

Full Paper submitted to Dalton Transactions

Supporting Information

Five different types of η^8 -cyclooctatetraenyl-lanthanide half-sandwich complexes from one ligand set, including a "giant neodymium wheel"

Farid M. Sroor^a, Cristian G. Hrib^b, Phil Liebing^b, Liane Hilfert^b, Sabine Busse^b,
and Frank T. Edelmann^{*b}

a *Organometallic and Organometalloid Chemistry Department, National Research Centre, 12622 Cairo, Egypt; E-Mail: faridsroor@gmx.de.*

b *Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany; E-Mail: frank.edelmann@ovgu.de*

E-mail: frank.edelmann@ovgu.de

Table of contents

Crystal Data Collection, Structure Solution and Refinement	S3
Table S1 (Crystal data and structure refinement of 2)	S4
Table S2 (Bond lengths [Å] and angles [°] of 2)	S5
Figures S1 and S2 (Molecular structure of 2 in the crystal)	S9
Table S3 (Crystal data and structure refinement of 3)	S10
Table S4 (Bond lengths [Å] and angles [°] of 3)	S11
Figures S3 and S4 (Molecular structure of 3 in the crystal)	S18
Table S5 (Crystal data and structure refinement of 7)	S19
Table S6 (Bond lengths [Å] and angles [°] of 7)	S20
Figures S5 and S6 (Molecular structure of 7 in the crystal)	S25
Table S7 (Crystal data and structure refinement of 8)	S26
Table S8 (Bond lengths [Å] and angles [°] of 8)	S27
Figures S7 and S8 (Molecular structure of 8 in the crystal)	S39
Figures S9 and S10 (¹ H and ¹³ C NMR spectrum of 9).....	S40
Figure S11 (HSQC spectrum of 9).....	S41
Table S9 (Crystal data and structure refinement of 10)	S42
Table S10 (Bond lengths [Å] and angles [°] of 10)	S43
Figures S12 and S13 (Molecular structure of 10 in the crystal)	S49
Figure S14 (HSQC spectrum of 10).....	S50
Table S11 (Crystal data and structure refinement of 11)	S51
Table S12 (Bond lengths [Å] and angles [°] of 11)	S52
Figures S15 and S16 (Molecular structure of 11 in the crystal)	S58
Table S13 (Crystal data and structure refinement of 12)	S59
Table S14 (Bond lengths [Å] and angles [°] of 12)	S60
Figures S17 and S18 (Molecular structure of 12 in the crystal)	S65
Figure S19 (HSQC spectrum of compound 12).....	S66
Figure S20 (EI Mass Spectrum of 13).....	S66
Table S15 (Crystal data and structure refinement of 14)	S67
Table S16 (Bond lengths [Å] and angles [°] of 14)	S68
Figures S21 and S22 (Molecular structure of 14 in the crystal)	S71
Figure S23 (EI Mass Spectrum EI of 14).....	S72
Table S17 (Crystal data and structure refinement of 15)	S73
Table S18 (Bond lengths [Å] and angles [°] of 15)	S74
Figures S24 and S25 (Molecular structure of 15 in the crystal)	S84
Figure S26 (HSQC spectrum of compound 15).....	S85
References.....	S86

Crystal Data Collection, Structure Solution and Refinement

The crystallographic data of compounds **2**, **3**, **7**, **8** and **14** were collected on a STOE IPDS 2T diffractometer at -140 to -120°C using graphite monochromated Mo-K_{α} radiation. Data collection, data reduction, space group determination and spherical absorption correction were performed with the STOE software X-AREA and X-RED32.¹

The intensity data of compounds **10**, **11**, **12** and **15** were registered on Xcalibur Atlas Nova diffractometer using mirror-focussed Cu-K_{α} radiation. Data collection, data reduction and space group determination were performed with the Agilent software CrysAlisPro.² Absorption corrections were applied using the multi-scan method.

The structures were solved by direct methods (SHELXS-97)³ and refined by full matrix least-squares methods on F^2 using SHELXL-97.⁴

Table S1. Crystal data and structure refinement (2).

Identification code	ip400	
Empirical formula	C ₄₈ H ₇₂ LiN ₄ OPr	
Formula weight	868.95	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 21.425(4) Å	α = 90°
	b = 20.113(4) Å	β = 90°
	c = 21.502(4) Å	γ = 90°
Volume	9266(3) Å ³	
Z	8	
Density (calculated)	1.246 Mg/m ³	
Absorption coefficient	1.089 mm ⁻¹	
F(000)	3664	
Crystal size	0.46 x 0.35 x 0.14 mm ³	
Theta range for data collection	2.15 to 26.37°	
Index ranges	-26 ≤ h ≤ 26, -25 ≤ k ≤ 21, -24 ≤ l ≤ 26	
Reflections collected	41749	
Independent reflections	9346 [R(int) = 0.0663]	
Completeness to theta = 26.37°	98.7 %	
Absorption correction	Sphere	
Max. and min. transmission	0.4912 and 0.4819	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9346 / 0 / 496	
Goodness-of-fit on F ²	1.014	
Final R indices [I > 2σ(I)]	R1 = 0.0355, wR2 = 0.0790	
R indices (all data)	R1 = 0.0515, wR2 = 0.0839	
Largest diff. peak and hole	0.887 and -1.490 e.Å ⁻³	

Table S2. Bond lengths [Å] and angles [°] (**2**).

