Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Data for:

Direct reaction of iodine-activated lanthanoid metals with 2,6-di*iso*propylphenol

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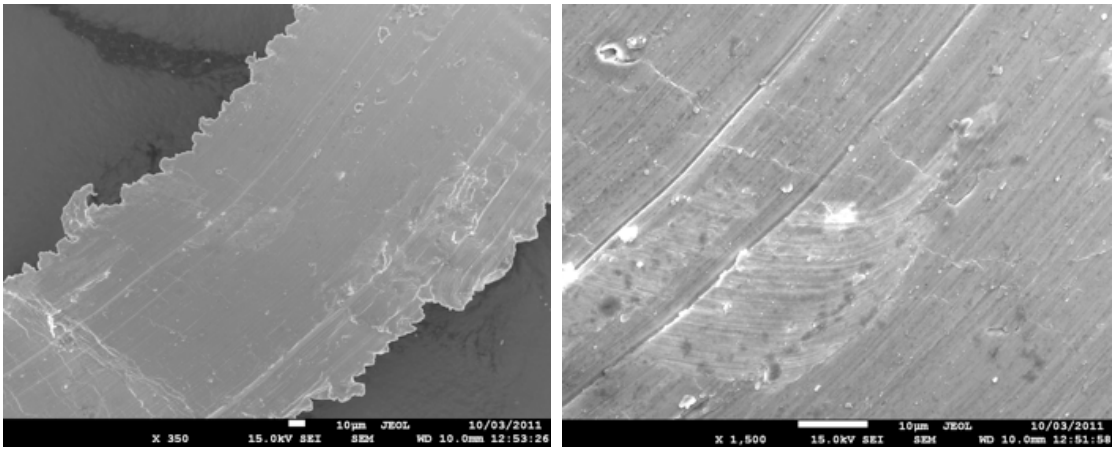
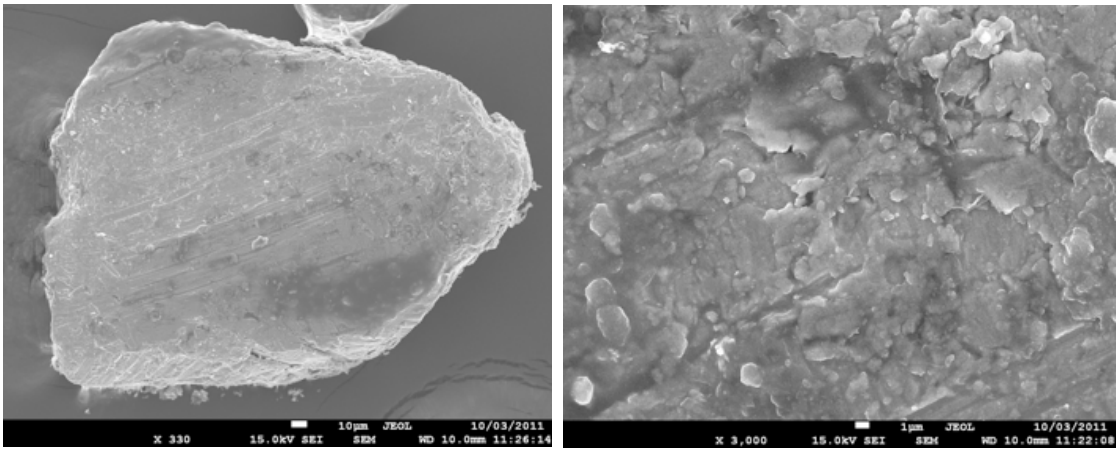
SEM Images:

Figure S1: Lanthanum after treatment with iodine: The surface of the metal lanthanum is smooth while cracks and gaps can be observed on the surface of the residual lanthanum with iodine. It is interesting that I_2 treatment affects the surface morphology in this way, after washing with a solvent in which LaI_3 is soluble.



SEM images of the surface of the metal lanthanum: Magnification x350 LHS, x1500 RHS



SEM images of the surface of the residual lanthanum with iodine: Magnification x350 LHS, x3000 RHS

X-ray Data for $[Nd(Odip)_3(thf)_3].C_7H_8$ (2b) and $[La(Odip)_3(thf)_3].thf$ (1)

Crystal data for **$[Nd(Odip)_3(thf)_3].C_7H_8$ (2b)**: $C_{55}H_{83}NdO_6$, M = 984.45, 0.15 × 0.10 × 0.05 mm^3, monoclinic, space group $P2_1/n$ (No. 14), a = 10.9370(4), b = 35.5722(15), c = 13.3069(6) Å, β = 95.671(2)°, V = 5151.8(4) $Å^3$, Z = 4, D_c = 1.269 g/cm^3, F_{000} = 2084, Bruker X8 Apex II CCD, MoKα radiation, λ = 0.71073 Å, T = 123(1)K, $2\theta_{max}$ = 53.2º, 31755 reflections collected, 10651 unique (R_{int} = 0.0753). Final *GooF* = 1.037, *R1* = 0.0542, *wR2* = 0.0819, *R* indices based on 7359 reflections with I > 2σ(I) (refinement on F^2), 572 parameters, 0 restraints. Lp and absorption corrections applied, μ = 1.054 mm^{-1}. *Variata*: Carbon atom 39 has slightly higher thermal motion than its neighbours. This may be expected for a carbon on a THF molecule.

