-P(1)-Sc(1)	91.48(7)
C(17)-P(1)-Sc(1)	125.78(8)
C(21)-P(1)-Sc(1)	115.04(7)
C(16)-P(2)-C(29)	104.80(11)
C(16)-P(2)-C(25)	103.72(11)
C(29)-P(2)-C(25)	110.89(11)
C(16)-P(2)-Sc(1)	91.66(7)
C(29)-P(2)-Sc(1)	124.34(8)
C(25)-P(2)-Sc(1)	116.09(7)
N(1)-Sc(1)-C(6)	119.65(10)
N(1)-Sc(1)-C(1)	119.81(11)
C(6)-Sc(1)-C(1)	119.35(13)
N(1)-Sc(1)-P(1)	70.11(5)
C(6)-Sc(1)-P(1)	94.11(8)
C(1)-Sc(1)-P(1)	95.00(9)
N(1)-Sc(1)-P(2)	70.71(5)
C(6)-Sc(1)-P(2)	109.19(8)
C(1)-Sc(1)-P(2)	100.23(9)
P(1)-Sc(1)-P(2)	140.53(2)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5

C(7)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
C(7)-C(8A)-H(8A1)	109.5
C(7)-C(8A)-H(8A2)	109.5
H(8A1)-C(8A)-H(8A2)	109.5
C(7)-C(8A)-H(8A3)	109.5
H(8A1)-C(8A)-H(8A3)	109.5
H(8A2)-C(8A)-H(8A3)	109.5
C(7)-C(9A)-H(9A1)	109.5
C(7)-C(9A)-H(9A2)	109.5
H(9A1)-C(9A)-H(9A2)	109.5
C(7)-C(9A)-H(9A3)	109.5
H(9A1)-C(9A)-H(9A3)	109.5
H(9A2)-C(9A)-H(9A3)	109.5
C(7)-C(10A)-H(10D)	109.5
C(7)-C(10A)-H(10E)	109.5
H(10D)-C(10A)-H(10E)	109.5
C(7)-C(10A)-H(10F)	109.5
H(10D)-C(10A)-H(10F)	109.5
H(10E)-C(10A)-H(10F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-*t*Bu)ScNp₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	29(2)	70(2)	37(2)	-5(2)	11(1)	20(2)
C(2)	26(1)	40(2)	48(2)	2(1)	20(1)	9(1)
C(3)	66(2)	87(3)	44(2)	-2(2)	26(2)	37(2)
C(4)	53(2)	56(2)	49(2)	15(2)	22(2)	22(2)
C(5)	31(2)	93(3)	79(3)	9(2)	23(2)	16(2)
C(6)	59(2)	21(1)	27(2)	-1(1)	7(1)	-5(1)
C(7)	58(2)	18(1)	38(2)	-9(1)	26(1)	-11(1)
C(11)	14(1)	22(1)	16(1)	0(1)	7(1)	1(1)
C(12)	13(1)	20(1)	16(1)	0(1)	6(1)	-1(1)
C(13)	20(1)	27(1)	21(1)	0(1)	7(1)	9(1)
C(14)	26(1)	23(1)	20(1)	-6(1)	9(1)	6(1)
C(15)	19(1)	17(1)	14(1)	-2(1)	7(1)	-2(1)
C(16)	22(1)	18(1)	15(1)	-2(1)	6(1)	-1(1)
C(17)	19(1)	23(1)	12(1)	-2(1)	7(1)	-3(1)
C(18)	23(1)	24(1)	15(1)	-3(1)	6(1)	-5(1)
C(19)	27(1)	36(2)	26(1)	-14(1)	14(1)	-3(1)
C(20)	33(2)	37(2)	14(1)	4(1)	4(1)	-10(1)
C(21)	18(1)	17(1)	20(1)	1(1)	8(1)	-4(1)
C(22)	23(1)	35(2)	30(1)	-7(1)	14(1)	-14(1)
C(23)	35(2)	17(1)	38(2)	7(1)	11(1)	-1(1)
C(24)	26(1)	20(1)	24(1)	-6(1)	7(1)	-10(1)
C(25)	17(1)	26(1)	17(1)	1(1)	7(1)	-2(1)
C(26)	19(1)	48(2)	27(1)	9(1)	2(1)	-10(1)
C(28)	24(1)	39(2)	31(1)	-2(1)	15(1)	3(1)
C(27)	30(2)	31(2)	42(2)	8(1)	17(1)	-5(1)
C(29)	19(1)	27(1)	20(1)	3(1)	6(1)	5(1)
C(30)	29(2)	62(2)	17(1)	6(1)	4(1)	9(1)
C(31)	25(1)	26(1)	43(2)	11(1)	11(1)	6(1)
C(32)	20(1)	30(1)	29(1)	2(1)	4(1)	3(1)
N(1)	16(1)	14(1)	14(1)	0(1)	8(1)	0(1)
P(1)	13(1)	13(1)	11(1)	1(1)	5(1)	0(1)

P(2)	17(1)	16(1)	12(1)	0(1)	6(1)	0(1)
Sc(1)	23(1)	12(1)	13(1)	0(1)	9(1)	3(1)
C(8)	65(8)	22(5)	53(6)	3(4)	36(6)	-4(5)
C(9)	48(7)	8(4)	52(7)	-1(4)	13(5)	2(4)
C(10)	76(5)	33(2)	53(5)	-21(3)	-16(3)	14(3)
C(8A)	141(9)	40(4)	136(8)	-1(4)	101(8)	-19(4)
C(9A)	66(5)	37(4)	84(6)	25(4)	-27(4)	-17(3)
C(10A)	76(5)	33(2)	53(5)	-21(3)	-16(3)	14(3)

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-*t*Bu)ScNp₂.

	x	y	z	U(eq)
H(1A)	4272	5261	1419	54
H(1B)	4439	4881	2166	54
H(3A)	4125	2778	891	95
H(3B)	5206	2671	983	95
H(3C)	4643	3783	632	95
H(4A)	4334	2436	2056	77
H(4B)	5114	3116	2622	77
H(4C)	5405	2208	2153	77
H(5A)	6355	3630	1888	100
H(5B)	6051	4542	2348	100
H(5C)	5979	4865	1593	100
H(6A)	1268	3300	856	45
H(6B)	2065	3044	556	45
H(15A)	802	6943	116	20
H(15B)	649	5639	306	20
H(17)	516	8115	1168	27
H(18)	1330	8042	2432	27
H(20A)	2452	6415	3259	22
H(20B)	3273	6397	2932	22
H(22A)	515	5007	-747	31
H(22B)	1171	4003	-340	31
H(22C)	985	4133	-1130	31
H(23A)	2606	4334	-1077	42
H(23B)	2838	3980	-306	42
H(23C)	3296	5105	-504	42
H(24A)	1489	5881	-1564	43
H(24B)	2207	6749	-1076	43
H(24C)	1152	6724	-1087	43
H(26A)	4030	7887	202	42
H(26B)	3421	7036	-364	42

H(26C)	4061	6536	339	42
H(27A)	1747	8407	278	45
H(27B)	1956	8150	-408	45
H(27C)	2609	9008	132	45
H(28A)	3655	8281	1209	35
H(28B)	3669	6946	1388	35
H(28C)	2780	7709	1352	35
H(30A)	884	3861	1940	49
H(30B)	660	5132	2132	49
H(30C)	104	4062	2290	49
H(31A)	562	4766	3476	45
H(31B)	1144	5783	3290	45
H(31C)	1633	4930	3895	45
H(32A)	1818	2863	3646	49
H(32B)	1637	2449	2889	49
H(32C)	781	2739	3149	49
H(34A)	3986	4110	4661	55
H(34B)	2904	3852	4329	55
H(34C)	3288	5129	4328	55
H(35A)	3873	2654	3127	47
H(35B)	3215	2357	3566	47
H(35C)	4300	2559	3925	47
H(36A)	4396	5542	3736	41
H(36B)	4520	4700	3170	41
H(36C)	4994	4394	3945	41
H(8A)	1248	1803	1860	64
H(8B)	2336	1555	2069	64
H(8C)	1611	549	1760	64
H(9A)	2726	267	1131	55
H(9B)	3248	1418	1459	55
H(9C)	2932	1245	663	55
H(10A)	1074	348	669	94
H(10B)	997	1320	116	94
H(10C)	433	1448	638	94
H(8A1)	454	2115	1139	139
H(8A2)	1207	1670	1812	139

H(8A3)	698	778	1234	139
H(9A1)	2329	291	1404	111
H(9A2)	2751	1417	1825	111
H(9A3)	2982	1129	1151	111
H(10D)	1143	421	304	94
H(10E)	1666	1370	8	94
H(10F)	667	1640	73	94

Table S16. Crystal data and structure refinement for [(PNP-Cy)ScCl₂]₂.

Empirical formula	C ₆₀ H ₁₀₀ Cl ₄ N ₂ P ₄ Sc ₂	
Formula weight	1205.02	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 15.4534(9) Å	α = 90°.
	b = 14.4104(8) Å	β = 104.156(2)°.
	c = 30.3498(18) Å	γ = 90°.
Volume	6553.4(7) Å ³	
Z	4	
Density (calculated)	1.221 Mg/m ³	
Absorption coefficient	0.504 mm ⁻¹	
F(000)	2576	
Crystal size	0.100 x 0.070 x 0.050 mm ³	
Theta range for data collection	1.573 to 25.366°.	
Index ranges	-18 ≤ h ≤ 18, -17 ≤ k ≤ 17, -36 ≤ l ≤ 34	
Reflections collected	103924	
Independent reflections	11986 [R(int) = 0.0840]	
Completeness to theta = 25.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8620 and 0.8239	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11986 / 0 / 688	
Goodness-of-fit on F ²	1.022	
Final R indices [I > 2σ(I)]	R ₁ = 0.0644, wR ₂ = 0.1539	
R indices (all data)	R ₁ = 0.0839, wR ₂ = 0.1642	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.134 and -0.530 e.Å ⁻³	

Table S17. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [(PNP-Cy)ScCl₂]₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sc(1)	3942(1)	2977(1)	1463(1)	20(1)
Sc(2)	1810(1)	1431(1)	972(1)	24(1)
Cl(3)	3308(1)	1372(1)	1579(1)	26(1)
Cl(4)	2421(1)	3069(1)	921(1)	30(1)
P(1)	4216(1)	4363(1)	888(1)	24(1)
P(2)	5385(1)	2211(1)	2071(1)	28(1)
Cl(1)	3796(1)	4083(1)	2017(1)	32(1)
P(3)	1049(1)	1523(1)	1693(1)	28(1)
P(4)	2357(1)	341(1)	359(1)	30(1)
Cl(2)	554(1)	1832(1)	384(1)	40(1)
N(2)	1373(2)	57(2)	1065(1)	25(1)
C(24)	5368(3)	1568(3)	2599(2)	40(1)
C(1)	4344(3)	3572(3)	434(1)	30(1)
N(1)	4874(2)	2509(2)	1089(1)	25(1)
C(7)	5246(3)	5082(3)	1015(1)	30(1)
C(6)	5670(3)	1378(3)	1672(2)	35(1)
C(18)	6367(3)	3001(3)	2244(2)	41(1)
C(2)	4906(3)	2777(3)	653(1)	26(1)
C(4)	5935(3)	1671(3)	870(2)	36(1)
C(3)	5538(3)	2275(3)	512(2)	35(1)
C(5)	5531(3)	1823(3)	1218(2)	30(1)
C(8)	6097(3)	4545(3)	1018(2)	40(1)
C(25)	4624(3)	1917(3)	2799(1)	42(1)
C(13)	3302(3)	5138(3)	601(1)	29(1)
C(26)	4649(4)	1454(3)	3257(2)	54(1)
C(14)	3472(3)	5674(4)	199(2)	47(1)
C(23)	6213(4)	3679(4)	2609(2)	56(2)
C(15)	2632(3)	6175(4)	-54(2)	52(1)
C(27)	4618(4)	419(3)	3220(2)	51(1)
C(17)	2970(4)	5768(4)	924(2)	51(1)
C(12)	5359(3)	5585(4)	1470(2)	63(2)

C(28)	5354(4)	57(4)	3007(2)	60(2)
C(10)	7009(3)	5730(4)	1535(2)	53(1)
C(29)	5332(3)	516(3)	2552(2)	51(1)
C(21)	7870(5)	3868(6)	2903(2)	105(3)
C(9)	6905(3)	5198(3)	1102(2)	45(1)
C(11)	6178(4)	6231(5)	1558(3)	85(2)
C(22)	6985(4)	4369(4)	2752(2)	78(2)
C(20)	8023(4)	3233(5)	2540(3)	94(3)
C(16)	2127(4)	6293(4)	672(2)	60(2)
C(19)	7272(3)	2514(4)	2396(2)	72(2)
C(102)	1209(3)	-638(3)	736(1)	29(1)
C(105)	1055(3)	-278(3)	1421(2)	33(1)
C(101)	1427(3)	-481(3)	288(1)	32(1)
C(103)	813(3)	-1375(3)	884(2)	44(1)
C(106)	1158(3)	285(3)	1845(1)	36(1)
C(107)	2395(4)	784(3)	-209(2)	47(1)
C(104)	714(4)	-1148(3)	1319(2)	54(1)
C(30)	2270(4)	6807(3)	261(2)	56(2)
C(109)	2738(5)	1759(3)	-170(2)	67(2)
C(110)	2851(5)	2145(4)	-621(2)	79(2)
C(108)	1586(6)	689(9)	-564(2)	161(5)
C(121)	3416(3)	-962(4)	932(2)	56(1)
C(118)	3353(3)	-424(4)	508(2)	56(1)
C(120)	5005(4)	-598(5)	626(3)	91(2)
C(117)	2029(5)	2064(7)	-969(3)	113(3)
C(116)	1733(6)	1043(9)	-1027(2)	155(5)
C(301)	1614(3)	3161(3)	2173(1)	39(1)
C(302)	2002(4)	3676(4)	2607(2)	56(1)
C(300)	1498(4)	2146(3)	2230(2)	56(2)
C(401)	-316(3)	2746(3)	1316(2)	34(1)
C(400)	-158(3)	1764(3)	1514(2)	50(1)
C(402)	-1293(3)	2955(4)	1131(2)	62(2)
C(202)	4256(4)	-1616(5)	1029(3)	87(2)
C(201)	5062(4)	-1073(6)	1057(3)	98(3)
C(119)	4198(4)	97(4)	529(3)	79(2)
C(304)	2142(18)	2150(20)	3053(10)	54(4)

C(303)	2481(8)	3114(8)	2976(3)	43(2)
C(305)	1949(9)	1576(7)	2603(3)	43(2)
C(34B)	1838(13)	2389(14)	3070(7)	54(4)
C(33B)	1787(6)	3414(6)	3019(3)	43(2)
C(35B)	1297(6)	1888(6)	2649(2)	43(2)
C(45)	-797(5)	1413(6)	1736(3)	49(2)
C(43)	-1891(6)	2635(6)	1345(4)	57(3)
C(44)	-1753(6)	1596(6)	1477(4)	51(3)
C(45B)	-682(6)	1043(7)	1318(4)	32(3)
C(43B)	-1845(7)	2188(8)	940(5)	48(4)
C(44B)	-1675(9)	1266(11)	1186(6)	60(4)

Table S18. Bond lengths [Å] and angles [°] for [(PNP-Cy)ScCl₂]₂.

Sc(1)-N(1)	2.150(3)
Sc(1)-Cl(1)	2.3661(11)
Sc(1)-Cl(4)	2.5222(11)
Sc(1)-Cl(3)	2.5695(11)
Sc(1)-P(1)	2.7531(12)
Sc(1)-P(2)	2.7540(12)
Sc(2)-N(2)	2.133(3)
Sc(2)-Cl(2)	2.3632(12)
Sc(2)-Cl(4)	2.5606(11)
Sc(2)-Cl(3)	2.5851(11)
Sc(2)-P(4)	2.7228(13)
Sc(2)-P(3)	2.7288(13)
P(1)-C(1)	1.838(4)
P(1)-C(13)	1.843(4)
P(1)-C(7)	1.859(4)
P(2)-C(6)	1.833(4)
P(2)-C(24)	1.855(4)
P(2)-C(18)	1.867(4)
P(3)-C(106)	1.840(4)
P(3)-C(300)	1.843(5)
P(3)-C(400)	1.843(4)
P(4)-C(101)	1.835(4)
P(4)-C(107)	1.852(5)
P(4)-C(118)	1.857(5)
N(2)-C(105)	1.380(5)
N(2)-C(102)	1.394(5)
C(24)-C(25)	1.512(7)
C(24)-C(29)	1.522(6)
C(24)-H(24)	1.0000
C(1)-C(2)	1.491(6)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
N(1)-C(2)	1.390(5)
N(1)-C(5)	1.403(5)

C(7)-C(8)	1.524(6)
C(7)-C(12)	1.529(6)
C(7)-H(7)	1.0000
C(6)-C(5)	1.488(6)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(18)-C(19)	1.531(7)
C(18)-C(23)	1.538(7)
C(18)-H(18)	1.0000
C(2)-C(3)	1.366(6)
C(4)-C(5)	1.370(6)
C(4)-C(3)	1.410(6)
C(4)-H(4)	0.9500
C(3)-H(3)	0.9500
C(8)-C(9)	1.534(6)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(25)-C(26)	1.534(6)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(13)-C(17)	1.517(6)
C(13)-C(14)	1.519(6)
C(13)-H(13)	1.0000
C(26)-C(27)	1.496(7)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(14)-C(15)	1.520(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(23)-C(22)	1.532(7)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(15)-C(30)	1.523(8)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(27)-C(28)	1.530(7)

C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(17)-C(16)	1.538(6)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(12)-C(11)	1.541(7)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(28)-C(29)	1.524(7)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(10)-C(11)	1.490(8)
C(10)-C(9)	1.496(7)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(21)-C(20)	1.494(12)
C(21)-C(22)	1.515(10)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(20)-C(19)	1.538(8)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(16)-C(30)	1.512(8)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(102)-C(103)	1.357(6)

C(102)-C(101)	1.496(6)
C(105)-C(104)	1.366(6)
C(105)-C(106)	1.494(6)
C(101)-H(10C)	0.9900
C(101)-H(10D)	0.9900
C(103)-C(104)	1.405(7)
C(103)-H(103)	0.9500
C(106)-H(10E)	0.9900
C(106)-H(10F)	0.9900
C(107)-C(108)	1.444(8)
C(107)-C(109)	1.496(7)
C(107)-H(107)	1.0000
C(104)-H(104)	0.9500
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(109)-C(110)	1.527(7)
C(109)-H(10G)	0.9900
C(109)-H(10H)	0.9900
C(110)-C(117)	1.443(10)
C(110)-H(11C)	0.9900
C(110)-H(11D)	0.9900
C(108)-C(116)	1.563(9)
C(108)-H(10I)	0.9900
C(108)-H(10J)	0.9900
C(121)-C(118)	1.485(7)
C(121)-C(202)	1.573(8)
C(121)-H(12C)	0.9900
C(121)-H(12D)	0.9900
C(118)-C(119)	1.493(7)
C(118)-H(118)	1.0000
C(120)-C(201)	1.460(11)
C(120)-C(119)	1.570(8)
C(120)-H(12E)	0.9900
C(120)-H(12F)	0.9900
C(117)-C(116)	1.539(13)
C(117)-H(11E)	0.9900

C(117)-H(11F)	0.9900
C(116)-H(11G)	0.9900
C(116)-H(11H)	0.9900
C(301)-C(300)	1.489(7)
C(301)-C(302)	1.505(6)
C(301)-H(30C)	0.9900
C(301)-H(30D)	0.9900
C(302)-C(33B)	1.421(10)
C(302)-C(303)	1.433(12)
C(302)-H(30E)	0.9900
C(302)-H(30F)	0.9900
C(300)-C(35B)	1.429(9)
C(300)-C(305)	1.433(11)
C(300)-H(300)	1.0000
C(401)-C(402)	1.507(6)
C(401)-C(400)	1.534(6)
C(401)-H(40A)	0.9900
C(401)-H(40B)	0.9900
C(400)-C(45B)	1.361(11)
C(400)-C(45)	1.418(10)
C(400)-H(400)	1.0000
C(402)-C(43)	1.334(11)
C(402)-C(43B)	1.430(14)
C(402)-H(40C)	0.9900
C(402)-H(40D)	0.9900
C(202)-C(201)	1.456(10)
C(202)-H(20C)	0.9900
C(202)-H(20D)	0.9900
C(201)-H(20E)	0.9900
C(201)-H(20F)	0.9900
C(119)-H(11I)	0.9900
C(119)-H(11J)	0.9900
C(304)-C(303)	1.53(4)
C(304)-C(305)	1.56(3)
C(304)-H(30G)	0.9900
C(304)-H(30H)	0.9900

C(303)-H(30I)	0.9900
C(303)-H(30J)	0.9900
C(305)-H(30K)	0.9900
C(305)-H(30L)	0.9900
C(34B)-C(33B)	1.49(2)
C(34B)-C(35B)	1.53(2)
C(34B)-H(34A)	0.9900
C(34B)-H(34B)	0.9900
C(33B)-H(33A)	0.9900
C(33B)-H(33B)	0.9900
C(35B)-H(35A)	0.9900
C(35B)-H(35B)	0.9900
C(45)-C(44)	1.517(11)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(43)-C(44)	1.551(11)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45B)-C(44B)	1.523(16)
C(45B)-H(45C)	0.9900
C(45B)-H(45D)	0.9900
C(43B)-C(44B)	1.515(16)
C(43B)-H(43C)	0.9900
C(43B)-H(43D)	0.9900
C(44B)-H(44C)	0.9900
C(44B)-H(44D)	0.9900
N(1)-Sc(1)-Cl(1)	141.20(9)
N(1)-Sc(1)-Cl(4)	108.02(9)
Cl(1)-Sc(1)-Cl(4)	101.09(4)
N(1)-Sc(1)-Cl(3)	96.72(9)
Cl(1)-Sc(1)-Cl(3)	113.79(4)
Cl(4)-Sc(1)-Cl(3)	79.11(3)
N(1)-Sc(1)-P(1)	70.46(9)

Cl(1)-Sc(1)-P(1)	91.01(4)
Cl(4)-Sc(1)-P(1)	79.13(3)
Cl(3)-Sc(1)-P(1)	149.65(4)
N(1)-Sc(1)-P(2)	72.02(9)
Cl(1)-Sc(1)-P(2)	89.80(4)
Cl(4)-Sc(1)-P(2)	158.63(4)
Cl(3)-Sc(1)-P(2)	79.67(3)
P(1)-Sc(1)-P(2)	119.40(4)
N(2)-Sc(2)-Cl(2)	95.70(9)
N(2)-Sc(2)-Cl(4)	175.47(9)
Cl(2)-Sc(2)-Cl(4)	88.63(4)
N(2)-Sc(2)-Cl(3)	97.57(9)
Cl(2)-Sc(2)-Cl(3)	166.72(5)
Cl(4)-Sc(2)-Cl(3)	78.12(3)
N(2)-Sc(2)-P(4)	73.54(9)
Cl(2)-Sc(2)-P(4)	87.77(4)
Cl(4)-Sc(2)-P(4)	108.06(4)
Cl(3)-Sc(2)-P(4)	95.40(4)
N(2)-Sc(2)-P(3)	74.09(9)
Cl(2)-Sc(2)-P(3)	99.07(4)
Cl(4)-Sc(2)-P(3)	103.94(4)
Cl(3)-Sc(2)-P(3)	85.19(4)
P(4)-Sc(2)-P(3)	147.41(4)
Sc(1)-Cl(3)-Sc(2)	100.22(4)
Sc(1)-Cl(4)-Sc(2)	102.17(4)
C(1)-P(1)-C(13)	103.38(18)
C(1)-P(1)-C(7)	104.89(19)
C(13)-P(1)-C(7)	106.19(18)
C(1)-P(1)-Sc(1)	94.98(13)
C(13)-P(1)-Sc(1)	121.39(14)
C(7)-P(1)-Sc(1)	121.98(13)
C(6)-P(2)-C(24)	107.4(2)
C(6)-P(2)-C(18)	105.9(2)
C(24)-P(2)-C(18)	104.14(19)
C(6)-P(2)-Sc(1)	96.06(13)
C(24)-P(2)-Sc(1)	126.74(15)

C(18)-P(2)-Sc(1)	114.40(13)
C(106)-P(3)-C(300)	105.0(2)
C(106)-P(3)-C(400)	106.3(2)
C(300)-P(3)-C(400)	107.6(3)
C(106)-P(3)-Sc(2)	97.08(14)
C(300)-P(3)-Sc(2)	126.2(2)
C(400)-P(3)-Sc(2)	112.14(19)
C(101)-P(4)-C(107)	108.4(2)
C(101)-P(4)-C(118)	103.0(2)
C(107)-P(4)-C(118)	102.7(3)
C(101)-P(4)-Sc(2)	95.01(14)
C(107)-P(4)-Sc(2)	121.48(17)
C(118)-P(4)-Sc(2)	123.61(19)
C(105)-N(2)-C(102)	105.9(3)
C(105)-N(2)-Sc(2)	127.9(3)
C(102)-N(2)-Sc(2)	125.4(3)
C(25)-C(24)-C(29)	110.7(4)
C(25)-C(24)-P(2)	110.7(3)
C(29)-C(24)-P(2)	115.2(4)
C(25)-C(24)-H(24)	106.6
C(29)-C(24)-H(24)	106.6
P(2)-C(24)-H(24)	106.6
C(2)-C(1)-P(1)	107.4(3)
C(2)-C(1)-H(1A)	110.2
P(1)-C(1)-H(1A)	110.2
C(2)-C(1)-H(1B)	110.2
P(1)-C(1)-H(1B)	110.2
H(1A)-C(1)-H(1B)	108.5
C(2)-N(1)-C(5)	105.7(3)
C(2)-N(1)-Sc(1)	126.9(2)
C(5)-N(1)-Sc(1)	127.3(3)
C(8)-C(7)-C(12)	109.1(4)
C(8)-C(7)-P(1)	114.4(3)
C(12)-C(7)-P(1)	110.7(3)
C(8)-C(7)-H(7)	107.5
C(12)-C(7)-H(7)	107.5

P(1)-C(7)-H(7)	107.5
C(5)-C(6)-P(2)	109.1(3)
C(5)-C(6)-H(6A)	109.9
P(2)-C(6)-H(6A)	109.9
C(5)-C(6)-H(6B)	109.9
P(2)-C(6)-H(6B)	109.9
H(6A)-C(6)-H(6B)	108.3
C(19)-C(18)-C(23)	111.4(4)
C(19)-C(18)-P(2)	115.1(3)
C(23)-C(18)-P(2)	109.3(3)
C(19)-C(18)-H(18)	106.8
C(23)-C(18)-H(18)	106.8
P(2)-C(18)-H(18)	106.8
C(3)-C(2)-N(1)	110.2(4)
C(3)-C(2)-C(1)	130.5(4)
N(1)-C(2)-C(1)	119.1(3)
C(5)-C(4)-C(3)	107.5(4)
C(5)-C(4)-H(4)	126.2
C(3)-C(4)-H(4)	126.2
C(2)-C(3)-C(4)	107.2(4)
C(2)-C(3)-H(3)	126.4
C(4)-C(3)-H(3)	126.4
C(4)-C(5)-N(1)	109.4(4)
C(4)-C(5)-C(6)	131.0(4)
N(1)-C(5)-C(6)	119.5(4)
C(7)-C(8)-C(9)	110.8(4)
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
C(9)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(24)-C(25)-C(26)	111.4(4)
C(24)-C(25)-H(25A)	109.3
C(26)-C(25)-H(25A)	109.3
C(24)-C(25)-H(25B)	109.3
C(26)-C(25)-H(25B)	109.3

H(25A)-C(25)-H(25B)	108.0
C(17)-C(13)-C(14)	111.5(4)
C(17)-C(13)-P(1)	113.4(3)
C(14)-C(13)-P(1)	115.2(3)
C(17)-C(13)-H(13)	105.2
C(14)-C(13)-H(13)	105.2
P(1)-C(13)-H(13)	105.2
C(27)-C(26)-C(25)	111.8(4)
C(27)-C(26)-H(26A)	109.2
C(25)-C(26)-H(26A)	109.2
C(27)-C(26)-H(26B)	109.2
C(25)-C(26)-H(26B)	109.2
H(26A)-C(26)-H(26B)	107.9
C(13)-C(14)-C(15)	110.8(4)
C(13)-C(14)-H(14A)	109.5
C(15)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
C(15)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	108.1
C(22)-C(23)-C(18)	111.7(5)
C(22)-C(23)-H(23A)	109.3
C(18)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23B)	109.3
C(18)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	107.9
C(14)-C(15)-C(30)	111.4(4)
C(14)-C(15)-H(15A)	109.4
C(30)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15B)	109.4
C(30)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(26)-C(27)-C(28)	111.0(4)
C(26)-C(27)-H(27A)	109.4
C(28)-C(27)-H(27A)	109.4
C(26)-C(27)-H(27B)	109.4
C(28)-C(27)-H(27B)	109.4

H(27A)-C(27)-H(27B)	108.0
C(13)-C(17)-C(16)	110.6(4)
C(13)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	108.1
C(7)-C(12)-C(11)	110.6(5)
C(7)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(29)-C(28)-C(27)	112.3(4)
C(29)-C(28)-H(28A)	109.1
C(27)-C(28)-H(28A)	109.1
C(29)-C(28)-H(28B)	109.1
C(27)-C(28)-H(28B)	109.1
H(28A)-C(28)-H(28B)	107.9
C(11)-C(10)-C(9)	112.4(4)
C(11)-C(10)-H(10A)	109.1
C(9)-C(10)-H(10A)	109.1
C(11)-C(10)-H(10B)	109.1
C(9)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.8
C(24)-C(29)-C(28)	110.9(5)
C(24)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29A)	109.5
C(24)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	108.0
C(20)-C(21)-C(22)	111.3(5)
C(20)-C(21)-H(21A)	109.4
C(22)-C(21)-H(21A)	109.4
C(20)-C(21)-H(21B)	109.4
C(22)-C(21)-H(21B)	109.4

H(21A)-C(21)-H(21B)	108.0
C(10)-C(9)-C(8)	111.6(4)
C(10)-C(9)-H(9A)	109.3
C(8)-C(9)-H(9A)	109.3
C(10)-C(9)-H(9B)	109.3
C(8)-C(9)-H(9B)	109.3
H(9A)-C(9)-H(9B)	108.0
C(10)-C(11)-C(12)	112.2(5)
C(10)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11A)	109.2
C(10)-C(11)-H(11B)	109.2
C(12)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
C(21)-C(22)-C(23)	111.0(5)
C(21)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22A)	109.4
C(21)-C(22)-H(22B)	109.4
C(23)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
C(21)-C(20)-C(19)	112.2(6)
C(21)-C(20)-H(20A)	109.2
C(19)-C(20)-H(20A)	109.2
C(21)-C(20)-H(20B)	109.2
C(19)-C(20)-H(20B)	109.2
H(20A)-C(20)-H(20B)	107.9
C(30)-C(16)-C(17)	112.0(5)
C(30)-C(16)-H(16A)	109.2
C(17)-C(16)-H(16A)	109.2
C(30)-C(16)-H(16B)	109.2
C(17)-C(16)-H(16B)	109.2
H(16A)-C(16)-H(16B)	107.9
C(18)-C(19)-C(20)	110.3(5)
C(18)-C(19)-H(19A)	109.6
C(20)-C(19)-H(19A)	109.6
C(18)-C(19)-H(19B)	109.6
C(20)-C(19)-H(19B)	109.6

H(19A)-C(19)-H(19B)	108.1
C(103)-C(102)-N(2)	110.0(4)
C(103)-C(102)-C(101)	129.8(4)
N(2)-C(102)-C(101)	120.2(3)
C(104)-C(105)-N(2)	109.6(4)
C(104)-C(105)-C(106)	130.3(4)
N(2)-C(105)-C(106)	120.0(4)
C(102)-C(101)-P(4)	109.5(3)
C(102)-C(101)-H(10C)	109.8
P(4)-C(101)-H(10C)	109.8
C(102)-C(101)-H(10D)	109.8
P(4)-C(101)-H(10D)	109.8
H(10C)-C(101)-H(10D)	108.2
C(102)-C(103)-C(104)	106.9(4)
C(102)-C(103)-H(103)	126.5
C(104)-C(103)-H(103)	126.5
C(105)-C(106)-P(3)	109.0(3)
C(105)-C(106)-H(10E)	109.9
P(3)-C(106)-H(10E)	109.9
C(105)-C(106)-H(10F)	109.9
P(3)-C(106)-H(10F)	109.9
H(10E)-C(106)-H(10F)	108.3
C(108)-C(107)-C(109)	112.0(6)
C(108)-C(107)-P(4)	116.3(4)
C(109)-C(107)-P(4)	110.0(3)
C(108)-C(107)-H(107)	105.9
C(109)-C(107)-H(107)	105.9
P(4)-C(107)-H(107)	105.9
C(105)-C(104)-C(103)	107.6(4)
C(105)-C(104)-H(104)	126.2
C(103)-C(104)-H(104)	126.2
C(16)-C(30)-C(15)	112.1(4)
C(16)-C(30)-H(30A)	109.2
C(15)-C(30)-H(30A)	109.2
C(16)-C(30)-H(30B)	109.2
C(15)-C(30)-H(30B)	109.2