Pr-N(2)	2.569(2)	C(10)-C(11)	1.525(5)
Pr-N(3)	2.595(2)	C(11)-C(12)	1.525(4)
Pr-N(4)	2.599(2)	C(13)-C(14)	1.515(4)
Pr-C(43)	2.697(3)	C(13)-C(18)	1.525(4)
Pr-C(44)	2.707(3)	C(14)-C(15)	1.522(4)
Pr-C(47)	2.715(3)	C(15)-C(16)	1.511(5)
Pr-C(42)	2.731(3)	C(16)-C(17)	1.523(4)
Pr-C(45)	2.734(3)	C(17)-C(18)	1.525(4)
Pr-C(48)	2.735(3)	C(21)-C(22)	1.463(4)
Pr-C(41)	2.742(3)	C(22)-C(23)	1.186(4)
Pr-C(46)	2.743(3)	C(23)-C(24)	1.443(4)
Pr-N(1)	2.771(2)	C(24)-C(25)	1.472(6)
Li-O	1.894(5)	C(24)-C(26)	1.502(6)
Li-N(4)	2.106(5)	C(25)-C(26)	1.427(6)
Li-N(2)	2.130(6)	C(27)-C(32)	1.521(4)
Li-N(1)	2.152(6)	C(27)-C(28)	1.532(3)
Li-C(1)	2.401(6)	C(28)-C(29)	1.523(4)
O-C(53)	1.400(4)	C(29)-C(30)	1.522(4)
O-C(52)	1.445(4)	C(30)-C(31)	1.518(4)
N(1)-C(1)	1.326(3)	C(31)-C(32)	1.518(4)
N(1)-C(7)	1.474(3)	C(33)-C(38)	1.516(4)
N(2)-C(1)	1.338(3)	C(33)-C(34)	1.518(4)
N(2)-C(13)	1.476(3)	C(34)-C(35)	1.526(4)
N(3)-C(21)	1.305(3)	C(35)-C(36)	1.518(5)
N(3)-C(27)	1.475(3)	C(36)-C(37)	1.511(5)
N(4)-C(21)	1.362(4)	C(37)-C(38)	1.522(4)
N(4)-C(33)	1.470(3)	C(41)-C(48)	1.400(5)
C(1)-C(2)	1.453(4)	C(41)-C(42)	1.404(4)
C(2)-C(3)	1.188(4)	C(42)-C(43)	1.405(4)
C(3)-C(4)	1.438(4)	C(43)-C(44)	1.404(4)
C(4)-C(6)	1.498(6)	C(44)-C(45)	1.405(5)
C(4)-C(5)	1.503(6)	C(45)-C(46)	1.403(5)
C(5)-C(6)	1.453(7)	C(46)-C(47)	1.403(5)
C(7)-C(12)	1.521(4)	C(47)-C(48)	1.410(5)
C(7)-C(8)	1.533(4)	C(51)-C(52)	1.486(5)
C(8)-C(9)	1.524(4)	C(53)-C(54)	1.487(5)
C(9)-C(10)	1.521(5)		

N(2)-Pr-N(3)	88.49(7)	N(4)-Pr-C(41)	113.13(8)
N(2)-Pr-N(4)	83.43(7)	C(43)-Pr-C(41)	57.04(9)
N(3)-Pr-N(4)	52.39(7)	C(44)-Pr-C(41)	77.04(9)
N(2)-Pr-C(43)	99.04(8)	C(47)-Pr-C(41)	56.60(10)
N(3)-Pr-C(43)	96.13(9)	C(42)-Pr-C(41)	29.72(9)
N(4)-Pr-C(43)	148.48(9)	C(45)-Pr-C(41)	84.04(9)
N(2)-Pr-C(44)	84.16(8)	C(48)-Pr-C(41)	29.62(10)
N(3)-Pr-C(44)	121.85(9)	N(2)-Pr-C(46)	107.03(8)
N(4)-Pr-C(44)	166.44(8)	N(3)-Pr-C(46)	163.69(8)
C(43)-Pr-C(44)	30.12(9)	N(4)-Pr-C(46)	132.78(9)
N(2)-Pr-C(47)	134.57(9)	C(43)-Pr-C(46)	76.84(10)
N(3)-Pr-C(47)	136.31(9)	C(44)-Pr-C(46)	56.81(10)
N(4)-Pr-C(47)	115.28(9)	C(47)-Pr-C(46)	29.79(10)
C(43)-Pr-C(47)	85.36(9)	C(42)-Pr-C(46)	83.72(9)
C(44)-Pr-C(47)	77.56(10)	C(45)-Pr-C(46)	29.68(10)
N(2)-Pr-C(42)	125.47(8)	C(48)-Pr-C(46)	56.66(10)
N(3)-Pr-C(42)	83.10(8)	C(41)-Pr-C(46)	75.97(9)
N(4)-Pr-C(42)	127.98(8)	N(2)-Pr-N(1)	49.79(7)
C(43)-Pr-C(42)	29.99(8)	N(3)-Pr-N(1)	116.65(7)
C(44)-Pr-C(42)	56.99(9)	N(4)-Pr-N(1)	74.53(7)
C(47)-Pr-C(42)	76.79(9)	C(43)-Pr-N(1)	130.40(8)
N(2)-Pr-C(45)	87.71(8)	C(44)-Pr-N(1)	101.33(8)
N(3)-Pr-C(45)	151.78(9)	C(47)-Pr-N(1)	93.57(9)
N(4)-Pr-C(45)	154.14(9)	C(42)-Pr-N(1)	157.48(8)
C(43)-Pr-C(45)	57.00(10)	C(45)-Pr-N(1)	81.19(8)
C(44)-Pr-C(45)	29.93(10)	C(48)-Pr-N(1)	120.82(9)
C(47)-Pr-C(45)	56.94(10)	C(41)-Pr-N(1)	150.00(8)
C(42)-Pr-C(45)	76.49(9)	C(46)-Pr-N(1)	78.30(8)
N(2)-Pr-C(48)	163.66(9)	O-Li-N(4)	125.5(3)
N(3)-Pr-C(48)	107.70(9)	O-Li-N(2)	114.9(2)
N(4)-Pr-C(48)	107.97(8)	N(4)-Li-N(2)	108.5(2)
C(43)-Pr-C(48)	77.51(9)	O-Li-N(1)	128.1(3)
C(44)-Pr-C(48)	85.31(9)	N(4)-Li-N(1)	99.7(2)
C(47)-Pr-C(48)	29.99(10)	N(2)-Li-N(1)	63.56(16)
C(42)-Pr-C(48)	56.70(10)	O-Li-C(1)	116.8(2)
C(45)-Pr-C(48)	76.98(10)	N(4)-Li-C(1)	117.6(2)
N(2)-Pr-C(41)	155.18(8)	N(2)-Li-C(1)	33.68(11)
N(3)-Pr-C(41)	87.84(8)	N(1)-Li-C(1)	33.30(11)