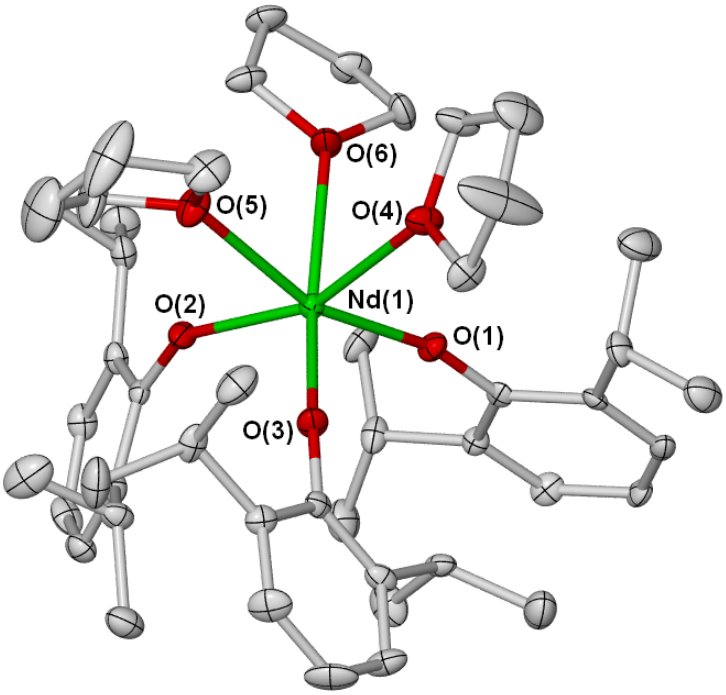


Figure S2. Molecular structure of $[Nd(Odip)_3(thf)_3].C_7H_8$ (**2b**) shown with 50% thermal ellipsoids.

Selected (i) Bond Lengths (Å) and (ii) Angles (°) for **[Nd(Odip)$_3$(thf)$_3$].C$_7$H$_8$ (2b)**

(i) Bond Lengths

Atoms	**Distance**	**Atoms**	**Distance**
Nd1-O1	2.205(3)	Nd1-O2	2.222(3)
Nd1-O3	2.185(3)	Nd1-O4	2.575(3)
Nd1-O5	2.558(3)	Nd1 O6	2.523(3)
O1-C1	1.343(5)	O2-C13	1.344(5)
O3-C25	1.337(5)		

(ii) Bond Angles

Atoms	**Angle**	**Atoms**	**Angle**
O1-Nd1-O2	104.61(11)	O1-Nd1-O3	101.45(11)
O1-Nd1-O4	91.90(10)	O1-Nd1-O5	162.01(11)
O1-Nd1-O6	85.81(10)	O2-Nd1-O3	103.60(11)
O2-Nd1-O4	159.17(10)	O2-Nd1-O5	82.41(10)
O2-Nd1-O6	90.08(10)	O3-Nd1-O4	85.04(10)
O3-Nd1-O5	92.73(11)	O3-Nd1-O6	162.13(10)
O4-Nd1-O5	78.23(10)	O4-Nd1-O6	78.36(10)
O5-Nd1-O6	77.54(10)	C1-O1-Nd1	165.0(3)
C13-O2-Nd1	147.1(3)	C25-O3-Nd1	168.3(3)

Crystal data for **[La(Odip)$_3$(thf)$_3$].thf (1)**: $C_{52}H_{83}LaO_7$, M = 959.09, 0.14 × 0.12 × 0.06 mm^3, monoclinic, space group $P2_1/n$ (No. 14), a = 11.4044(15), b = 35.747(5), c = 13.3608(18) Å, β = 97.540(5)°, V = 5399.8(12) Å^3, Z = 4, D_c = 1.180 g/cm^3, F_{000} = 2032, Bruker X8 Apex II CCD, MoKα radiation, λ = 0.71073 Å, T = 123(1)K, $2\theta_{max}$ = 55.0º, 32284 reflections collected, 12385 unique (R_{int} = 0.0755). Final *GooF* = 1.040, *R1* = 0.1117, *wR2* = 0.2402, *R* indices based on 6485 reflections reflections with $I > 2\sigma(I)$ (refinement on F^2), 388 parameters, 65 restraints. Lp and absorption corrections applied, μ = 0.835 mm^{-1}.

Variata: Carbon atoms 34 and 43 have higher thermal motion than their neighbours.

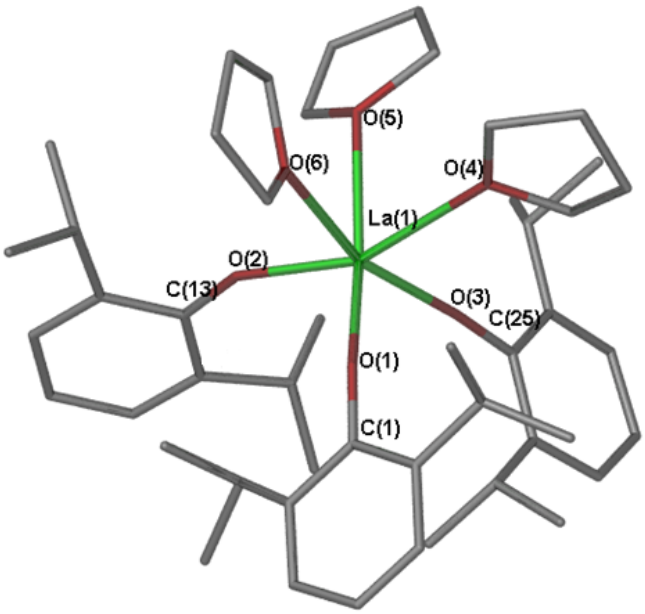


Figure S3. Molecular structure of [La(Odip)$_3$(thf)$_3$].thf (**1**)