H(30A)-C(30)-H(30B)	107.9
C(107)-C(109)-C(110)	112.8(4)
C(107)-C(109)-H(10G)	109.0
C(110)-C(109)-H(10G)	109.0
C(107)-C(109)-H(10H)	109.0
C(110)-C(109)-H(10H)	109.0
H(10G)-C(109)-H(10H)	107.8
C(117)-C(110)-C(109)	110.6(6)
C(117)-C(110)-H(11C)	109.5
C(109)-C(110)-H(11C)	109.5
C(117)-C(110)-H(11D)	109.5
C(109)-C(110)-H(11D)	109.5
H(11C)-C(110)-H(11D)	108.1
C(107)-C(108)-C(116)	110.6(6)
C(107)-C(108)-H(10I)	109.5
C(116)-C(108)-H(10I)	109.5
C(107)-C(108)-H(10J)	109.5
C(116)-C(108)-H(10J)	109.5
H(10I)-C(108)-H(10J)	108.1
C(118)-C(121)-C(202)	110.5(5)
C(118)-C(121)-H(12C)	109.5
C(202)-C(121)-H(12C)	109.5
C(118)-C(121)-H(12D)	109.5
C(202)-C(121)-H(12D)	109.5
H(12C)-C(121)-H(12D)	108.1
C(121)-C(118)-C(119)	110.7(5)
C(121)-C(118)-P(4)	113.3(4)
C(119)-C(118)-P(4)	112.0(4)
C(121)-C(118)-H(118)	106.8
C(119)-C(118)-H(118)	106.8
P(4)-C(118)-H(118)	106.8
C(201)-C(120)-C(119)	109.7(6)
C(201)-C(120)-H(12E)	109.7
C(119)-C(120)-H(12E)	109.7
C(201)-C(120)-H(12F)	109.7
C(119)-C(120)-H(12F)	109.7

H(12E)-C(120)-H(12F)	108.2
C(110)-C(117)-C(116)	110.2(6)
C(110)-C(117)-H(11E)	109.6
C(116)-C(117)-H(11E)	109.6
C(110)-C(117)-H(11F)	109.6
C(116)-C(117)-H(11F)	109.6
H(11E)-C(117)-H(11F)	108.1
C(117)-C(116)-C(108)	108.2(8)
C(117)-C(116)-H(11G)	110.1
C(108)-C(116)-H(11G)	110.1
C(117)-C(116)-H(11H)	110.1
C(108)-C(116)-H(11H)	110.1
H(11G)-C(116)-H(11H)	108.4
C(300)-C(301)-C(302)	114.5(4)
C(300)-C(301)-H(30C)	108.6
C(302)-C(301)-H(30C)	108.6
C(300)-C(301)-H(30D)	108.6
C(302)-C(301)-H(30D)	108.6
H(30C)-C(301)-H(30D)	107.6
C(33B)-C(302)-C(301)	120.7(5)
C(303)-C(302)-C(301)	115.2(6)
C(303)-C(302)-H(30E)	108.5
C(301)-C(302)-H(30E)	108.5
C(303)-C(302)-H(30F)	108.5
C(301)-C(302)-H(30F)	108.5
H(30E)-C(302)-H(30F)	107.5
C(35B)-C(300)-C(301)	114.7(5)
C(305)-C(300)-C(301)	127.3(6)
C(35B)-C(300)-P(3)	123.0(5)
C(305)-C(300)-P(3)	115.2(5)
C(301)-C(300)-P(3)	113.9(3)
C(305)-C(300)-H(300)	96.4
C(301)-C(300)-H(300)	96.4
P(3)-C(300)-H(300)	96.4
C(402)-C(401)-C(400)	112.3(4)
C(402)-C(401)-H(40A)	109.1

C(400)-C(401)-H(40A)	109.1
C(402)-C(401)-H(40B)	109.1
C(400)-C(401)-H(40B)	109.1
H(40A)-C(401)-H(40B)	107.9
C(45B)-C(400)-C(401)	120.8(6)
C(45)-C(400)-C(401)	116.9(5)
C(45B)-C(400)-P(3)	115.8(5)
C(45)-C(400)-P(3)	124.4(4)
C(401)-C(400)-P(3)	110.0(3)
C(45)-C(400)-H(400)	99.8
C(401)-C(400)-H(400)	99.8
P(3)-C(400)-H(400)	99.8
C(43)-C(402)-C(401)	120.0(6)
C(43B)-C(402)-C(401)	116.2(6)
C(43)-C(402)-H(40C)	107.3
C(401)-C(402)-H(40C)	107.3
C(43)-C(402)-H(40D)	107.3
C(401)-C(402)-H(40D)	107.3
H(40C)-C(402)-H(40D)	106.9
C(201)-C(202)-C(121)	110.2(6)
C(201)-C(202)-H(20C)	109.6
C(121)-C(202)-H(20C)	109.6
C(201)-C(202)-H(20D)	109.6
C(121)-C(202)-H(20D)	109.6
H(20C)-C(202)-H(20D)	108.1
C(202)-C(201)-C(120)	109.7(6)
C(202)-C(201)-H(20E)	109.7
C(120)-C(201)-H(20E)	109.7
C(202)-C(201)-H(20F)	109.7
C(120)-C(201)-H(20F)	109.7
H(20E)-C(201)-H(20F)	108.2
C(118)-C(119)-C(120)	109.5(5)
C(118)-C(119)-H(11I)	109.8
C(120)-C(119)-H(11I)	109.8
C(118)-C(119)-H(11J)	109.8
C(120)-C(119)-H(11J)	109.8

H(11I)-C(119)-H(11J)	108.2
C(303)-C(304)-C(305)	110(2)
C(303)-C(304)-H(30G)	109.6
C(305)-C(304)-H(30G)	109.6
C(303)-C(304)-H(30H)	109.6
C(305)-C(304)-H(30H)	109.6
H(30G)-C(304)-H(30H)	108.1
C(302)-C(303)-C(304)	120.3(13)
C(302)-C(303)-H(30I)	107.2
C(304)-C(303)-H(30I)	107.2
C(302)-C(303)-H(30J)	107.2
C(304)-C(303)-H(30J)	107.2
H(30I)-C(303)-H(30J)	106.9
C(300)-C(305)-C(304)	110.1(12)
C(300)-C(305)-H(30K)	109.6
C(304)-C(305)-H(30K)	109.6
C(300)-C(305)-H(30L)	109.6
C(304)-C(305)-H(30L)	109.6
H(30K)-C(305)-H(30L)	108.2
C(33B)-C(34B)-C(35B)	112.2(12)
C(33B)-C(34B)-H(34A)	109.2
C(35B)-C(34B)-H(34A)	109.2
C(33B)-C(34B)-H(34B)	109.2
C(35B)-C(34B)-H(34B)	109.2
H(34A)-C(34B)-H(34B)	107.9
C(302)-C(33B)-C(34B)	109.8(10)
C(302)-C(33B)-H(33A)	109.7
C(34B)-C(33B)-H(33A)	109.7
C(302)-C(33B)-H(33B)	109.7
C(34B)-C(33B)-H(33B)	109.7
H(33A)-C(33B)-H(33B)	108.2
C(300)-C(35B)-C(34B)	115.4(11)
C(300)-C(35B)-H(35A)	108.4
C(34B)-C(35B)-H(35A)	108.4
C(300)-C(35B)-H(35B)	108.4
C(34B)-C(35B)-H(35B)	108.4

H(35A)-C(35B)-H(35B)	107.5
C(400)-C(45)-C(44)	113.3(7)
C(400)-C(45)-H(45A)	108.9
C(44)-C(45)-H(45A)	108.9
C(400)-C(45)-H(45B)	108.9
C(44)-C(45)-H(45B)	108.9
H(45A)-C(45)-H(45B)	107.7
C(402)-C(43)-C(44)	113.1(7)
C(402)-C(43)-H(43A)	109.0
C(44)-C(43)-H(43A)	109.0
C(402)-C(43)-H(43B)	109.0
C(44)-C(43)-H(43B)	109.0
H(43A)-C(43)-H(43B)	107.8
C(45)-C(44)-C(43)	110.9(7)
C(45)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44A)	109.5
C(45)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	108.0
C(400)-C(45B)-C(44B)	114.1(10)
C(400)-C(45B)-H(45C)	108.7
C(44B)-C(45B)-H(45C)	108.7
C(400)-C(45B)-H(45D)	108.7
C(44B)-C(45B)-H(45D)	108.7
H(45C)-C(45B)-H(45D)	107.6
C(402)-C(43B)-C(44B)	117.6(11)
C(402)-C(43B)-H(43C)	107.9
C(44B)-C(43B)-H(43C)	107.9
C(402)-C(43B)-H(43D)	107.9
C(44B)-C(43B)-H(43D)	107.9
H(43C)-C(43B)-H(43D)	107.2
C(43B)-C(44B)-C(45B)	110.9(11)
C(43B)-C(44B)-H(44C)	109.5
C(45B)-C(44B)-H(44C)	109.5
C(43B)-C(44B)-H(44D)	109.5
C(45B)-C(44B)-H(44D)	109.5

H(44C)-C(44B)-H(44D) 108.1

Symmetry transformations used to generate equivalent atoms:

Table S19. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [(PNP-Cy)ScCl₂]₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Sc(1)	18(1)	19(1)	18(1)	-1(1)	-1(1)	-2(1)
Sc(2)	21(1)	28(1)	20(1)	-2(1)	-2(1)	-7(1)
Cl(3)	23(1)	24(1)	25(1)	2(1)	-6(1)	-6(1)
Cl(4)	23(1)	24(1)	34(1)	4(1)	-7(1)	-2(1)
P(1)	26(1)	22(1)	20(1)	0(1)	0(1)	-2(1)
P(2)	22(1)	24(1)	31(1)	5(1)	-6(1)	-4(1)
Cl(1)	40(1)	29(1)	27(1)	-9(1)	8(1)	-3(1)
P(3)	28(1)	31(1)	22(1)	4(1)	0(1)	10(1)
P(4)	23(1)	40(1)	24(1)	-2(1)	2(1)	-9(1)
Cl(2)	32(1)	48(1)	29(1)	5(1)	-12(1)	-9(1)
N(2)	18(2)	28(2)	27(2)	1(1)	2(1)	0(1)
C(24)	32(2)	36(2)	42(3)	17(2)	-8(2)	-8(2)
C(1)	34(2)	32(2)	22(2)	-4(2)	4(2)	-9(2)
N(1)	22(2)	20(2)	30(2)	-4(1)	2(1)	-1(1)
C(7)	31(2)	26(2)	30(2)	2(2)	1(2)	-5(2)
C(6)	24(2)	26(2)	52(3)	3(2)	1(2)	2(2)
C(18)	31(2)	39(2)	41(3)	16(2)	-13(2)	-12(2)
C(2)	25(2)	25(2)	28(2)	-7(2)	5(2)	-11(2)
C(4)	23(2)	32(2)	56(3)	-9(2)	14(2)	-1(2)
C(3)	29(2)	37(2)	43(3)	-13(2)	15(2)	-8(2)
C(5)	21(2)	21(2)	46(3)	-5(2)	4(2)	-1(2)
C(8)	30(2)	36(2)	52(3)	-7(2)	10(2)	-8(2)
C(25)	67(3)	30(2)	27(2)	1(2)	6(2)	5(2)
C(13)	25(2)	28(2)	29(2)	4(2)	-1(2)	1(2)
C(26)	78(4)	44(3)	39(3)	7(2)	14(3)	-4(3)
C(14)	44(3)	55(3)	39(3)	22(2)	3(2)	10(2)
C(23)	66(3)	51(3)	37(3)	4(2)	-16(2)	-30(3)
C(15)	49(3)	56(3)	44(3)	20(2)	-3(2)	7(2)
C(27)	58(3)	37(3)	58(3)	10(2)	13(3)	-11(2)
C(17)	62(3)	53(3)	33(3)	1(2)	3(2)	32(3)
C(12)	36(3)	74(4)	80(4)	-47(3)	14(3)	-16(3)

C(28)	54(3)	44(3)	87(4)	37(3)	25(3)	9(2)
C(10)	39(3)	63(3)	53(3)	-8(3)	2(2)	-19(2)
C(29)	49(3)	35(2)	74(4)	21(2)	27(3)	14(2)
C(21)	91(5)	112(6)	75(5)	55(5)	-52(4)	-79(5)
C(9)	31(2)	44(3)	57(3)	-3(2)	7(2)	-11(2)
C(11)	50(3)	79(4)	121(6)	-67(4)	10(4)	-22(3)
C(22)	103(5)	61(4)	46(3)	14(3)	-25(3)	-48(4)
C(20)	41(3)	98(5)	121(6)	54(5)	-24(4)	-35(4)
C(16)	62(3)	66(4)	47(3)	2(3)	5(3)	37(3)
C(19)	33(3)	66(4)	100(5)	33(3)	-14(3)	-15(3)
C(102)	22(2)	26(2)	38(2)	-5(2)	4(2)	-3(2)
C(105)	36(2)	26(2)	40(2)	9(2)	15(2)	9(2)
C(101)	24(2)	36(2)	34(2)	-8(2)	4(2)	-8(2)
C(103)	51(3)	27(2)	63(3)	-7(2)	29(3)	-7(2)
C(106)	38(2)	35(2)	35(2)	16(2)	10(2)	18(2)
C(107)	64(3)	48(3)	28(2)	-5(2)	11(2)	-15(2)
C(104)	80(4)	27(2)	71(4)	9(2)	45(3)	1(2)
C(30)	56(3)	36(3)	59(3)	5(2)	-19(3)	12(2)
C(109)	136(6)	34(3)	39(3)	-5(2)	34(3)	-19(3)
C(110)	142(7)	41(3)	61(4)	-4(3)	41(4)	-19(4)
C(108)	113(7)	296(14)	52(4)	62(6)	-20(4)	-108(8)
C(121)	38(3)	77(4)	51(3)	4(3)	6(2)	6(3)
C(118)	30(3)	67(3)	68(4)	7(3)	9(2)	1(2)
C(120)	34(3)	90(5)	150(8)	-14(5)	26(4)	8(3)
C(117)	71(5)	175(9)	90(6)	90(6)	13(4)	34(5)
C(116)	109(6)	305(14)	33(4)	52(6)	-18(4)	-116(8)
C(301)	35(2)	53(3)	25(2)	-2(2)	0(2)	-16(2)
C(302)	73(4)	57(3)	35(3)	-11(2)	5(3)	0(3)
C(300)	102(4)	40(3)	21(2)	-2(2)	4(3)	20(3)
C(401)	31(2)	25(2)	37(2)	-2(2)	-10(2)	6(2)
C(400)	25(2)	46(3)	78(4)	26(3)	11(2)	15(2)
C(402)	42(3)	37(3)	91(4)	12(3)	-15(3)	13(2)
C(202)	63(4)	87(5)	95(5)	3(4)	-12(4)	18(4)
C(201)	46(4)	117(6)	117(7)	-34(6)	-10(4)	14(4)
C(119)	48(3)	59(4)	126(6)	-27(4)	16(4)	-16(3)
C(304)	71(13)	64(11)	20(3)	3(6)	-1(7)	-4(7)

C(303)	42(4)	56(4)	27(3)	-12(3)	1(3)	-12(3)
C(305)	65(5)	36(4)	26(3)	2(3)	5(4)	-1(3)
C(34B)	71(13)	64(11)	20(3)	3(6)	-1(7)	-4(7)
C(33B)	42(4)	56(4)	27(3)	-12(3)	1(3)	-12(3)
C(35B)	65(5)	36(4)	26(3)	2(3)	5(4)	-1(3)
C(45)	40(5)	45(5)	57(6)	6(4)	5(4)	10(4)
C(43)	34(5)	36(5)	89(8)	-4(5)	-10(5)	11(4)
C(44)	21(4)	34(5)	93(8)	6(5)	4(5)	1(3)
C(45B)	15(5)	27(5)	56(7)	18(5)	10(5)	-6(4)
C(43B)	29(6)	46(7)	67(9)	33(7)	6(6)	12(5)
C(44B)	39(8)	49(9)	88(12)	32(8)	11(8)	17(6)

Table S20. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for [(PNP-Cy)ScCl₂]₂.

	x	y	z	U(eq)
H(24)	5940	1719	2824	48
H(1A)	3753	3347	261	36
H(1B)	4636	3896	221	36
H(7)	5174	5567	773	36
H(6A)	6300	1183	1782	42
H(6B)	5288	820	1651	42
H(18)	6387	3382	1971	49
H(4)	6399	1238	870	43
H(3)	5683	2324	226	42
H(8A)	6032	4227	723	47
H(8B)	6195	4067	1259	47
H(25A)	4042	1787	2584	51
H(25B)	4679	2598	2841	51
H(13)	2790	4717	469	35
H(26A)	5202	1641	3481	65
H(26B)	4135	1672	3369	65
H(14A)	3669	5241	-10	57
H(14B)	3954	6132	309	57
H(23A)	5651	4024	2489	67
H(23B)	6149	3324	2878	67
H(15A)	2171	5712	-192	62
H(15B)	2767	6549	-303	62
H(27A)	4029	225	3031	62
H(27B)	4692	145	3526	62
H(17A)	3442	6219	1062	61
H(17B)	2833	5393	1172	61
H(12A)	5434	5123	1718	76
H(12B)	4816	5953	1466	76
H(28A)	5942	172	3219	72
H(28B)	5285	-622	2963	72

H(10A)	7174	5295	1795	64
H(10B)	7500	6183	1563	64
H(29A)	5847	299	2440	61
H(29B)	4779	334	2328	61
H(21A)	8360	4328	2978	127
H(21B)	7878	3504	3180	127
H(9A)	7453	4830	1116	53
H(9B)	6832	5639	845	53
H(11A)	6067	6737	1331	102
H(11B)	6261	6517	1863	102
H(22A)	7000	4782	2493	93
H(22B)	6889	4759	3004	93
H(20A)	8598	2906	2652	113
H(20B)	8066	3605	2272	113
H(16A)	1631	5847	574	72
H(16B)	1955	6742	883	72
H(19A)	7380	2133	2143	86
H(19B)	7268	2096	2654	86
H(10C)	897	-231	67	39
H(10D)	1592	-1078	168	39
H(103)	636	-1937	724	53
H(10E)	1751	166	2052	43
H(10F)	694	107	2003	43
H(107)	2856	404	-307	56
H(104)	457	-1530	1508	65
H(30A)	2695	7323	363	68
H(30B)	1696	7078	92	68
H(10G)	3321	1779	56	81
H(10H)	2319	2160	-57	81
H(11C)	3030	2805	-583	94
H(11D)	3330	1800	-716	94
H(10I)	1102	1050	-484	193
H(10J)	1404	29	-593	193
H(12C)	2869	-1340	902	68
H(12D)	3460	-530	1190	68
H(118)	3290	-886	256	67

H(12E)	4923	-1058	377	109
H(12F)	5566	-255	639	109
H(11E)	2117	2306	-1260	135
H(11F)	1559	2439	-883	135
H(11G)	2196	665	-1118	186
H(11H)	1172	989	-1267	186
H(30C)	1025	3434	2028	47
H(30D)	2007	3255	1963	47
H(30E)	2410	4161	2545	67
H(30F)	1511	3993	2704	67
H(300)	921	2190	2322	67
H(40A)	-58	3203	1556	41
H(40B)	-3	2815	1070	41
H(400)	-317	1393	1227	60
H(40C)	-1358	3638	1113	75
H(40D)	-1464	2718	816	75
H(20C)	4302	-1951	1319	104
H(20D)	4190	-2081	783	104
H(20E)	5589	-1487	1126	118
H(20F)	5132	-612	1305	118
H(11I)	4287	568	774	94
H(11J)	4159	421	238	94
H(30G)	1589	2198	3161	65
H(30H)	2595	1819	3290	65
H(30I)	2526	3471	3259	52
H(30J)	3096	3041	2938	52
H(30K)	2517	1348	2548	52
H(30L)	1574	1032	2630	52
H(34A)	1612	2207	3336	65
H(34B)	2469	2192	3129	65
H(33A)	1177	3629	3017	52
H(33B)	2210	3710	3280	52
H(35A)	1397	1212	2693	52
H(35B)	656	2007	2624	52
H(45A)	-695	1701	2041	59
H(45B)	-709	736	1779	59

H(43A)	-2497	2718	1145	69
H(43B)	-1854	3007	1623	69
H(44A)	-2163	1419	1668	61
H(44B)	-1898	1210	1199	61
H(45C)	-581	513	1532	39
H(45D)	-495	848	1042	39
H(43C)	-1782	2093	626	58
H(43D)	-2474	2364	918	58
H(44C)	-1998	769	987	71
H(44D)	-1906	1290	1463	71

Table S21. Crystal data and structure refinement for (PNP-Cy)Sc(CH₂SiMe₃)₂.

Empirical formula	C _{28.50} H ₅₄ N _{0.75} P _{1.50} Sc _{0.75} Si _{1.50}	
Formula weight	529.53	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 14.0824(7) Å	α = 90°.
	b = 16.2330(7) Å	β = 95.3980(10)°.
	c = 55.407(3) Å	γ = 90°.
Volume	12609.8(10) Å ³	
Z	16	
Density (calculated)	1.116 Mg/m ³	
Absorption coefficient	0.333 mm ⁻¹	
F(000)	4632	
Crystal size	0.080 x 0.080 x 0.050 mm ³	
Theta range for data collection	1.477 to 25.350°.	
Index ranges	-16 ≤ h ≤ 16, -19 ≤ k ≤ 19, -65 ≤ l ≤ 66	
Reflections collected	109591	
Independent reflections	11428 [R(int) = 0.0723]	
Completeness to theta = 25.000°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9833 and 0.9735	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11428 / 0 / 642	
Goodness-of-fit on F ²	1.026	
Final R indices [I > 2σ(I)]	R ₁ = 0.0426, wR ₂ = 0.0884	
R indices (all data)	R ₁ = 0.0603, wR ₂ = 0.0958	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.820 and -0.591 e.Å ⁻³	

Table S22. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)Sc(CH₂SiMe₃)₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sc(1)	0	2532(1)	2500	17(1)
Sc(2)	6758(1)	2078(1)	857(1)	14(1)
P(1)	1895(1)	2031(1)	2477(1)	27(1)
P(2)	8212(1)	1854(1)	1231(1)	16(1)
P(3)	6184(1)	3433(1)	576(1)	15(1)
Si(1)	44(1)	4154(1)	2035(1)	25(1)
Si(2)	7630(1)	429(1)	508(1)	21(1)
Si(3)	4576(1)	1441(1)	1106(1)	21(1)
N(1)	0	1208(2)	2500	29(1)
N(2)	6704(1)	3129(1)	1102(1)	16(1)
C(110)	7213(2)	3263(1)	1328(1)	18(1)
C(123)	7778(2)	-421(1)	1560(1)	24(1)
C(131)	3758(2)	2749(2)	123(1)	25(1)
C(127)	5351(2)	3359(1)	295(1)	17(1)
C(9)	1580(2)	1142(1)	2041(1)	19(1)
C(113)	6200(2)	3861(1)	1048(1)	17(1)
C(8)	2310(2)	1711(1)	2184(1)	18(1)
C(132)	4436(2)	2900(2)	351(1)	22(1)
C(116)	9972(2)	1658(2)	1031(1)	26(1)
C(125)	9374(2)	105(1)	1746(1)	24(1)
C(122)	7554(2)	434(1)	1451(1)	21(1)
C(118)	10805(2)	2843(2)	840(1)	31(1)
C(111)	7053(2)	4046(1)	1408(1)	24(1)
C(112)	6408(2)	4429(1)	1229(1)	25(1)
C(128)	5830(2)	2897(2)	95(1)	25(1)
C(101)	5494(2)	1291(1)	889(1)	21(1)
C(105)	7628(2)	1543(1)	574(1)	19(1)
C(120)	9285(2)	3105(1)	1038(1)	23(1)
C(121)	8479(2)	881(1)	1398(1)	18(1)
C(134)	6711(2)	5062(1)	436(1)	22(1)
C(126)	9159(2)	956(1)	1632(1)	21(1)

C(106)	7894(2)	-222(2)	788(1)	32(1)
C(129)	5138(2)	2779(2)	-133(1)	29(1)
C(115)	9399(2)	2271(1)	1171(1)	20(1)
C(133)	7104(2)	4227(1)	533(1)	20(1)
C(10)	1893(2)	909(2)	1793(1)	23(1)
C(109)	7786(2)	2574(1)	1454(1)	19(1)
C(12)	2839(2)	2214(2)	1782(1)	28(1)
C(1)	-231(2)	3106(2)	2135(1)	31(1)
C(136)	8345(2)	5431(2)	314(1)	35(1)
C(137)	8724(2)	4587(2)	404(1)	29(1)
C(124)	8456(2)	-351(2)	1792(1)	24(1)
C(117)	10931(2)	2015(2)	972(1)	30(1)
C(107)	8569(2)	144(2)	301(1)	27(1)
C(114)	5555(2)	3930(1)	816(1)	19(1)
C(130)	4248(2)	2312(2)	-76(1)	28(1)
C(7)	-493(3)	-117(2)	2459(1)	81(2)
C(11)	2092(2)	1667(2)	1644(1)	26(1)
C(19)	3833(2)	1974(2)	2687(1)	35(1)
C(13)	2524(2)	2462(2)	2029(1)	25(1)
C(119)	10260(2)	3453(2)	985(1)	30(1)
C(4)	1282(2)	4490(2)	2152(1)	34(1)
C(108)	6434(2)	103(2)	359(1)	38(1)
C(3)	-20(2)	4244(2)	1695(1)	51(1)
C(135)	7501(2)	5712(2)	448(1)	31(1)
C(103)	5148(2)	1745(2)	1412(1)	35(1)
C(104)	3863(2)	481(2)	1150(1)	31(1)
C(138)	7927(2)	3938(2)	391(1)	25(1)
C(2)	-802(2)	4933(2)	2145(1)	43(1)
C(102)	3706(2)	2282(2)	1004(1)	36(1)
C(6)	-779(3)	693(2)	2435(1)	45(1)
C(5)	1746(2)	1057(2)	2637(1)	52(1)
C(16)	3640(2)	3551(2)	2945(1)	40(1)
C(17)	4433(5)	2985(4)	3042(2)	38(2)
C(18)	4722(4)	2509(5)	2823(1)	39(2)
C(15)	2766(3)	3133(3)	2842(1)	26(1)
C(14)	3032(4)	2624(4)	2625(1)	16(1)

C(17A)	4614(5)	3057(5)	2907(2)	27(2)
C(18A)	4491(6)	2132(6)	2892(2)	27(2)
C(15A)	2940(5)	3239(4)	2694(2)	20(2)
C(14A)	2804(5)	2306(6)	2695(2)	16(2)

Table S23. Bond lengths [Å] and angles [°] for (PNP-Cy)Sc(CH₂SiMe₃)₂.

Sc(1)-N(1)	2.150(3)
Sc(1)-C(1)	2.225(3)
Sc(1)-C(1)#1	2.225(3)
Sc(1)-P(1)#1	2.8032(7)
Sc(1)-P(1)	2.8033(7)
Sc(2)-N(2)	2.1868(18)
Sc(2)-C(101)	2.211(2)
Sc(2)-C(105)	2.251(2)
Sc(2)-P(3)	2.7698(7)
Sc(2)-P(2)	2.7978(7)
P(1)-C(14A)	1.733(7)
P(1)-C(5)	1.835(3)
P(1)-C(8)	1.855(2)
P(1)-C(14)	1.978(5)
P(2)-C(109)	1.843(2)
P(2)-C(121)	1.852(2)
P(2)-C(115)	1.860(2)
P(3)-C(114)	1.850(2)
P(3)-C(133)	1.859(2)
P(3)-C(127)	1.860(2)
Si(1)-C(1)	1.841(3)
Si(1)-C(2)	1.879(3)
Si(1)-C(4)	1.882(3)
Si(1)-C(3)	1.886(3)
Si(2)-C(105)	1.844(2)
Si(2)-C(108)	1.881(3)
Si(2)-C(107)	1.885(2)
Si(2)-C(106)	1.886(3)
Si(3)-C(101)	1.865(2)
Si(3)-C(103)	1.874(3)
Si(3)-C(104)	1.882(2)
Si(3)-C(102)	1.885(3)
N(1)-C(6)	1.398(3)
N(1)-C(6)#1	1.398(3)

N(2)-C(110)	1.399(3)
N(2)-C(113)	1.402(3)
C(110)-C(111)	1.372(3)
C(110)-C(109)	1.510(3)
C(123)-C(124)	1.532(3)
C(123)-C(122)	1.533(3)
C(123)-H(00A)	0.9900
C(123)-H(00B)	0.9900
C(131)-C(130)	1.527(4)
C(131)-C(132)	1.531(3)
C(131)-H(00C)	0.9900
C(131)-H(00D)	0.9900
C(127)-C(128)	1.544(3)
C(127)-C(132)	1.545(3)
C(127)-H(004)	1.0000
C(9)-C(10)	1.529(3)
C(9)-C(8)	1.543(3)
C(9)-H(00E)	0.9900
C(9)-H(00F)	0.9900
C(113)-C(112)	1.375(3)
C(113)-C(114)	1.508(3)
C(8)-C(13)	1.535(3)
C(8)-H(007)	1.0000
C(132)-H(00G)	0.9900
C(132)-H(00H)	0.9900
C(116)-C(117)	1.532(3)
C(116)-C(115)	1.538(3)
C(116)-H(00I)	0.9900
C(116)-H(00J)	0.9900
C(125)-C(124)	1.531(3)
C(125)-C(126)	1.538(3)
C(125)-H(01A)	0.9900
C(125)-H(01B)	0.9900
C(122)-C(121)	1.544(3)
C(122)-H(01C)	0.9900
C(122)-H(01D)	0.9900

C(118)-C(119)	1.527(4)
C(118)-C(117)	1.533(4)
C(118)-H(01E)	0.9900
C(118)-H(01F)	0.9900
C(111)-C(112)	1.422(3)
C(111)-H(013)	0.9500
C(112)-H(014)	0.9500
C(128)-C(129)	1.537(3)
C(128)-H(01G)	0.9900
C(128)-H(01H)	0.9900
C(101)-H(01I)	0.9900
C(101)-H(01J)	0.9900
C(105)-H(01K)	0.9900
C(105)-H(01L)	0.9900
C(120)-C(119)	1.539(3)
C(120)-C(115)	1.544(3)
C(120)-H(01M)	0.9900
C(120)-H(01N)	0.9900
C(121)-C(126)	1.542(3)
C(121)-H(019)	1.0000
C(134)-C(135)	1.532(3)
C(134)-C(133)	1.541(3)
C(134)-H(02A)	0.9900
C(134)-H(02B)	0.9900
C(126)-H(02C)	0.9900
C(126)-H(02D)	0.9900
C(106)-H(02E)	0.9800
C(106)-H(02F)	0.9800
C(106)-H(02G)	0.9800
C(129)-C(130)	1.525(3)
C(129)-H(02H)	0.9900
C(129)-H(02I)	0.9900
C(115)-H(024)	1.0000
C(133)-C(138)	1.535(3)
C(133)-H(025)	1.0000
C(10)-C(11)	1.523(3)

C(10)-H(02J)	0.9900
C(10)-H(02K)	0.9900
C(109)-H(02L)	0.9900
C(109)-H(02M)	0.9900
C(12)-C(11)	1.524(4)
C(12)-C(13)	1.536(4)
C(12)-H(02N)	0.9900
C(12)-H(02O)	0.9900
C(1)-H(02P)	0.9900
C(1)-H(02Q)	0.9900
C(136)-C(135)	1.528(4)
C(136)-C(137)	1.537(4)
C(136)-H(03A)	0.9900
C(136)-H(03B)	0.9900
C(137)-C(138)	1.536(3)
C(137)-H(03C)	0.9900
C(137)-H(03D)	0.9900
C(124)-H(03E)	0.9900
C(124)-H(03F)	0.9900
C(117)-H(03G)	0.9900
C(117)-H(03H)	0.9900
C(107)-H(03I)	0.9800
C(107)-H(03J)	0.9800
C(107)-H(03K)	0.9800
C(114)-H(03L)	0.9900
C(114)-H(03M)	0.9900
C(130)-H(03N)	0.9900
C(130)-H(03O)	0.9900
C(7)-C(6)	1.377(5)
C(7)-C(7)#1	1.420(9)
C(7)-H(037)	0.9500
C(11)-H(03P)	0.9900
C(11)-H(03Q)	0.9900
C(19)-C(18A)	1.422(8)
C(19)-C(14A)	1.549(7)
C(19)-C(14)	1.558(5)