O-Li-Pr	164.8(3)	C(3)-C(2)-C(1)	175.4(3)
N(4)-Li-Pr	56.43(13)	C(2)-C(3)-C(4)	178.2(4)
N(2)-Li-Pr	55.52(12)	C(3)-C(4)-C(6)	118.1(3)
N(1)-Li-Pr	60.91(13)	C(3)-C(4)-C(5)	118.9(4)
C(1)-Li-Pr	62.90(13)	C(6)-C(4)-C(5)	57.9(3)
C(53)-O-C(52)	112.7(3)	C(6)-C(5)-C(4)	60.9(3)
C(53)-O-Li	124.1(3)	C(5)-C(6)-C(4)	61.2(3)
C(52)-O-Li	123.2(3)	N(1)-C(7)-C(12)	110.9(2)
C(1)-N(1)-C(7)	117.5(2)	N(1)-C(7)-C(8)	111.3(2)
C(1)-N(1)-Li	83.7(2)	C(12)-C(7)-C(8)	109.0(2)
C(7)-N(1)-Li	141.8(2)	C(9)-C(8)-C(7)	112.0(3)
C(1)-N(1)-Pr	82.83(15)	C(10)-C(9)-C(8)	111.4(3)
C(7)-N(1)-Pr	134.18(17)	C(9)-C(10)-C(11)	110.3(3)
Li-N(1)-Pr	76.35(14)	C(12)-C(11)-C(10)	111.2(3)
C(1)-N(2)-C(13)	118.4(2)	C(7)-C(12)-C(11)	111.5(3)
C(1)-N(2)-Li	84.3(2)	N(2)-C(13)-C(14)	109.0(2)
C(13)-N(2)-Li	137.7(2)	N(2)-C(13)-C(18)	111.9(2)
C(1)-N(2)-Pr	91.07(15)	C(14)-C(13)-C(18)	109.9(2)
C(13)-N(2)-Pr	129.01(16)	C(13)-C(14)-C(15)	112.5(2)
Li-N(2)-Pr	81.37(14)	C(16)-C(15)-C(14)	111.0(3)
C(21)-N(3)-C(27)	117.5(2)	C(15)-C(16)-C(17)	111.0(3)
C(21)-N(3)-Pr	92.92(16)	C(16)-C(17)-C(18)	111.2(2)
C(27)-N(3)-Pr	144.43(17)	C(13)-C(18)-C(17)	111.1(3)
C(21)-N(4)-C(33)	116.9(2)	N(3)-C(21)-N(4)	118.5(2)
C(21)-N(4)-Li	120.8(2)	N(3)-C(21)-C(22)	122.2(2)
C(33)-N(4)-Li	110.4(2)	N(4)-C(21)-C(22)	119.3(2)
C(21)-N(4)-Pr	91.41(16)	N(3)-C(21)-Pr	60.99(14)
C(33)-N(4)-Pr	132.57(18)	N(4)-C(21)-Pr	61.23(14)
Li-N(4)-Pr	81.10(15)	C(22)-C(21)-Pr	160.92(18)
N(1)-C(1)-N(2)	115.7(2)	C(23)-C(22)-C(21)	177.3(3)
N(1)-C(1)-C(2)	122.1(3)	C(22)-C(23)-C(24)	175.7(4)
N(2)-C(1)-C(2)	122.2(2)	C(23)-C(24)-C(25)	118.9(4)
N(1)-C(1)-Li	62.98(19)	C(23)-C(24)-C(26)	118.2(3)
N(2)-C(1)-Li	61.98(19)	C(25)-C(24)-C(26)	57.3(3)
C(2)-C(1)-Li	152.3(2)	C(26)-C(25)-C(24)	62.4(3)
N(1)-C(1)-Pr	70.37(14)	C(25)-C(26)-C(24)	60.3(3)
N(2)-C(1)-Pr	61.65(13)	N(3)-C(27)-C(32)	110.4(2)
C(2)-C(1)-Pr	137.50(19)	N(3)-C(27)-C(28)	111.7(2)
Li-C(1)-Pr	70.02(13)	C(32)-C(27)-C(28)	110.3(2)

C(29)-C(28)-C(27)	111.5(2)
C(30)-C(29)-C(28)	110.4(2)
C(31)-C(30)-C(29)	110.3(3)
C(30)-C(31)-C(32)	111.1(3)
C(31)-C(32)-C(27)	112.1(2)
N(4)-C(33)-C(38)	110.5(2)
N(4)-C(33)-C(34)	112.2(2)
C(38)-C(33)-C(34)	111.3(2)
C(33)-C(34)-C(35)	110.4(2)
C(36)-C(35)-C(34)	112.1(3)
C(37)-C(36)-C(35)	111.1(3)
C(36)-C(37)-C(38)	111.4(3)
C(33)-C(38)-C(37)	111.3(3)
C(48)-C(41)-C(42)	135.5(3)
C(48)-C(41)-Pr	74.88(17)
C(42)-C(41)-Pr	74.67(16)
C(41)-C(42)-C(43)	135.3(3)
C(41)-C(42)-Pr	75.61(17)
C(43)-C(42)-Pr	73.67(17)
C(44)-C(43)-C(42)	134.9(3)
C(44)-C(43)-Pr	75.34(17)
C(42)-C(43)-Pr	76.34(17)
C(43)-C(44)-C(45)	134.6(3)
C(43)-C(44)-Pr	74.54(17)
C(45)-C(44)-Pr	76.11(18)
C(46)-C(45)-C(44)	134.8(3)
C(46)-C(45)-Pr	75.52(18)
C(44)-C(45)-Pr	73.96(18)
C(45)-C(46)-C(47)	135.6(3)
C(45)-C(46)-Pr	74.80(18)
C(47)-C(46)-Pr	73.98(18)
C(46)-C(47)-C(48)	135.0(3)
C(46)-C(47)-Pr	76.23(17)
C(48)-C(47)-Pr	75.79(17)
C(41)-C(48)-C(47)	134.0(3)
C(41)-C(48)-Pr	75.50(16)
C(47)-C(48)-Pr	74.22(16)
O-C(52)-C(51)	112.7(3)
O-C(53)-C(54)	110.5(3)

