

ELECTRONIC SUPPORTING INFORMATION

**A Base-Free Synthetic Route to Anti-Bimetallic Lanthanide
Pentalene Complexes.**

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Table of contents

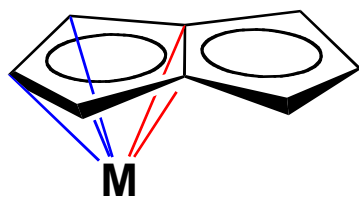
1. Additional X-ray crystallographic data	S2
2. Additional SQUID magnetometry data	S6
3. Additional cyclic voltammetry data	S7

1. Additional X-ray crystallographic data

Table S1 Crystallographic details for **1–4**.

Complex	1. (SiMe ₄) ₂	2. (C ₇ H ₈)	3	4
CCDC	1518413	1518414	1518415	1518416
Formula	2(C ₂₇ H ₅₀ Si ₂ Yb)	C ₅₃ H ₈₄ Eu ₂ Si ₂	C ₄₆ H ₇₆ Sm ₂ Si ₂	C ₄₆ H ₄₅ BF ₂₀ O ₃ Yb
<i>M_r</i>	603.89	1081.30	985.95	1209.67
Crystal System	monoclinic	monoclinic	triclinic	monoclinic
Space Group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>
Crystal Morphology	brown block	orange block	brown needle	yellow block
<i>a</i> , <i>b</i> , <i>c</i> / Å	13.133(3) 17.767(4) 13.725(3)	16.8151(6) 15.4458(7) 20.1800(7)	8.3909(10) 11.4240(15) 24.064(3)	12.660(3) 28.204(6) 13.915(3)
<i>α</i> , <i>β</i> , <i>γ</i> / °	90 114.10(3) 90	90 99.859(3) 90	94.072(7) 94.267(7) 92.703(7)	90 103.12(3) 90
Volume / Å ³	2923.2(10)	5163.8(4)	2291.3(5)	4838.8(17)
Temperature / K	173	173	100	173
<i>Z</i>	4	4	2	4
<i>R</i> _{int}	0.0821	0.0715	0.1189	0.0966
<i>λ</i> / Å	0.71073	1.54184	0.71073	0.71075
<i>θ</i> _{max} / °	27.48	71.404	25.03	27.47
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0464	0.0533	0.0699	0.0470
<i>wR</i> ₂ (all data)	0.0952	0.1308	0.1492	0.0921
<i>Goof</i>	1.015	1.077	1.049	1.028

Ring slippage (Δ)



$$\Delta = \Sigma(\text{M-C}_{\text{bridge}})/2 - \Sigma(\text{M-C}_{\text{wing}})/3$$

Fold angle (FA)

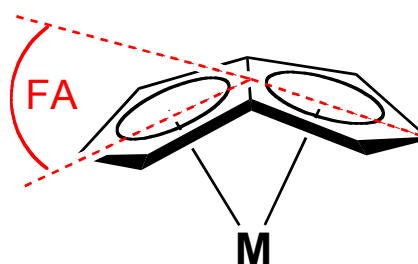


Figure S1 Definition of geometric parameters Δ and FA.

Table S2. Short intermolecular contacts (less than the sum of the van der Waals radii, Σr_{vdw}) for **1**.(SiMe₄)₂.

Atom1	Atom2	Distance / Å	Distance – Σr_{vdw} / Å
Yb1	C31 (TMS solvent)	2.930	–0.770

Table S3. Short intermolecular contacts (less than the sum of the van der Waals radii) for **2**.(C₇H₈).

Atom1	Atom2	Distance / Å	Distance – Σr_{vdw} / Å
Eu2	C52 (toluene solvent)	3.627	–0.073
Eu2	C47 (toluene solvent)	3.060	–0.640
Eu2	C48 (toluene solvent)	3.214	–0.486

Table S4. Short intermolecular contacts (less than the sum of the van der Waals radii) for **3**.