C(19)-C(18)	1.647(6)
C(19)-H(03R)	0.9900
C(19)-H(03S)	0.9900
C(13)-H(04A)	0.9900
C(13)-H(04B)	0.9900
C(119)-H(04C)	0.9900
C(119)-H(04D)	0.9900
C(4)-H(04E)	0.9800
C(4)-H(04F)	0.9800
C(4)-H(04G)	0.9800
C(108)-H(04H)	0.9800
C(108)-H(04I)	0.9800
C(108)-H(04J)	0.9800
C(3)-H(04K)	0.9800
C(3)-H(04L)	0.9800
C(3)-H(04M)	0.9800
C(135)-H(04N)	0.9900
C(135)-H(04O)	0.9900
C(103)-H(04P)	0.9800
C(103)-H(04Q)	0.9800
C(103)-H(04R)	0.9800
C(104)-H(04S)	0.9800
C(104)-H(04T)	0.9800
C(104)-H(04U)	0.9800
C(138)-H(04V)	0.9900
C(138)-H(04W)	0.9900
C(2)-H(04\$)	0.9800
C(2)-H(04)	0.9800
C(2)-H(04X)	0.9800
C(102)-H(05A)	0.9800
C(102)-H(05B)	0.9800
C(102)-H(05C)	0.9800
C(6)-C(5)#1	1.504(5)
C(5)-C(6)#1	1.504(5)
C(5)-H(05D)	0.9900
C(5)-H(05E)	0.9900

C(16)-C(15)	1.474(5)
C(16)-C(17)	1.506(6)
C(16)-C(17A)	1.620(9)
C(16)-C(15A)	1.703(8)
C(16)-H(05F)	0.9900
C(16)-H(05G)	0.9900
C(17)-C(18)	1.526(11)
C(17)-H(05L)	0.9900
C(17)-H(05M)	0.9900
C(18)-H(05H)	0.9900
C(18)-H(05I)	0.9900
C(15)-C(14)	1.534(8)
C(15)-H(05J)	0.9900
C(15)-H(05K)	0.9900
C(14)-H(057)	1.0000
C(17A)-C(18A)	1.513(13)
C(17A)-H(53A)	0.9900
C(17A)-H(53B)	0.9900
C(18A)-H(55A)	0.9900
C(18A)-H(55B)	0.9900
C(15A)-C(14A)	1.528(12)
C(15A)-H(56A)	0.9900
C(15A)-H(56B)	0.9900
C(14A)-H(57A)	1.0000
N(1)-Sc(1)-C(1)	114.75(7)
N(1)-Sc(1)-C(1)#1	114.75(7)
C(1)-Sc(1)-C(1)#1	130.49(14)
N(1)-Sc(1)-P(1)#1	73.132(19)
C(1)-Sc(1)-P(1)#1	95.98(7)
C(1)#1-Sc(1)-P(1)#1	97.98(7)
N(1)-Sc(1)-P(1)	73.131(19)
C(1)-Sc(1)-P(1)	97.99(7)
C(1)#1-Sc(1)-P(1)	95.97(7)
P(1)#1-Sc(1)-P(1)	146.26(4)
N(2)-Sc(2)-C(101)	108.98(8)

N(2)-Sc(2)-C(105)	141.87(8)
C(101)-Sc(2)-C(105)	109.11(9)
N(2)-Sc(2)-P(3)	72.85(5)
C(101)-Sc(2)-P(3)	108.04(6)
C(105)-Sc(2)-P(3)	93.77(6)
N(2)-Sc(2)-P(2)	72.91(5)
C(101)-Sc(2)-P(2)	113.80(7)
C(105)-Sc(2)-P(2)	93.22(6)
P(3)-Sc(2)-P(2)	132.38(2)
C(14A)-P(1)-C(5)	89.8(4)
C(14A)-P(1)-C(8)	114.1(3)
C(5)-P(1)-C(8)	104.05(13)
C(5)-P(1)-C(14)	110.2(2)
C(8)-P(1)-C(14)	100.84(19)
C(14A)-P(1)-Sc(1)	122.6(2)
C(5)-P(1)-Sc(1)	94.36(10)
C(8)-P(1)-Sc(1)	120.04(7)
C(14)-P(1)-Sc(1)	125.28(14)
C(109)-P(2)-C(121)	105.65(11)
C(109)-P(2)-C(115)	104.04(11)
C(121)-P(2)-C(115)	104.81(10)
C(109)-P(2)-Sc(2)	98.76(7)
C(121)-P(2)-Sc(2)	125.55(7)
C(115)-P(2)-Sc(2)	115.38(8)
C(114)-P(3)-C(133)	100.10(11)
C(114)-P(3)-C(127)	108.78(10)
C(133)-P(3)-C(127)	109.33(11)
C(114)-P(3)-Sc(2)	94.40(7)
C(133)-P(3)-Sc(2)	116.86(7)
C(127)-P(3)-Sc(2)	123.06(7)
C(1)-Si(1)-C(2)	111.56(13)
C(1)-Si(1)-C(4)	112.24(12)
C(2)-Si(1)-C(4)	106.76(13)
C(1)-Si(1)-C(3)	112.33(14)
C(2)-Si(1)-C(3)	107.56(15)
C(4)-Si(1)-C(3)	106.03(14)

C(105)-Si(2)-C(108)	110.19(12)
C(105)-Si(2)-C(107)	112.12(11)
C(108)-Si(2)-C(107)	108.33(12)
C(105)-Si(2)-C(106)	112.89(11)
C(108)-Si(2)-C(106)	107.56(13)
C(107)-Si(2)-C(106)	105.48(12)
C(101)-Si(3)-C(103)	110.69(11)
C(101)-Si(3)-C(104)	112.70(12)
C(103)-Si(3)-C(104)	106.92(13)
C(101)-Si(3)-C(102)	111.80(12)
C(103)-Si(3)-C(102)	106.99(14)
C(104)-Si(3)-C(102)	107.44(12)
C(6)-N(1)-C(6)#1	106.6(4)
C(6)-N(1)-Sc(1)	126.70(18)
C(6)#1-N(1)-Sc(1)	126.70(18)
C(110)-N(2)-C(113)	105.39(18)
C(110)-N(2)-Sc(2)	129.30(14)
C(113)-N(2)-Sc(2)	125.02(15)
C(111)-C(110)-N(2)	110.3(2)
C(111)-C(110)-C(109)	129.3(2)
N(2)-C(110)-C(109)	120.26(19)
C(124)-C(123)-C(122)	110.56(19)
C(124)-C(123)-H(00A)	109.5
C(122)-C(123)-H(00A)	109.5
C(124)-C(123)-H(00B)	109.5
C(122)-C(123)-H(00B)	109.5
H(00A)-C(123)-H(00B)	108.1
C(130)-C(131)-C(132)	112.3(2)
C(130)-C(131)-H(00C)	109.1
C(132)-C(131)-H(00C)	109.1
C(130)-C(131)-H(00D)	109.1
C(132)-C(131)-H(00D)	109.1
H(00C)-C(131)-H(00D)	107.9
C(128)-C(127)-C(132)	109.72(19)
C(128)-C(127)-P(3)	110.33(15)
C(132)-C(127)-P(3)	109.65(16)

C(128)-C(127)-H(004)	109.0
C(132)-C(127)-H(004)	109.0
P(3)-C(127)-H(004)	109.0
C(10)-C(9)-C(8)	111.87(19)
C(10)-C(9)-H(00E)	109.2
C(8)-C(9)-H(00E)	109.2
C(10)-C(9)-H(00F)	109.2
C(8)-C(9)-H(00F)	109.2
H(00E)-C(9)-H(00F)	107.9
C(112)-C(113)-N(2)	110.1(2)
C(112)-C(113)-C(114)	130.0(2)
N(2)-C(113)-C(114)	119.85(19)
C(13)-C(8)-C(9)	110.30(19)
C(13)-C(8)-P(1)	111.17(16)
C(9)-C(8)-P(1)	111.48(15)
C(13)-C(8)-H(007)	107.9
C(9)-C(8)-H(007)	107.9
P(1)-C(8)-H(007)	107.9
C(131)-C(132)-C(127)	112.3(2)
C(131)-C(132)-H(00G)	109.2
C(127)-C(132)-H(00G)	109.2
C(131)-C(132)-H(00H)	109.2
C(127)-C(132)-H(00H)	109.2
H(00G)-C(132)-H(00H)	107.9
C(117)-C(116)-C(115)	112.1(2)
C(117)-C(116)-H(00I)	109.2
C(115)-C(116)-H(00I)	109.2
C(117)-C(116)-H(00J)	109.2
C(115)-C(116)-H(00J)	109.2
H(00I)-C(116)-H(00J)	107.9
C(124)-C(125)-C(126)	111.44(19)
C(124)-C(125)-H(01A)	109.3
C(126)-C(125)-H(01A)	109.3
C(124)-C(125)-H(01B)	109.3
C(126)-C(125)-H(01B)	109.3
H(01A)-C(125)-H(01B)	108.0

C(123)-C(122)-C(121)	110.71(18)
C(123)-C(122)-H(01C)	109.5
C(121)-C(122)-H(01C)	109.5
C(123)-C(122)-H(01D)	109.5
C(121)-C(122)-H(01D)	109.5
H(01C)-C(122)-H(01D)	108.1
C(119)-C(118)-C(117)	111.0(2)
C(119)-C(118)-H(01E)	109.4
C(117)-C(118)-H(01E)	109.4
C(119)-C(118)-H(01F)	109.4
C(117)-C(118)-H(01F)	109.4
H(01E)-C(118)-H(01F)	108.0
C(110)-C(111)-C(112)	107.1(2)
C(110)-C(111)-H(013)	126.5
C(112)-C(111)-H(013)	126.5
C(113)-C(112)-C(111)	107.0(2)
C(113)-C(112)-H(014)	126.5
C(111)-C(112)-H(014)	126.5
C(129)-C(128)-C(127)	111.54(19)
C(129)-C(128)-H(01G)	109.3
C(127)-C(128)-H(01G)	109.3
C(129)-C(128)-H(01H)	109.3
C(127)-C(128)-H(01H)	109.3
H(01G)-C(128)-H(01H)	108.0
Si(3)-C(101)-Sc(2)	126.10(12)
Si(3)-C(101)-H(01I)	105.8
Sc(2)-C(101)-H(01I)	105.8
Si(3)-C(101)-H(01J)	105.8
Sc(2)-C(101)-H(01J)	105.8
H(01I)-C(101)-H(01J)	106.2
Si(2)-C(105)-Sc(2)	121.92(12)
Si(2)-C(105)-H(01K)	106.8
Sc(2)-C(105)-H(01K)	106.8
Si(2)-C(105)-H(01L)	106.8
Sc(2)-C(105)-H(01L)	106.8
H(01K)-C(105)-H(01L)	106.7

C(119)-C(120)-C(115)	111.03(19)
C(119)-C(120)-H(01M)	109.4
C(115)-C(120)-H(01M)	109.4
C(119)-C(120)-H(01N)	109.4
C(115)-C(120)-H(01N)	109.4
H(01M)-C(120)-H(01N)	108.0
C(126)-C(121)-C(122)	110.19(19)
C(126)-C(121)-P(2)	115.66(15)
C(122)-C(121)-P(2)	111.17(15)
C(126)-C(121)-H(019)	106.4
C(122)-C(121)-H(019)	106.4
P(2)-C(121)-H(019)	106.4
C(135)-C(134)-C(133)	110.84(19)
C(135)-C(134)-H(02A)	109.5
C(133)-C(134)-H(02A)	109.5
C(135)-C(134)-H(02B)	109.5
C(133)-C(134)-H(02B)	109.5
H(02A)-C(134)-H(02B)	108.1
C(125)-C(126)-C(121)	110.90(19)
C(125)-C(126)-H(02C)	109.5
C(121)-C(126)-H(02C)	109.5
C(125)-C(126)-H(02D)	109.5
C(121)-C(126)-H(02D)	109.5
H(02C)-C(126)-H(02D)	108.0
Si(2)-C(106)-H(02E)	109.5
Si(2)-C(106)-H(02F)	109.5
H(02E)-C(106)-H(02F)	109.5
Si(2)-C(106)-H(02G)	109.5
H(02E)-C(106)-H(02G)	109.5
H(02F)-C(106)-H(02G)	109.5
C(130)-C(129)-C(128)	110.9(2)
C(130)-C(129)-H(02H)	109.4
C(128)-C(129)-H(02H)	109.4
C(130)-C(129)-H(02I)	109.4
C(128)-C(129)-H(02I)	109.4
H(02H)-C(129)-H(02I)	108.0

C(116)-C(115)-C(120)	111.1(2)
C(116)-C(115)-P(2)	112.14(16)
C(120)-C(115)-P(2)	110.45(15)
C(116)-C(115)-H(024)	107.7
C(120)-C(115)-H(024)	107.7
P(2)-C(115)-H(024)	107.7
C(138)-C(133)-C(134)	110.8(2)
C(138)-C(133)-P(3)	114.95(16)
C(134)-C(133)-P(3)	114.95(15)
C(138)-C(133)-H(025)	105.0
C(134)-C(133)-H(025)	105.0
P(3)-C(133)-H(025)	105.0
C(11)-C(10)-C(9)	111.8(2)
C(11)-C(10)-H(02J)	109.3
C(9)-C(10)-H(02J)	109.3
C(11)-C(10)-H(02K)	109.3
C(9)-C(10)-H(02K)	109.3
H(02J)-C(10)-H(02K)	107.9
C(110)-C(109)-P(2)	110.72(16)
C(110)-C(109)-H(02L)	109.5
P(2)-C(109)-H(02L)	109.5
C(110)-C(109)-H(02M)	109.5
P(2)-C(109)-H(02M)	109.5
H(02L)-C(109)-H(02M)	108.1
C(11)-C(12)-C(13)	110.9(2)
C(11)-C(12)-H(02N)	109.5
C(13)-C(12)-H(02N)	109.5
C(11)-C(12)-H(02O)	109.5
C(13)-C(12)-H(02O)	109.5
H(02N)-C(12)-H(02O)	108.1
Si(1)-C(1)-Sc(1)	130.02(15)
Si(1)-C(1)-H(02P)	104.8
Sc(1)-C(1)-H(02P)	104.8
Si(1)-C(1)-H(02Q)	104.8
Sc(1)-C(1)-H(02Q)	104.8
H(02P)-C(1)-H(02Q)	105.8

C(135)-C(136)-C(137)	111.9(2)
C(135)-C(136)-H(03A)	109.2
C(137)-C(136)-H(03A)	109.2
C(135)-C(136)-H(03B)	109.2
C(137)-C(136)-H(03B)	109.2
H(03A)-C(136)-H(03B)	107.9
C(138)-C(137)-C(136)	111.5(2)
C(138)-C(137)-H(03C)	109.3
C(136)-C(137)-H(03C)	109.3
C(138)-C(137)-H(03D)	109.3
C(136)-C(137)-H(03D)	109.3
H(03C)-C(137)-H(03D)	108.0
C(125)-C(124)-C(123)	111.4(2)
C(125)-C(124)-H(03E)	109.3
C(123)-C(124)-H(03E)	109.3
C(125)-C(124)-H(03F)	109.3
C(123)-C(124)-H(03F)	109.3
H(03E)-C(124)-H(03F)	108.0
C(116)-C(117)-C(118)	111.6(2)
C(116)-C(117)-H(03G)	109.3
C(118)-C(117)-H(03G)	109.3
C(116)-C(117)-H(03H)	109.3
C(118)-C(117)-H(03H)	109.3
H(03G)-C(117)-H(03H)	108.0
Si(2)-C(107)-H(03I)	109.5
Si(2)-C(107)-H(03J)	109.5
H(03I)-C(107)-H(03J)	109.5
Si(2)-C(107)-H(03K)	109.5
H(03I)-C(107)-H(03K)	109.5
H(03J)-C(107)-H(03K)	109.5
C(113)-C(114)-P(3)	106.86(15)
C(113)-C(114)-H(03L)	110.3
P(3)-C(114)-H(03L)	110.3
C(113)-C(114)-H(03M)	110.3
P(3)-C(114)-H(03M)	110.3
H(03L)-C(114)-H(03M)	108.6

C(129)-C(130)-C(131)	110.8(2)
C(129)-C(130)-H(03N)	109.5
C(131)-C(130)-H(03N)	109.5
C(129)-C(130)-H(03O)	109.5
C(131)-C(130)-H(03O)	109.5
H(03N)-C(130)-H(03O)	108.1
C(6)-C(7)-C(7)#1	107.4(2)
C(6)-C(7)-H(037)	126.3
C(7)#1-C(7)-H(037)	126.3
C(10)-C(11)-C(12)	110.6(2)
C(10)-C(11)-H(03P)	109.5
C(12)-C(11)-H(03P)	109.5
C(10)-C(11)-H(03Q)	109.5
C(12)-C(11)-H(03Q)	109.5
H(03P)-C(11)-H(03Q)	108.1
C(18A)-C(19)-C(14A)	117.0(5)
C(14)-C(19)-C(18)	104.3(4)
C(14)-C(19)-H(03R)	110.9
C(18)-C(19)-H(03R)	110.9
C(14)-C(19)-H(03S)	110.9
C(18)-C(19)-H(03S)	110.9
H(03R)-C(19)-H(03S)	108.9
C(8)-C(13)-C(12)	112.2(2)
C(8)-C(13)-H(04A)	109.2
C(12)-C(13)-H(04A)	109.2
C(8)-C(13)-H(04B)	109.2
C(12)-C(13)-H(04B)	109.2
H(04A)-C(13)-H(04B)	107.9
C(118)-C(119)-C(120)	111.2(2)
C(118)-C(119)-H(04C)	109.4
C(120)-C(119)-H(04C)	109.4
C(118)-C(119)-H(04D)	109.4
C(120)-C(119)-H(04D)	109.4
H(04C)-C(119)-H(04D)	108.0
Si(1)-C(4)-H(04E)	109.5
Si(1)-C(4)-H(04F)	109.5

H(04E)-C(4)-H(04F)	109.5
Si(1)-C(4)-H(04G)	109.5
H(04E)-C(4)-H(04G)	109.5
H(04F)-C(4)-H(04G)	109.5
Si(2)-C(108)-H(04H)	109.5
Si(2)-C(108)-H(04I)	109.5
H(04H)-C(108)-H(04I)	109.5
Si(2)-C(108)-H(04J)	109.5
H(04H)-C(108)-H(04J)	109.5
H(04I)-C(108)-H(04J)	109.5
Si(1)-C(3)-H(04K)	109.5
Si(1)-C(3)-H(04L)	109.5
H(04K)-C(3)-H(04L)	109.5
Si(1)-C(3)-H(04M)	109.5
H(04K)-C(3)-H(04M)	109.5
H(04L)-C(3)-H(04M)	109.5
C(136)-C(135)-C(134)	111.7(2)
C(136)-C(135)-H(04N)	109.3
C(134)-C(135)-H(04N)	109.3
C(136)-C(135)-H(04O)	109.3
C(134)-C(135)-H(04O)	109.3
H(04N)-C(135)-H(04O)	108.0
Si(3)-C(103)-H(04P)	109.5
Si(3)-C(103)-H(04Q)	109.5
H(04P)-C(103)-H(04Q)	109.5
Si(3)-C(103)-H(04R)	109.5
H(04P)-C(103)-H(04R)	109.5
H(04Q)-C(103)-H(04R)	109.5
Si(3)-C(104)-H(04S)	109.5
Si(3)-C(104)-H(04T)	109.5
H(04S)-C(104)-H(04T)	109.5
Si(3)-C(104)-H(04U)	109.5
H(04S)-C(104)-H(04U)	109.5
H(04T)-C(104)-H(04U)	109.5
C(133)-C(138)-C(137)	110.5(2)
C(133)-C(138)-H(04V)	109.5

C(137)-C(138)-H(04V)	109.5
C(133)-C(138)-H(04W)	109.5
C(137)-C(138)-H(04W)	109.5
H(04V)-C(138)-H(04W)	108.1
Si(1)-C(2)-H(04\$)	109.5
Si(1)-C(2)-H(04)	109.5
H(04\$)-C(2)-H(04)	109.5
Si(1)-C(2)-H(04X)	109.5
H(04\$)-C(2)-H(04X)	109.5
H(04)-C(2)-H(04X)	109.5
Si(3)-C(102)-H(05A)	109.5
Si(3)-C(102)-H(05B)	109.5
H(05A)-C(102)-H(05B)	109.5
Si(3)-C(102)-H(05C)	109.5
H(05A)-C(102)-H(05C)	109.5
H(05B)-C(102)-H(05C)	109.5
C(7)-C(6)-N(1)	109.3(3)
C(7)-C(6)-C(5)#1	130.5(3)
N(1)-C(6)-C(5)#1	120.1(3)
C(6)#1-C(5)-P(1)	110.56(19)
C(6)#1-C(5)-H(05D)	109.5
P(1)-C(5)-H(05D)	109.5
C(6)#1-C(5)-H(05E)	109.5
P(1)-C(5)-H(05E)	109.5
H(05D)-C(5)-H(05E)	108.1
C(15)-C(16)-C(17)	115.0(3)
C(17A)-C(16)-C(15A)	100.3(5)
C(15)-C(16)-H(05F)	108.5
C(17)-C(16)-H(05F)	108.5
C(15)-C(16)-H(05G)	108.5
C(17)-C(16)-H(05G)	108.5
H(05F)-C(16)-H(05G)	107.5
C(16)-C(17)-C(18)	105.6(6)
C(16)-C(17)-H(05L)	110.6
C(18)-C(17)-H(05L)	110.6
C(16)-C(17)-H(05M)	110.6

C(18)-C(17)-H(05M)	110.6
H(05L)-C(17)-H(05M)	108.7
C(17)-C(18)-C(19)	112.5(5)
C(17)-C(18)-H(05H)	109.1
C(19)-C(18)-H(05H)	109.1
C(17)-C(18)-H(05I)	109.1
C(19)-C(18)-H(05I)	109.1
H(05H)-C(18)-H(05I)	107.8
C(16)-C(15)-C(14)	107.2(5)
C(16)-C(15)-H(05J)	110.3
C(14)-C(15)-H(05J)	110.3
C(16)-C(15)-H(05K)	110.3
C(14)-C(15)-H(05K)	110.3
H(05J)-C(15)-H(05K)	108.5
C(15)-C(14)-C(19)	114.7(4)
C(15)-C(14)-P(1)	109.7(4)
C(19)-C(14)-P(1)	107.6(3)
C(15)-C(14)-H(057)	108.2
C(19)-C(14)-H(057)	108.2
P(1)-C(14)-H(057)	108.2
C(18A)-C(17A)-C(16)	113.8(7)
C(18A)-C(17A)-H(53A)	108.8
C(16)-C(17A)-H(53A)	108.8
C(18A)-C(17A)-H(53B)	108.8
C(16)-C(17A)-H(53B)	108.8
H(53A)-C(17A)-H(53B)	107.7
C(19)-C(18A)-C(17A)	106.5(7)
C(19)-C(18A)-H(55A)	110.4
C(17A)-C(18A)-H(55A)	110.4
C(19)-C(18A)-H(55B)	110.4
C(17A)-C(18A)-H(55B)	110.4
H(55A)-C(18A)-H(55B)	108.6
C(14A)-C(15A)-C(16)	110.8(6)
C(14A)-C(15A)-H(56A)	109.5
C(16)-C(15A)-H(56A)	109.5
C(14A)-C(15A)-H(56B)	109.5

C(16)-C(15A)-H(56B)	109.5
H(56A)-C(15A)-H(56B)	108.1
C(15A)-C(14A)-C(19)	103.1(7)
C(15A)-C(14A)-P(1)	109.7(6)
C(19)-C(14A)-P(1)	121.4(4)
C(15A)-C(14A)-H(57A)	107.3
C(19)-C(14A)-H(57A)	107.3
P(1)-C(14A)-H(57A)	107.3

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table S24. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)Sc(CH₂SiMe₃)₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Sc(1)	14(1)	19(1)	18(1)	0	3(1)	0
Sc(2)	14(1)	12(1)	16(1)	-1(1)	1(1)	2(1)
P(1)	23(1)	41(1)	16(1)	-7(1)	-3(1)	16(1)
P(2)	15(1)	15(1)	17(1)	1(1)	-1(1)	2(1)
P(3)	13(1)	14(1)	18(1)	1(1)	1(1)	1(1)
Si(1)	22(1)	23(1)	30(1)	5(1)	0(1)	2(1)
Si(2)	21(1)	19(1)	23(1)	-6(1)	2(1)	3(1)
Si(3)	17(1)	21(1)	26(1)	0(1)	4(1)	-2(1)
N(1)	48(2)	21(2)	22(2)	0	20(2)	0
N(2)	16(1)	13(1)	18(1)	-2(1)	2(1)	0(1)
C(110)	16(1)	18(1)	19(1)	-1(1)	2(1)	0(1)
C(123)	23(1)	20(1)	29(2)	2(1)	2(1)	-6(1)
C(131)	20(1)	25(1)	28(2)	0(1)	-3(1)	-4(1)
C(127)	16(1)	14(1)	20(1)	2(1)	-2(1)	0(1)
C(9)	20(1)	17(1)	21(1)	0(1)	3(1)	-1(1)
C(113)	16(1)	13(1)	22(1)	-1(1)	5(1)	2(1)
C(8)	13(1)	22(1)	18(1)	-4(1)	-1(1)	4(1)
C(132)	19(1)	24(1)	21(1)	1(1)	-1(1)	-2(1)
C(116)	20(1)	27(1)	32(2)	6(1)	4(1)	6(1)
C(125)	21(1)	24(1)	25(2)	6(1)	-3(1)	0(1)
C(122)	18(1)	23(1)	21(1)	2(1)	-2(1)	-2(1)
C(118)	24(1)	44(2)	26(2)	6(1)	4(1)	-6(1)
C(111)	27(1)	21(1)	24(2)	-8(1)	-3(1)	-1(1)
C(112)	28(1)	16(1)	30(2)	-4(1)	0(1)	6(1)
C(128)	21(1)	33(1)	22(2)	-2(1)	1(1)	0(1)
C(101)	21(1)	20(1)	22(1)	-2(1)	0(1)	2(1)
C(105)	20(1)	19(1)	18(1)	-1(1)	1(1)	4(1)
C(120)	24(1)	20(1)	24(2)	5(1)	2(1)	0(1)
C(121)	17(1)	15(1)	21(1)	0(1)	1(1)	1(1)
C(134)	26(1)	20(1)	20(1)	2(1)	-1(1)	-2(1)
C(126)	19(1)	21(1)	22(1)	4(1)	-2(1)	-2(1)

C(106)	42(2)	22(1)	34(2)	-1(1)	13(1)	4(1)
C(129)	29(1)	38(2)	21(2)	-4(1)	3(1)	-2(1)
C(115)	16(1)	23(1)	18(1)	3(1)	-1(1)	-1(1)
C(133)	18(1)	17(1)	24(1)	3(1)	0(1)	-3(1)
C(10)	20(1)	29(1)	21(1)	-7(1)	-2(1)	0(1)
C(109)	17(1)	21(1)	19(1)	-3(1)	1(1)	0(1)
C(12)	24(1)	30(1)	33(2)	8(1)	11(1)	0(1)
C(1)	25(1)	32(2)	36(2)	8(1)	8(1)	9(1)
C(136)	35(2)	34(2)	34(2)	5(1)	0(1)	-19(1)
C(137)	22(1)	39(2)	28(2)	0(1)	3(1)	-10(1)
C(124)	25(1)	21(1)	25(2)	6(1)	1(1)	0(1)
C(117)	18(1)	42(2)	30(2)	4(1)	5(1)	3(1)
C(107)	30(1)	25(1)	27(2)	-5(1)	3(1)	9(1)
C(114)	19(1)	16(1)	21(1)	2(1)	3(1)	5(1)
C(130)	32(1)	26(1)	26(2)	-2(1)	-6(1)	-4(1)
C(7)	185(5)	24(2)	47(3)	-15(2)	78(4)	-30(2)
C(11)	24(1)	40(2)	16(1)	4(1)	5(1)	7(1)
C(19)	20(1)	44(2)	41(2)	3(1)	-5(1)	9(1)
C(13)	19(1)	22(1)	33(2)	-5(1)	4(1)	-4(1)
C(119)	31(1)	32(2)	26(2)	7(1)	2(1)	-9(1)
C(4)	28(1)	31(2)	41(2)	-8(1)	-2(1)	4(1)
C(108)	30(2)	43(2)	43(2)	-22(1)	4(1)	-4(1)
C(3)	56(2)	57(2)	36(2)	12(2)	-7(2)	-22(2)
C(135)	39(2)	24(1)	30(2)	6(1)	-3(1)	-8(1)
C(103)	26(1)	49(2)	31(2)	-9(1)	9(1)	-7(1)
C(104)	31(1)	28(1)	33(2)	6(1)	5(1)	-7(1)
C(138)	20(1)	27(1)	29(2)	-1(1)	6(1)	-3(1)
C(2)	32(2)	31(2)	64(2)	9(2)	3(2)	13(1)
C(102)	23(1)	31(2)	56(2)	11(1)	16(1)	3(1)
C(6)	83(2)	36(2)	23(2)	-16(1)	36(2)	-29(2)
C(5)	61(2)	72(2)	26(2)	24(2)	22(2)	49(2)
C(16)	37(2)	35(2)	47(2)	-1(1)	-4(1)	-7(1)
C(17)	42(3)	41(3)	30(4)	3(3)	-11(3)	-16(2)
C(18)	22(3)	29(4)	62(5)	-4(3)	-20(3)	-4(3)
C(15)	29(3)	26(3)	23(4)	-5(2)	3(2)	-2(2)
C(14)	12(2)	16(3)	18(3)	-4(2)	0(2)	-4(2)

C(17A)	21(4)	28(5)	28(6)	-5(4)	-11(4)	-9(3)
C(18A)	24(4)	23(5)	32(5)	3(3)	-8(3)	2(3)
C(15A)	15(3)	20(4)	24(5)	-3(3)	-2(3)	-5(2)
C(14A)	8(3)	17(4)	25(4)	-6(3)	5(3)	-7(3)

Table S25. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)Sc(CH₂SiMe₃)₂.

	x	y	z	U(eq)
H(00A)	7179	-691	1597	29
H(00B)	8075	-766	1440	29
H(00C)	3213	2412	166	30
H(00D)	3504	3284	60	30
H(004)	5177	3927	237	20
H(00E)	1500	634	2136	23
H(00F)	954	1424	2019	23
H(007)	2917	1394	2219	21
H(00G)	4614	2364	428	26
H(00H)	4102	3227	468	26
H(00I)	10086	1150	1128	31
H(00J)	9592	1507	877	31
H(01A)	9737	-228	1636	28
H(01B)	9775	173	1901	28
H(01C)	7215	765	1566	25
H(01D)	7130	376	1299	25
H(01E)	11439	3073	815	38
H(01F)	10453	2757	679	38
H(013)	7323	4288	1555	29
H(014)	6165	4974	1234	30
H(01G)	6393	3212	54	30
H(01H)	6052	2352	158	30
H(01I)	5141	1284	726	25
H(01J)	5744	726	918	25
H(01K)	7426	1827	420	23
H(01L)	8299	1704	620	23
H(01M)	8880	3030	883	28
H(01N)	8962	3502	1138	28
H(019)	8805	514	1286	21
H(02A)	6434	4996	266	26

H(02B)	6197	5247	534	26
H(02C)	9762	1218	1594	25
H(02D)	8864	1312	1749	25
H(02E)	8515	-66	870	48
H(02F)	7906	-805	742	48
H(02G)	7397	-135	898	48
H(02H)	4952	3324	-203	35
H(02I)	5462	2470	-256	35
H(024)	9768	2373	1332	23
H(025)	7405	4348	700	24
H(02J)	2476	567	1816	28
H(02K)	1386	576	1704	28
H(02L)	7386	2274	1562	23
H(02M)	8339	2809	1555	23
H(02N)	2938	2715	1685	34
H(02O)	3453	1914	1805	34
H(02P)	102	2737	2028	37
H(02Q)	-920	3034	2086	37
H(03A)	8863	5843	339	42
H(03B)	8145	5399	139	42
H(03C)	9230	4404	303	35
H(03D)	9011	4637	573	35
H(03E)	8132	-52	1917	29
H(03F)	8617	-909	1855	29
H(03G)	11247	1621	869	36
H(03H)	11347	2092	1125	36
H(03I)	8485	479	154	41
H(03J)	8506	-441	258	41
H(03K)	9203	245	385	41
H(03L)	5425	4515	775	22
H(03M)	4941	3649	832	22
H(03N)	4427	1747	-22	34
H(03O)	3800	2269	-224	34
H(037)	-884	-589	2427	98
H(03P)	1495	1983	1607	32
H(03Q)	2323	1493	1489	32

H(03R)	4023	1710	2538	42
H(03S)	3618	1544	2796	42
H(04A)	3034	2794	2118	30
H(04B)	1946	2810	2005	30
H(04C)	10165	3974	893	35
H(04D)	10641	3578	1140	35
H(04E)	1363	4435	2328	50
H(04F)	1377	5066	2107	50
H(04G)	1752	4143	2080	50
H(04H)	5950	169	473	58
H(04I)	6462	-476	310	58
H(04J)	6266	446	216	58
H(04K)	401	3833	1631	76
H(04L)	183	4797	1650	76
H(04M)	-677	4149	1625	76
H(04N)	7241	6231	375	37
H(04O)	7723	5825	619	37
H(04P)	5611	1323	1471	52
H(04Q)	4658	1797	1526	52
H(04R)	5476	2274	1400	52
H(04S)	3508	327	996	46
H(04T)	3415	583	1272	46
H(04U)	4296	31	1205	46
H(04V)	7687	3841	220	30
H(04W)	8185	3411	460	30
H(04\$)	-1460	4757	2100	64
H(04)	-693	5469	2071	64
H(04X)	-692	4980	2322	64
H(05A)	4025	2818	1023	54
H(05B)	3166	2270	1104	54
H(05C)	3475	2196	834	54
H(05D)	2247	663	2599	63
H(05E)	1818	1155	2815	63
H(05F)	3475	3916	3078	48
H(05G)	3878	3905	2818	48
H(05L)	4209	2604	3164	46

H(05M)	4979	3306	3118	46
H(05H)	5252	2130	2876	47
H(05I)	4958	2902	2705	47
H(05J)	2270	3544	2788	31
H(05K)	2515	2770	2964	31
H(057)	3251	3011	2501	19
H(53A)	4862	3253	2756	32
H(53B)	5097	3189	3043	32
H(55A)	5109	1861	2873	32
H(55B)	4240	1920	3041	32
H(56A)	2311	3513	2690	24
H(56B)	3240	3404	2547	24
H(57A)	2594	2153	2857	20

Table S26. Crystal data and structure refinement for (PNP-Cy)ScNp₂.