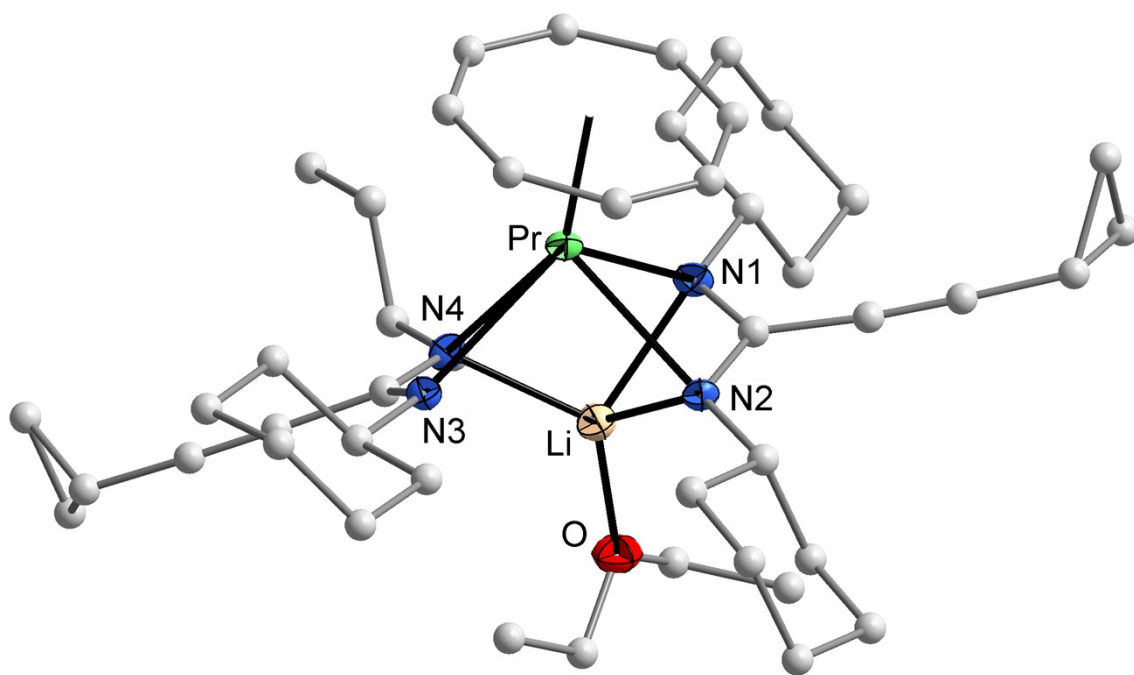


Figure S1. Molecular structure of complex (COT)Pr[μ -*c*-C₃H₅-C $\equiv$ C-C(NCy)₂]₂Li(Et₂O) (**2**) in the crystal. Ellipsoids of the heavier atoms and Li with 50% probability, H atoms omitted for clarity.

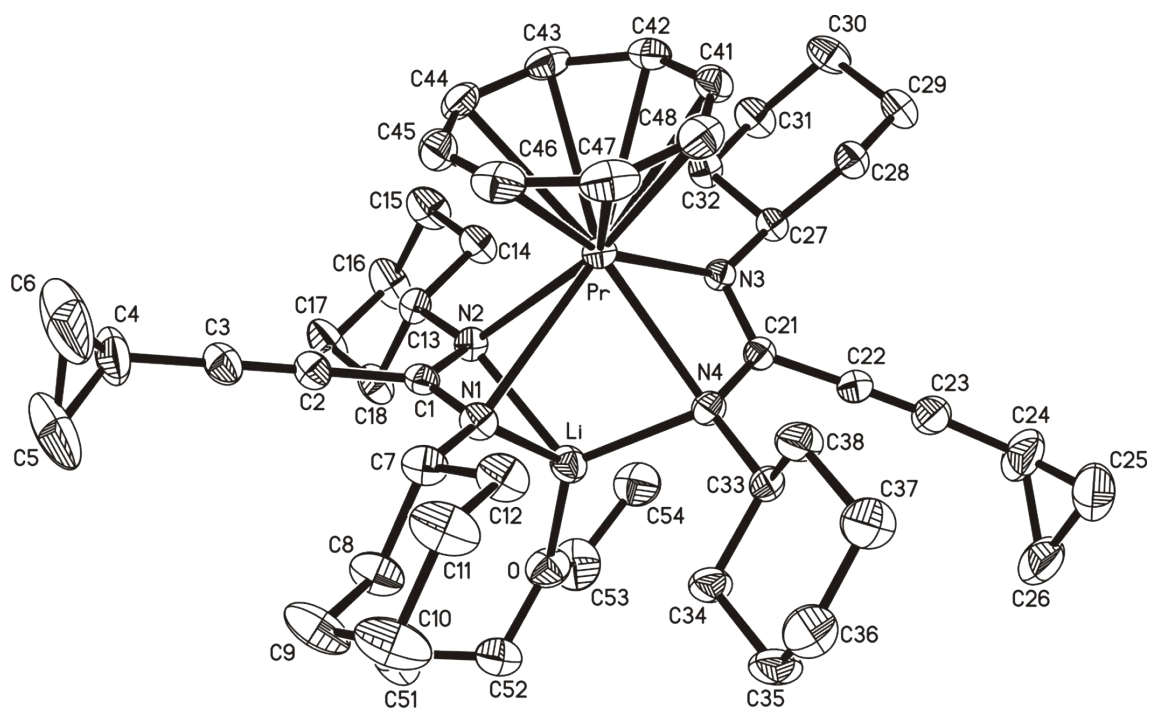


Figure S2. ORTEP drawing of (COT)Pr[μ -*c*-C₃H₅-C $\equiv$ C-C(NCy)₂]₂Li(Et₂O)(**2**).