Atom1	Atom2	Distance / Å	Distance – Σr_{vdw} / Å
Sm1	C31 (iPr-CH ₃ neighbour)	3.435	–0.265
Sm2	C37 (iPr-CH ₃ neighbour)	3.394	–0.306
C32	C32	3.356	–0.044

Table S5. Short intermolecular contacts (less than the sum of the van der Waals radii) for **4**.

Atom1	Atom2	Distance / Å	Distance – Σr_{vdw} / Å
C14	F20	3.167	–0.003
C26	F3	3.166	–0.004
C27	F3	3.141	–0.029
C38	C39	3.303	–0.097

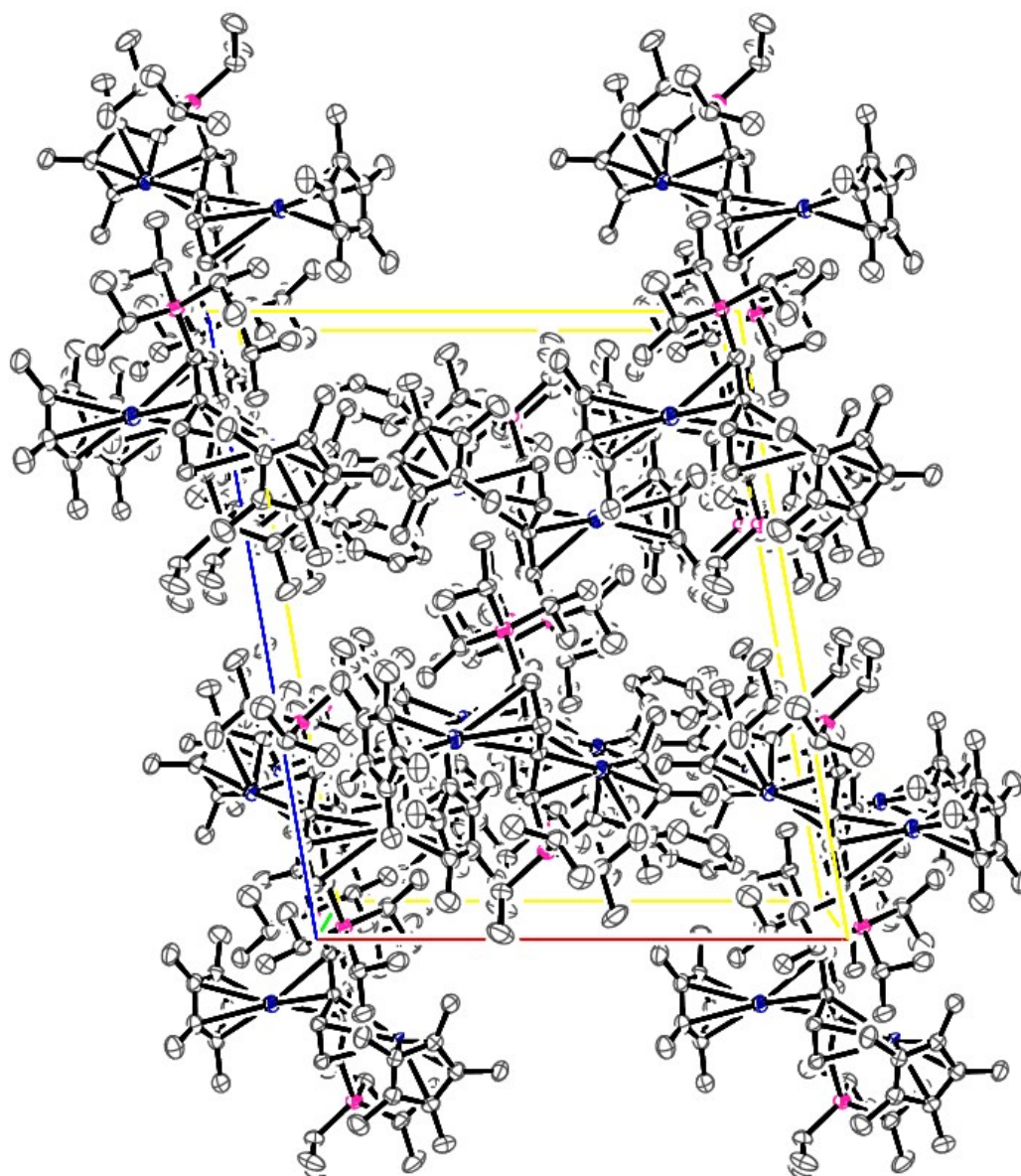


Figure S2. ORTEP view of the unit cell of 2.C₇H₈ (50% ellipsoids).