Empirical formula	C ₄₀ H ₇₂ N ₁ P ₂ Sc ₁	
Formula weight	673.88	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 13.9103(4) Å	α = 90°.
	b = 15.5320(4) Å	β = 95.279(2)°.
	c = 55.3947(14) Å	γ = 90°.
Volume	11917.5(5) Å ³	
Z	12	
Density (calculated)	1.127 Mg/m ³	
Absorption coefficient	0.292 mm ⁻¹	
F(000)	4440	
Crystal size	0.08 x 0.06 x 0.05 mm ³	
Theta range for data collection	1.48 to 25.49°.	
Index ranges	-16 ≤ h ≤ 16, -18 ≤ k ≤ 16, -66 ≤ l ≤ 67	
Reflections collected	67786	
Independent reflections	10987 [R(int) = 0.0692]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9855 and 0.9770	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10987 / 0 / 605	
Goodness-of-fit on F ²	1.040	
Final R indices [I > 2σ(I)]	R ₁ = 0.0495, wR ₂ = 0.0891	
R indices (all data)	R ₁ = 0.0805, wR ₂ = 0.0994	
Largest diff. peak and hole	0.353 and -0.512 e.Å ⁻³	

Table S27. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)ScNp₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	625(2)	950(2)	801(1)	15(1)
C(2)	1265(2)	1035(2)	1033(1)	14(1)
C(3)	1535(2)	435(2)	1206(1)	19(1)
C(4)	2155(2)	849(2)	1387(1)	18(1)
C(5)	2232(2)	1687(2)	1316(1)	14(1)
C(6)	2766(2)	2416(2)	1446(1)	16(1)
C(7)	3450(2)	4185(2)	1397(1)	16(1)
C(8)	2514(2)	4644(2)	1452(1)	18(1)
C(9)	2733(2)	5518(2)	1570(1)	21(1)
C(10)	3404(2)	5414(2)	1801(1)	22(1)
C(11)	4333(2)	4956(2)	1752(1)	22(1)
C(12)	4129(2)	4083(2)	1630(1)	19(1)
C(13)	4389(2)	2763(2)	1165(1)	16(1)
C(14)	4918(2)	3372(2)	1005(1)	22(1)
C(15)	5920(2)	3032(2)	961(1)	26(1)
C(16)	5859(2)	2129(2)	856(1)	25(1)
C(17)	5341(2)	1521(2)	1015(1)	25(1)
C(18)	4332(2)	1857(2)	1055(1)	22(1)
C(19)	2206(2)	832(2)	518(1)	16(1)
C(20)	3042(2)	1242(2)	395(1)	20(1)
C(21)	3902(2)	626(2)	405(1)	24(1)
C(22)	3614(2)	-242(2)	289(1)	31(1)
C(23)	2764(2)	-641(2)	402(1)	29(1)
C(24)	1906(2)	-24(2)	394(1)	21(1)
C(25)	344(2)	1579(2)	294(1)	15(1)
C(26)	813(2)	1958(2)	77(1)	21(1)
C(27)	89(2)	2027(2)	-148(1)	24(1)
C(28)	-782(2)	2569(2)	-96(1)	24(1)
C(29)	-1257(2)	2200(2)	118(1)	21(1)
C(30)	-549(2)	2116(2)	343(1)	19(1)
C(31)	362(2)	3729(2)	934(1)	18(1)

C(32)	-411(2)	3564(2)	1113(1)	18(1)
C(33)	79(2)	3321(2)	1362(1)	28(1)
C(34)	-1065(2)	2819(2)	1022(1)	32(1)
C(35)	-1037(2)	4362(2)	1143(1)	26(1)
C(36)	2425(2)	3653(2)	579(1)	18(1)
C(37)	2499(2)	4635(2)	537(1)	17(1)
C(38)	1506(2)	4995(2)	448(1)	30(1)
C(39)	3207(2)	4833(2)	349(1)	25(1)
C(40)	2858(2)	5098(2)	773(1)	24(1)
C(41)	1149(2)	3036(2)	2306(1)	30(1)
C(42)	262(2)	2594(2)	2176(1)	34(1)
C(43)	522(2)	2150(2)	1948(1)	34(1)
C(44)	2200(2)	1905(2)	2138(1)	28(1)
C(45)	3264(2)	3871(2)	2342(1)	19(1)
C(46)	4234(2)	4245(2)	2423(1)	17(1)
C(47)	4513(2)	5089(2)	2451(1)	18(1)
C(48)	4866(2)	1695(2)	2135(1)	23(1)
C(49)	5061(2)	789(2)	2038(1)	27(1)
C(50)	4326(2)	151(2)	2123(1)	51(1)
C(51)	6067(2)	492(2)	2135(1)	37(1)
C(52)	2706(2)	3304(2)	2809(1)	16(1)
C(53)	3494(2)	3853(2)	2947(1)	19(1)
C(54)	2405(2)	2564(2)	2971(1)	19(1)
C(60)	1305(2)	1489(2)	2007(1)	30(1)
C(61)	2101(2)	2894(2)	3213(1)	23(1)
C(62)	2898(2)	3426(2)	3346(1)	23(1)
C(63)	3175(2)	4167(2)	3187(1)	21(1)
C(64)	4996(3)	778(2)	1761(1)	51(1)
C(140)	1970(2)	2400(2)	2365(1)	16(1)
N(1)	1706(1)	1823(1)	1093(1)	13(1)
N(2)	5000	3703(2)	2500	15(1)
P(3)	3183(1)	3182(1)	1224(1)	14(1)
P(4)	1199(1)	1564(1)	569(1)	14(1)
P(5)	3081(1)	2885(1)	2518(1)	15(1)
Sc(1)	1651(1)	2977(1)	865(1)	12(1)
Sc(2)	5000	2303(1)	2500	16(1)

Table S27. Bond lengths [Å] and angles [°] for (PNP-Cy)ScNp₂.

C(1)-C(2)	1.503(3)
C(1)-P(4)	1.838(2)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.366(4)
C(2)-N(1)	1.394(3)
C(3)-C(4)	1.415(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.367(4)
C(4)-H(4)	0.9500
C(5)-N(1)	1.394(3)
C(5)-C(6)	1.499(3)
C(6)-P(3)	1.840(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(12)	1.537(3)
C(7)-C(8)	1.538(3)
C(7)-P(3)	1.848(3)
C(7)-H(7)	1.0000
C(8)-C(9)	1.525(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.524(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.521(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.531(4)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.530(4)

C(13)-C(18)	1.534(4)
C(13)-P(3)	1.856(2)
C(13)-H(13)	1.0000
C(14)-C(15)	1.531(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.519(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.517(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.532(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(24)	1.538(4)
C(19)-C(20)	1.539(3)
C(19)-P(4)	1.846(3)
C(19)-H(19)	1.0000
C(20)-C(21)	1.529(4)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.530(4)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.519(4)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.528(4)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.540(3)

C(25)-C(30)	1.540(3)
C(25)-P(4)	1.845(3)
C(25)-H(25)	1.0000
C(26)-C(27)	1.531(4)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.524(4)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.522(4)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.520(3)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(32)	1.549(3)
C(31)-Sc(1)	2.202(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.527(4)
C(32)-C(34)	1.529(4)
C(32)-C(35)	1.533(4)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.549(4)
C(36)-Sc(1)	2.256(3)
C(36)-H(36A)	0.9900

C(36)-H(36B)	0.9900
C(37)-C(38)	1.528(4)
C(37)-C(39)	1.531(3)
C(37)-C(40)	1.534(4)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(140)	1.523(4)
C(41)-C(42)	1.534(4)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.512(4)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(60)	1.510(4)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(60)	1.525(4)
C(44)-C(140)	1.534(4)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(46)	1.499(4)
C(45)-P(5)	1.846(3)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.372(4)
C(46)-N(2)	1.394(3)
C(47)-C(47)#1	1.411(5)
C(47)-H(47)	0.9500
C(48)-C(49)	1.538(4)

C(48)-Sc(2)	2.223(3)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(51)	1.523(4)
C(49)-C(50)	1.530(4)
C(49)-C(64)	1.531(4)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-C(53)	1.535(3)
C(52)-C(54)	1.539(4)
C(52)-P(5)	1.858(3)
C(52)-H(52)	1.0000
C(53)-C(63)	1.520(4)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-C(61)	1.534(4)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(61)-C(62)	1.518(4)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900
C(62)-C(63)	1.522(4)
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(140)-P(5)	1.852(3)

C(140)-H(140)	1.0000
N(1)-Sc(1)	2.188(2)
N(2)-C(46)#1	1.394(3)
N(2)-Sc(2)	2.174(3)
P(3)-Sc(1)	2.7955(8)
P(4)-Sc(1)	2.7773(8)
P(5)-Sc(2)	2.8291(7)
Sc(2)-C(48)#1	2.223(3)
Sc(2)-P(5)#1	2.8291(7)

C(2)-C(1)-P(4)	106.84(17)
C(2)-C(1)-H(1A)	110.4
P(4)-C(1)-H(1A)	110.4
C(2)-C(1)-H(1B)	110.4
P(4)-C(1)-H(1B)	110.4
H(1A)-C(1)-H(1B)	108.6
C(3)-C(2)-N(1)	110.2(2)
C(3)-C(2)-C(1)	130.1(2)
N(1)-C(2)-C(1)	119.6(2)
C(2)-C(3)-C(4)	107.2(2)
C(2)-C(3)-H(3)	126.4
C(4)-C(3)-H(3)	126.4
C(5)-C(4)-C(3)	106.8(2)
C(5)-C(4)-H(4)	126.6
C(3)-C(4)-H(4)	126.6
C(4)-C(5)-N(1)	110.5(2)
C(4)-C(5)-C(6)	129.1(2)
N(1)-C(5)-C(6)	120.5(2)
C(5)-C(6)-P(3)	109.99(17)
C(5)-C(6)-H(6A)	109.7
P(3)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6B)	109.7
P(3)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
C(12)-C(7)-C(8)	110.3(2)
C(12)-C(7)-P(3)	115.24(18)

C(8)-C(7)-P(3)	111.06(18)
C(12)-C(7)-H(7)	106.6
C(8)-C(7)-H(7)	106.6
P(3)-C(7)-H(7)	106.6
C(9)-C(8)-C(7)	111.0(2)
C(9)-C(8)-H(8A)	109.4
C(7)-C(8)-H(8A)	109.4
C(9)-C(8)-H(8B)	109.4
C(7)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
C(10)-C(9)-C(8)	110.5(2)
C(10)-C(9)-H(9A)	109.6
C(8)-C(9)-H(9A)	109.6
C(10)-C(9)-H(9B)	109.6
C(8)-C(9)-H(9B)	109.6
H(9A)-C(9)-H(9B)	108.1
C(11)-C(10)-C(9)	111.3(2)
C(11)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10A)	109.4
C(11)-C(10)-H(10B)	109.4
C(9)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
C(10)-C(11)-C(12)	111.5(2)
C(10)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11A)	109.3
C(10)-C(11)-H(11B)	109.3
C(12)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-C(7)	110.8(2)
C(11)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(18)	110.3(2)
C(14)-C(13)-P(3)	112.08(18)

C(18)-C(13)-P(3)	112.21(18)
C(14)-C(13)-H(13)	107.3
C(18)-C(13)-H(13)	107.3
P(3)-C(13)-H(13)	107.3
C(13)-C(14)-C(15)	111.9(2)
C(13)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14A)	109.2
C(13)-C(14)-H(14B)	109.2
C(15)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9
C(16)-C(15)-C(14)	111.1(2)
C(16)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15B)	109.4
C(14)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(17)-C(16)-C(15)	111.4(2)
C(17)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16B)	109.4
C(15)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(16)-C(17)-C(18)	111.2(2)
C(16)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
C(17)-C(18)-C(13)	110.8(2)
C(17)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	108.1
C(24)-C(19)-C(20)	110.2(2)
C(24)-C(19)-P(4)	114.93(18)

C(20)-C(19)-P(4)	115.31(18)
C(24)-C(19)-H(19)	105.1
C(20)-C(19)-H(19)	105.1
P(4)-C(19)-H(19)	105.1
C(21)-C(20)-C(19)	110.2(2)
C(21)-C(20)-H(20A)	109.6
C(19)-C(20)-H(20A)	109.6
C(21)-C(20)-H(20B)	109.6
C(19)-C(20)-H(20B)	109.6
H(20A)-C(20)-H(20B)	108.1
C(20)-C(21)-C(22)	111.3(2)
C(20)-C(21)-H(21A)	109.4
C(22)-C(21)-H(21A)	109.4
C(20)-C(21)-H(21B)	109.4
C(22)-C(21)-H(21B)	109.4
H(21A)-C(21)-H(21B)	108.0
C(23)-C(22)-C(21)	111.7(2)
C(23)-C(22)-H(22A)	109.3
C(21)-C(22)-H(22A)	109.3
C(23)-C(22)-H(22B)	109.3
C(21)-C(22)-H(22B)	109.3
H(22A)-C(22)-H(22B)	107.9
C(22)-C(23)-C(24)	111.6(2)
C(22)-C(23)-H(23A)	109.3
C(24)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23B)	109.3
C(24)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	108.0
C(23)-C(24)-C(19)	110.5(2)
C(23)-C(24)-H(24A)	109.6
C(19)-C(24)-H(24A)	109.6
C(23)-C(24)-H(24B)	109.6
C(19)-C(24)-H(24B)	109.6
H(24A)-C(24)-H(24B)	108.1
C(26)-C(25)-C(30)	109.6(2)
C(26)-C(25)-P(4)	111.36(17)

C(30)-C(25)-P(4)	109.35(17)
C(26)-C(25)-H(25)	108.8
C(30)-C(25)-H(25)	108.8
P(4)-C(25)-H(25)	108.8
C(27)-C(26)-C(25)	111.6(2)
C(27)-C(26)-H(26A)	109.3
C(25)-C(26)-H(26A)	109.3
C(27)-C(26)-H(26B)	109.3
C(25)-C(26)-H(26B)	109.3
H(26A)-C(26)-H(26B)	108.0
C(28)-C(27)-C(26)	111.1(2)
C(28)-C(27)-H(27A)	109.4
C(26)-C(27)-H(27A)	109.4
C(28)-C(27)-H(27B)	109.4
C(26)-C(27)-H(27B)	109.4
H(27A)-C(27)-H(27B)	108.0
C(29)-C(28)-C(27)	110.4(2)
C(29)-C(28)-H(28A)	109.6
C(27)-C(28)-H(28A)	109.6
C(29)-C(28)-H(28B)	109.6
C(27)-C(28)-H(28B)	109.6
H(28A)-C(28)-H(28B)	108.1
C(30)-C(29)-C(28)	112.1(2)
C(30)-C(29)-H(29A)	109.2
C(28)-C(29)-H(29A)	109.2
C(30)-C(29)-H(29B)	109.2
C(28)-C(29)-H(29B)	109.2
H(29A)-C(29)-H(29B)	107.9
C(29)-C(30)-C(25)	112.1(2)
C(29)-C(30)-H(30A)	109.2
C(25)-C(30)-H(30A)	109.2
C(29)-C(30)-H(30B)	109.2
C(25)-C(30)-H(30B)	109.2
H(30A)-C(30)-H(30B)	107.9
C(32)-C(31)-Sc(1)	130.34(18)
C(32)-C(31)-H(31A)	104.7

Sc(1)-C(31)-H(31A)	104.7
C(32)-C(31)-H(31B)	104.7
Sc(1)-C(31)-H(31B)	104.7
H(31A)-C(31)-H(31B)	105.7
C(33)-C(32)-C(34)	108.3(2)
C(33)-C(32)-C(35)	108.2(2)
C(34)-C(32)-C(35)	108.8(2)
C(33)-C(32)-C(31)	109.8(2)
C(34)-C(32)-C(31)	109.9(2)
C(35)-C(32)-C(31)	111.8(2)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(37)-C(36)-Sc(1)	127.37(18)
C(37)-C(36)-H(36A)	105.5
Sc(1)-C(36)-H(36A)	105.5
C(37)-C(36)-H(36B)	105.5
Sc(1)-C(36)-H(36B)	105.5
H(36A)-C(36)-H(36B)	106.0
C(38)-C(37)-C(39)	109.1(2)
C(38)-C(37)-C(40)	108.5(2)

C(39)-C(37)-C(40)	107.9(2)
C(38)-C(37)-C(36)	109.7(2)
C(39)-C(37)-C(36)	110.9(2)
C(40)-C(37)-C(36)	110.7(2)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(140)-C(41)-C(42)	111.4(2)
C(140)-C(41)-H(41A)	109.3
C(42)-C(41)-H(41A)	109.3
C(140)-C(41)-H(41B)	109.3
C(42)-C(41)-H(41B)	109.3
H(41A)-C(41)-H(41B)	108.0
C(43)-C(42)-C(41)	110.7(3)
C(43)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42A)	109.5
C(43)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	108.1
C(60)-C(43)-C(42)	110.5(2)
C(60)-C(43)-H(43A)	109.5

C(42)-C(43)-H(43A)	109.6
C(60)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	108.1
C(60)-C(44)-C(140)	112.2(2)
C(60)-C(44)-H(44A)	109.2
C(140)-C(44)-H(44A)	109.2
C(60)-C(44)-H(44B)	109.2
C(140)-C(44)-H(44B)	109.2
H(44A)-C(44)-H(44B)	107.9
C(46)-C(45)-P(5)	109.13(18)
C(46)-C(45)-H(45A)	109.9
P(5)-C(45)-H(45A)	109.9
C(46)-C(45)-H(45B)	109.9
P(5)-C(45)-H(45B)	109.9
H(45A)-C(45)-H(45B)	108.3
C(47)-C(46)-N(2)	110.0(2)
C(47)-C(46)-C(45)	129.9(2)
N(2)-C(46)-C(45)	119.9(2)
C(46)-C(47)-C(47)#1	107.16(15)
C(46)-C(47)-H(47)	126.4
C(47)#1-C(47)-H(47)	126.4
C(49)-C(48)-Sc(2)	134.6(2)
C(49)-C(48)-H(48A)	103.5
Sc(2)-C(48)-H(48A)	103.5
C(49)-C(48)-H(48B)	103.5
Sc(2)-C(48)-H(48B)	103.5
H(48A)-C(48)-H(48B)	105.3
C(51)-C(49)-C(50)	108.3(3)
C(51)-C(49)-C(64)	108.6(3)
C(50)-C(49)-C(64)	108.8(3)
C(51)-C(49)-C(48)	109.9(2)
C(50)-C(49)-C(48)	109.9(2)
C(64)-C(49)-C(48)	111.3(3)
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5

H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-C(54)	110.2(2)
C(53)-C(52)-P(5)	112.41(17)
C(54)-C(52)-P(5)	110.86(18)
C(53)-C(52)-H(52)	107.7
C(54)-C(52)-H(52)	107.7
P(5)-C(52)-H(52)	107.7
C(63)-C(53)-C(52)	111.1(2)
C(63)-C(53)-H(53A)	109.4
C(52)-C(53)-H(53A)	109.4
C(63)-C(53)-H(53B)	109.4
C(52)-C(53)-H(53B)	109.4
H(53A)-C(53)-H(53B)	108.0
C(61)-C(54)-C(52)	111.8(2)
C(61)-C(54)-H(54A)	109.2
C(52)-C(54)-H(54A)	109.2
C(61)-C(54)-H(54B)	109.2
C(52)-C(54)-H(54B)	109.2
H(54A)-C(54)-H(54B)	107.9
C(43)-C(60)-C(44)	110.9(3)
C(43)-C(60)-H(60A)	109.5
C(44)-C(60)-H(60A)	109.5
C(43)-C(60)-H(60B)	109.5
C(44)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	108.0
C(62)-C(61)-C(54)	111.0(2)
C(62)-C(61)-H(61A)	109.4

C(54)-C(61)-H(61A)	109.4
C(62)-C(61)-H(61B)	109.4
C(54)-C(61)-H(61B)	109.4
H(61A)-C(61)-H(61B)	108.0
C(61)-C(62)-C(63)	110.0(2)
C(61)-C(62)-H(62A)	109.7
C(63)-C(62)-H(62A)	109.7
C(61)-C(62)-H(62B)	109.7
C(63)-C(62)-H(62B)	109.7
H(62A)-C(62)-H(62B)	108.2
C(53)-C(63)-C(62)	112.0(2)
C(53)-C(63)-H(63A)	109.2
C(62)-C(63)-H(63A)	109.2
C(53)-C(63)-H(63B)	109.2
C(62)-C(63)-H(63B)	109.2
H(63A)-C(63)-H(63B)	107.9
C(49)-C(64)-H(64A)	109.5
C(49)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(49)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(41)-C(140)-C(44)	111.0(2)
C(41)-C(140)-P(5)	114.35(19)
C(44)-C(140)-P(5)	110.49(18)
C(41)-C(140)-H(140)	106.9
C(44)-C(140)-H(140)	106.9
P(5)-C(140)-H(140)	106.9
C(2)-N(1)-C(5)	105.2(2)
C(2)-N(1)-Sc(1)	126.19(16)
C(5)-N(1)-Sc(1)	128.46(16)
C(46)#1-N(2)-C(46)	105.6(3)
C(46)#1-N(2)-Sc(2)	127.20(15)
C(46)-N(2)-Sc(2)	127.20(15)
C(6)-P(3)-C(7)	105.16(12)
C(6)-P(3)-C(13)	103.68(12)

C(7)-P(3)-C(13)	104.19(12)
C(6)-P(3)-Sc(1)	97.68(8)
C(7)-P(3)-Sc(1)	124.57(8)
C(13)-P(3)-Sc(1)	118.47(9)
C(1)-P(4)-C(25)	107.08(11)
C(1)-P(4)-C(19)	99.84(12)
C(25)-P(4)-C(19)	108.81(12)
C(1)-P(4)-Sc(1)	95.03(9)
C(25)-P(4)-Sc(1)	124.90(9)
C(19)-P(4)-Sc(1)	116.27(9)
C(45)-P(5)-C(140)	104.24(12)
C(45)-P(5)-C(52)	103.36(12)
C(140)-P(5)-C(52)	104.49(12)
C(45)-P(5)-Sc(2)	93.99(9)
C(140)-P(5)-Sc(2)	127.20(9)
C(52)-P(5)-Sc(2)	118.92(9)
N(1)-Sc(1)-C(31)	108.72(9)
N(1)-Sc(1)-C(36)	142.38(9)
C(31)-Sc(1)-C(36)	108.87(10)
N(1)-Sc(1)-P(4)	71.75(6)
C(31)-Sc(1)-P(4)	112.20(7)
C(36)-Sc(1)-P(4)	92.81(7)
N(1)-Sc(1)-P(3)	72.55(6)
C(31)-Sc(1)-P(3)	113.34(7)
C(36)-Sc(1)-P(3)	93.71(7)
P(4)-Sc(1)-P(3)	128.78(3)
N(2)-Sc(2)-C(48)	115.13(7)
N(2)-Sc(2)-C(48)#1	115.13(7)
C(48)-Sc(2)-C(48)#1	129.74(15)
N(2)-Sc(2)-P(5)#1	71.37(2)
C(48)-Sc(2)-P(5)#1	95.97(7)
C(48)#1-Sc(2)-P(5)#1	99.63(7)
N(2)-Sc(2)-P(5)	71.37(2)
C(48)-Sc(2)-P(5)	99.63(7)
C(48)#1-Sc(2)-P(5)	95.97(7)
P(5)#1-Sc(2)-P(5)	142.74(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1,y,-z+1/2$

Table S29. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)ScNp₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	16(1)	14(2)	16(1)	1(1)	1(1)	-2(1)
C(2)	14(1)	14(2)	13(1)	2(1)	2(1)	0(1)
C(3)	22(2)	13(2)	23(2)	3(1)	3(1)	-4(1)
C(4)	20(2)	21(2)	12(1)	4(1)	-2(1)	1(1)
C(5)	16(1)	15(2)	12(1)	2(1)	3(1)	1(1)
C(6)	19(1)	16(2)	12(1)	1(1)	-3(1)	-1(1)
C(7)	17(1)	14(2)	16(2)	-2(1)	1(1)	0(1)
C(8)	16(1)	20(2)	18(2)	-1(1)	-1(1)	2(1)
C(9)	22(2)	17(2)	24(2)	-5(1)	1(1)	6(1)
C(10)	26(2)	15(2)	23(2)	-6(1)	1(1)	3(1)
C(11)	24(2)	21(2)	22(2)	-7(1)	-4(1)	2(1)
C(12)	19(2)	20(2)	19(2)	-6(1)	-4(1)	2(1)
C(13)	14(1)	17(2)	17(2)	-4(1)	-1(1)	4(1)
C(14)	18(2)	18(2)	31(2)	-6(1)	4(1)	-1(1)
C(15)	20(2)	24(2)	34(2)	-4(1)	6(1)	0(1)
C(16)	22(2)	29(2)	24(2)	-4(1)	5(1)	6(1)
C(17)	27(2)	19(2)	30(2)	-5(1)	5(1)	7(1)
C(18)	26(2)	15(2)	25(2)	-3(1)	5(1)	0(1)
C(19)	20(1)	14(2)	14(1)	0(1)	-2(1)	1(1)
C(20)	18(2)	23(2)	20(2)	1(1)	1(1)	4(1)
C(21)	19(2)	30(2)	24(2)	2(1)	2(1)	8(1)
C(22)	35(2)	33(2)	23(2)	-5(1)	-2(1)	20(2)
C(23)	39(2)	22(2)	24(2)	-8(1)	-7(1)	9(1)
C(24)	27(2)	17(2)	17(2)	-2(1)	-2(1)	3(1)
C(25)	17(1)	13(2)	14(1)	-1(1)	-4(1)	-2(1)
C(26)	19(2)	28(2)	16(2)	2(1)	-1(1)	0(1)
C(27)	25(2)	30(2)	16(2)	4(1)	-1(1)	-1(1)
C(28)	25(2)	22(2)	24(2)	7(1)	-6(1)	0(1)
C(29)	18(1)	22(2)	23(2)	2(1)	-4(1)	2(1)
C(30)	19(1)	19(2)	18(2)	0(1)	-2(1)	2(1)
C(31)	19(2)	18(2)	16(2)	1(1)	1(1)	0(1)

C(32)	17(1)	19(2)	18(2)	0(1)	4(1)	3(1)
C(33)	23(2)	41(2)	23(2)	6(2)	8(1)	7(1)
C(34)	27(2)	30(2)	39(2)	-4(2)	10(1)	-6(1)
C(35)	26(2)	28(2)	26(2)	3(1)	10(1)	9(1)
C(36)	19(1)	18(2)	16(2)	0(1)	1(1)	-1(1)
C(37)	20(2)	14(2)	17(2)	2(1)	2(1)	-1(1)
C(38)	28(2)	30(2)	31(2)	14(2)	2(1)	2(1)
C(39)	33(2)	19(2)	24(2)	4(1)	10(1)	-5(1)
C(40)	30(2)	16(2)	26(2)	2(1)	5(1)	-2(1)
C(41)	24(2)	21(2)	42(2)	-4(2)	-7(1)	1(1)
C(42)	24(2)	27(2)	50(2)	-3(2)	-13(2)	3(1)
C(43)	35(2)	34(2)	30(2)	6(2)	-11(1)	-14(2)
C(44)	25(2)	36(2)	21(2)	-9(1)	2(1)	-5(1)
C(45)	21(2)	19(2)	17(2)	3(1)	3(1)	1(1)
C(46)	18(1)	17(2)	17(2)	4(1)	5(1)	2(1)
C(47)	23(1)	13(2)	19(2)	3(1)	6(1)	4(1)
C(48)	21(2)	21(2)	27(2)	-4(1)	4(1)	-2(1)
C(49)	22(2)	23(2)	34(2)	-8(1)	1(1)	-1(1)
C(50)	36(2)	25(2)	94(3)	-14(2)	12(2)	-10(2)
C(51)	31(2)	24(2)	56(2)	2(2)	4(2)	-1(2)
C(52)	16(1)	16(2)	15(1)	-1(1)	1(1)	2(1)
C(53)	21(2)	17(2)	18(2)	-1(1)	2(1)	-2(1)
C(54)	19(2)	20(2)	17(2)	-3(1)	2(1)	-2(1)
C(60)	32(2)	37(2)	21(2)	-11(2)	2(1)	-7(2)
C(61)	23(2)	26(2)	19(2)	2(1)	5(1)	1(1)
C(62)	24(2)	30(2)	14(2)	-3(1)	2(1)	1(1)
C(63)	19(2)	24(2)	21(2)	-7(1)	1(1)	1(1)
C(64)	52(2)	64(3)	37(2)	-28(2)	-4(2)	18(2)
C(140)	16(1)	16(2)	16(2)	-2(1)	-1(1)	-2(1)
N(1)	14(1)	13(1)	12(1)	1(1)	-2(1)	0(1)
N(2)	14(2)	16(2)	16(2)	0	3(1)	0
P(3)	15(1)	12(1)	14(1)	-2(1)	0(1)	0(1)
P(4)	14(1)	13(1)	13(1)	1(1)	-1(1)	-1(1)
P(5)	16(1)	16(1)	14(1)	0(1)	1(1)	0(1)
Sc(1)	13(1)	11(1)	12(1)	1(1)	0(1)	0(1)
Sc(2)	17(1)	13(1)	18(1)	0	3(1)	0

Table S30. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)ScNp₂.

	x	y	z	U(eq)
H(1A)	-26	1183	820	18
H(1B)	559	337	753	18
H(3)	1341	-152	1206	23
H(4)	2458	594	1530	22
H(6A)	3327	2188	1549	19
H(6B)	2336	2714	1551	19
H(7)	3784	4578	1288	19
H(8A)	2094	4724	1299	22
H(8B)	2163	4281	1562	22
H(9A)	3040	5896	1455	25
H(9B)	2123	5792	1608	25
H(10A)	3561	5989	1872	26
H(10B)	3072	5080	1921	26
H(11A)	4736	4869	1907	27
H(11B)	4701	5321	1647	27
H(12A)	3829	3693	1743	23
H(12B)	4744	3821	1591	23
H(13)	4784	2722	1325	19
H(14A)	4985	3944	1084	26
H(14B)	4530	3446	847	26
H(15A)	6219	3421	848	31
H(15B)	6335	3027	1116	31
H(16A)	5509	2146	692	30
H(16B)	6518	1910	840	30
H(17A)	5724	1458	1174	30
H(17B)	5285	947	938	30
H(18A)	4022	1462	1164	26
H(18B)	3929	1872	898	26
H(19)	2492	669	684	19
H(20A)	2825	1379	224	24

H(20B)	3240	1787	479	24
H(21A)	4157	535	576	29
H(21B)	4422	886	318	29
H(22A)	3441	-161	113	37
H(22B)	4172	-640	309	37
H(23A)	2965	-796	573	35
H(23B)	2566	-1176	314	35
H(24A)	1380	-290	478	25
H(24B)	1659	85	224	25
H(25)	135	975	254	18
H(26A)	1073	2537	120	25
H(26B)	1359	1588	39	25
H(27A)	408	2291	-282	29
H(27B)	-129	1443	-200	29
H(28A)	-575	3168	-60	29
H(28B)	-1255	2578	-241	29
H(29A)	-1796	2579	155	26
H(29B)	-1528	1626	74	26
H(30A)	-879	1840	474	23
H(30B)	-339	2697	399	23
H(31A)	611	4313	975	21
H(31B)	-8	3782	774	21
H(33A)	-413	3223	1474	43
H(33B)	507	3790	1422	43
H(33C)	458	2795	1347	43
H(34A)	-1366	2954	859	47
H(34B)	-1568	2733	1132	47
H(34C)	-680	2293	1015	47
H(35A)	-1349	4536	985	39
H(35B)	-631	4834	1212	39
H(35C)	-1532	4228	1252	39
H(36A)	3100	3444	602	21
H(36B)	2147	3412	423	21
H(38A)	1061	4907	573	44
H(38B)	1260	4696	299	44
H(38C)	1562	5612	415	44

H(39A)	2992	4546	196	38
H(39B)	3851	4623	407	38
H(39C)	3233	5456	322	38
H(40A)	2922	5715	741	35
H(40B)	3486	4862	835	35
H(40C)	2393	5011	894	35
H(41A)	1370	3500	2202	35
H(41B)	969	3303	2458	35
H(42A)	4	2166	2285	41
H(42B)	-248	3028	2133	41
H(43A)	-57	1864	1867	40
H(43B)	749	2582	1834	40
H(44A)	2488	2305	2025	33
H(44B)	2683	1452	2185	33
H(45A)	3230	3732	2167	23
H(45B)	2752	4295	2367	23
H(47)	4124	5582	2412	22
H(48A)	4186	1806	2074	27
H(48B)	5255	2075	2039	27
H(50A)	4396	119	2301	76
H(50B)	4437	-419	2056	76
H(50C)	3671	345	2068	76
H(51A)	6110	471	2313	55
H(51B)	6549	896	2084	55
H(51C)	6189	-83	2072	55
H(52)	2129	3680	2771	19
H(53A)	4090	3506	2977	22
H(53B)	3641	4354	2846	22
H(54A)	1860	2245	2884	22
H(54B)	2952	2159	3002	22
H(60A)	1477	1214	1856	36
H(60B)	1061	1036	2111	36
H(61A)	1511	3250	3184	27
H(61B)	1947	2398	3315	27
H(62A)	3469	3057	3389	28
H(62B)	2675	3655	3498	28

H(63A)	2614	4557	3155	26
H(63B)	3706	4499	3274	26
H(64A)	5181	208	1705	77
H(64B)	5433	1213	1704	77
H(64C)	4332	906	1696	77
H(140)	1734	1968	2480	20

Table S31. Crystal data and structure refinement for (PNP-tBu)ScNHAr.