Table S3. Crystal data and structure refinement (3).

Identification code	ip359	
Empirical formula	C ₃₆ H ₅₄ LiN ₄ NdO	
Formula weight	710.01	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 17.592(3) Å	α = 90°
	b = 20.156(4) Å	β = 90°
	c = 20.206(4) Å	γ = 90°
Volume	7165(2) Å ³	
Z	8	
Density (calculated)	1.316 Mg/m ³	
Absorption coefficient	1.481 mm ⁻¹	
F(000)	2952	
Crystal size	0.36 x 0.31 x 0.16 mm ³	
Theta range for data collection	2.25 to 26.37°	
Index ranges	-21 ≤ h ≤ 21, -25 ≤ k ≤ 23, -23 ≤ l ≤ 25	
Reflections collected	40920	
Independent reflections	14633 [R(int) = 0.0849]	
Completeness to theta = 26.37°	99.9 %	
Absorption correction	Sphere	
Max. and min. transmission	0.4912 and 0.4819	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	14633 / 0 / 775	
Goodness-of-fit on F ²	0.917	
Final R indices [I > 2σ(I)]	R1 = 0.0442, wR2 = 0.0771	
R indices (all data)	R1 = 0.0641, wR2 = 0.0815	
Absolute structure parameter	0.490(14)	
Largest diff. peak and hole	0.843 and -1.068 e.Å ⁻³	

Table S4. Bond lengths [Å] and angles [°] (**3**).

Nd(1)-N(3)	2.549(5)	C(50)-C(51)	1.517(8)
Nd(1)-N(2)	2.555(5)	C(50)-C(52)	1.526(9)
Nd(1)-N(1)	2.603(4)	C(53)-C(54)	1.401(11)
Nd(1)-C(14)	2.684(7)	C(53)-C(60)	1.413(12)
Nd(1)-C(18)	2.701(6)	C(54)-C(55)	1.412(11)
Nd(1)-C(19)	2.702(6)	C(55)-C(56)	1.348(13)
Nd(1)-C(17)	2.709(7)	C(56)-C(57)	1.421(12)
Nd(1)-C(15)	2.709(7)	C(57)-C(58)	1.407(10)
Nd(1)-C(20)	2.720(7)	C(58)-C(59)	1.401(10)
Nd(1)-C(16)	2.724(7)	C(59)-C(60)	1.383(11)
Nd(1)-C(13)	2.724(7)	C(61)-N(8)	1.294(8)
Nd(1)-N(4)	2.771(5)	C(61)-N(7)	1.348(7)
Nd(2)-N(8)	2.557(5)	C(61)-C(62)	1.465(9)
Nd(2)-N(6)	2.570(4)	C(62)-C(63)	1.190(9)
Nd(2)-N(7)	2.622(5)	C(63)-C(64)	1.449(9)
Nd(2)-C(53)	2.686(7)	C(64)-C(65)	1.488(8)
Nd(2)-C(54)	2.687(7)	C(64)-C(66)	1.516(9)
Nd(2)-C(57)	2.690(6)	C(65)-C(66)	1.467(11)
Nd(2)-C(60)	2.697(7)	C(67)-N(7)	1.479(8)
Nd(2)-C(59)	2.707(7)	C(67)-C(69)	1.516(10)
Nd(2)-C(55)	2.710(8)	C(67)-C(68)	1.542(10)
Nd(2)-C(58)	2.715(6)	C(70)-N(8)	1.493(7)
Nd(2)-C(56)	2.721(6)	C(70)-C(72)	1.519(8)
Nd(2)-N(5)	2.745(5)	C(70)-C(71)	1.526(9)
C(41)-N(5)	1.326(7)	C(73)-O(2)	1.419(9)
C(41)-N(6)	1.333(6)	C(73)-C(74)	1.516(11)
C(41)-C(42)	1.457(9)	C(74)-C(75)	1.407(15)
C(41)-Li(2)	2.368(13)	C(75)-C(76)	1.451(13)
C(42)-C(43)	1.192(9)	C(76)-O(2)	1.433(8)
C(43)-C(44)	1.425(9)	N(1)-C(1)	1.319(8)
C(44)-C(46)	1.509(9)	N(1)-C(7)	1.487(6)
C(44)-C(45)	1.510(8)	N(1)-Li(1)	2.048(13)
C(45)-C(46)	1.472(10)	N(2)-C(1)	1.331(7)
C(47)-N(6)	1.486(7)	N(2)-C(10)	1.466(8)
C(47)-C(48)	1.522(11)	N(3)-C(21)	1.315(8)
C(47)-C(49)	1.529(9)	N(3)-C(27)	1.470(7)
C(50)-N(5)	1.486(7)	N(3)-Li(1)	2.175(12)

