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Supporting Information

Substitution reaction of triphenylphosphine oxide with rare-earth metal phosphido methyl complexes

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Table S1 Crystallographic Data and Refinement for **1**, **3**, **7** and **8**.

Complex	**1**	**3**
Empirical formula	$C_{40}H_{67}N_3PSc$	$C_{30}H_{47}N_3PSc$
Formula weight	665.90	525.63
Colour	orange	orange
Crystal system	Orthorhombic	monoclinic
Space group	Pbca	P2(1)/n
a/Å	13.925(2)	10.710(2)
b/Å	22.628(3)	13.537(2)
c/Å	25.869(4)	20.887(3)
α/^{o}	90.00	90.00
β/^{o}	90.00	93.806(3)
γ/^{o}	90.00	90.00
Volume/Å^3	8151(2)	3021(1)
Z	8	4
Density (calculated)/g cm^{-3}	1.085	1.156
F(000)	2912	1136
T(K)	143(2)	133(2)
Θ range/^{o}	1.57 to 27.56	1.79 to 27.00
Reflections collected	62632	18804
Unique reflections	9402	6540
Unique reflections [I >2σ(I)]	5419	4411
Parameters	428	327
Goodness of fit	1.020	1.041
Final R indices [I >2σ(I)]	0.0569, 0.1285	0.0728, 0.1917
$\Delta\rho_{max, min}$/ eÅ^{-3}	0.629, -0.550	2.048, -0.607

Complex	**7**	**8**
Empirical formula	$C_{40}H_{51}N_3OPLu$	$C_{40}H_{52}N_3OPClSc$
Formula weight	795.78	702.22
Colour	yellow	yellow
Crystal system	monoclinic	monoclinic
Space group	P2(1)/n	P2(1)/n
a/Å	9.591(1)	27.730(4)
b/Å	23.000(2)	9.843(2)
c/Å	17.017(2)	27.805(4)
α/°	90.00	90.00
β/°	97.618(2)	92.963(3)
γ/°	90.00	90.00
Volume/Å^3	3720.8(5)	7579(2)
Z	4	8
Density (calculated)/g cm^{-3}	1.421	1.231
F(000)	1624	2992
T(K)	143(2)	140(2)
Θ range/°	1.50 to 30.03	1.06 to 25.10
Reflections collected	34993	48937
Unique reflections	10798	13486
Unique reflections [I >2σ(I)]	7776	8022
Parameters	423	846
Goodness of fit	0.984	0.947
Final R indices [I >2σ(I)]	0.0371, 0.0693	0.0769, 0.2140
$\Delta\rho_{max,\ min}$/ eÅ^{-3}	1.911, -0.740	1.826, -0.627

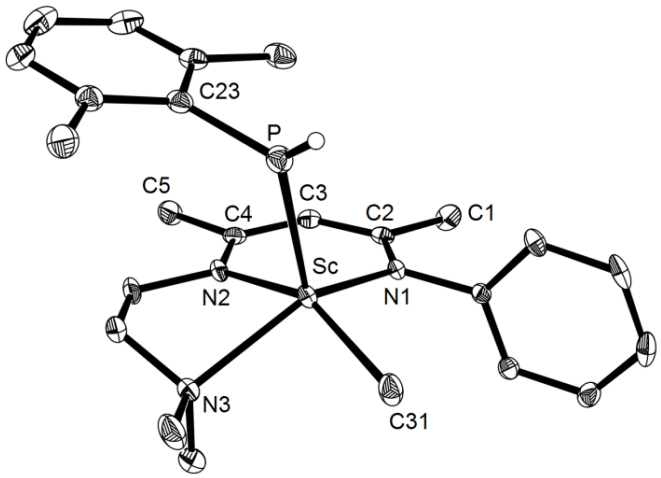

Fig. S1 Molecular structure of **3** with thermal ellipsoids set at 30% probability. Isopropyl groups on the arene and all H-atoms (except the phosphido hydrogen atom) are omitted for clarity. Selected bond lengths (Å) and angles (◦): Sc–N1 2.169(3), Sc–N2 2.200(3), Sc–N3 2.328(3), Sc–P 2.664(1), Sc–C 1.839(4), C2–N1 1.352(5), C4–N2 1.326(5), C2–C3 1.391(6), C3–C4 1.411(5), N1–Sc–N2 83.54(12) P–Sc–C22 99.91(13), Sc–P–C23 106.47(13).