Empirical formula	C ₄₁ H ₅₇ N ₂ P ₂ Sc	
Formula weight	684.79	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 14.3460(19) Å	$\alpha = 90^\circ$.
	b = 13.9805(19) Å	$\beta = 104.687(7)^\circ$.
	c = 19.889(3) Å	$\gamma = 90^\circ$.
Volume	3858.7(9) Å ³	
Z	4	
Density (calculated)	1.179 Mg/m ³	
Absorption coefficient	0.303 mm ⁻¹	
F(000)	1472	
Crystal size	0.07 x 0.07 x 0.01 mm ³	
Theta range for data collection	1.80 to 25.43°.	
Index ranges	-16 ≤ h ≤ 17, -16 ≤ k ≤ 16, -24 ≤ l ≤ 23	
Reflections collected	55555	
Independent reflections	7073 [R(int) = 0.0999]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9801 and 0.8970	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7073 / 0 / 459	
Goodness-of-fit on F ²	1.013	
Final R indices [I > 2σ(I)]	R ₁ = 0.0462, wR ₂ = 0.0877	
R indices (all data)	R ₁ = 0.0891, wR ₂ = 0.1026	
Largest diff. peak and hole	0.409 and -0.284 e.Å ⁻³	

Table S32. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-tBu)ScNHAr. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	-1662(2)	7281(2)	1681(1)	16(1)
C(2)	-2046(2)	6352(2)	1720(1)	17(1)
C(3)	-3039(2)	6285(2)	1676(1)	20(1)
C(4)	-3658(2)	7063(2)	1597(1)	21(1)
C(5)	-3273(2)	7957(2)	1528(1)	21(1)
C(6)	-2304(2)	8071(2)	1548(1)	18(1)
C(7)	-4715(2)	6935(2)	1578(2)	29(1)
C(8)	-1940(2)	9037(2)	1418(1)	18(1)
C(9)	-1593(2)	9188(2)	836(1)	23(1)
C(10)	-1251(2)	10079(2)	699(2)	27(1)
C(11)	-1253(2)	10832(2)	1144(2)	28(1)
C(12)	-1595(2)	10696(2)	1727(2)	28(1)
C(13)	-1934(2)	9805(2)	1862(1)	24(1)
C(14)	-1464(2)	5457(2)	1798(1)	17(1)
C(15)	-1915(2)	4591(2)	1541(1)	24(1)
C(16)	-1428(2)	3730(2)	1625(2)	29(1)
C(17)	-459(2)	3700(2)	1960(2)	31(1)
C(18)	0(2)	4546(2)	2203(2)	28(1)
C(19)	-461(2)	5445(2)	2133(1)	20(1)
C(20)	2758(2)	6495(2)	1989(1)	24(1)
C(21)	2804(2)	6516(2)	2747(1)	21(1)
C(22)	3602(2)	6553(2)	3297(2)	28(1)
C(23)	3274(2)	6510(2)	3904(2)	29(1)
C(24)	2285(2)	6446(2)	3697(1)	23(1)
C(25)	1567(2)	6387(2)	4129(2)	30(1)
C(26)	1374(2)	6369(2)	630(1)	28(1)
C(27)	556(2)	6852(2)	84(2)	38(1)
C(28)	2259(2)	6232(2)	335(2)	41(1)
C(29)	1021(2)	5382(2)	793(2)	36(1)
C(30)	1935(2)	8332(2)	1359(2)	26(1)
C(31)	2416(3)	8714(2)	2082(2)	53(1)

C(32)	1000(2)	8898(2)	1086(2)	35(1)
C(33)	2603(2)	8507(2)	885(2)	45(1)
C(34)	-459(2)	6671(2)	4141(1)	23(1)
C(35)	-1388(2)	7232(2)	3854(2)	49(1)
C(36)	-657(2)	5634(2)	3911(2)	39(1)
C(37)	-185(2)	6697(3)	4930(2)	58(1)
C(38)	875(2)	8386(2)	4030(2)	37(1)
N(1)	1970(1)	6461(2)	2981(1)	20(1)
N(2)	-674(1)	7436(2)	1786(1)	21(1)
P(1)	1633(1)	7044(1)	1470(1)	20(1)
P(2)	502(1)	7129(1)	3743(1)	20(1)
Sc(1)	466(1)	6696(1)	2372(1)	16(1)
C(39)	1466(6)	8703(5)	3515(4)	39(2)
C(40)	1639(6)	8349(5)	4775(3)	52(2)
C(41)	92(5)	9017(4)	4027(5)	55(2)
C(39A)	1835(7)	8641(6)	3945(6)	47(3)
C(40A)	795(6)	8696(5)	4754(4)	44(3)
C(41A)	91(6)	9081(5)	3491(5)	52(3)

Table S33. Bond lengths [Å] and angles [°] for (PNP-tBu)ScNHAr.

C(1)-N(2)	1.397(3)
C(1)-C(6)	1.420(3)
C(1)-C(2)	1.420(3)
C(2)-C(3)	1.409(3)
C(2)-C(14)	1.491(3)
C(3)-C(4)	1.387(4)
C(3)-H(21)	0.9500
C(4)-C(5)	1.387(4)
C(4)-C(7)	1.518(3)
C(5)-C(6)	1.390(3)
C(5)-H(23)	0.9500
C(6)-C(8)	1.494(3)
C(7)-H(32A)	0.9800
C(7)-H(32B)	0.9800
C(7)-H(32C)	0.9800
C(8)-C(9)	1.387(4)
C(8)-C(13)	1.390(4)
C(9)-C(10)	1.390(4)
C(9)-H(26)	0.9500
C(10)-C(11)	1.375(4)
C(10)-H(25)	0.9500
C(11)-C(12)	1.381(4)
C(11)-H(38)	0.9500
C(12)-C(13)	1.388(4)
C(12)-H(37)	0.9500
C(13)-H(36)	0.9500
C(14)-C(15)	1.406(3)
C(14)-C(19)	1.424(3)
C(15)-C(16)	1.382(4)
C(15)-H(33)	0.9500
C(16)-C(17)	1.381(4)
C(16)-H(34)	0.9500
C(17)-C(18)	1.380(4)
C(17)-H(35)	0.9500

C(18)-C(19)	1.410(4)
C(18)-H(29)	0.9500
C(19)-Sc(1)	2.176(3)
C(20)-C(21)	1.493(4)
C(20)-P(1)	1.848(2)
C(20)-H(1A)	0.9900
C(20)-H(1B)	0.9900
C(21)-C(22)	1.369(3)
C(21)-N(1)	1.390(3)
C(22)-C(23)	1.405(4)
C(22)-H(3)	0.9500
C(23)-C(24)	1.377(3)
C(23)-H(4)	0.9500
C(24)-N(1)	1.382(3)
C(24)-C(25)	1.502(4)
C(25)-P(2)	1.844(3)
C(25)-H(6A)	0.9900
C(25)-H(6B)	0.9900
C(26)-C(29)	1.532(4)
C(26)-C(27)	1.538(4)
C(26)-C(28)	1.539(4)
C(26)-P(1)	1.874(3)
C(27)-H(15A)	0.9800
C(27)-H(15B)	0.9800
C(27)-H(15C)	0.9800
C(28)-H(13A)	0.9800
C(28)-H(13B)	0.9800
C(28)-H(13C)	0.9800
C(29)-H(14A)	0.9800
C(29)-H(14B)	0.9800
C(29)-H(14C)	0.9800
C(30)-C(33)	1.525(4)
C(30)-C(31)	1.525(4)
C(30)-C(32)	1.534(4)
C(30)-P(1)	1.878(3)
C(31)-H(18A)	0.9800

C(31)-H(18B)	0.9800
C(31)-H(18C)	0.9800
C(32)-H(17A)	0.9800
C(32)-H(17B)	0.9800
C(32)-H(17C)	0.9800
C(33)-H(30A)	0.9800
C(33)-H(30B)	0.9800
C(33)-H(30C)	0.9800
C(34)-C(37)	1.518(4)
C(34)-C(36)	1.525(4)
C(34)-C(35)	1.526(4)
C(34)-P(2)	1.869(3)
C(35)-H(9A)	0.9800
C(35)-H(9B)	0.9800
C(35)-H(9C)	0.9800
C(36)-H(8A)	0.9800
C(36)-H(8B)	0.9800
C(36)-H(8C)	0.9800
C(37)-H(10A)	0.9800
C(37)-H(10B)	0.9800
C(37)-H(10C)	0.9800
C(38)-C(41)	1.427(7)
C(38)-C(39A)	1.471(9)
C(38)-C(40A)	1.535(8)
C(38)-C(39)	1.550(8)
C(38)-C(40)	1.604(7)
C(38)-C(41A)	1.658(8)
C(38)-P(2)	1.883(3)
N(1)-Sc(1)	2.215(2)
N(2)-Sc(1)	2.034(2)
N(2)-H(2)	0.8800
P(1)-Sc(1)	2.7886(9)
P(2)-Sc(1)	2.7810(9)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800

C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(39A)-H(39D)	0.9800
C(39A)-H(39E)	0.9800
C(39A)-H(39F)	0.9800
C(40A)-H(40D)	0.9800
C(40A)-H(40E)	0.9800
C(40A)-H(40F)	0.9800
C(41A)-H(41D)	0.9800
C(41A)-H(41E)	0.9800
C(41A)-H(41F)	0.9800

N(2)-C(1)-C(6)	119.5(2)
N(2)-C(1)-C(2)	121.8(2)
C(6)-C(1)-C(2)	118.6(2)
C(3)-C(2)-C(1)	117.3(2)
C(3)-C(2)-C(14)	118.8(2)
C(1)-C(2)-C(14)	123.9(2)
C(4)-C(3)-C(2)	124.2(2)
C(4)-C(3)-H(21)	117.9
C(2)-C(3)-H(21)	117.9
C(3)-C(4)-C(5)	117.3(2)
C(3)-C(4)-C(7)	121.1(2)
C(5)-C(4)-C(7)	121.5(2)
C(4)-C(5)-C(6)	121.4(2)
C(4)-C(5)-H(23)	119.3
C(6)-C(5)-H(23)	119.3
C(5)-C(6)-C(1)	120.9(2)
C(5)-C(6)-C(8)	119.3(2)
C(1)-C(6)-C(8)	119.8(2)
C(4)-C(7)-H(32A)	109.5
C(4)-C(7)-H(32B)	109.5

H(32A)-C(7)-H(32B)	109.5
C(4)-C(7)-H(32C)	109.5
H(32A)-C(7)-H(32C)	109.5
H(32B)-C(7)-H(32C)	109.5
C(9)-C(8)-C(13)	117.9(2)
C(9)-C(8)-C(6)	119.8(2)
C(13)-C(8)-C(6)	122.3(2)
C(8)-C(9)-C(10)	121.2(3)
C(8)-C(9)-H(26)	119.4
C(10)-C(9)-H(26)	119.4
C(11)-C(10)-C(9)	120.1(3)
C(11)-C(10)-H(25)	120.0
C(9)-C(10)-H(25)	120.0
C(10)-C(11)-C(12)	119.6(3)
C(10)-C(11)-H(38)	120.2
C(12)-C(11)-H(38)	120.2
C(11)-C(12)-C(13)	120.2(3)
C(11)-C(12)-H(37)	119.9
C(13)-C(12)-H(37)	119.9
C(12)-C(13)-C(8)	121.0(3)
C(12)-C(13)-H(36)	119.5
C(8)-C(13)-H(36)	119.5
C(15)-C(14)-C(19)	118.5(2)
C(15)-C(14)-C(2)	119.3(2)
C(19)-C(14)-C(2)	122.1(2)
C(16)-C(15)-C(14)	122.3(2)
C(16)-C(15)-H(33)	118.9
C(14)-C(15)-H(33)	118.9
C(17)-C(16)-C(15)	120.0(3)
C(17)-C(16)-H(34)	120.0
C(15)-C(16)-H(34)	120.0
C(18)-C(17)-C(16)	118.4(3)
C(18)-C(17)-H(35)	120.8
C(16)-C(17)-H(35)	120.8
C(17)-C(18)-C(19)	123.9(2)
C(17)-C(18)-H(29)	118.0

C(19)-C(18)-H(29)	118.0
C(18)-C(19)-C(14)	116.8(2)
C(18)-C(19)-Sc(1)	116.67(18)
C(14)-C(19)-Sc(1)	125.56(18)
C(21)-C(20)-P(1)	111.37(18)
C(21)-C(20)-H(1A)	109.4
P(1)-C(20)-H(1A)	109.4
C(21)-C(20)-H(1B)	109.4
P(1)-C(20)-H(1B)	109.4
H(1A)-C(20)-H(1B)	108.0
C(22)-C(21)-N(1)	110.6(2)
C(22)-C(21)-C(20)	128.4(2)
N(1)-C(21)-C(20)	121.0(2)
C(21)-C(22)-C(23)	106.9(2)
C(21)-C(22)-H(3)	126.5
C(23)-C(22)-H(3)	126.5
C(24)-C(23)-C(22)	106.8(2)
C(24)-C(23)-H(4)	126.6
C(22)-C(23)-H(4)	126.6
C(23)-C(24)-N(1)	110.5(2)
C(23)-C(24)-C(25)	129.6(3)
N(1)-C(24)-C(25)	119.9(2)
C(24)-C(25)-P(2)	110.30(18)
C(24)-C(25)-H(6A)	109.6
P(2)-C(25)-H(6A)	109.6
C(24)-C(25)-H(6B)	109.6
P(2)-C(25)-H(6B)	109.6
H(6A)-C(25)-H(6B)	108.1
C(29)-C(26)-C(27)	108.2(2)
C(29)-C(26)-C(28)	108.6(2)
C(27)-C(26)-C(28)	109.9(2)
C(29)-C(26)-P(1)	105.40(19)
C(27)-C(26)-P(1)	110.6(2)
C(28)-C(26)-P(1)	113.9(2)
C(26)-C(27)-H(15A)	109.5
C(26)-C(27)-H(15B)	109.5

H(15A)-C(27)-H(15B)	109.5
C(26)-C(27)-H(15C)	109.5
H(15A)-C(27)-H(15C)	109.5
H(15B)-C(27)-H(15C)	109.5
C(26)-C(28)-H(13A)	109.5
C(26)-C(28)-H(13B)	109.5
H(13A)-C(28)-H(13B)	109.5
C(26)-C(28)-H(13C)	109.5
H(13A)-C(28)-H(13C)	109.5
H(13B)-C(28)-H(13C)	109.5
C(26)-C(29)-H(14A)	109.5
C(26)-C(29)-H(14B)	109.5
H(14A)-C(29)-H(14B)	109.5
C(26)-C(29)-H(14C)	109.5
H(14A)-C(29)-H(14C)	109.5
H(14B)-C(29)-H(14C)	109.5
C(33)-C(30)-C(31)	108.8(3)
C(33)-C(30)-C(32)	109.2(2)
C(31)-C(30)-C(32)	107.4(3)
C(33)-C(30)-P(1)	115.3(2)
C(31)-C(30)-P(1)	106.73(19)
C(32)-C(30)-P(1)	109.21(18)
C(30)-C(31)-H(18A)	109.5
C(30)-C(31)-H(18B)	109.5
H(18A)-C(31)-H(18B)	109.5
C(30)-C(31)-H(18C)	109.5
H(18A)-C(31)-H(18C)	109.5
H(18B)-C(31)-H(18C)	109.5
C(30)-C(32)-H(17A)	109.5
C(30)-C(32)-H(17B)	109.5
H(17A)-C(32)-H(17B)	109.5
C(30)-C(32)-H(17C)	109.5
H(17A)-C(32)-H(17C)	109.5
H(17B)-C(32)-H(17C)	109.5
C(30)-C(33)-H(30A)	109.5
C(30)-C(33)-H(30B)	109.5

H(30A)-C(33)-H(30B)	109.5
C(30)-C(33)-H(30C)	109.5
H(30A)-C(33)-H(30C)	109.5
H(30B)-C(33)-H(30C)	109.5
C(37)-C(34)-C(36)	108.2(3)
C(37)-C(34)-C(35)	110.3(3)
C(36)-C(34)-C(35)	107.4(2)
C(37)-C(34)-P(2)	113.75(19)
C(36)-C(34)-P(2)	107.50(19)
C(35)-C(34)-P(2)	109.5(2)
C(34)-C(35)-H(9A)	109.5
C(34)-C(35)-H(9B)	109.5
H(9A)-C(35)-H(9B)	109.5
C(34)-C(35)-H(9C)	109.5
H(9A)-C(35)-H(9C)	109.5
H(9B)-C(35)-H(9C)	109.5
C(34)-C(36)-H(8A)	109.5
C(34)-C(36)-H(8B)	109.5
H(8A)-C(36)-H(8B)	109.5
C(34)-C(36)-H(8C)	109.5
H(8A)-C(36)-H(8C)	109.5
H(8B)-C(36)-H(8C)	109.5
C(34)-C(37)-H(10A)	109.5
C(34)-C(37)-H(10B)	109.5
H(10A)-C(37)-H(10B)	109.5
C(34)-C(37)-H(10C)	109.5
H(10A)-C(37)-H(10C)	109.5
H(10B)-C(37)-H(10C)	109.5
C(41)-C(38)-C(39A)	127.5(5)
C(41)-C(38)-C(40A)	65.4(5)
C(39A)-C(38)-C(40A)	109.5(5)
C(41)-C(38)-C(39)	112.5(5)
C(39A)-C(38)-C(39)	34.1(4)
C(40A)-C(38)-C(39)	136.2(4)
C(41)-C(38)-C(40)	112.1(5)
C(39A)-C(38)-C(40)	71.0(5)

C(40A)-C(38)-C(40)	48.7(4)
C(39)-C(38)-C(40)	105.1(4)
C(41)-C(38)-C(41A)	39.6(4)
C(39A)-C(38)-C(41A)	106.6(5)
C(40A)-C(38)-C(41A)	103.9(5)
C(39)-C(38)-C(41A)	78.5(4)
C(40)-C(38)-C(41A)	144.0(4)
C(41)-C(38)-P(2)	114.4(3)
C(39A)-C(38)-P(2)	113.1(4)
C(40A)-C(38)-P(2)	117.7(3)
C(39)-C(38)-P(2)	103.2(3)
C(40)-C(38)-P(2)	108.9(3)
C(41A)-C(38)-P(2)	104.9(3)
C(24)-N(1)-C(21)	105.2(2)
C(24)-N(1)-Sc(1)	125.75(17)
C(21)-N(1)-Sc(1)	127.62(17)
C(1)-N(2)-Sc(1)	130.16(17)
C(1)-N(2)-H(2)	114.9
Sc(1)-N(2)-H(2)	114.9
C(20)-P(1)-C(26)	103.65(12)
C(20)-P(1)-C(30)	105.61(12)
C(26)-P(1)-C(30)	112.17(13)
C(20)-P(1)-Sc(1)	98.65(9)
C(26)-P(1)-Sc(1)	118.05(9)
C(30)-P(1)-Sc(1)	115.94(9)
C(25)-P(2)-C(34)	104.68(12)
C(25)-P(2)-C(38)	104.89(14)
C(34)-P(2)-C(38)	112.04(13)
C(25)-P(2)-Sc(1)	95.38(10)
C(34)-P(2)-Sc(1)	120.51(9)
C(38)-P(2)-Sc(1)	115.69(10)
N(2)-Sc(1)-C(19)	85.74(9)
N(2)-Sc(1)-N(1)	156.77(8)
C(19)-Sc(1)-N(1)	117.21(9)
N(2)-Sc(1)-P(2)	105.30(7)
C(19)-Sc(1)-P(2)	104.34(7)

N(1)-Sc(1)-P(2)	73.90(6)
N(2)-Sc(1)-P(1)	93.95(6)
C(19)-Sc(1)-P(1)	115.69(7)
N(1)-Sc(1)-P(1)	73.55(6)
P(2)-Sc(1)-P(1)	136.66(3)
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
C(38)-C(41)-H(41A)	109.5
C(38)-C(41)-H(41B)	109.5
C(38)-C(41)-H(41C)	109.5
C(38)-C(39A)-H(39D)	109.5
C(38)-C(39A)-H(39E)	109.5
H(39D)-C(39A)-H(39E)	109.5
C(38)-C(39A)-H(39F)	109.5
H(39D)-C(39A)-H(39F)	109.5
H(39E)-C(39A)-H(39F)	109.5
C(38)-C(40A)-H(40D)	109.5
C(38)-C(40A)-H(40E)	109.5
H(40D)-C(40A)-H(40E)	109.5
C(38)-C(40A)-H(40F)	109.5
H(40D)-C(40A)-H(40F)	109.5
H(40E)-C(40A)-H(40F)	109.5
C(38)-C(41A)-H(41D)	109.5
C(38)-C(41A)-H(41E)	109.5
H(41D)-C(41A)-H(41E)	109.5
C(38)-C(41A)-H(41F)	109.5
H(41D)-C(41A)-H(41F)	109.5
H(41E)-C(41A)-H(41F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S34. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-tBu)ScNHAr. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	15(1)	22(2)	12(1)	-1(1)	2(1)	-1(1)
C(2)	15(1)	22(2)	14(1)	-1(1)	2(1)	-1(1)
C(3)	20(1)	21(2)	18(1)	1(1)	5(1)	-4(1)
C(4)	15(1)	29(2)	19(2)	1(1)	5(1)	-2(1)
C(5)	17(1)	24(2)	21(2)	2(1)	3(1)	6(1)
C(6)	16(1)	21(2)	15(1)	0(1)	1(1)	0(1)
C(7)	18(1)	34(2)	35(2)	6(1)	6(1)	1(1)
C(8)	11(1)	20(1)	18(2)	3(1)	-2(1)	3(1)
C(9)	24(2)	24(2)	20(2)	2(1)	4(1)	5(1)
C(10)	25(2)	32(2)	25(2)	13(1)	8(1)	6(1)
C(11)	24(2)	22(2)	33(2)	10(1)	1(1)	-1(1)
C(12)	29(2)	23(2)	30(2)	-3(1)	2(1)	-3(1)
C(13)	22(2)	27(2)	22(2)	3(1)	3(1)	-2(1)
C(14)	20(1)	19(1)	15(1)	0(1)	7(1)	-5(1)
C(15)	16(1)	28(2)	29(2)	-5(1)	8(1)	-6(1)
C(16)	29(2)	19(2)	40(2)	-9(1)	12(1)	-5(1)
C(17)	33(2)	16(2)	46(2)	2(1)	15(2)	5(1)
C(18)	22(2)	23(2)	39(2)	3(1)	6(1)	1(1)
C(19)	20(1)	17(1)	23(2)	2(1)	7(1)	1(1)
C(20)	17(1)	28(2)	31(2)	6(1)	11(1)	3(1)
C(21)	15(1)	20(2)	29(2)	7(1)	7(1)	0(1)
C(22)	12(1)	38(2)	34(2)	11(2)	3(1)	-1(1)
C(23)	20(2)	35(2)	28(2)	7(1)	-2(1)	-1(1)
C(24)	20(1)	24(2)	25(2)	8(1)	3(1)	3(1)
C(25)	24(2)	40(2)	28(2)	13(1)	7(1)	8(1)
C(26)	28(2)	32(2)	26(2)	1(1)	11(1)	1(1)
C(27)	39(2)	42(2)	29(2)	1(2)	2(1)	-1(2)
C(28)	46(2)	47(2)	36(2)	2(2)	20(2)	6(2)
C(29)	40(2)	31(2)	36(2)	-2(2)	9(2)	-4(2)
C(30)	21(1)	24(2)	34(2)	9(1)	8(1)	-1(1)
C(31)	71(2)	23(2)	53(2)	2(2)	-5(2)	-13(2)

C(32)	30(2)	25(2)	54(2)	14(2)	18(2)	2(1)
C(33)	28(2)	36(2)	77(3)	24(2)	26(2)	6(2)
C(34)	21(1)	26(2)	24(2)	0(1)	9(1)	0(1)
C(35)	31(2)	44(2)	80(3)	16(2)	28(2)	10(2)
C(36)	29(2)	29(2)	63(2)	-6(2)	21(2)	-7(1)
C(37)	54(2)	94(3)	32(2)	-3(2)	18(2)	-37(2)
C(38)	54(2)	27(2)	35(2)	-7(2)	18(2)	-12(2)
N(1)	14(1)	20(1)	25(1)	6(1)	4(1)	0(1)
N(2)	14(1)	21(1)	27(1)	8(1)	4(1)	-2(1)
P(1)	14(1)	22(1)	24(1)	4(1)	6(1)	1(1)
P(2)	20(1)	18(1)	21(1)	2(1)	4(1)	1(1)
Sc(1)	12(1)	16(1)	21(1)	2(1)	3(1)	0(1)
C(39)	60(5)	20(3)	35(4)	2(3)	10(4)	-18(3)
C(40)	74(6)	43(4)	39(4)	-11(3)	14(4)	-39(4)
C(41)	74(5)	23(4)	77(7)	-4(4)	34(5)	-3(3)
C(39A)	66(7)	28(5)	56(7)	-14(5)	31(5)	-15(4)
C(40A)	59(6)	33(4)	45(5)	-15(4)	23(4)	-18(4)
C(41A)	85(6)	18(4)	52(6)	8(4)	17(5)	8(4)

Table S35. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-tBu)ScNHAr.

	x	y	z	U(eq)
H(21)	-3303	5667	1704	24
H(23)	-3680	8503	1466	25
H(32A)	-5008	7563	1605	44
H(32B)	-4773	6541	1972	44
H(32C)	-5047	6620	1142	44
H(26)	-1589	8673	525	27
H(25)	-1016	10168	298	33
H(38)	-1021	11441	1051	33
H(37)	-1599	11213	2035	34
H(36)	-2166	9719	2265	29
H(33)	-2579	4600	1301	29
H(34)	-1759	3157	1452	34
H(35)	-117	3112	2022	37
H(29)	667	4522	2432	34
H(1A)	2794	5824	1839	29
H(1B)	3317	6844	1904	29
H(3)	4253	6600	3272	34
H(4)	3661	6523	4369	35
H(6A)	1868	6612	4607	36
H(6B)	1366	5714	4157	36
H(15A)	367	6443	-328	57
H(15B)	779	7471	-47	57
H(15C)	1	6951	279	57
H(13A)	2794	5974	698	62
H(13B)	2447	6850	177	62
H(13C)	2100	5786	-57	62
H(14A)	929	4970	383	54
H(14B)	408	5450	921	54
H(14C)	1500	5094	1181	54
H(18A)	3042	8401	2257	79

H(18B)	2005	8581	2397	79
H(18C)	2511	9406	2057	79
H(17A)	1154	9572	1031	52
H(17B)	599	8846	1417	52
H(17C)	648	8638	636	52
H(30A)	2758	9189	886	67
H(30B)	2282	8305	411	67
H(30C)	3198	8138	1053	67
H(9A)	-1911	6944	4019	74
H(9B)	-1552	7216	3344	74
H(9C)	-1296	7897	4013	74
H(8A)	-82	5247	4105	58
H(8B)	-819	5599	3403	58
H(8C)	-1197	5389	4079	58
H(10A)	-114	7364	5088	88
H(10B)	427	6359	5107	88
H(10C)	-689	6387	5104	88
H(2)	-520	7932	1564	25
H(39A)	1052	8693	3040	59
H(39B)	2008	8264	3549	59
H(39C)	1712	9353	3631	59
H(40A)	1800	9001	4944	78
H(40B)	2224	8020	4731	78
H(40C)	1358	8001	5104	78
H(41A)	333	9675	4103	83
H(41B)	-209	8835	4398	83
H(41C)	-384	8975	3577	83
H(39D)	1906	9338	3957	71
H(39E)	1905	8396	3499	71
H(39F)	2331	8357	4324	71
H(40D)	1027	9355	4844	66
H(40E)	1185	8270	5106	66
H(40F)	120	8662	4773	66
H(41D)	-561	8942	3535	78
H(41E)	124	8960	3013	78
H(41F)	245	9754	3608	78

Table S36. Crystal data and structure refinement for (PNP-tBu)ScNHAr(DMAP)₂.