H atoms and ⁱPr groups removed for clarity.

Crystal data for **5**: $C_{52}H_{92}KSi_4Yb$, $M_r = 1041.78$, monoclinic, apparent space group $P2_1/n$, green plate, $a = 14.0303(10) \text{ \AA}$, $b = 35.391(3) \text{ \AA}$, $c = 23.0682(16) \text{ \AA}$, $\alpha = \gamma = 90^\circ$, $\beta = 93.8875(16)^\circ$, $V = 11428(12) \text{ \AA}^3$.

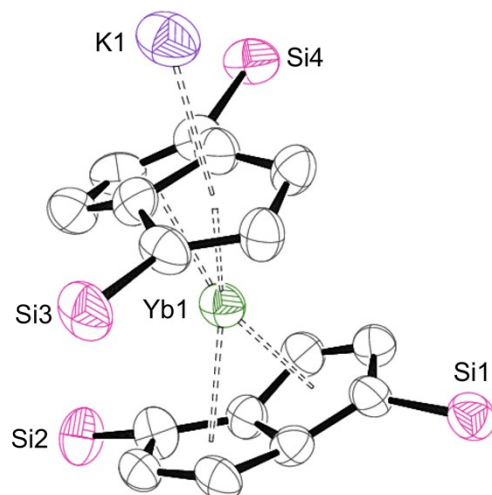


Figure S3. Partially refined ($R_1 = 0.1271$) model of **5**.
H atoms and ^iPr groups omitted for clarity.

2. Additional SQUID magnetometry data

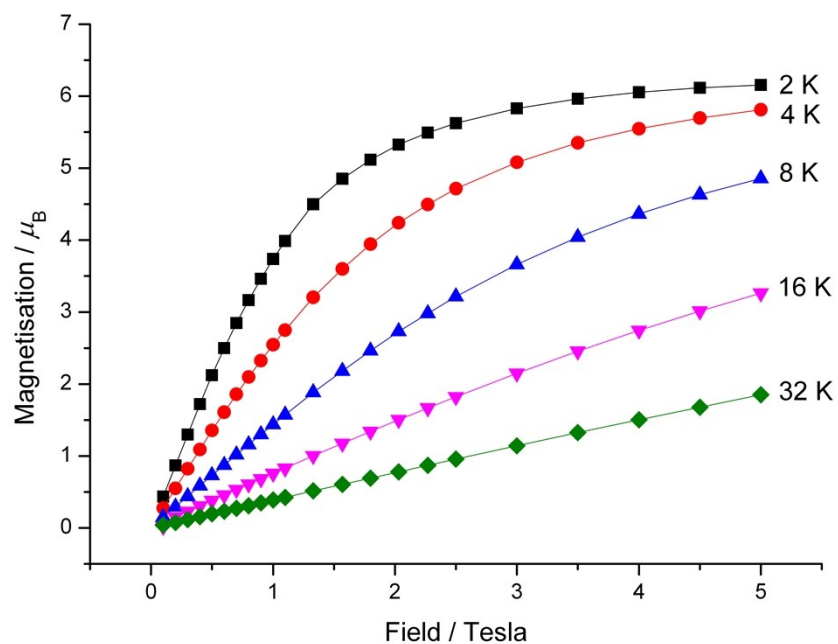


Figure S4. Field dependence of the solid state magnetisation for **2**.

