Electronic Supplementary Information for Dalton Transactions

†Supplementary Material

Mono-Phosphacyclopentadienyl Bis(tetramethylaluminate) Lanthanide Complexes†

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Molecular drawing and bonding parameters for the 2nd isomer of complex **1b**:

X-ray Crystallography and Crystal Structure Determination. *Crystal data:* for **1b**: from hexane. $C_{16}H_{36}Al_2NdP$, M = 457.62, monoclinic, space group $P2_1/c$, a = 14.7933(18), b = 16.262(2), c = 18.559(2) Å, β = 103.493(2), V = 4341.4(9) Å^3, Z = 8, ρ_{calcd} = 1.400 g.cm^{-3}, F(000) = 1864, μ(Mo-K$_\alpha$) = 2.538 mm^{-1}, λ = 0.71073 Å, T = 103(2) K. The 31111 reflections measured on a Bruker SMART 2K CCD area detector yielded 11998 unique data (θ_{max} = 30.07°, R_{int} = 0.0443) [9945 observed reflections ($I > 2\sigma(I)$]. $R1$ = 0.0411, $wR2$ = 0.1164. CCDC reference number 647979.

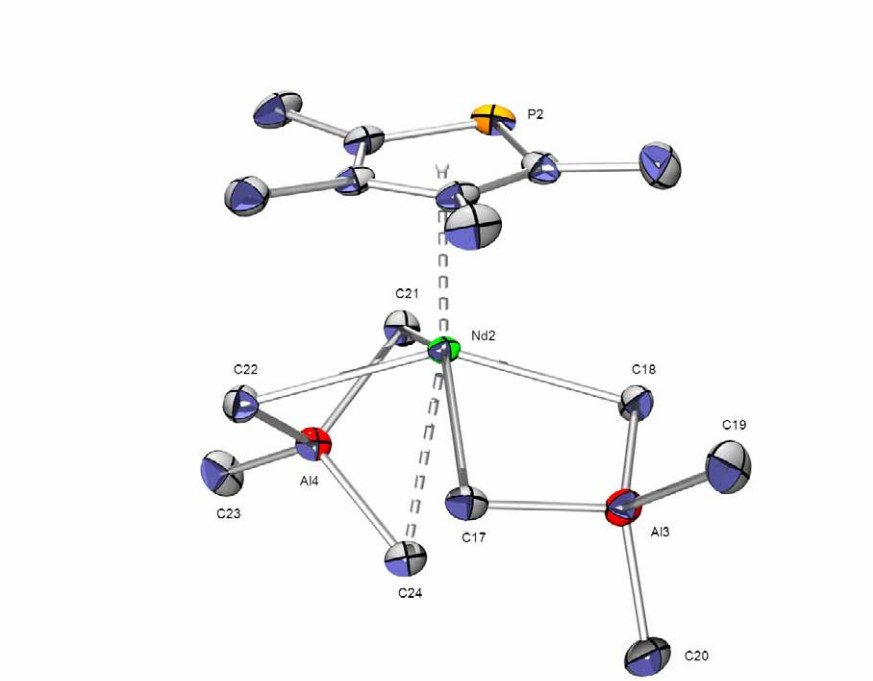

Figure S1 Molecular structure of [(η^5-PC_4Me_4)Nd((μ-Me)$_2$AlMe$_2$)$_2$)] (**1b**). Hydrogen atoms have been omitted. Selected bond lengths (Å) and angles (°) for the 2nd isomer: Nd2-P2, 2.9257(10); Nd2---Ct2, 2.500; Nd2-C18, 2.655(4); Nd2-C17, 2.645(4); Nd2-C22, 2.776(4); Nd2-C21, 2.723(4); Al3-C18(C17), 2.084(4) (2.079(4)); Al4-C22(C21), 2.057(4) (2.065((4)); Nd2---C24, 3.112(4); Nd2---Al3, 3.2034(11); Nd2---Al4, 2.9510(11); Ct2-Nd2-Al3, 111.45; Ct2-Nd2-Al4, 131.10; Nd2-C18-Al3, 84.16; Nd2-Ct2-P2, 90.05; Ct2-Nd2-C17, 107.55; Ct2-Nd2-C18, 107.55; Ct2-Nd2-C21, 108.25; Ct2-Nd2-C22, 103.92; Ct2-Nd2-C24, 169.14; C18-Nd2-C22, 148.52; C17-Nd2-C21, 143.47.