Empirical formula	C ₅₅ H ₇₇ N ₆ P ₂ Sc	
Formula weight	929.12	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2 ₁	
Unit cell dimensions	a = 23.1810(9) Å	α = 90°.
	b = 22.5100(8) Å	β = 90°.
	c = 25.2361(10) Å	γ = 90°.
Volume	13168.3(9) Å ³	
Z	8	
Density (calculated)	0.937 Mg/m ³	
Absorption coefficient	0.193 mm ⁻¹	
F(000)	4000	
Crystal size	0.080 x 0.080 x 0.030 mm ³	
Theta range for data collection	1.497 to 25.405°.	
Index ranges	-27 ≤ h ≤ 27, -18 ≤ k ≤ 27, -30 ≤ l ≤ 30	
Reflections collected	92497	
Independent reflections	23416 [R(int) = 0.0507]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7452 and 0.6462	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	23416 / 1 / 1188	
Goodness-of-fit on F ²	1.033	
Final R indices [I > 2σ(I)]	R1 = 0.0760, wR2 = 0.1899	
R indices (all data)	R1 = 0.0991, wR2 = 0.2067	
Absolute structure parameter	0.52(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.973 and -0.870 e.Å ⁻³	

Table S37. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-tBu)ScNHAr(DMAP)₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2583(3)	3435(3)	2513(3)	30(2)
C(2)	3017(3)	3803(3)	2358(3)	28(2)
C(3)	2916(3)	4426(3)	2319(3)	26(2)
C(4)	2365(3)	4613(3)	2467(4)	34(2)
C(5)	1964(3)	4210(3)	2627(3)	31(2)
C(6)	3927(3)	4602(4)	2105(4)	38(2)
C(7)	3198(4)	5417(3)	2050(4)	36(2)
C(8)	1625(3)	1674(3)	2599(4)	27(2)
C(9)	1810(3)	1157(3)	2340(4)	33(2)
C(10)	2101(3)	1200(3)	1861(3)	32(2)
C(11)	2197(3)	1778(3)	1667(3)	31(2)
C(12)	2005(3)	2258(3)	1940(3)	30(2)
C(13)	2563(5)	793(5)	1064(4)	61(3)
C(14)	2099(4)	125(3)	1746(5)	51(3)
C(15)	564(4)	671(3)	1130(3)	33(2)
C(16)	453(3)	1166(3)	1518(3)	33(2)
C(17)	582(3)	1752(3)	1377(3)	28(2)
C(18)	224(3)	1072(3)	2008(3)	27(2)
C(19)	163(3)	1513(3)	2383(3)	29(2)
C(20)	367(3)	2104(3)	2268(3)	25(2)
C(21)	-84(3)	1372(3)	2902(3)	29(2)
C(22)	71(3)	864(3)	3192(3)	34(2)
C(23)	-166(4)	732(4)	3666(4)	52(3)
C(24)	-596(4)	1096(4)	3885(4)	47(2)
C(25)	-777(4)	1585(4)	3610(4)	47(2)
C(26)	-524(3)	1725(4)	3125(4)	37(2)
C(27)	543(3)	2218(3)	1732(3)	25(2)
C(28)	686(3)	2842(3)	1536(3)	27(2)
C(29)	501(4)	2971(3)	1024(3)	36(2)
C(30)	622(4)	3513(3)	795(4)	36(2)
C(31)	944(4)	3932(4)	1078(3)	37(2)

C(32)	1117(3)	3797(3)	1595(3)	31(2)
C(33)	997(3)	3260(3)	1853(3)	24(2)
C(34)	1589(4)	3512(3)	3963(3)	33(2)
C(35)	1114(3)	3873(3)	3719(3)	26(2)
C(36)	843(3)	4351(3)	3926(3)	29(2)
C(37)	408(3)	4510(3)	3559(3)	31(2)
C(38)	422(3)	4118(3)	3144(3)	24(2)
C(39)	98(3)	4089(3)	2643(3)	26(2)
C(40)	2649(4)	2582(4)	3619(4)	54(3)
C(41)	2243(4)	2428(3)	4066(4)	41(2)
C(42)	2236(4)	1730(4)	4099(4)	50(2)
C(43)	2448(6)	2692(5)	4586(6)	92(5)
C(44)	1091(7)	2501(7)	4876(5)	96(5)
C(45)	375(4)	2777(4)	4150(4)	54(3)
C(46)	930(4)	2460(4)	4297(4)	47(2)
C(47)	817(5)	1794(4)	4158(6)	74(4)
C(48)	-1722(4)	3986(4)	2937(5)	55(3)
C(49)	-1103(3)	3768(4)	2818(4)	35(2)
C(50)	-860(4)	3492(4)	3317(4)	42(2)
C(51)	-1157(4)	3291(3)	2375(4)	51(3)
C(52)	-1350(4)	4904(4)	1904(4)	48(2)
C(53)	-738(3)	4694(3)	1980(3)	29(2)
C(54)	-341(4)	5238(4)	1930(4)	45(2)
C(55)	-576(4)	4260(4)	1531(4)	39(2)
C(101)	-1005(3)	7263(3)	3933(3)	33(2)
C(102)	-1209(3)	6787(3)	4213(3)	31(2)
C(103)	-1091(3)	6206(3)	4013(3)	24(2)
C(104)	-777(3)	6173(3)	3546(3)	25(2)
C(105)	-598(4)	6680(3)	3300(3)	33(2)
C(106)	-1118(4)	5115(3)	4102(4)	43(2)
C(107)	-1572(5)	5770(4)	4778(3)	48(3)
C(108)	-1545(3)	8501(3)	3352(3)	33(2)
C(109)	-1972(4)	8889(4)	3489(4)	38(2)
C(110)	-1836(4)	9508(4)	3510(4)	39(2)
C(111)	-1292(4)	9669(3)	3353(3)	34(2)
C(112)	-897(3)	9244(3)	3204(4)	29(2)

C(113)	-2081(4)	10529(4)	3761(4)	49(2)
C(114)	-2831(4)	9739(4)	3763(5)	60(3)
C(115)	674(4)	7145(3)	3696(3)	35(2)
C(116)	913(4)	6560(3)	3605(3)	36(2)
C(117)	507(5)	6849(4)	4614(4)	62(3)
C(118)	498(4)	7280(4)	4218(4)	41(2)
C(119)	921(5)	6150(4)	4020(4)	60(3)
C(120)	1161(4)	6391(3)	3083(4)	37(2)
C(121)	1583(3)	6720(3)	2835(3)	32(2)
C(122)	1825(4)	6554(4)	2372(4)	38(2)
C(123)	1653(4)	6031(4)	2129(4)	42(2)
C(124)	1238(4)	5685(4)	2360(4)	40(2)
C(125)	993(4)	5861(4)	2840(4)	38(2)
C(126)	312(4)	7890(4)	4384(3)	35(2)
C(127)	480(4)	8067(4)	4903(3)	42(2)
C(128)	307(4)	8611(4)	5112(4)	43(2)
C(129)	8(4)	9000(4)	4795(3)	40(2)
C(130)	-134(4)	8845(3)	4288(4)	35(2)
C(131)	6(3)	8282(3)	4053(3)	26(2)
C(132)	953(3)	9091(3)	3251(3)	26(2)
C(133)	583(3)	9118(3)	2752(3)	25(2)
C(134)	625(3)	9519(3)	2336(4)	33(2)
C(135)	196(3)	9351(3)	1964(3)	29(2)
C(136)	-68(3)	8844(3)	2166(3)	26(2)
C(137)	-538(3)	8490(3)	1912(4)	32(2)
C(138)	2181(4)	8319(4)	3459(4)	46(2)
C(139)	2145(3)	8803(4)	3050(3)	34(2)
C(140)	1880(4)	8533(4)	2546(4)	50(3)
C(141)	2741(4)	9064(4)	2914(4)	48(2)
C(142)	1735(3)	9692(4)	3928(4)	34(2)
C(143)	1338(4)	10231(4)	3979(4)	49(2)
C(144)	2364(4)	9930(4)	3993(4)	43(2)
C(145)	1601(5)	9240(4)	4341(4)	49(3)
C(146)	258(4)	6762(3)	1833(4)	38(2)
C(147)	117(3)	7398(3)	1649(3)	31(2)
C(148)	652(4)	7765(4)	1749(4)	37(2)

C(149)	-27(4)	7395(4)	1065(4)	44(2)
C(150)	-1198(4)	7403(4)	1854(4)	40(2)
C(151)	-1625(4)	7564(3)	2297(4)	41(2)
C(152)	-1427(4)	7673(4)	1338(4)	43(2)
C(153)	723(6)	6267(4)	4519(5)	78(4)
C(154)	-1196(4)	6717(4)	1804(4)	45(2)
C(155)	718(9)	5805(6)	4963(6)	124(8)
N(1)	2042(2)	3614(2)	2649(3)	28(1)
N(2)	3341(3)	4798(3)	2166(3)	31(2)
N(3)	1723(3)	2234(2)	2413(3)	27(1)
N(4)	2282(4)	717(3)	1582(3)	44(2)
N(5)	873(3)	3717(2)	3238(3)	27(1)
N(6)	436(3)	2524(3)	2657(3)	30(1)
N(7)	-999(3)	8652(3)	3211(3)	32(2)
N(8)	-2243(3)	9904(3)	3671(3)	43(2)
N(9)	-705(3)	7235(3)	3482(3)	31(2)
N(10)	-1292(3)	5708(3)	4272(3)	30(2)
N(11)	169(2)	8696(2)	2643(2)	22(1)
N(12)	581(3)	7531(3)	3275(3)	30(1)
P(1)	1509(1)	2706(1)	3832(1)	29(1)
P(2)	-634(1)	4434(1)	2683(1)	25(1)
P(3)	1651(1)	9457(1)	3206(1)	27(1)
P(4)	-474(1)	7690(1)	2086(1)	28(1)
Sc(1)	1192(1)	3028(1)	2697(1)	23(1)
Sc(2)	-163(1)	8036(1)	3204(1)	25(1)

Table S38. Bond lengths [Å] and angles [°] for (PNP-tBu)ScNHAr(DMAP)₂.

C(1)-N(1)	1.362(9)
C(1)-C(2)	1.363(11)
C(1)-H(1)	0.9500
C(2)-C(3)	1.425(10)
C(2)-H(2)	0.9500
C(3)-N(2)	1.349(9)
C(3)-C(4)	1.395(11)
C(4)-C(5)	1.359(11)
C(4)-H(4)	0.9500
C(5)-N(1)	1.356(9)
C(5)-H(5)	0.9500
C(6)-N(2)	1.437(10)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-N(2)	1.463(10)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-N(3)	1.365(9)
C(8)-C(9)	1.401(11)
C(8)-H(8)	0.9500
C(9)-C(10)	1.386(12)
C(9)-H(9)	0.9500
C(10)-N(4)	1.361(10)
C(10)-C(11)	1.407(11)
C(11)-C(12)	1.357(11)
C(11)-H(11)	0.9500
C(12)-N(3)	1.362(10)
C(12)-H(12A)	0.9500
C(13)-N(4)	1.471(13)
C(13)-H(13H)	0.9800
C(13)-H(13I)	0.9800
C(13)-H(13J)	0.9800

C(14)-N(4)	1.458(11)
C(14)-H(14S)	0.9800
C(14)-H(14T)	0.9800
C(14)-H(14U)	0.9800
C(15)-C(16)	1.508(11)
C(15)-H(15D)	0.9800
C(15)-H(15E)	0.9800
C(15)-H(15F)	0.9800
C(16)-C(18)	1.362(12)
C(16)-C(17)	1.399(10)
C(17)-C(27)	1.382(11)
C(17)-H(17)	0.9500
C(18)-C(19)	1.378(11)
C(18)-H(18)	0.9500
C(19)-C(20)	1.441(10)
C(19)-C(21)	1.466(11)
C(20)-N(6)	1.373(10)
C(20)-C(27)	1.435(11)
C(21)-C(22)	1.403(11)
C(21)-C(26)	1.408(11)
C(22)-C(23)	1.350(13)
C(22)-H(22)	0.9500
C(23)-C(24)	1.405(13)
C(23)-H(23)	0.9500
C(24)-C(25)	1.369(13)
C(24)-H(24)	0.9500
C(25)-C(26)	1.393(13)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(28)	1.526(10)
C(28)-C(29)	1.394(12)
C(28)-C(33)	1.430(10)
C(29)-C(30)	1.377(11)
C(29)-H(29)	0.9500
C(30)-C(31)	1.399(12)
C(30)-H(30)	0.9500

C(31)-C(32)	1.400(12)
C(31)-H(31)	0.9500
C(32)-C(33)	1.400(10)
C(32)-H(32)	0.9500
C(33)-Sc(1)	2.238(8)
C(34)-C(35)	1.500(11)
C(34)-P(1)	1.853(8)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.350(11)
C(35)-N(5)	1.382(10)
C(36)-C(37)	1.415(11)
C(36)-H(36)	0.9500
C(37)-C(38)	1.370(11)
C(37)-H(37)	0.9500
C(38)-N(5)	1.400(9)
C(38)-C(39)	1.472(11)
C(39)-P(2)	1.869(7)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.509(13)
C(40)-H(40D)	0.9800
C(40)-H(40E)	0.9800
C(40)-H(40F)	0.9800
C(41)-C(43)	1.517(14)
C(41)-C(42)	1.575(11)
C(41)-P(1)	1.905(9)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-C(46)	1.510(16)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800

C(44)-H(44C)	0.9800
C(45)-C(46)	1.518(13)
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.562(14)
C(46)-P(1)	1.867(10)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-C(49)	1.547(12)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-C(50)	1.513(12)
C(49)-C(51)	1.555(12)
C(49)-P(2)	1.884(8)
C(50)-H(50D)	0.9800
C(50)-H(50E)	0.9800
C(50)-H(50F)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-C(53)	1.508(11)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-C(54)	1.539(11)
C(53)-C(55)	1.542(11)
C(53)-P(2)	1.884(8)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800

C(101)-N(9)	1.335(10)
C(101)-C(102)	1.369(11)
C(101)-H(101)	0.9500
C(102)-C(103)	1.428(11)
C(102)-H(102)	0.9500
C(103)-N(10)	1.379(9)
C(103)-C(104)	1.387(11)
C(104)-C(105)	1.365(11)
C(104)-H(104)	0.9500
C(105)-N(9)	1.355(10)
C(105)-H(105)	0.9500
C(106)-N(10)	1.461(10)
C(106)-H(10D)	0.9800
C(106)-H(10E)	0.9800
C(106)-H(10F)	0.9800
C(107)-N(10)	1.437(11)
C(107)-H(10A)	0.9800
C(107)-H(10B)	0.9800
C(107)-H(10C)	0.9800
C(108)-N(7)	1.358(10)
C(108)-C(109)	1.366(11)
C(108)-H(108)	0.9500
C(109)-C(110)	1.429(12)
C(109)-H(109)	0.9500
C(110)-N(8)	1.361(10)
C(110)-C(111)	1.372(12)
C(111)-C(112)	1.377(11)
C(111)-H(111)	0.9500
C(112)-N(7)	1.354(9)
C(112)-H(112)	0.9500
C(113)-N(8)	1.475(11)
C(113)-H(11A)	0.9800
C(113)-H(11B)	0.9800
C(113)-H(11C)	0.9800
C(114)-N(8)	1.430(12)
C(114)-H(11D)	0.9800

C(114)-H(11E)	0.9800
C(114)-H(11F)	0.9800
C(115)-N(12)	1.389(10)
C(115)-C(118)	1.411(12)
C(115)-C(116)	1.447(11)
C(116)-C(119)	1.396(12)
C(116)-C(120)	1.486(12)
C(117)-C(118)	1.394(12)
C(117)-C(153)	1.421(13)
C(117)-H(117)	0.9500
C(118)-C(126)	1.501(11)
C(119)-C(153)	1.367(14)
C(119)-H(119)	0.9500
C(120)-C(121)	1.378(12)
C(120)-C(125)	1.396(12)
C(121)-C(122)	1.347(12)
C(121)-H(121)	0.9500
C(122)-C(123)	1.388(12)
C(122)-H(122)	0.9500
C(123)-C(124)	1.368(13)
C(123)-H(123)	0.9500
C(124)-C(125)	1.395(12)
C(124)-H(124)	0.9500
C(125)-H(125)	0.9500
C(126)-C(131)	1.407(11)
C(126)-C(127)	1.422(12)
C(127)-C(128)	1.392(12)
C(127)-H(127)	0.9500
C(128)-C(129)	1.373(13)
C(128)-H(128)	0.9500
C(129)-C(130)	1.367(12)
C(129)-H(129)	0.9500
C(130)-C(131)	1.437(10)
C(130)-H(130)	0.9500
C(131)-Sc(2)	2.249(8)
C(132)-C(133)	1.527(11)

C(132)-P(3)	1.820(7)
C(132)-H(13A)	0.9900
C(132)-H(13B)	0.9900
C(133)-N(11)	1.378(9)
C(133)-C(134)	1.387(11)
C(134)-C(135)	1.418(11)
C(134)-H(134)	0.9500
C(135)-C(136)	1.390(10)
C(135)-H(135)	0.9500
C(136)-N(11)	1.364(10)
C(136)-C(137)	1.494(10)
C(137)-P(4)	1.860(8)
C(137)-H(13C)	0.9900
C(137)-H(13D)	0.9900
C(138)-C(139)	1.503(12)
C(138)-H(13E)	0.9800
C(138)-H(13F)	0.9800
C(138)-H(13G)	0.9800
C(139)-C(140)	1.537(12)
C(139)-C(141)	1.541(11)
C(139)-P(3)	1.906(8)
C(140)-H(14G)	0.9800
C(140)-H(14H)	0.9800
C(140)-H(14I)	0.9800
C(141)-H(14P)	0.9800
C(141)-H(14Q)	0.9800
C(141)-H(14R)	0.9800
C(142)-C(145)	1.490(12)
C(142)-C(143)	1.529(11)
C(142)-C(144)	1.562(11)
C(142)-P(3)	1.908(9)
C(143)-H(14\$)	0.9800
C(143)-H(14Y)	0.9800
C(143)-H(14D)	0.9800
C(144)-H(14J)	0.9800
C(144)-H(14K)	0.9800

C(144)-H(14L)	0.9800
C(145)-H(14M)	0.9800
C(145)-H(14N)	0.9800
C(145)-H(14O)	0.9800
C(146)-C(147)	1.539(10)
C(146)-H(14A)	0.9800
C(146)-H(14B)	0.9800
C(146)-H(14C)	0.9800
C(147)-C(149)	1.511(12)
C(147)-C(148)	1.512(11)
C(147)-P(4)	1.878(8)
C(148)-H(14X)	0.9800
C(148)-H(14E)	0.9800
C(148)-H(14F)	0.9800
C(149)-H(14Z)	0.9800
C(149)-H(14V)	0.9800
C(149)-H(14W)	0.9800
C(150)-C(152)	1.532(13)
C(150)-C(151)	1.536(13)
C(150)-C(154)	1.551(11)
C(150)-P(4)	1.892(8)
C(151)-H(15J)	0.9800
C(151)-H(15K)	0.9800
C(151)-H(15L)	0.9800
C(152)-H(15G)	0.9800
C(152)-H(15H)	0.9800
C(152)-H(15I)	0.9800
C(153)-C(155)	1.528(15)
C(154)-H(15M)	0.9800
C(154)-H(15N)	0.9800
C(154)-H(15O)	0.9800
C(155)-H(15A)	0.9800
C(155)-H(15B)	0.9800
C(155)-H(15C)	0.9800
N(1)-Sc(1)	2.375(6)
N(3)-Sc(1)	2.285(6)

N(5)-Sc(1)	2.194(6)
N(6)-Sc(1)	2.088(6)
N(6)-H(6)	0.8800
N(7)-Sc(2)	2.383(6)
N(9)-Sc(2)	2.306(6)
N(11)-Sc(2)	2.192(6)
N(12)-Sc(2)	2.074(6)
N(12)-H(12)	0.8800
P(1)-Sc(1)	3.045(3)
P(4)-Sc(2)	3.014(3)

N(1)-C(1)-C(2)	125.0(7)
N(1)-C(1)-H(1)	117.5
C(2)-C(1)-H(1)	117.5
C(1)-C(2)-C(3)	119.8(6)
C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
N(2)-C(3)-C(4)	123.9(7)
N(2)-C(3)-C(2)	120.6(7)
C(4)-C(3)-C(2)	115.5(7)
C(5)-C(4)-C(3)	120.3(7)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
N(1)-C(5)-C(4)	125.5(7)
N(1)-C(5)-H(5)	117.2
C(4)-C(5)-H(5)	117.2
N(2)-C(6)-H(6A)	109.5
N(2)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
N(2)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
N(2)-C(7)-H(7A)	109.5
N(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
N(2)-C(7)-H(7C)	109.5

H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(3)-C(8)-C(9)	123.7(8)
N(3)-C(8)-H(8)	118.2
C(9)-C(8)-H(8)	118.2
C(10)-C(9)-C(8)	119.9(7)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
N(4)-C(10)-C(9)	123.0(8)
N(4)-C(10)-C(11)	120.6(8)
C(9)-C(10)-C(11)	116.3(7)
C(12)-C(11)-C(10)	120.5(8)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(11)-C(12)-N(3)	124.8(7)
C(11)-C(12)-H(12A)	117.6
N(3)-C(12)-H(12A)	117.6
N(4)-C(13)-H(13H)	109.5
N(4)-C(13)-H(13I)	109.5
H(13H)-C(13)-H(13I)	109.5
N(4)-C(13)-H(13J)	109.5
H(13H)-C(13)-H(13J)	109.5
H(13I)-C(13)-H(13J)	109.5
N(4)-C(14)-H(14S)	109.5
N(4)-C(14)-H(14T)	109.5
H(14S)-C(14)-H(14T)	109.5
N(4)-C(14)-H(14U)	109.5
H(14S)-C(14)-H(14U)	109.5
H(14T)-C(14)-H(14U)	109.5
C(16)-C(15)-H(15D)	109.5
C(16)-C(15)-H(15E)	109.5
H(15D)-C(15)-H(15E)	109.5
C(16)-C(15)-H(15F)	109.5
H(15D)-C(15)-H(15F)	109.5
H(15E)-C(15)-H(15F)	109.5
C(18)-C(16)-C(17)	117.5(7)

C(18)-C(16)-C(15)	122.8(7)
C(17)-C(16)-C(15)	119.7(8)
C(27)-C(17)-C(16)	122.3(8)
C(27)-C(17)-H(17)	118.9
C(16)-C(17)-H(17)	118.9
C(16)-C(18)-C(19)	123.4(7)
C(16)-C(18)-H(18)	118.3
C(19)-C(18)-H(18)	118.3
C(18)-C(19)-C(20)	119.5(7)
C(18)-C(19)-C(21)	119.8(7)
C(20)-C(19)-C(21)	120.6(7)
N(6)-C(20)-C(27)	121.1(6)
N(6)-C(20)-C(19)	122.1(7)
C(27)-C(20)-C(19)	116.6(7)
C(22)-C(21)-C(26)	116.0(7)
C(22)-C(21)-C(19)	122.8(7)
C(26)-C(21)-C(19)	121.1(7)
C(23)-C(22)-C(21)	122.4(8)
C(23)-C(22)-H(22)	118.8
C(21)-C(22)-H(22)	118.8
C(22)-C(23)-C(24)	120.7(9)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	119.1(9)
C(25)-C(24)-H(24)	120.5
C(23)-C(24)-H(24)	120.5
C(24)-C(25)-C(26)	119.9(8)
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0
C(25)-C(26)-C(21)	121.8(8)
C(25)-C(26)-H(26)	119.1
C(21)-C(26)-H(26)	119.1
C(17)-C(27)-C(20)	119.7(7)
C(17)-C(27)-C(28)	118.2(7)
C(20)-C(27)-C(28)	122.1(6)
C(29)-C(28)-C(33)	122.4(7)

C(29)-C(28)-C(27)	115.3(7)
C(33)-C(28)-C(27)	122.4(7)
C(30)-C(29)-C(28)	120.8(8)
C(30)-C(29)-H(29)	119.6
C(28)-C(29)-H(29)	119.6
C(29)-C(30)-C(31)	119.4(8)
C(29)-C(30)-H(30)	120.3
C(31)-C(30)-H(30)	120.3
C(30)-C(31)-C(32)	118.9(8)
C(30)-C(31)-H(31)	120.6
C(32)-C(31)-H(31)	120.6
C(31)-C(32)-C(33)	124.3(8)
C(31)-C(32)-H(32)	117.9
C(33)-C(32)-H(32)	117.9
C(32)-C(33)-C(28)	114.2(7)
C(32)-C(33)-Sc(1)	127.1(6)
C(28)-C(33)-Sc(1)	118.6(5)
C(35)-C(34)-P(1)	112.6(5)
C(35)-C(34)-H(34A)	109.1
P(1)-C(34)-H(34A)	109.1
C(35)-C(34)-H(34B)	109.1
P(1)-C(34)-H(34B)	109.1
H(34A)-C(34)-H(34B)	107.8
C(36)-C(35)-N(5)	110.8(7)
C(36)-C(35)-C(34)	127.8(7)
N(5)-C(35)-C(34)	121.3(7)
C(35)-C(36)-C(37)	106.2(7)
C(35)-C(36)-H(36)	126.9
C(37)-C(36)-H(36)	126.9
C(38)-C(37)-C(36)	108.7(7)
C(38)-C(37)-H(37)	125.7
C(36)-C(37)-H(37)	125.7
C(37)-C(38)-N(5)	107.8(7)
C(37)-C(38)-C(39)	132.2(7)
N(5)-C(38)-C(39)	119.8(6)
C(38)-C(39)-P(2)	113.5(5)

C(38)-C(39)-H(39A)	108.9
P(2)-C(39)-H(39A)	108.9
C(38)-C(39)-H(39B)	108.9
P(2)-C(39)-H(39B)	108.9
H(39A)-C(39)-H(39B)	107.7
C(41)-C(40)-H(40D)	109.5
C(41)-C(40)-H(40E)	109.5
H(40D)-C(40)-H(40E)	109.5
C(41)-C(40)-H(40F)	109.5
H(40D)-C(40)-H(40F)	109.5
H(40E)-C(40)-H(40F)	109.5
C(40)-C(41)-C(43)	111.2(9)
C(40)-C(41)-C(42)	105.9(7)
C(43)-C(41)-C(42)	110.3(8)
C(40)-C(41)-P(1)	104.5(6)
C(43)-C(41)-P(1)	114.7(7)
C(42)-C(41)-P(1)	109.7(6)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(46)-C(44)-H(44A)	109.5
C(46)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(46)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(46)-C(45)-H(45A)	109.5

C(46)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(46)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-C(45)	114.6(10)
C(44)-C(46)-C(47)	108.5(10)
C(45)-C(46)-C(47)	104.7(8)
C(44)-C(46)-P(1)	114.3(8)
C(45)-C(46)-P(1)	108.5(6)
C(47)-C(46)-P(1)	105.4(7)
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(49)-C(48)-H(48A)	109.5
C(49)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(49)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-C(48)	108.3(8)
C(50)-C(49)-C(51)	110.1(7)
C(48)-C(49)-C(51)	106.6(7)
C(50)-C(49)-P(2)	105.1(5)
C(48)-C(49)-P(2)	108.6(6)
C(51)-C(49)-P(2)	117.9(6)
C(49)-C(50)-H(50D)	109.5
C(49)-C(50)-H(50E)	109.5
H(50D)-C(50)-H(50E)	109.5
C(49)-C(50)-H(50F)	109.5
H(50D)-C(50)-H(50F)	109.5
H(50E)-C(50)-H(50F)	109.5
C(49)-C(51)-H(51A)	109.5

C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-H(52A)	109.5
C(53)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(53)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(52)-C(53)-C(54)	107.6(7)
C(52)-C(53)-C(55)	109.5(7)
C(54)-C(53)-C(55)	107.3(7)
C(52)-C(53)-P(2)	109.8(6)
C(54)-C(53)-P(2)	104.3(6)
C(55)-C(53)-P(2)	117.7(5)
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
N(9)-C(101)-C(102)	125.8(7)
N(9)-C(101)-H(101)	117.1
C(102)-C(101)-H(101)	117.1
C(101)-C(102)-C(103)	117.8(7)
C(101)-C(102)-H(102)	121.1
C(103)-C(102)-H(102)	121.1
N(10)-C(103)-C(104)	122.4(7)

N(10)-C(103)-C(102)	120.7(7)
C(104)-C(103)-C(102)	116.8(7)
C(105)-C(104)-C(103)	120.1(7)
C(105)-C(104)-H(104)	119.9
C(103)-C(104)-H(104)	119.9
N(9)-C(105)-C(104)	124.2(7)
N(9)-C(105)-H(105)	117.9
C(104)-C(105)-H(105)	117.9
N(10)-C(106)-H(10D)	109.5
N(10)-C(106)-H(10E)	109.5
H(10D)-C(106)-H(10E)	109.5
N(10)-C(106)-H(10F)	109.5
H(10D)-C(106)-H(10F)	109.5
H(10E)-C(106)-H(10F)	109.5
N(10)-C(107)-H(10A)	109.5
N(10)-C(107)-H(10B)	109.5
H(10A)-C(107)-H(10B)	109.5
N(10)-C(107)-H(10C)	109.5
H(10A)-C(107)-H(10C)	109.5
H(10B)-C(107)-H(10C)	109.5
N(7)-C(108)-C(109)	125.5(7)
N(7)-C(108)-H(108)	117.2
C(109)-C(108)-H(108)	117.2
C(108)-C(109)-C(110)	118.3(8)
C(108)-C(109)-H(109)	120.9
C(110)-C(109)-H(109)	120.9
N(8)-C(110)-C(111)	123.5(8)
N(8)-C(110)-C(109)	119.8(8)
C(111)-C(110)-C(109)	116.8(7)
C(110)-C(111)-C(112)	120.5(7)
C(110)-C(111)-H(111)	119.8
C(112)-C(111)-H(111)	119.8
N(7)-C(112)-C(111)	124.3(7)
N(7)-C(112)-H(112)	117.9
C(111)-C(112)-H(112)	117.9
N(8)-C(113)-H(11A)	109.5

N(8)-C(113)-H(11B)	109.5
H(11A)-C(113)-H(11B)	109.5
N(8)-C(113)-H(11C)	109.5
H(11A)-C(113)-H(11C)	109.5
H(11B)-C(113)-H(11C)	109.5
N(8)-C(114)-H(11D)	109.5
N(8)-C(114)-H(11E)	109.5
H(11D)-C(114)-H(11E)	109.5
N(8)-C(114)-H(11F)	109.5
H(11D)-C(114)-H(11F)	109.5
H(11E)-C(114)-H(11F)	109.5
N(12)-C(115)-C(118)	122.3(7)
N(12)-C(115)-C(116)	120.4(7)
C(118)-C(115)-C(116)	117.0(7)
C(119)-C(116)-C(115)	119.1(8)
C(119)-C(116)-C(120)	119.3(7)
C(115)-C(116)-C(120)	121.5(7)
C(118)-C(117)-C(153)	121.7(9)
C(118)-C(117)-H(117)	119.2
C(153)-C(117)-H(117)	119.2
C(117)-C(118)-C(115)	121.1(8)
C(117)-C(118)-C(126)	116.1(8)
C(115)-C(118)-C(126)	122.8(7)
C(153)-C(119)-C(116)	124.0(8)
C(153)-C(119)-H(119)	118.0
C(116)-C(119)-H(119)	118.0
C(121)-C(120)-C(125)	117.2(8)
C(121)-C(120)-C(116)	122.6(8)
C(125)-C(120)-C(116)	120.1(8)
C(122)-C(121)-C(120)	122.7(8)
C(122)-C(121)-H(121)	118.6
C(120)-C(121)-H(121)	118.6
C(121)-C(122)-C(123)	120.0(8)
C(121)-C(122)-H(122)	120.0
C(123)-C(122)-H(122)	120.0
C(124)-C(123)-C(122)	119.7(9)

C(124)-C(123)-H(123)	120.2
C(122)-C(123)-H(123)	120.2
C(123)-C(124)-C(125)	119.7(8)
C(123)-C(124)-H(124)	120.2
C(125)-C(124)-H(124)	120.2
C(124)-C(125)-C(120)	120.7(8)
C(124)-C(125)-H(125)	119.6
C(120)-C(125)-H(125)	119.6
C(131)-C(126)-C(127)	120.6(7)
C(131)-C(126)-C(118)	123.5(7)
C(127)-C(126)-C(118)	115.9(7)
C(128)-C(127)-C(126)	121.1(8)
C(128)-C(127)-H(127)	119.5
C(126)-C(127)-H(127)	119.5
C(129)-C(128)-C(127)	119.1(9)
C(129)-C(128)-H(128)	120.5
C(127)-C(128)-H(128)	120.5
C(130)-C(129)-C(128)	120.3(8)
C(130)-C(129)-H(129)	119.8
C(128)-C(129)-H(129)	119.8
C(129)-C(130)-C(131)	123.7(8)
C(129)-C(130)-H(130)	118.1
C(131)-C(130)-H(130)	118.1
C(126)-C(131)-C(130)	115.0(7)
C(126)-C(131)-Sc(2)	120.0(5)
C(130)-C(131)-Sc(2)	124.8(6)
C(133)-C(132)-P(3)	115.4(5)
C(133)-C(132)-H(13A)	108.4
P(3)-C(132)-H(13A)	108.4
C(133)-C(132)-H(13B)	108.4
P(3)-C(132)-H(13B)	108.4
H(13A)-C(132)-H(13B)	107.5
N(11)-C(133)-C(134)	110.3(7)
N(11)-C(133)-C(132)	121.9(6)
C(134)-C(133)-C(132)	127.7(6)
C(133)-C(134)-C(135)	106.1(6)

C(133)-C(134)-H(134)	126.9
C(135)-C(134)-H(134)	126.9
C(136)-C(135)-C(134)	106.6(7)
C(136)-C(135)-H(135)	126.7
C(134)-C(135)-H(135)	126.7
N(11)-C(136)-C(135)	110.3(6)
N(11)-C(136)-C(137)	122.8(7)
C(135)-C(136)-C(137)	127.0(7)
C(136)-C(137)-P(4)	110.9(5)
C(136)-C(137)-H(13C)	109.5
P(4)-C(137)-H(13C)	109.5
C(136)-C(137)-H(13D)	109.5
P(4)-C(137)-H(13D)	109.5
H(13C)-C(137)-H(13D)	108.0
C(139)-C(138)-H(13E)	109.5
C(139)-C(138)-H(13F)	109.5
H(13E)-C(138)-H(13F)	109.5
C(139)-C(138)-H(13G)	109.5
H(13E)-C(138)-H(13G)	109.5
H(13F)-C(138)-H(13G)	109.5
C(138)-C(139)-C(140)	107.7(7)
C(138)-C(139)-C(141)	112.4(7)
C(140)-C(139)-C(141)	108.8(7)
C(138)-C(139)-P(3)	116.9(6)
C(140)-C(139)-P(3)	103.7(5)
C(141)-C(139)-P(3)	106.8(6)
C(139)-C(140)-H(14G)	109.5
C(139)-C(140)-H(14H)	109.5
H(14G)-C(140)-H(14H)	109.5
C(139)-C(140)-H(14I)	109.5
H(14G)-C(140)-H(14I)	109.5
H(14H)-C(140)-H(14I)	109.5
C(139)-C(141)-H(14P)	109.5
C(139)-C(141)-H(14Q)	109.5
H(14P)-C(141)-H(14Q)	109.5
C(139)-C(141)-H(14R)	109.5