N(4)-C(21)	1.335(8)	C(17)-C(18)	1.421(11)
N(4)-C(30)	1.475(8)	C(18)-C(19)	1.363(13)
N(4)-Li(1)	2.152(14)	C(19)-C(20)	1.395(12)
N(5)-Li(2)	2.081(12)	C(21)-C(22)	1.455(9)
N(6)-Li(2)	2.154(12)	C(21)-Li(1)	2.409(14)
N(7)-Li(2)	2.071(12)	C(22)-C(23)	1.189(9)
C(1)-C(2)	1.468(9)	C(23)-C(24)	1.451(10)
C(2)-C(3)	1.181(9)	C(24)-C(25)	1.490(9)
C(3)-C(4)	1.438(10)	C(24)-C(26)	1.494(10)
C(4)-C(5)	1.475(13)	C(25)-C(26)	1.483(11)
C(4)-C(6)	1.475(9)	C(27)-C(28)	1.503(10)
C(5)-C(6)	1.407(17)	C(27)-C(29)	1.526(9)
C(7)-C(8)	1.507(10)	C(30)-C(31)	1.522(10)
C(7)-C(9)	1.515(9)	C(30)-C(32)	1.530(11)
C(10)-C(12)	1.524(8)	C(33)-O(1)	1.417(9)
C(10)-C(11)	1.528(9)	C(33)-C(34)	1.516(13)
C(13)-C(14)	1.393(11)	C(34)-C(35)	1.469(13)
C(13)-C(20)	1.426(11)	C(35)-C(36)	1.506(12)
C(14)-C(15)	1.373(12)	C(36)-O(1)	1.444(8)
C(15)-C(16)	1.422(12)	O(1)-Li(1)	1.875(13)
C(16)-C(17)	1.385(10)	O(2)-Li(2)	1.884(12)
N(3)-Nd(1)-N(2)	82.71(18)	N(1)-Nd(1)-C(17)	116.5(2)
N(3)-Nd(1)-N(1)	84.62(17)	C(14)-Nd(1)-C(17)	76.8(3)
N(2)-Nd(1)-N(1)	52.32(14)	C(18)-Nd(1)-C(17)	30.5(2)
N(3)-Nd(1)-C(14)	132.5(2)	C(19)-Nd(1)-C(17)	56.9(3)
N(2)-Nd(1)-C(14)	142.2(2)	N(3)-Nd(1)-C(15)	161.2(2)
N(1)-Nd(1)-C(14)	109.8(2)	N(2)-Nd(1)-C(15)	113.5(2)
N(3)-Nd(1)-C(18)	112.0(2)	N(1)-Nd(1)-C(15)	97.8(2)
N(2)-Nd(1)-C(18)	94.2(2)	C(14)-Nd(1)-C(15)	29.5(3)
N(1)-Nd(1)-C(18)	141.7(2)	C(18)-Nd(1)-C(15)	77.4(2)
C(14)-Nd(1)-C(18)	84.8(2)	C(19)-Nd(1)-C(15)	85.0(2)
N(3)-Nd(1)-C(19)	96.0(2)	C(17)-Nd(1)-C(15)	56.9(2)
N(2)-Nd(1)-C(19)	117.4(2)	N(3)-Nd(1)-C(20)	94.4(3)
N(1)-Nd(1)-C(19)	169.6(2)	N(2)-Nd(1)-C(20)	146.9(2)
C(14)-Nd(1)-C(19)	77.5(3)	N(1)-Nd(1)-C(20)	160.6(2)
C(18)-Nd(1)-C(19)	29.2(3)	C(14)-Nd(1)-C(20)	57.5(3)
N(3)-Nd(1)-C(17)	137.99(19)	C(18)-Nd(1)-C(20)	56.2(3)
N(2)-Nd(1)-C(17)	83.5(2)	C(19)-Nd(1)-C(20)	29.8(3)

C(17)-Nd(1)-C(20)	76.8(3)	N(6)-Nd(2)-C(54)	89.6(2)
C(15)-Nd(1)-C(20)	77.2(3)	N(7)-Nd(2)-C(54)	173.9(2)
N(3)-Nd(1)-C(16)	167.2(2)	C(53)-Nd(2)-C(54)	30.2(2)
N(2)-Nd(1)-C(16)	91.0(2)	N(8)-Nd(2)-C(57)	130.0(2)
N(1)-Nd(1)-C(16)	100.3(2)	N(6)-Nd(2)-C(57)	143.96(19)
C(14)-Nd(1)-C(16)	57.0(3)	N(7)-Nd(2)-C(57)	106.2(2)
C(18)-Nd(1)-C(16)	57.2(2)	C(53)-Nd(2)-C(57)	85.5(2)
C(19)-Nd(1)-C(16)	77.0(2)	C(54)-Nd(2)-C(57)	77.9(3)
C(17)-Nd(1)-C(16)	29.5(2)	N(8)-Nd(2)-C(60)	85.45(19)
C(15)-Nd(1)-C(16)	30.3(3)	N(6)-Nd(2)-C(60)	124.4(2)
C(20)-Nd(1)-C(16)	84.9(3)	N(7)-Nd(2)-C(60)	127.4(2)
N(3)-Nd(1)-C(13)	108.7(2)	C(53)-Nd(2)-C(60)	30.4(3)
N(2)-Nd(1)-C(13)	167.3(2)	C(54)-Nd(2)-C(60)	57.5(3)
N(1)-Nd(1)-C(13)	132.4(2)	C(57)-Nd(2)-C(60)	76.5(2)
C(14)-Nd(1)-C(13)	29.8(2)	N(8)-Nd(2)-C(59)	85.76(19)
C(18)-Nd(1)-C(13)	76.5(3)	N(6)-Nd(2)-C(59)	153.1(2)
C(19)-Nd(1)-C(13)	57.2(3)	N(7)-Nd(2)-C(59)	108.2(2)
C(17)-Nd(1)-C(13)	84.3(3)	C(53)-Nd(2)-C(59)	57.5(3)
C(15)-Nd(1)-C(13)	56.4(3)	C(54)-Nd(2)-C(59)	77.8(3)
C(20)-Nd(1)-C(13)	30.4(2)	C(57)-Nd(2)-C(59)	56.6(2)
C(16)-Nd(1)-C(13)	76.8(3)	C(60)-Nd(2)-C(59)	29.7(2)
N(3)-Nd(1)-N(4)	49.78(16)	N(8)-Nd(2)-C(55)	158.8(2)
N(2)-Nd(1)-N(4)	112.77(17)	N(6)-Nd(2)-C(55)	96.8(2)
N(1)-Nd(1)-N(4)	75.56(16)	N(7)-Nd(2)-C(55)	149.3(2)
C(14)-Nd(1)-N(4)	89.1(2)	C(53)-Nd(2)-C(55)	57.2(3)
C(18)-Nd(1)-N(4)	141.7(2)	C(54)-Nd(2)-C(55)	30.3(3)
C(19)-Nd(1)-N(4)	112.7(2)	C(57)-Nd(2)-C(55)	56.6(3)
C(17)-Nd(1)-N(4)	163.8(2)	C(60)-Nd(2)-C(55)	76.7(2)
C(15)-Nd(1)-N(4)	112.7(2)	C(59)-Nd(2)-C(55)	84.2(2)
C(20)-Nd(1)-N(4)	88.9(2)	N(8)-Nd(2)-C(58)	102.2(2)
C(16)-Nd(1)-N(4)	142.8(2)	N(6)-Nd(2)-C(58)	173.87(19)
C(13)-Nd(1)-N(4)	79.5(2)	N(7)-Nd(2)-C(58)	99.0(2)
N(8)-Nd(2)-N(6)	83.92(15)	C(53)-Nd(2)-C(58)	78.7(3)
N(8)-Nd(2)-N(7)	51.84(15)	C(54)-Nd(2)-C(58)	86.8(3)
N(6)-Nd(2)-N(7)	84.50(19)	C(57)-Nd(2)-C(58)	30.2(2)
N(8)-Nd(2)-C(53)	101.7(2)	C(60)-Nd(2)-C(58)	57.1(2)
N(6)-Nd(2)-C(53)	100.5(2)	C(59)-Nd(2)-C(58)	29.9(2)
N(7)-Nd(2)-C(53)	152.8(2)	C(55)-Nd(2)-C(58)	77.6(3)
N(8)-Nd(2)-C(54)	128.9(2)	N(8)-Nd(2)-C(56)	159.9(2)