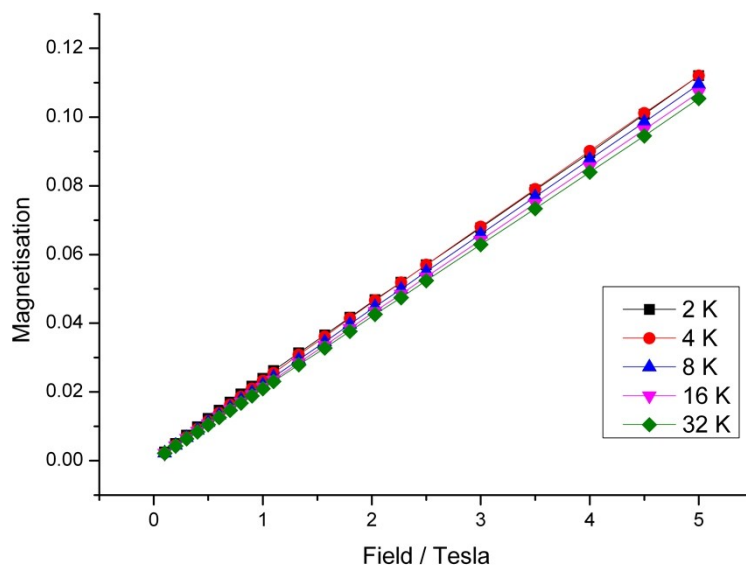


Figure S5. Field dependence of the solid state magnetisation for **3**.

3. Additional cyclic voltammetry data

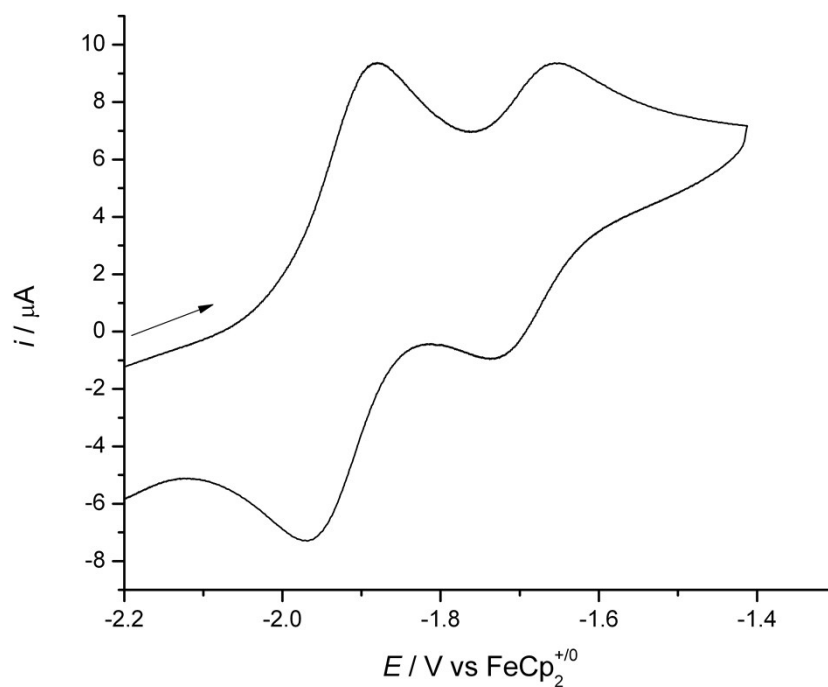


Figure S6. CV scan of **1** in MeCN / 0.1 M [$n\text{Bu}_4\text{N}$][PF₆], scan rate 100 mV s⁻¹.

Table S6. Peak potentials (E_p vs FeCp₂⁺⁰) and limiting currents (i_p) for process I of complex **3** in THF / 0.1 M [$n\text{Bu}_4\text{N}$][PF₆] at scan rate 50 mV s⁻¹

Scan Rate / mV s ⁻¹	E_{pa} / mV	E_{pc} / mV	ΔE_{pp} / mV	i_{pa} / μA	i_{pc} / μA	$ i_{pa}/i_{pc} $
20	-16185	-17295	111	0.5521	0.5341	1.03
50	-1593.5	-1708.5	115	1.1292	1.1389	0.99
100	-1581.5	-1702.5	121	1.8097	1.5024	1.20
200	-1579.5	-1712.5	133	2.5364	1.76	1.44
500	-1568.5	-1731.5	163	*	*	*

*Noise levels too high for accurate peak current determination