^{31}P VT NMR and ^{31}P MAS NMR spectra of complex **1a**:

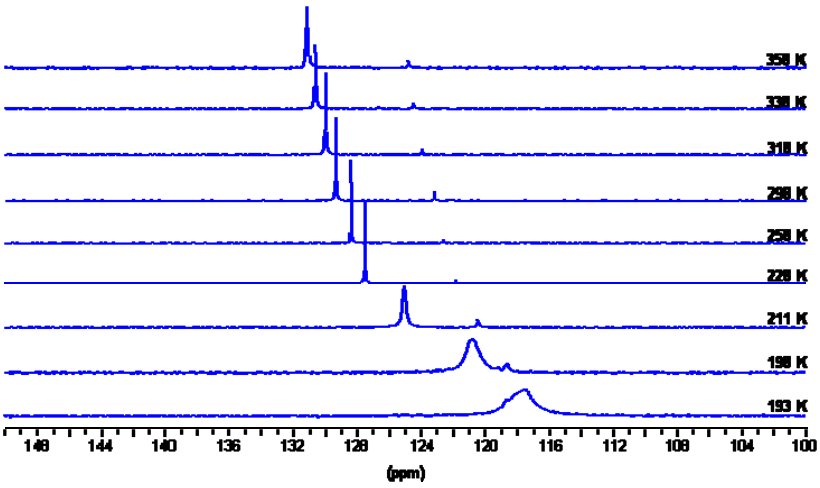

Figure S2 Variable temperature ^{31}P NMR spectra of **1a** in toluene-d_8.

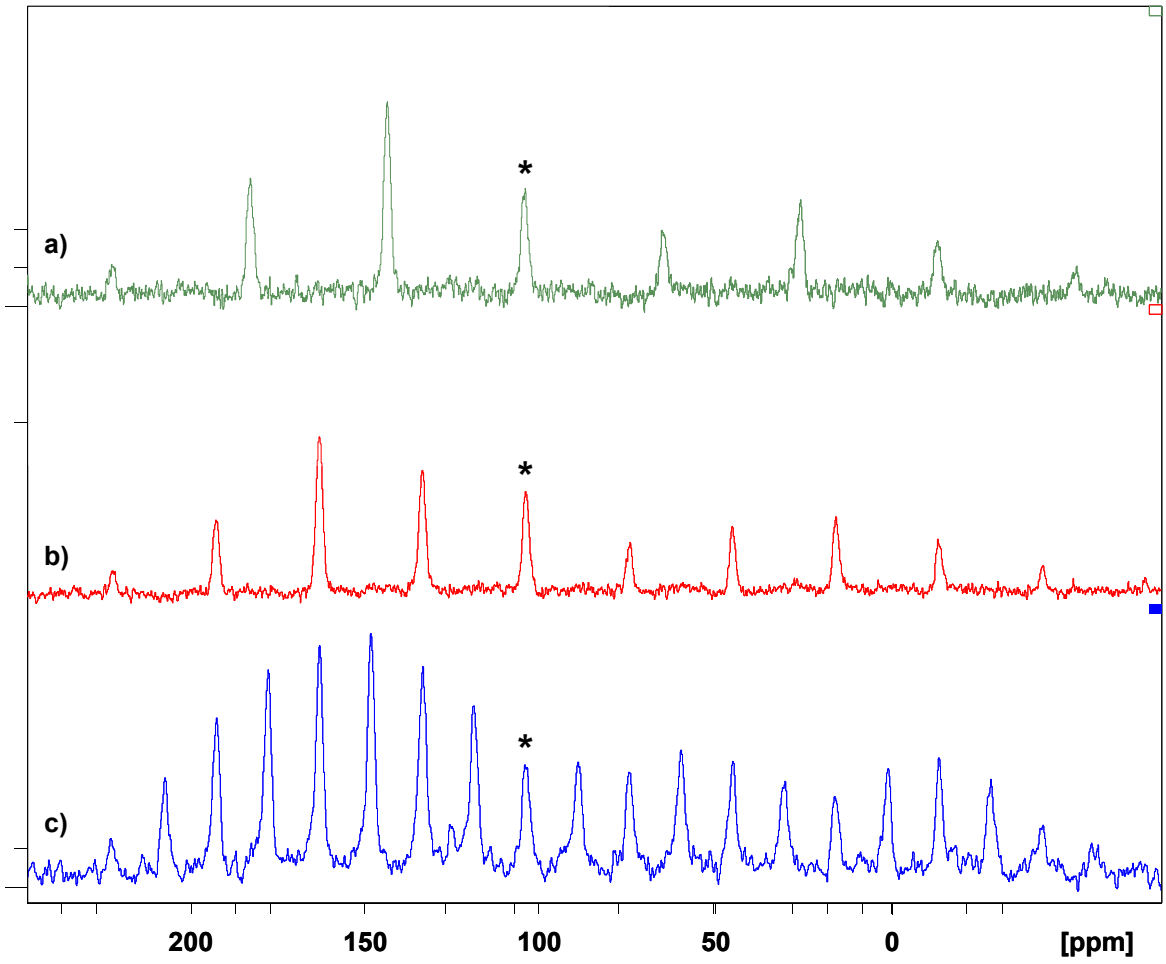

Figure S3 ^{31}P MAS NMR spectra of solid **1a** at 298 K (NS 16, D1 = 5 s, P1 = 4.5 μs, LB = 50 Hz), not optimized. a) 8 KHz. b) 6 KHz. c) 3 KHz. Asterisks indicate the signal and the unlabelled signals correspond to the spinning side bands.