N(6)-Nd(2)-C(56)	116.1(2)	C(48)-C(47)-C(49)	111.0(6)
N(7)-Nd(2)-C(56)	125.3(2)	N(5)-C(50)-C(51)	110.0(5)
C(53)-Nd(2)-C(56)	76.7(3)	N(5)-C(50)-C(52)	109.9(5)
C(54)-Nd(2)-C(56)	56.6(3)	C(51)-C(50)-C(52)	110.5(5)
C(57)-Nd(2)-C(56)	30.4(3)	C(54)-C(53)-C(60)	133.9(7)
C(60)-Nd(2)-C(56)	83.7(2)	C(54)-C(53)-Nd(2)	74.9(4)
C(59)-Nd(2)-C(56)	76.5(2)	C(60)-C(53)-Nd(2)	75.2(4)
C(55)-Nd(2)-C(56)	28.7(3)	C(53)-C(54)-C(55)	133.5(8)
C(58)-Nd(2)-C(56)	57.8(3)	C(53)-C(54)-Nd(2)	74.8(4)
N(8)-Nd(2)-N(5)	112.78(15)	C(55)-C(54)-Nd(2)	75.7(4)
N(6)-Nd(2)-N(5)	49.82(14)	C(56)-C(55)-C(54)	136.4(8)
N(7)-Nd(2)-N(5)	74.80(16)	C(56)-C(55)-Nd(2)	76.1(5)
C(53)-Nd(2)-N(5)	128.6(2)	C(54)-C(55)-Nd(2)	73.9(4)
C(54)-Nd(2)-N(5)	100.4(2)	C(55)-C(56)-C(57)	135.3(7)
C(57)-Nd(2)-N(5)	98.94(18)	C(55)-C(56)-Nd(2)	75.2(4)
C(60)-Nd(2)-N(5)	157.8(2)	C(57)-C(56)-Nd(2)	73.6(4)
C(59)-Nd(2)-N(5)	155.45(17)	C(58)-C(57)-C(56)	136.4(7)
C(55)-Nd(2)-N(5)	82.7(2)	C(58)-C(57)-Nd(2)	75.9(3)
C(58)-Nd(2)-N(5)	126.15(17)	C(56)-C(57)-Nd(2)	76.0(4)
C(56)-Nd(2)-N(5)	82.10(19)	C(59)-C(58)-C(57)	131.3(8)
N(5)-C(41)-N(6)	115.1(5)	C(59)-C(58)-Nd(2)	74.7(4)
N(5)-C(41)-C(42)	122.5(5)	C(57)-C(58)-Nd(2)	73.9(4)
N(6)-C(41)-C(42)	122.2(5)	C(60)-C(59)-C(58)	136.6(7)
N(5)-C(41)-Li(2)	61.1(4)	C(60)-C(59)-Nd(2)	74.8(4)
N(6)-C(41)-Li(2)	64.2(5)	C(58)-C(59)-Nd(2)	75.4(4)
C(42)-C(41)-Li(2)	152.1(5)	C(59)-C(60)-C(53)	136.4(7)
N(5)-C(41)-Nd(2)	68.3(3)	C(59)-C(60)-Nd(2)	75.6(4)
N(6)-C(41)-Nd(2)	60.8(3)	C(53)-C(60)-Nd(2)	74.4(4)
C(42)-C(41)-Nd(2)	139.8(4)	N(8)-C(61)-N(7)	117.9(6)
Li(2)-C(41)-Nd(2)	68.1(3)	N(8)-C(61)-C(62)	121.7(5)
C(43)-C(42)-C(41)	175.5(6)	N(7)-C(61)-C(62)	120.4(6)
C(42)-C(43)-C(44)	177.9(8)	N(8)-C(61)-Nd(2)	60.0(3)
C(43)-C(44)-C(46)	119.4(6)	N(7)-C(61)-Nd(2)	62.9(3)
C(43)-C(44)-C(45)	119.3(5)	C(62)-C(61)-Nd(2)	157.7(4)
C(46)-C(44)-C(45)	58.4(4)	C(63)-C(62)-C(61)	173.3(7)
C(46)-C(45)-C(44)	60.8(4)	C(62)-C(63)-C(64)	176.9(7)
C(45)-C(46)-C(44)	60.8(4)	C(63)-C(64)-C(65)	121.1(6)
N(6)-C(47)-C(48)	112.6(6)	C(63)-C(64)-C(66)	117.8(6)
N(6)-C(47)-C(49)	108.0(6)	C(65)-C(64)-C(66)	58.4(5)