H(14P)-C(141)-H(14R)	109.5
H(14Q)-C(141)-H(14R)	109.5
C(145)-C(142)-C(143)	111.0(8)
C(145)-C(142)-C(144)	110.8(8)
C(143)-C(142)-C(144)	106.3(7)
C(145)-C(142)-P(3)	117.3(6)
C(143)-C(142)-P(3)	103.8(6)
C(144)-C(142)-P(3)	106.8(6)
C(142)-C(143)-H(14\$)	109.5
C(142)-C(143)-H(14Y)	109.5
H(14\$)-C(143)-H(14Y)	109.5
C(142)-C(143)-H(14D)	109.5
H(14\$)-C(143)-H(14D)	109.5
H(14Y)-C(143)-H(14D)	109.5
C(142)-C(144)-H(14J)	109.5
C(142)-C(144)-H(14K)	109.5
H(14J)-C(144)-H(14K)	109.5
C(142)-C(144)-H(14L)	109.5
H(14J)-C(144)-H(14L)	109.5
H(14K)-C(144)-H(14L)	109.5
C(142)-C(145)-H(14M)	109.5
C(142)-C(145)-H(14N)	109.5
H(14M)-C(145)-H(14N)	109.5
C(142)-C(145)-H(14O)	109.5
H(14M)-C(145)-H(14O)	109.5
H(14N)-C(145)-H(14O)	109.5
C(147)-C(146)-H(14A)	109.5
C(147)-C(146)-H(14B)	109.5
H(14A)-C(146)-H(14B)	109.5
C(147)-C(146)-H(14C)	109.5
H(14A)-C(146)-H(14C)	109.5
H(14B)-C(146)-H(14C)	109.5
C(149)-C(147)-C(148)	110.4(7)
C(149)-C(147)-C(146)	109.7(7)
C(148)-C(147)-C(146)	106.4(7)
C(149)-C(147)-P(4)	114.4(6)

C(148)-C(147)-P(4)	108.0(6)
C(146)-C(147)-P(4)	107.7(6)
C(147)-C(148)-H(14X)	109.5
C(147)-C(148)-H(14E)	109.5
H(14X)-C(148)-H(14E)	109.5
C(147)-C(148)-H(14F)	109.5
H(14X)-C(148)-H(14F)	109.5
H(14E)-C(148)-H(14F)	109.5
C(147)-C(149)-H(14Z)	109.5
C(147)-C(149)-H(14V)	109.5
H(14Z)-C(149)-H(14V)	109.5
C(147)-C(149)-H(14W)	109.5
H(14Z)-C(149)-H(14W)	109.5
H(14V)-C(149)-H(14W)	109.5
C(152)-C(150)-C(151)	107.7(7)
C(152)-C(150)-C(154)	109.1(7)
C(151)-C(150)-C(154)	107.2(7)
C(152)-C(150)-P(4)	115.8(6)
C(151)-C(150)-P(4)	105.4(6)
C(154)-C(150)-P(4)	111.3(6)
C(150)-C(151)-H(15J)	109.5
C(150)-C(151)-H(15K)	109.5
H(15J)-C(151)-H(15K)	109.5
C(150)-C(151)-H(15L)	109.5
H(15J)-C(151)-H(15L)	109.5
H(15K)-C(151)-H(15L)	109.5
C(150)-C(152)-H(15G)	109.5
C(150)-C(152)-H(15H)	109.5
H(15G)-C(152)-H(15H)	109.5
C(150)-C(152)-H(15I)	109.5
H(15G)-C(152)-H(15I)	109.5
H(15H)-C(152)-H(15I)	109.5
C(119)-C(153)-C(117)	116.8(8)
C(119)-C(153)-C(155)	123.1(9)
C(117)-C(153)-C(155)	120.1(10)
C(150)-C(154)-H(15M)	109.5

C(150)-C(154)-H(15N)	109.5
H(15M)-C(154)-H(15N)	109.5
C(150)-C(154)-H(15O)	109.5
H(15M)-C(154)-H(15O)	109.5
H(15N)-C(154)-H(15O)	109.5
C(153)-C(155)-H(15A)	109.5
C(153)-C(155)-H(15B)	109.5
H(15A)-C(155)-H(15B)	109.5
C(153)-C(155)-H(15C)	109.5
H(15A)-C(155)-H(15C)	109.5
H(15B)-C(155)-H(15C)	109.5
C(5)-N(1)-C(1)	114.0(6)
C(5)-N(1)-Sc(1)	116.2(4)
C(1)-N(1)-Sc(1)	127.7(5)
C(3)-N(2)-C(6)	122.1(6)
C(3)-N(2)-C(7)	118.9(6)
C(6)-N(2)-C(7)	119.0(6)
C(12)-N(3)-C(8)	114.7(6)
C(12)-N(3)-Sc(1)	120.2(5)
C(8)-N(3)-Sc(1)	121.7(5)
C(10)-N(4)-C(14)	119.6(8)
C(10)-N(4)-C(13)	120.2(8)
C(14)-N(4)-C(13)	119.2(8)
C(35)-N(5)-C(38)	106.5(6)
C(35)-N(5)-Sc(1)	126.2(5)
C(38)-N(5)-Sc(1)	127.0(5)
C(20)-N(6)-Sc(1)	120.4(5)
C(20)-N(6)-H(6)	119.8
Sc(1)-N(6)-H(6)	119.8
C(112)-N(7)-C(108)	114.5(6)
C(112)-N(7)-Sc(2)	115.4(5)
C(108)-N(7)-Sc(2)	127.9(5)
C(110)-N(8)-C(114)	122.6(8)
C(110)-N(8)-C(113)	119.6(7)
C(114)-N(8)-C(113)	117.7(7)
C(101)-N(9)-C(105)	115.3(7)

C(101)-N(9)-Sc(2)	120.4(5)
C(105)-N(9)-Sc(2)	121.3(5)
C(103)-N(10)-C(107)	119.7(7)
C(103)-N(10)-C(106)	120.7(7)
C(107)-N(10)-C(106)	118.3(7)
C(136)-N(11)-C(133)	106.7(6)
C(136)-N(11)-Sc(2)	126.5(5)
C(133)-N(11)-Sc(2)	125.6(5)
C(115)-N(12)-Sc(2)	122.5(5)
C(115)-N(12)-H(12)	118.8
Sc(2)-N(12)-H(12)	118.8
C(34)-P(1)-C(46)	104.5(4)
C(34)-P(1)-C(41)	100.3(4)
C(46)-P(1)-C(41)	110.5(4)
C(34)-P(1)-Sc(1)	87.7(3)
C(46)-P(1)-Sc(1)	119.2(3)
C(41)-P(1)-Sc(1)	125.8(3)
C(39)-P(2)-C(53)	101.3(3)
C(39)-P(2)-C(49)	101.8(3)
C(53)-P(2)-C(49)	110.0(4)
C(132)-P(3)-C(139)	101.3(3)
C(132)-P(3)-C(142)	99.0(4)
C(139)-P(3)-C(142)	110.5(4)
C(137)-P(4)-C(147)	105.0(4)
C(137)-P(4)-C(150)	100.8(4)
C(147)-P(4)-C(150)	110.3(4)
C(137)-P(4)-Sc(2)	89.4(3)
C(147)-P(4)-Sc(2)	117.8(3)
C(150)-P(4)-Sc(2)	126.1(3)
N(6)-Sc(1)-N(5)	97.6(2)
N(6)-Sc(1)-C(33)	84.9(3)
N(5)-Sc(1)-C(33)	111.0(2)
N(6)-Sc(1)-N(3)	90.7(2)
N(5)-Sc(1)-N(3)	158.3(2)
C(33)-Sc(1)-N(3)	89.6(2)
N(6)-Sc(1)-N(1)	174.3(3)

N(5)-Sc(1)-N(1)	85.3(2)
C(33)-Sc(1)-N(1)	89.4(2)
N(3)-Sc(1)-N(1)	88.4(2)
N(6)-Sc(1)-P(1)	96.9(2)
N(5)-Sc(1)-P(1)	70.36(18)
C(33)-Sc(1)-P(1)	177.59(18)
N(3)-Sc(1)-P(1)	88.78(18)
N(1)-Sc(1)-P(1)	88.77(18)
N(12)-Sc(2)-N(11)	97.7(2)
N(12)-Sc(2)-C(131)	84.7(3)
N(11)-Sc(2)-C(131)	112.8(2)
N(12)-Sc(2)-N(9)	89.9(2)
N(11)-Sc(2)-N(9)	156.5(2)
C(131)-Sc(2)-N(9)	89.8(3)
N(12)-Sc(2)-N(7)	174.2(3)
N(11)-Sc(2)-N(7)	84.1(2)
C(131)-Sc(2)-N(7)	89.5(3)
N(9)-Sc(2)-N(7)	90.6(2)
N(12)-Sc(2)-P(4)	97.9(2)
N(11)-Sc(2)-P(4)	69.76(16)
C(131)-Sc(2)-P(4)	176.10(19)
N(9)-Sc(2)-P(4)	87.28(18)
N(7)-Sc(2)-P(4)	87.88(18)

Symmetry transformations used to generate equivalent atoms:

Table S39. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-tBu)ScNHAr(DMAP)₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	17(4)	21(4)	52(5)	1(3)	-3(3)	4(3)
C(2)	12(3)	22(4)	50(5)	2(3)	3(3)	11(3)
C(3)	15(3)	27(4)	35(4)	-3(3)	-2(3)	-4(3)
C(4)	21(4)	17(3)	64(6)	-1(4)	0(4)	-7(3)
C(5)	24(4)	19(3)	51(5)	0(4)	0(4)	0(3)
C(6)	13(4)	38(4)	61(5)	-5(4)	10(4)	-6(3)
C(7)	40(5)	23(4)	44(5)	10(4)	-2(4)	-4(4)
C(8)	12(3)	17(3)	53(5)	4(3)	-4(3)	4(3)
C(9)	28(4)	11(3)	60(6)	-2(3)	-11(4)	4(3)
C(10)	32(4)	24(4)	41(5)	-9(3)	-7(4)	6(3)
C(11)	25(4)	24(4)	44(5)	-2(3)	-1(3)	8(3)
C(12)	29(4)	23(4)	39(5)	2(3)	-3(3)	5(3)
C(13)	81(8)	43(6)	57(6)	-10(5)	2(6)	14(5)
C(14)	37(5)	16(4)	101(8)	-10(5)	-23(5)	-2(4)
C(15)	33(4)	21(4)	47(5)	3(3)	-10(4)	4(3)
C(16)	19(4)	21(4)	59(6)	-4(4)	-2(4)	0(3)
C(17)	28(4)	18(3)	37(4)	2(3)	-3(3)	-4(3)
C(18)	21(4)	12(3)	48(5)	-2(3)	1(3)	1(3)
C(19)	23(4)	14(3)	50(5)	6(3)	0(3)	2(3)
C(20)	10(3)	17(3)	47(5)	-1(3)	2(3)	-5(3)
C(21)	20(4)	19(4)	49(5)	-2(3)	6(3)	-10(3)
C(22)	27(4)	32(4)	42(5)	2(4)	2(4)	7(3)
C(23)	38(5)	44(5)	75(7)	19(5)	4(5)	-2(4)
C(24)	34(5)	45(5)	61(6)	7(5)	16(4)	-6(4)
C(25)	31(5)	36(5)	72(7)	-4(5)	25(5)	-1(4)
C(26)	26(4)	25(4)	60(6)	1(4)	9(4)	-2(3)
C(27)	12(3)	19(3)	44(5)	2(3)	3(3)	1(3)
C(28)	28(4)	14(3)	39(4)	-1(3)	5(3)	-3(3)
C(29)	42(5)	19(4)	49(5)	-3(4)	1(4)	11(3)
C(30)	40(5)	20(4)	47(5)	5(3)	10(4)	5(3)
C(31)	36(5)	28(4)	46(5)	4(4)	8(4)	3(4)

C(32)	28(4)	22(4)	42(5)	-3(3)	3(3)	1(3)
C(33)	12(3)	14(3)	45(5)	-1(3)	7(3)	5(3)
C(34)	35(4)	19(4)	44(5)	4(3)	-5(4)	2(3)
C(35)	24(4)	21(4)	33(4)	0(3)	1(3)	-11(3)
C(36)	26(4)	14(3)	45(5)	3(3)	-1(4)	0(3)
C(37)	27(4)	18(4)	48(5)	-2(3)	6(4)	7(3)
C(38)	18(3)	15(3)	37(4)	2(3)	5(3)	-1(3)
C(39)	16(3)	13(3)	49(5)	2(3)	12(3)	7(3)
C(40)	24(5)	37(5)	101(8)	14(5)	-10(5)	1(4)
C(41)	46(5)	20(4)	56(6)	0(4)	-5(4)	9(4)
C(42)	50(6)	29(5)	70(7)	11(4)	17(5)	14(4)
C(43)	90(9)	67(8)	119(11)	-41(8)	-58(9)	48(7)
C(44)	112(12)	115(12)	60(8)	3(8)	36(8)	-27(9)
C(45)	39(5)	50(6)	74(7)	15(5)	35(5)	3(5)
C(46)	46(5)	33(5)	60(6)	14(4)	-1(5)	-1(4)
C(47)	52(7)	30(5)	138(11)	20(6)	16(7)	8(5)
C(48)	24(5)	45(5)	94(8)	1(5)	-1(5)	-13(4)
C(49)	22(4)	31(4)	53(6)	-6(4)	4(4)	-13(3)
C(50)	37(5)	41(5)	47(5)	15(4)	1(4)	-14(4)
C(51)	58(6)	12(4)	84(7)	-4(4)	-14(5)	-8(4)
C(52)	30(5)	52(6)	61(6)	3(5)	8(4)	19(4)
C(53)	19(4)	23(4)	46(5)	0(3)	1(3)	6(3)
C(54)	52(6)	32(5)	52(6)	13(4)	-3(5)	-8(4)
C(55)	24(4)	38(5)	55(6)	-6(4)	-8(4)	6(4)
C(101)	30(4)	19(4)	49(5)	-1(3)	9(4)	9(3)
C(102)	30(4)	27(4)	36(5)	1(3)	4(4)	-1(3)
C(103)	11(3)	17(3)	45(5)	8(3)	-5(3)	-6(3)
C(104)	24(4)	13(3)	39(4)	-1(3)	0(3)	1(3)
C(105)	40(5)	24(4)	34(4)	2(3)	7(4)	4(3)
C(106)	36(5)	23(4)	68(6)	15(4)	15(4)	3(4)
C(107)	76(7)	40(5)	30(5)	12(4)	-7(5)	-27(5)
C(108)	32(4)	19(4)	49(5)	-7(3)	5(4)	3(3)
C(109)	26(4)	36(5)	51(5)	5(4)	14(4)	11(4)
C(110)	41(5)	23(4)	54(5)	-9(4)	-3(4)	11(4)
C(111)	45(5)	20(4)	35(4)	-2(3)	-1(4)	2(3)
C(112)	17(4)	19(3)	51(5)	-2(4)	2(4)	1(3)

C(113)	36(5)	31(5)	79(7)	-6(5)	-4(5)	23(4)
C(114)	43(6)	43(5)	95(8)	8(6)	18(5)	25(5)
C(115)	34(5)	23(4)	48(5)	4(4)	9(4)	4(3)
C(116)	39(5)	25(4)	45(5)	5(4)	14(4)	18(4)
C(117)	96(9)	38(5)	51(6)	15(5)	42(6)	24(5)
C(118)	51(6)	25(4)	47(5)	5(4)	10(4)	13(4)
C(119)	87(8)	27(5)	64(7)	16(4)	38(6)	30(5)
C(120)	36(5)	20(4)	56(6)	1(4)	-3(4)	7(3)
C(121)	30(4)	22(4)	46(5)	-1(3)	-4(4)	10(3)
C(122)	23(4)	34(4)	58(6)	1(4)	3(4)	11(4)
C(123)	41(5)	36(5)	50(5)	-4(4)	4(4)	12(4)
C(124)	26(4)	30(4)	65(6)	-3(4)	-4(4)	-2(4)
C(125)	34(4)	24(4)	55(6)	6(4)	3(4)	13(3)
C(126)	41(5)	33(4)	31(4)	-2(3)	15(4)	10(4)
C(127)	41(5)	47(5)	39(5)	7(4)	6(4)	21(4)
C(128)	54(6)	34(5)	40(5)	-2(4)	4(4)	3(4)
C(129)	52(5)	34(5)	34(5)	-2(4)	15(4)	7(4)
C(130)	41(5)	17(4)	49(5)	-2(4)	10(4)	7(3)
C(131)	22(4)	19(3)	37(4)	-2(3)	13(3)	0(3)
C(132)	21(4)	23(4)	33(4)	-5(3)	-4(3)	4(3)
C(133)	16(3)	9(3)	49(5)	-3(3)	2(3)	1(3)
C(134)	21(4)	16(3)	61(5)	8(4)	-2(4)	-2(3)
C(135)	31(4)	15(3)	42(5)	11(3)	-4(4)	0(3)
C(136)	19(4)	12(3)	47(5)	-3(3)	-3(3)	4(3)
C(137)	23(4)	20(4)	54(5)	-3(4)	1(4)	-2(3)
C(138)	30(5)	36(5)	72(7)	2(5)	3(4)	22(4)
C(139)	21(4)	37(4)	45(5)	-7(4)	0(3)	5(3)
C(140)	30(5)	46(5)	73(7)	-23(5)	-5(4)	18(4)
C(141)	22(4)	51(5)	71(6)	-10(5)	11(4)	2(4)
C(142)	23(4)	30(4)	51(5)	-5(4)	-7(4)	6(3)
C(143)	46(5)	29(5)	73(7)	-11(5)	-4(5)	9(4)
C(144)	32(5)	44(5)	54(6)	2(4)	-17(4)	-1(4)
C(145)	67(7)	45(6)	34(5)	5(4)	10(5)	-7(5)
C(146)	42(5)	20(4)	53(5)	4(4)	-2(4)	6(3)
C(147)	23(4)	23(4)	47(5)	-3(3)	-2(3)	0(3)
C(148)	33(5)	27(4)	51(5)	-6(4)	-7(4)	2(4)

C(149)	50(6)	34(5)	47(5)	-3(4)	-5(4)	-2(4)
C(150)	31(4)	26(4)	61(6)	-1(4)	-12(4)	-6(4)
C(151)	30(4)	17(4)	75(6)	-5(4)	4(4)	-4(3)
C(152)	39(5)	32(4)	58(6)	1(4)	-7(4)	-7(4)
C(153)	114(10)	38(6)	81(8)	31(5)	49(7)	50(6)
C(154)	38(5)	23(4)	75(7)	-10(4)	-3(5)	-4(4)
C(155)	230(20)	52(7)	87(10)	29(7)	75(12)	63(10)
N(1)	16(3)	14(3)	55(4)	4(3)	-4(3)	0(2)
N(2)	15(3)	25(3)	53(4)	3(3)	3(3)	-10(3)
N(3)	21(3)	13(3)	46(4)	-1(3)	-2(3)	1(2)
N(4)	49(5)	23(4)	59(5)	-11(3)	-7(4)	16(3)
N(5)	20(3)	13(3)	48(4)	0(3)	4(3)	0(2)
N(6)	20(3)	22(3)	47(4)	-3(3)	11(3)	-3(2)
N(7)	26(3)	20(3)	50(4)	-1(3)	3(3)	4(3)
N(8)	31(4)	33(4)	64(5)	4(4)	12(3)	11(3)
N(9)	37(4)	17(3)	40(4)	-3(3)	3(3)	-2(3)
N(10)	28(3)	21(3)	39(4)	3(3)	2(3)	-3(3)
N(11)	16(3)	16(3)	33(3)	-1(3)	-1(3)	4(2)
N(12)	33(4)	17(3)	40(4)	8(3)	7(3)	1(3)
P(1)	28(1)	18(1)	42(1)	0(1)	-1(1)	4(1)
P(2)	18(1)	18(1)	40(1)	-1(1)	3(1)	2(1)
P(3)	21(1)	21(1)	41(1)	1(1)	-2(1)	2(1)
P(4)	25(1)	16(1)	42(1)	-1(1)	-1(1)	-1(1)
Sc(1)	16(1)	12(1)	41(1)	0(1)	2(1)	1(1)
Sc(2)	25(1)	14(1)	37(1)	0(1)	5(1)	3(1)

Table S40. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for (PNP-tBu)ScNHAr(DMAP)₂.

	x	y	z	U(eq)
H(1)	2663	3021	2527	36
H(2)	3387	3645	2276	34
H(4)	2270	5023	2456	41
H(5)	1598	4360	2732	38
H(6A)	4039	4363	2413	56
H(6B)	4181	4949	2078	56
H(6C)	3960	4362	1783	56
H(7A)	2844	5433	1838	54
H(7B)	3515	5600	1852	54
H(7C)	3139	5634	2383	54
H(8)	1419	1631	2922	33
H(9)	1737	779	2491	40
H(11)	2397	1832	1342	37
H(12A)	2072	2639	1790	36
H(13H)	2300	1000	822	91
H(13I)	2660	402	917	91
H(13J)	2916	1027	1107	91
H(14S)	2118	95	2133	77
H(14T)	2353	-173	1586	77
H(14U)	1701	56	1629	77
H(15D)	803	365	1298	50
H(15E)	765	829	819	50
H(15F)	196	496	1020	50
H(17)	701	1833	1024	33
H(18)	99	682	2096	32
H(22)	354	604	3048	40
H(23)	-41	389	3852	63
H(24)	-759	1004	4221	56
H(25)	-1075	1830	3749	56
H(26)	-651	2067	2939	44

H(29)	290	2683	829	44
H(30)	487	3601	449	43
H(31)	1043	4302	921	44
H(32)	1330	4089	1784	37
H(34A)	1591	3580	4351	39
H(34B)	1964	3649	3820	39
H(36)	928	4542	4253	34
H(37)	149	4834	3595	37
H(39A)	56	3668	2538	31
H(39B)	323	4293	2364	31
H(40D)	2631	3010	3549	81
H(40E)	2537	2363	3300	81
H(40F)	3044	2472	3719	81
H(42A)	2631	1584	4148	75
H(42B)	2077	1566	3771	75
H(42C)	1998	1605	4400	75
H(43A)	2842	2558	4658	138
H(43B)	2192	2562	4873	138
H(43C)	2441	3127	4562	138
H(44A)	1205	2910	4960	144
H(44B)	1414	2232	4949	144
H(44C)	759	2388	5094	144
H(45A)	48	2576	4318	82
H(45B)	326	2769	3764	82
H(45C)	392	3190	4272	82
H(47A)	526	1632	4400	110
H(47B)	1176	1568	4195	110
H(47C)	677	1764	3793	110
H(48A)	-1973	3644	3004	82
H(48B)	-1869	4210	2632	82
H(48C)	-1717	4244	3250	82
H(50D)	-1132	3196	3454	63
H(50E)	-800	3802	3584	63
H(50F)	-491	3300	3236	63
H(51A)	-771	3171	2258	77
H(51B)	-1372	3456	2075	77

H(51C)	-1362	2943	2514	77
H(52A)	-1385	5102	1559	71
H(52B)	-1451	5184	2186	71
H(52C)	-1612	4562	1915	71
H(54A)	61	5106	1904	67
H(54B)	-386	5492	2243	67
H(54C)	-444	5463	1612	67
H(55A)	-873	3951	1502	58
H(55B)	-203	4075	1611	58
H(55C)	-549	4478	1196	58
H(101)	-1084	7647	4071	39
H(102)	-1423	6841	4531	37
H(104)	-687	5796	3397	31
H(105)	-384	6641	2980	39
H(10D)	-701	5069	4150	64
H(10E)	-1215	5061	3727	64
H(10F)	-1321	4816	4314	64
H(10A)	-1904	6036	4743	73
H(10B)	-1299	5935	5035	73
H(10C)	-1703	5379	4900	73
H(108)	-1638	8089	3357	40
H(109)	-2350	8752	3567	45
H(111)	-1187	10077	3347	40
H(112)	-528	9375	3089	35
H(11A)	-2029	10729	3420	73
H(11B)	-1720	10545	3963	73
H(11C)	-2387	10729	3962	73
H(11D)	-2855	9501	4088	90
H(11E)	-2973	9505	3463	90
H(11F)	-3067	10097	3803	90
H(117)	366	6946	4957	74
H(119)	1075	5767	3951	71
H(121)	1709	7078	2997	39
H(122)	2112	6796	2213	46
H(123)	1824	5912	1803	51
H(124)	1117	5328	2194	49

H(125)	708	5619	3002	45
H(127)	713	7810	5110	50
H(128)	394	8712	5468	52
H(129)	-101	9378	4929	48
H(130)	-337	9127	4078	43
H(13A)	1018	8668	3343	31
H(13B)	734	9273	3546	31
H(134)	887	9841	2307	39
H(135)	106	9546	1641	35
H(13C)	-517	8537	1522	39
H(13D)	-917	8642	2031	39
H(13E)	2284	8492	3803	69
H(13F)	2475	8030	3354	69
H(13G)	1806	8120	3488	69
H(14G)	2155	8256	2386	75
H(14H)	1791	8851	2294	75
H(14I)	1525	8321	2637	75
H(14P)	2993	8748	2782	72
H(14Q)	2911	9241	3232	72
H(14R)	2697	9370	2640	72
H(14\$)	1435	10523	3705	74
H(14Y)	1388	10412	4329	74
H(14D)	936	10105	3936	74
H(14J)	2397	10145	4329	65
H(14K)	2454	10200	3699	65
H(14L)	2634	9596	3990	65
H(14M)	1651	9416	4693	73
H(14N)	1864	8901	4303	73
H(14O)	1202	9105	4300	73
H(14A)	320	6761	2217	57
H(14B)	609	6624	1654	57
H(14C)	-63	6498	1744	57
H(14X)	590	8171	1621	56
H(14E)	980	7589	1562	56
H(14F)	733	7774	2130	56
H(14Z)	-82	7804	942	65

H(14V)	-383	7168	1007	65
H(14W)	289	7210	867	65
H(15J)	-1478	7416	2637	61
H(15K)	-2000	7382	2223	61
H(15L)	-1668	7997	2315	61
H(15G)	-1791	7480	1241	64
H(15H)	-1144	7611	1054	64
H(15I)	-1491	8100	1387	64
H(15M)	-1586	6578	1717	68
H(15N)	-1074	6541	2141	68
H(15O)	-928	6597	1524	68
H(15A)	1063	5555	4935	186
H(15B)	373	5557	4931	186
H(15C)	716	6007	5307	186
H(6)	160	2582	2890	36
H(12)	849	7563	3029	36

Table S41. Crystal data and structure refinement for (PNP-Cy)Sc(C#CCHMe₂)₂.

Empirical formula	C _{44.75} H _{69.25} N P ₂ Sc	
Formula weight	728.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.0240(5) Å	α = 73.2353(15)°.
	b = 17.1492(5) Å	β = 84.4873(18)°.
	c = 20.2172(7) Å	γ = 67.1130(14)°.
Volume	4288.4(3) Å ³	
Z	4	
Density (calculated)	1.128 Mg/m ³	
Absorption coefficient	0.276 mm ⁻¹	
F(000)	1583	
Crystal size	0.100 x 0.080 x 0.030 mm ³	
Theta range for data collection	1.052 to 25.399°.	
Index ranges	-16 ≤ h ≤ 16, -20 ≤ k ≤ 20, -24 ≤ l ≤ 24	
Reflections collected	112231	
Independent reflections	15695 [R(int) = 0.0610]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9280 and 0.8506	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	15695 / 0 / 904	
Goodness-of-fit on F ²	1.048	
Final R indices [I > 2σ(I)]	R ₁ = 0.0616, wR ₂ = 0.1495	
R indices (all data)	R ₁ = 0.0902, wR ₂ = 0.1680	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.557 and -0.678 e.Å ⁻³	

Table S42. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)Sc(C#CCHMe₂)₂. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(100)	6955(5)	9113(3)	7505(3)	74(2)
C(101)	6944(4)	9547(4)	6711(4)	73(2)
C(102)	7423(5)	9078(5)	6279(4)	94(2)
C(103)	7377(6)	9512(6)	5566(4)	98(2)
C(104)	6867(6)	10366(6)	5299(5)	108(3)
C(105)	6407(6)	10853(5)	5737(4)	99(2)
C(106)	6441(5)	10429(4)	6458(3)	74(2)
C(202)	4957(8)	431(7)	9810(8)	175(7)
C(201)	4942(7)	588(9)	9024(8)	171(6)
C(200)	4779(12)	1333(10)	8785(10)	117(7)
C(1)	1589(2)	6309(2)	3211(2)	17(1)
C(2)	1679(3)	5678(2)	3702(2)	25(1)
C(3)	1700(4)	4939(3)	4312(2)	52(1)
C(5)	2698(4)	4543(3)	4727(2)	44(1)
C(6)	364(2)	6312(2)	2205(2)	15(1)
C(7)	-510(3)	6358(2)	2335(2)	21(1)
C(8)	-1595(3)	6413(2)	2492(2)	29(1)
C(9)	-1941(3)	5973(3)	2059(3)	44(1)
C(10)	-1695(3)	6035(3)	3274(2)	44(1)
C(11)	-1346(3)	8108(2)	2846(2)	25(1)
C(12)	-2236(3)	8405(2)	3012(2)	31(1)
C(13)	-3331(3)	8773(3)	3231(2)	43(1)
C(14)	-3392(5)	8503(6)	3992(3)	116(3)
C(15)	-3819(4)	9768(3)	2932(4)	88(2)
C(16)	3070(3)	4212(2)	2901(2)	21(1)
C(17)	3544(3)	3451(2)	3201(2)	34(1)
C(18)	4105(5)	2513(3)	3565(3)	83(2)
C(19)	3897(6)	2266(4)	4269(3)	110(3)
C(20)	5008(5)	2061(3)	3275(3)	98(3)
C(21)	1948(3)	8092(2)	3336(2)	28(1)
C(22)	1958(3)	8411(2)	2568(2)	23(1)

C(23)	2487(3)	8891(2)	2157(2)	29(1)
C(24)	2203(3)	9041(2)	1463(2)	27(1)
C(25)	1507(2)	8654(2)	1484(2)	18(1)
C(26)	955(2)	8612(2)	905(2)	18(1)
C(27)	-654(2)	8202(2)	510(2)	18(1)
C(28)	-1534(3)	7864(2)	694(2)	22(1)
C(29)	-1706(3)	7493(2)	133(2)	26(1)
C(30)	-1902(3)	8179(2)	-573(2)	28(1)
C(31)	-1021(3)	8508(2)	-757(2)	28(1)
C(32)	-855(3)	8883(2)	-199(2)	21(1)
C(33)	-1157(2)	9735(2)	1056(2)	17(1)
C(34)	-2311(2)	9881(2)	1125(2)	21(1)
C(35)	-2986(3)	10865(2)	973(2)	26(1)
C(36)	-2685(3)	11310(2)	1424(2)	25(1)
C(37)	-1539(3)	11146(2)	1367(2)	23(1)
C(38)	-873(2)	10160(2)	1538(2)	19(1)
C(39)	-22(3)	9466(2)	3422(2)	29(1)
C(40)	-1156(3)	9743(2)	3623(2)	38(1)
C(41)	-1708(3)	10751(3)	3416(2)	43(1)
C(42)	-1165(4)	11168(3)	3729(3)	65(2)
C(43)	-38(4)	10889(3)	3532(4)	82(2)
C(44)	521(4)	9883(3)	3745(3)	63(2)
C(45)	567(5)	7824(3)	4532(2)	67(2)
C(46)	1573(5)	7132(3)	4849(2)	73(2)
C(47)	1494(10)	6767(4)	5648(3)	149(5)
C(48)	589(8)	6464(5)	5803(3)	138(5)
C(49)	-414(8)	7177(4)	5511(4)	174(6)
C(50)	-303(5)	7501(3)	4738(3)	96(3)
C(51)	3715(2)	6800(2)	1498(2)	20(1)
C(52)	3094(2)	6671(2)	1006(2)	18(1)
C(53)	3061(2)	6925(2)	296(2)	21(1)
C(54)	2311(2)	6680(2)	85(2)	20(1)
C(55)	1919(2)	6286(2)	674(2)	17(1)
C(56)	1172(2)	5832(2)	754(2)	16(1)
C(57)	4279(3)	6381(2)	2920(2)	27(1)
C(58)	4317(3)	5848(3)	3678(2)	35(1)

C(59)	4461(3)	6331(3)	4166(2)	54(1)
C(60)	5377(4)	6589(3)	3983(3)	63(2)
C(61)	5306(4)	7135(3)	3241(3)	63(2)
C(62)	5213(3)	6640(2)	2745(2)	39(1)
C(63)	5250(2)	5099(2)	2098(2)	22(1)
C(64)	5817(3)	4349(2)	2723(2)	30(1)
C(65)	6852(3)	3736(2)	2511(2)	37(1)
C(66)	6721(3)	3375(2)	1938(2)	31(1)
C(67)	6149(3)	4120(2)	1319(2)	29(1)
C(68)	5106(3)	4722(2)	1533(2)	24(1)
C(69)	754(3)	4301(2)	1615(2)	29(1)
C(70)	426(3)	4045(3)	1055(2)	37(1)
C(71)	-479(3)	3747(3)	1264(2)	33(1)
C(72)	-203(3)	2982(3)	1931(2)	40(1)
C(73)	93(3)	3238(3)	2495(2)	39(1)
C(74)	972(3)	3586(2)	2299(2)	21(1)
C(75)	2890(3)	4151(2)	1017(2)	20(1)
C(76)	3367(3)	3190(2)	1455(2)	29(1)
C(77)	4407(3)	2700(2)	1161(2)	30(1)
C(78)	4282(3)	2732(2)	417(2)	25(1)
C(79)	3795(3)	3684(2)	-28(2)	24(1)
C(80)	2760(3)	4192(2)	261(2)	20(1)
N(1)	1337(2)	8259(2)	2162(1)	17(1)
N(2)	2396(2)	6267(2)	1254(1)	14(1)
P(1)	-305(1)	8560(1)	1201(1)	14(1)
P(2)	609(1)	8252(1)	3580(1)	25(1)
P(3)	3994(1)	5893(1)	2297(1)	17(1)
P(4)	1739(1)	4804(1)	1435(1)	15(1)
Sc(1)	296(1)	7559(1)	2557(1)	14(1)
Sc(2)	2170(1)	5591(1)	2318(1)	12(1)
C(4)	1231(6)	4375(4)	4219(4)	33(2)
C(4A)	838(8)	5015(6)	4640(4)	44(3)

Table S43. Bond lengths [Å] and angles [°] for (PNP-Cy)Sc(C#CCHMe₂)₂.

C(100)-C(101)	1.561(8)
C(101)-C(102)	1.317(8)
C(101)-C(106)	1.357(8)
C(102)-C(103)	1.413(10)
C(103)-C(104)	1.324(10)
C(104)-C(105)	1.340(10)
C(105)-C(106)	1.425(9)
C(202)-C(202)#1	1.42(2)
C(202)-C(201)	1.533(18)
C(201)-C(200)	1.165(15)
C(1)-C(2)	1.212(4)
C(1)-Sc(1)	2.332(3)
C(1)-Sc(2)	2.380(3)
C(2)-C(3)	1.485(5)
C(2)-Sc(2)	2.851(3)
C(3)-C(4A)	1.300(10)
C(3)-C(4)	1.423(8)
C(3)-C(5)	1.510(6)
C(6)-C(7)	1.205(4)
C(6)-Sc(2)	2.346(3)
C(6)-Sc(1)	2.408(3)
C(7)-C(8)	1.496(5)
C(7)-Sc(1)	2.857(3)
C(8)-C(9)	1.521(6)
C(8)-C(10)	1.541(5)
C(11)-C(12)	1.206(5)
C(11)-Sc(1)	2.214(4)
C(12)-C(13)	1.493(5)
C(13)-C(14)	1.476(8)
C(13)-C(15)	1.524(6)
C(16)-C(17)	1.208(5)
C(16)-Sc(2)	2.221(3)
C(17)-C(18)	1.480(5)
C(18)-C(20)	1.381(7)

C(18)-C(19)	1.399(7)
C(21)-C(22)	1.491(5)
C(21)-P(2)	1.828(4)
C(22)-C(23)	1.371(5)
C(22)-N(1)	1.392(4)
C(23)-C(24)	1.418(5)
C(24)-C(25)	1.369(5)
C(25)-N(1)	1.387(4)
C(25)-C(26)	1.497(5)
C(26)-P(1)	1.837(3)
C(27)-C(28)	1.530(5)
C(27)-C(32)	1.534(4)
C(27)-P(1)	1.850(3)
C(28)-C(29)	1.530(5)
C(29)-C(30)	1.533(5)
C(30)-C(31)	1.523(5)
C(31)-C(32)	1.525(5)
C(33)-C(38)	1.531(4)
C(33)-C(34)	1.537(4)
C(33)-P(1)	1.851(3)
C(34)-C(35)	1.534(4)
C(35)-C(36)	1.522(5)
C(36)-C(37)	1.519(5)
C(37)-C(38)	1.532(4)
C(39)-C(44)	1.520(6)
C(39)-C(40)	1.523(5)
C(39)-P(2)	1.858(3)
C(40)-C(41)	1.538(5)
C(41)-C(42)	1.506(6)
C(42)-C(43)	1.513(8)
C(43)-C(44)	1.537(6)
C(45)-C(46)	1.497(7)
C(45)-C(50)	1.506(9)
C(45)-P(2)	1.856(4)
C(46)-C(47)	1.564(9)
C(47)-C(48)	1.523(14)

C(48)-C(49)	1.493(12)
C(49)-C(50)	1.514(8)
C(51)-C(52)	1.498(5)
C(51)-P(3)	1.838(3)
C(52)-C(53)	1.373(5)
C(52)-N(2)	1.386(4)
C(53)-C(54)	1.414(5)
C(54)-C(55)	1.370(5)
C(55)-N(2)	1.392(4)
C(55)-C(56)	1.502(4)
C(56)-P(4)	1.833(3)
C(57)-C(62)	1.520(5)
C(57)-C(58)	1.536(5)
C(57)-P(3)	1.848(3)
C(58)-C(59)	1.529(5)
C(59)-C(60)	1.496(7)
C(60)-C(61)	1.510(8)
C(61)-C(62)	1.531(6)
C(63)-C(68)	1.528(5)
C(63)-C(64)	1.530(5)
C(63)-P(3)	1.852(3)
C(64)-C(65)	1.533(5)
C(65)-C(66)	1.517(5)
C(66)-C(67)	1.522(5)
C(67)-C(68)	1.533(4)
C(69)-C(70)	1.495(5)
C(69)-C(74)	1.522(4)
C(69)-P(4)	1.852(4)
C(70)-C(71)	1.525(5)
C(71)-C(72)	1.541(5)
C(72)-C(73)	1.478(6)
C(73)-C(74)	1.542(5)
C(75)-C(80)	1.536(4)
C(75)-C(76)	1.537(4)
C(75)-P(4)	1.858(3)
C(76)-C(77)	1.535(5)

C(77)-C(78)	1.514(5)
C(78)-C(79)	1.532(5)
C(79)-C(80)	1.534(4)
N(1)-Sc(1)	2.190(3)
N(2)-Sc(2)	2.188(3)
P(1)-Sc(1)	2.7892(10)
P(2)-Sc(1)	2.8073(11)
P(3)-Sc(2)	2.7960(10)
P(4)-Sc(2)	2.7569(10)
Sc(1)-Sc(2)	3.5122(8)

C(102)-C(101)-C(106)	118.9(7)
C(102)-C(101)-C(100)	121.6(6)
C(106)-C(101)-C(100)	119.5(5)
C(101)-C(102)-C(103)	118.7(7)
C(104)-C(103)-C(102)	124.1(8)
C(103)-C(104)-C(105)	117.7(8)
C(104)-C(105)-C(106)	119.1(8)
C(101)-C(106)-C(105)	121.5(7)
C(202)#1-C(202)-C(201)	114.0(12)
C(200)-C(201)-C(202)	106.2(15)
C(2)-C(1)-Sc(1)	139.7(3)
C(2)-C(1)-Sc(2)	99.9(2)
Sc(1)-C(1)-Sc(2)	96.38(11)
C(1)-C(2)-C(3)	175.5(4)
C(1)-C(2)-Sc(2)	55.3(2)
C(3)-C(2)-Sc(2)	126.8(3)
C(4A)-C(3)-C(2)	117.0(5)
C(4)-C(3)-C(2)	116.2(4)
C(4A)-C(3)-C(5)	118.7(6)
C(4)-C(3)-C(5)	119.3(4)
C(2)-C(3)-C(5)	112.5(4)
C(7)-C(6)-Sc(2)	153.3(3)
C(7)-C(6)-Sc(1)	99.0(2)
Sc(2)-C(6)-Sc(1)	95.25(11)
C(6)-C(7)-C(8)	179.5(4)

C(6)-C(7)-Sc(1)	56.35(19)
C(8)-C(7)-Sc(1)	124.1(2)
C(7)-C(8)-C(9)	111.7(3)
C(7)-C(8)-C(10)	109.7(3)
C(9)-C(8)-C(10)	112.8(3)
C(12)-C(11)-Sc(1)	179.1(3)
C(11)-C(12)-C(13)	178.8(4)
C(14)-C(13)-C(12)	110.3(4)
C(14)-C(13)-C(15)	112.4(5)
C(12)-C(13)-C(15)	111.7(3)
C(17)-C(16)-Sc(2)	177.4(3)
C(16)-C(17)-C(18)	178.7(5)
C(20)-C(18)-C(19)	123.0(5)
C(20)-C(18)-C(17)	117.2(4)
C(19)-C(18)-C(17)	115.5(4)
C(22)-C(21)-P(2)	107.1(2)
C(23)-C(22)-N(1)	110.0(3)
C(23)-C(22)-C(21)	129.6(3)
N(1)-C(22)-C(21)	120.3(3)
C(22)-C(23)-C(24)	107.0(3)
C(25)-C(24)-C(23)	106.9(3)
C(24)-C(25)-N(1)	110.3(3)
C(24)-C(25)-C(26)	129.8(3)
N(1)-C(25)-C(26)	119.9(3)
C(25)-C(26)-P(1)	109.6(2)
C(28)-C(27)-C(32)	110.8(3)
C(28)-C(27)-P(1)	114.2(2)
C(32)-C(27)-P(1)	114.0(2)
C(29)-C(28)-C(27)	111.3(3)
C(28)-C(29)-C(30)	110.9(3)
C(31)-C(30)-C(29)	111.1(3)
C(30)-C(31)-C(32)	111.0(3)
C(31)-C(32)-C(27)	111.2(3)
C(38)-C(33)-C(34)	109.6(3)
C(38)-C(33)-P(1)	112.1(2)
C(34)-C(33)-P(1)	112.8(2)

C(35)-C(34)-C(33)	110.9(3)
C(36)-C(35)-C(34)	112.3(3)
C(37)-C(36)-C(35)	111.0(3)
C(36)-C(37)-C(38)	111.4(3)
C(33)-C(38)-C(37)	110.6(3)
C(44)-C(39)-C(40)	110.3(3)
C(44)-C(39)-P(2)	115.6(3)
C(40)-C(39)-P(2)	111.4(3)
C(39)-C(40)-C(41)	111.3(3)
C(42)-C(41)-C(40)	111.0(3)
C(41)-C(42)-C(43)	110.6(4)
C(42)-C(43)-C(44)	111.7(5)
C(39)-C(44)-C(43)	110.1(4)
C(46)-C(45)-C(50)	110.8(4)
C(46)-C(45)-P(2)	113.6(4)
C(50)-C(45)-P(2)	111.4(4)
C(45)-C(46)-C(47)	111.9(6)
C(48)-C(47)-C(46)	109.8(7)
C(49)-C(48)-C(47)	112.6(7)
C(48)-C(49)-C(50)	108.3(6)
C(45)-C(50)-C(49)	114.4(8)
C(52)-C(51)-P(3)	109.9(2)
C(53)-C(52)-N(2)	110.0(3)
C(53)-C(52)-C(51)	129.8(3)
N(2)-C(52)-C(51)	120.2(3)
C(52)-C(53)-C(54)	107.2(3)
C(55)-C(54)-C(53)	106.8(3)
C(54)-C(55)-N(2)	110.1(3)
C(54)-C(55)-C(56)	129.5(3)
N(2)-C(55)-C(56)	120.1(3)
C(55)-C(56)-P(4)	105.2(2)
C(62)-C(57)-C(58)	111.4(3)
C(62)-C(57)-P(3)	114.5(3)
C(58)-C(57)-P(3)	114.3(2)
C(59)-C(58)-C(57)	111.4(4)
C(60)-C(59)-C(58)	112.0(4)

C(59)-C(60)-C(61)	111.3(4)
C(60)-C(61)-C(62)	111.1(4)
C(57)-C(62)-C(61)	110.4(4)
C(68)-C(63)-C(64)	109.9(3)
C(68)-C(63)-P(3)	110.4(2)
C(64)-C(63)-P(3)	114.6(2)
C(63)-C(64)-C(65)	110.8(3)
C(66)-C(65)-C(64)	112.2(3)
C(65)-C(66)-C(67)	110.7(3)
C(66)-C(67)-C(68)	110.8(3)
C(63)-C(68)-C(67)	111.2(3)
C(70)-C(69)-C(74)	112.4(3)
C(70)-C(69)-P(4)	119.5(3)
C(74)-C(69)-P(4)	111.9(2)
C(69)-C(70)-C(71)	112.5(3)
C(70)-C(71)-C(72)	110.2(3)
C(73)-C(72)-C(71)	110.9(3)
C(72)-C(73)-C(74)	113.0(3)
C(69)-C(74)-C(73)	112.3(3)
C(80)-C(75)-C(76)	110.5(3)
C(80)-C(75)-P(4)	117.0(2)
C(76)-C(75)-P(4)	111.5(2)
C(77)-C(76)-C(75)	110.7(3)
C(78)-C(77)-C(76)	111.1(3)
C(77)-C(78)-C(79)	110.9(3)
C(78)-C(79)-C(80)	111.7(3)
C(79)-C(80)-C(75)	110.8(3)
C(25)-N(1)-C(22)	105.8(3)
C(25)-N(1)-Sc(1)	129.0(2)
C(22)-N(1)-Sc(1)	125.2(2)
C(52)-N(2)-C(55)	105.9(2)
C(52)-N(2)-Sc(2)	129.0(2)
C(55)-N(2)-Sc(2)	124.8(2)
C(26)-P(1)-C(27)	101.25(15)
C(26)-P(1)-C(33)	102.72(14)
C(27)-P(1)-C(33)	105.75(14)

C(26)-P(1)-Sc(1)	97.52(10)
C(27)-P(1)-Sc(1)	126.88(10)
C(33)-P(1)-Sc(1)	117.77(10)
C(21)-P(2)-C(45)	108.6(2)
C(21)-P(2)-C(39)	102.72(17)
C(45)-P(2)-C(39)	103.88(18)
C(21)-P(2)-Sc(1)	93.58(11)
C(45)-P(2)-Sc(1)	128.16(17)
C(39)-P(2)-Sc(1)	116.29(12)
C(51)-P(3)-C(57)	102.05(16)
C(51)-P(3)-C(63)	101.70(15)
C(57)-P(3)-C(63)	106.59(15)
C(51)-P(3)-Sc(2)	97.68(10)
C(57)-P(3)-Sc(2)	122.85(12)
C(63)-P(3)-Sc(2)	120.97(11)
C(56)-P(4)-C(69)	105.75(15)
C(56)-P(4)-C(75)	103.17(14)
C(69)-P(4)-C(75)	111.37(17)
C(56)-P(4)-Sc(2)	94.60(10)
C(69)-P(4)-Sc(2)	123.11(13)
C(75)-P(4)-Sc(2)	114.65(11)
N(1)-Sc(1)-C(11)	128.16(11)
N(1)-Sc(1)-C(1)	93.97(10)
C(11)-Sc(1)-C(1)	125.96(12)
N(1)-Sc(1)-C(6)	123.23(10)
C(11)-Sc(1)-C(6)	101.79(12)
C(1)-Sc(1)-C(6)	71.90(11)
N(1)-Sc(1)-P(1)	71.53(7)
C(11)-Sc(1)-P(1)	88.03(9)
C(1)-Sc(1)-P(1)	142.43(8)
C(6)-Sc(1)-P(1)	87.12(8)
N(1)-Sc(1)-P(2)	71.06(7)
C(11)-Sc(1)-P(2)	83.17(10)
C(1)-Sc(1)-P(2)	80.82(8)
C(6)-Sc(1)-P(2)	149.50(8)
P(1)-Sc(1)-P(2)	123.29(3)

N(1)-Sc(1)-C(7)	144.89(10)
C(11)-Sc(1)-C(7)	77.21(11)
C(1)-Sc(1)-C(7)	85.40(10)
C(6)-Sc(1)-C(7)	24.63(10)
P(1)-Sc(1)-C(7)	87.77(7)
P(2)-Sc(1)-C(7)	142.62(7)
N(1)-Sc(1)-Sc(2)	91.31(7)
C(11)-Sc(1)-Sc(2)	140.18(9)
C(1)-Sc(1)-Sc(2)	42.33(7)
C(6)-Sc(1)-Sc(2)	41.70(8)
P(1)-Sc(1)-Sc(2)	102.02(2)
P(2)-Sc(1)-Sc(2)	119.80(3)
C(7)-Sc(1)-Sc(2)	64.99(7)
N(2)-Sc(2)-C(16)	127.60(11)
N(2)-Sc(2)-C(6)	92.20(10)
C(16)-Sc(2)-C(6)	127.80(12)
N(2)-Sc(2)-C(1)	123.39(10)
C(16)-Sc(2)-C(1)	102.46(11)
C(6)-Sc(2)-C(1)	72.15(11)
N(2)-Sc(2)-P(4)	71.14(7)
C(16)-Sc(2)-P(4)	83.55(9)
C(6)-Sc(2)-P(4)	79.28(8)
C(1)-Sc(2)-P(4)	147.90(8)
N(2)-Sc(2)-P(3)	72.32(7)
C(16)-Sc(2)-P(3)	86.78(9)
C(6)-Sc(2)-P(3)	142.48(8)
C(1)-Sc(2)-P(3)	87.92(8)
P(4)-Sc(2)-P(3)	124.09(3)
N(2)-Sc(2)-C(2)	147.91(10)
C(16)-Sc(2)-C(2)	79.19(11)
C(6)-Sc(2)-C(2)	80.21(10)
C(1)-Sc(2)-C(2)	24.75(10)
P(4)-Sc(2)-C(2)	136.16(8)
P(3)-Sc(2)-C(2)	94.92(8)
N(2)-Sc(2)-Sc(1)	90.75(6)
C(16)-Sc(2)-Sc(1)	141.17(9)

C(6)-Sc(2)-Sc(1)	43.05(7)
C(1)-Sc(2)-Sc(1)	41.29(7)
P(4)-Sc(2)-Sc(1)	119.38(3)
P(3)-Sc(2)-Sc(1)	101.78(2)
C(2)-Sc(2)-Sc(1)	62.50(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2

Table S44. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)Sc(C#CCHMe₂)₂. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(100)	95(5)	45(3)	69(4)	-3(3)	-25(3)	-17(3)
C(101)	61(4)	68(4)	104(5)	-38(4)	18(3)	-32(3)
C(102)	88(5)	82(5)	127(7)	-48(5)	11(4)	-35(4)
C(103)	89(5)	126(7)	66(5)	-26(4)	13(4)	-29(5)
C(104)	91(5)	96(6)	111(6)	-27(5)	33(5)	-16(4)
C(105)	76(5)	105(6)	111(6)	-6(5)	-17(4)	-41(4)
C(106)	81(4)	68(4)	70(4)	-1(3)	-19(3)	-34(3)
C(202)	77(5)	232(16)	310(17)	-226(17)	70(8)	-64(9)
C(201)	63(5)	209(13)	296(17)	-173(14)	24(8)	-40(7)
C(200)	70(10)	69(9)	165(17)	11(10)	23(10)	-13(8)
C(1)	20(2)	14(2)	16(2)	-6(1)	-1(1)	-4(1)
C(2)	29(2)	24(2)	20(2)	-4(2)	-7(2)	-10(2)
C(3)	65(3)	52(3)	35(3)	25(2)	-25(2)	-38(2)
C(5)	59(3)	33(2)	29(2)	11(2)	-18(2)	-16(2)
C(6)	17(2)	14(2)	14(2)	-4(1)	3(1)	-6(1)
C(7)	22(2)	18(2)	22(2)	-4(1)	2(2)	-7(1)
C(8)	15(2)	31(2)	39(2)	-7(2)	6(2)	-10(2)
C(9)	25(2)	39(2)	74(3)	-17(2)	6(2)	-20(2)
C(10)	30(2)	48(2)	43(3)	9(2)	6(2)	-19(2)
C(11)	27(2)	19(2)	27(2)	-8(1)	8(2)	-7(2)
C(12)	30(2)	21(2)	42(2)	-13(2)	12(2)	-10(2)
C(13)	29(2)	36(2)	72(3)	-28(2)	24(2)	-17(2)
C(14)	48(4)	195(8)	72(4)	-37(5)	40(3)	-19(4)
C(15)	39(3)	44(3)	157(6)	-25(3)	45(4)	-3(2)
C(16)	22(2)	19(2)	18(2)	-5(1)	-2(1)	-5(1)
C(17)	39(2)	22(2)	25(2)	-1(2)	4(2)	1(2)
C(18)	78(4)	31(3)	70(4)	24(2)	28(3)	20(2)
C(19)	146(7)	48(3)	62(4)	8(3)	15(4)	21(4)
C(20)	111(5)	39(3)	67(4)	6(3)	10(4)	35(3)
C(21)	29(2)	19(2)	33(2)	-10(2)	-15(2)	1(1)
C(22)	19(2)	12(2)	33(2)	-5(1)	-10(2)	-1(1)

C(23)	21(2)	16(2)	50(2)	-4(2)	-13(2)	-7(1)
C(24)	18(2)	14(2)	40(2)	4(1)	-2(2)	-5(1)
C(25)	13(2)	12(1)	23(2)	2(1)	0(1)	-3(1)
C(26)	15(2)	14(2)	19(2)	0(1)	1(1)	-2(1)
C(27)	16(2)	16(2)	18(2)	-4(1)	-2(1)	-3(1)
C(28)	24(2)	21(2)	21(2)	-5(1)	-3(1)	-10(1)
C(29)	26(2)	25(2)	29(2)	-6(2)	-7(2)	-10(2)
C(30)	30(2)	28(2)	25(2)	-10(2)	-11(2)	-5(2)
C(31)	35(2)	24(2)	18(2)	-4(1)	-4(2)	-5(2)
C(32)	25(2)	18(2)	15(2)	-3(1)	-2(1)	-5(1)
C(33)	16(2)	11(1)	17(2)	0(1)	1(1)	-2(1)
C(34)	16(2)	16(2)	30(2)	-8(1)	-1(1)	-3(1)
C(35)	17(2)	20(2)	34(2)	-9(2)	-2(2)	1(1)
C(36)	19(2)	19(2)	31(2)	-10(1)	2(2)	1(1)
C(37)	25(2)	15(2)	27(2)	-8(1)	1(2)	-4(1)
C(38)	16(2)	15(2)	22(2)	-3(1)	0(1)	-3(1)
C(39)	35(2)	18(2)	33(2)	-9(2)	-5(2)	-6(2)
C(40)	43(2)	28(2)	42(2)	-21(2)	10(2)	-9(2)
C(41)	43(3)	30(2)	46(3)	-17(2)	-5(2)	2(2)
C(42)	69(4)	27(2)	91(4)	-27(2)	-37(3)	7(2)
C(43)	65(4)	19(2)	160(6)	-25(3)	-45(4)	-3(2)
C(44)	57(3)	23(2)	109(4)	-25(2)	-36(3)	0(2)
C(45)	132(5)	27(2)	21(2)	-8(2)	-10(3)	-6(3)
C(46)	130(5)	36(3)	38(3)	-10(2)	-30(3)	-8(3)
C(47)	323(15)	29(3)	43(4)	-16(3)	-63(6)	6(5)
C(48)	242(12)	52(4)	38(4)	-2(3)	24(5)	20(5)
C(49)	242(11)	62(4)	74(5)	26(4)	89(6)	43(5)
C(50)	127(6)	37(3)	67(4)	13(2)	66(4)	-4(3)
C(51)	11(2)	18(2)	28(2)	0(1)	-1(1)	-6(1)
C(52)	13(2)	11(1)	23(2)	-1(1)	1(1)	-1(1)
C(53)	18(2)	17(2)	19(2)	2(1)	7(1)	-4(1)
C(54)	19(2)	18(2)	14(2)	-1(1)	0(1)	0(1)
C(55)	16(2)	12(1)	16(2)	-3(1)	-3(1)	1(1)
C(56)	16(2)	14(1)	14(2)	-5(1)	0(1)	-3(1)
C(57)	19(2)	21(2)	42(2)	-15(2)	-9(2)	-1(1)
C(58)	27(2)	45(2)	33(2)	-17(2)	-8(2)	-6(2)

C(59)	37(3)	60(3)	53(3)	-36(2)	-28(2)	14(2)
C(60)	53(3)	45(3)	91(4)	-37(3)	-47(3)	5(2)
C(61)	53(3)	33(2)	109(5)	-22(3)	-44(3)	-10(2)
C(62)	27(2)	28(2)	63(3)	-9(2)	-19(2)	-12(2)
C(63)	15(2)	17(2)	31(2)	-6(1)	-1(1)	-3(1)
C(64)	27(2)	23(2)	31(2)	-8(2)	-11(2)	2(2)
C(65)	27(2)	25(2)	48(3)	-14(2)	-13(2)	7(2)
C(66)	19(2)	23(2)	46(2)	-15(2)	-3(2)	2(1)
C(67)	19(2)	27(2)	35(2)	-13(2)	5(2)	-1(2)
C(68)	17(2)	22(2)	26(2)	-6(1)	1(2)	-2(1)
C(69)	37(2)	25(2)	28(2)	3(2)	-11(2)	-18(2)
C(70)	41(2)	38(2)	31(2)	-7(2)	-4(2)	-16(2)
C(71)	30(2)	52(2)	23(2)	-4(2)	-6(2)	-26(2)
C(72)	39(2)	52(3)	36(2)	-4(2)	0(2)	-29(2)
C(73)	51(3)	37(2)	32(2)	2(2)	-8(2)	-28(2)
C(74)	26(2)	21(2)	18(2)	-5(1)	-4(1)	-9(1)
C(75)	19(2)	18(2)	21(2)	-9(1)	-4(1)	-1(1)
C(76)	35(2)	18(2)	20(2)	-7(1)	-7(2)	7(2)
C(77)	24(2)	23(2)	36(2)	-12(2)	-9(2)	5(2)
C(78)	18(2)	24(2)	33(2)	-14(2)	5(2)	-5(1)
C(79)	21(2)	25(2)	26(2)	-10(1)	6(2)	-8(1)
C(80)	20(2)	18(2)	18(2)	-5(1)	0(1)	-3(1)
N(1)	15(1)	12(1)	21(2)	-4(1)	-2(1)	-2(1)
N(2)	9(1)	14(1)	18(1)	-2(1)	0(1)	-2(1)
P(1)	13(1)	11(1)	15(1)	-2(1)	0(1)	-2(1)
P(2)	40(1)	16(1)	19(1)	-6(1)	-2(1)	-7(1)
P(3)	13(1)	15(1)	22(1)	-4(1)	-2(1)	-4(1)
P(4)	17(1)	11(1)	16(1)	-3(1)	-4(1)	-3(1)
Sc(1)	16(1)	10(1)	14(1)	-2(1)	1(1)	-3(1)
Sc(2)	12(1)	10(1)	13(1)	-2(1)	0(1)	-3(1)
C(4)	43(5)	27(4)	26(4)	0(3)	2(3)	-17(3)
C(4A)	59(7)	41(5)	29(5)	-4(4)	15(4)	-23(5)

Table S45. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (PNP-Cy)Sc(C#CCHMe₂)₂.

	x	y	z	U(eq)
H(10A)	6830	8569	7588	110
H(10B)	6411	9521	7722	110
H(10C)	7630	8977	7704	110
H(102)	7791	8461	6443	113
H(103)	7735	9169	5259	118
H(104)	6829	10625	4814	130
H(105)	6062	11473	5569	119
H(106)	6104	10772	6768	89
H(20A)	5545	542	9939	210
H(20B)	4312	860	9942	210
H(20C)	5617	224	8869	205
H(20D)	4393	437	8884	205
H(20E)	4177	1683	9006	175
H(20F)	4637	1493	8288	175
H(20G)	5384	1452	8859	175
H(5A)	2767	4986	4914	66
H(5B)	3284	4348	4427	66
H(5C)	2692	4039	5107	66
H(8)	-2058	7050	2366	35
H(9A)	-1769	6174	1575	65
H(9B)	-2691	6131	2097	65
H(9C)	-1587	5333	2226	65
H(10D)	-1228	5415	3417	67
H(10E)	-2410	6084	3375	67
H(10F)	-1509	6367	3526	67
H(13)	-3732	8511	3043	52
H(14A)	-3033	7863	4163	174
H(14B)	-4119	8670	4125	174
H(14C)	-3063	8795	4191	174
H(15A)	-3438	10045	3103	131

H(15B)	-4542	9984	3073	131
H(15C)	-3791	9914	2426	131
H(18)	3650	2277	3400	100
H(19A)	4171	1622	4440	165
H(19B)	3147	2498	4336	165
H(19C)	4226	2503	4524	165
H(20H)	5573	2204	3388	146
H(20I)	4915	2230	2772	146
H(20J)	5176	1426	3459	146
H(21A)	2202	8429	3549	34
H(21B)	2400	7462	3495	34
H(23)	2954	9086	2308	35
H(24)	2450	9350	1060	32
H(26A)	1377	8085	749	22
H(26B)	851	9139	510	22
H(27)	-29	7685	454	21
H(28A)	-1366	7398	1139	26
H(28B)	-2179	8352	753	26
H(29A)	-2307	7315	251	31
H(29B)	-1089	6964	110	31
H(30A)	-1972	7913	-932	34
H(30B)	-2559	8681	-564	34
H(31A)	-1183	8970	-1203	34
H(31B)	-376	8017	-811	34
H(32A)	-1475	9410	-177	25
H(32B)	-257	9065	-319	25
H(33)	-1052	10048	572	20
H(34A)	-2499	9629	798	26
H(34B)	-2441	9573	1599	26
H(35A)	-2919	11157	481	31
H(35B)	-3720	10938	1052	31
H(36A)	-3095	11952	1279	30
H(36B)	-2847	11080	1911	30
H(37A)	-1353	11406	1689	27
H(37B)	-1393	11439	892	27
H(38A)	-133	10074	1487	23

H(38B)	-982	9872	2023	23
H(39)	-16	9722	2911	35
H(40A)	-1203	9511	4128	45
H(40B)	-1507	9488	3392	45
H(41A)	-1722	10979	2906	51
H(41B)	-2432	10912	3574	51
H(42A)	-1217	10992	4238	78
H(42B)	-1508	11817	3565	78
H(43A)	310	11151	3758	98
H(43B)	10	11115	3026	98
H(44A)	1248	9722	3593	76
H(44B)	525	9658	4255	76
H(45)	416	8331	4729	80
H(46A)	2113	7385	4756	88
H(46B)	1783	6642	4633	88
H(47A)	2145	6266	5831	178
H(47B)	1391	7232	5876	178
H(48A)	729	5962	5608	166
H(48B)	531	6254	6309	166
H(49A)	-589	7667	5724	209
H(49B)	-976	6948	5608	209
H(50A)	-191	7015	4530	115
H(50B)	-960	7985	4543	115
H(51A)	3325	7367	1607	24
H(51B)	4372	6820	1281	24
H(53)	3467	7212	3	25
H(54)	2117	6771	-377	23
H(56A)	1095	5711	316	19
H(56B)	483	6200	889	19
H(57)	3673	6948	2883	33
H(58A)	3667	5744	3788	42
H(58B)	4897	5269	3749	42
H(59A)	3830	6865	4148	64
H(59B)	4552	5945	4645	64
H(60A)	6017	6052	4053	76
H(60B)	5416	6930	4292	76

H(61A)	5931	7280	3131	76
H(61B)	4695	7693	3179	76
H(62A)	5141	7019	2265	46
H(62B)	5848	6105	2779	46
H(63)	5707	5433	1909	26
H(64A)	5380	4009	2929	36
H(64B)	5943	4597	3076	36
H(65A)	7316	4063	2353	44
H(65B)	7185	3240	2918	44
H(66A)	6327	2988	2111	37
H(66B)	7409	3018	1795	37
H(67A)	6031	3871	963	34
H(67B)	6578	4469	1114	34
H(68A)	4758	5210	1125	28
H(68B)	4657	4383	1703	28
H(69)	114	4783	1705	35
H(70A)	1019	3561	935	44
H(70B)	224	4553	638	44
H(71A)	-645	3555	888	39
H(71B)	-1098	4246	1340	39
H(72A)	-805	2811	2072	48
H(72B)	378	2467	1843	48
H(73A)	316	2721	2905	47
H(73B)	-521	3698	2624	47
H(74A)	1065	3825	2668	25
H(74B)	1626	3092	2265	25
H(75)	3422	4407	1015	24
H(76A)	3472	3175	1937	34
H(76B)	2885	2892	1461	34
H(77A)	4905	2972	1188	36
H(77B)	4692	2079	1442	36
H(78A)	3839	2410	395	30
H(78B)	4968	2438	233	30
H(79A)	3681	3686	-505	29
H(79B)	4278	3985	-50	29
H(80A)	2248	3936	230	24

H(80B)	2493	4814	-20	24
H(4A)	548	4732	3997	49
H(4B)	1154	3994	4669	49
H(4C)	1668	4012	3926	49
H(4A1)	662	5482	4871	66
H(4A2)	919	4457	4985	66
H(4A3)	284	5164	4311	66