C(66)-C(65)-C(64)	61.7(4)	C(41)-N(6)-C(47)	118.8(5)
C(65)-C(66)-C(64)	59.8(5)	C(41)-N(6)-Li(2)	81.9(5)
N(7)-C(67)-C(69)	110.1(6)	C(47)-N(6)-Li(2)	133.9(5)
N(7)-C(67)-C(68)	110.7(6)	C(41)-N(6)-Nd(2)	92.3(3)
C(69)-C(67)-C(68)	110.6(5)	C(47)-N(6)-Nd(2)	134.8(4)
N(8)-C(70)-C(72)	113.3(5)	Li(2)-N(6)-Nd(2)	78.6(3)
N(8)-C(70)-C(71)	108.3(5)	C(61)-N(7)-C(67)	118.1(5)
C(72)-C(70)-C(71)	110.7(6)	C(61)-N(7)-Li(2)	117.0(5)
O(2)-C(73)-C(74)	106.1(7)	C(67)-N(7)-Li(2)	113.9(5)
C(75)-C(74)-C(73)	104.6(9)	C(61)-N(7)-Nd(2)	89.9(4)
C(74)-C(75)-C(76)	109.6(8)	C(67)-N(7)-Nd(2)	133.2(4)
O(2)-C(76)-C(75)	106.6(8)	Li(2)-N(7)-Nd(2)	78.8(4)
C(1)-N(1)-C(7)	117.2(5)	C(61)-N(8)-C(70)	118.8(5)
C(1)-N(1)-Li(1)	116.8(6)	C(61)-N(8)-Nd(2)	94.0(3)
C(7)-N(1)-Li(1)	112.7(5)	C(70)-N(8)-Nd(2)	141.4(4)
C(1)-N(1)-Nd(1)	89.8(3)	N(1)-C(1)-N(2)	118.3(6)
C(7)-N(1)-Nd(1)	135.4(4)	N(1)-C(1)-C(2)	121.4(5)
Li(1)-N(1)-Nd(1)	80.0(4)	N(2)-C(1)-C(2)	120.2(6)
C(1)-N(2)-C(10)	118.2(5)	N(1)-C(1)-Nd(1)	63.3(3)
C(1)-N(2)-Nd(1)	91.7(4)	N(2)-C(1)-Nd(1)	61.2(3)
C(10)-N(2)-Nd(1)	144.1(4)	C(2)-C(1)-Nd(1)	151.9(4)
C(21)-N(3)-C(27)	118.5(5)	C(3)-C(2)-C(1)	177.2(8)
C(21)-N(3)-Li(1)	83.4(5)	C(2)-C(3)-C(4)	179.2(9)
C(27)-N(3)-Li(1)	132.6(6)	C(3)-C(4)-C(5)	121.1(7)
C(21)-N(3)-Nd(1)	93.6(4)	C(3)-C(4)-C(6)	121.0(7)
C(27)-N(3)-Nd(1)	134.2(4)	C(5)-C(4)-C(6)	57.0(7)
Li(1)-N(3)-Nd(1)	79.0(4)	C(6)-C(5)-C(4)	61.5(7)
C(21)-N(4)-C(30)	118.1(5)	C(5)-C(6)-C(4)	61.5(6)
C(21)-N(4)-Li(1)	83.9(5)	N(1)-C(7)-C(8)	111.5(5)
C(30)-N(4)-Li(1)	137.6(5)	N(1)-C(7)-C(9)	108.6(5)
C(21)-N(4)-Nd(1)	83.7(4)	C(8)-C(7)-C(9)	110.2(7)
C(30)-N(4)-Nd(1)	139.0(4)	N(2)-C(10)-C(12)	109.8(5)
Li(1)-N(4)-Nd(1)	74.5(4)	N(2)-C(10)-C(11)	111.6(5)
C(41)-N(5)-C(50)	117.0(5)	C(12)-C(10)-C(11)	109.9(5)
C(41)-N(5)-Li(2)	85.0(4)	C(14)-C(13)-C(20)	134.4(8)
C(50)-N(5)-Li(2)	135.9(5)	C(14)-C(13)-Nd(1)	73.5(4)
C(41)-N(5)-Nd(2)	85.0(3)	C(20)-C(13)-Nd(1)	74.6(4)
C(50)-N(5)-Nd(2)	139.3(4)	C(15)-C(14)-C(13)	136.4(7)
Li(2)-N(5)-Nd(2)	75.8(3)	C(15)-C(14)-Nd(1)	76.2(4)

C(13)-C(14)-Nd(1)	76.7(4)	N(4)-C(30)-C(31)	111.0(6)
C(14)-C(15)-C(16)	134.7(7)	N(4)-C(30)-C(32)	109.8(6)
C(14)-C(15)-Nd(1)	74.3(4)	C(31)-C(30)-C(32)	109.3(6)
C(16)-C(15)-Nd(1)	75.4(4)	O(1)-C(33)-C(34)	106.6(7)
C(17)-C(16)-C(15)	133.9(8)	C(35)-C(34)-C(33)	102.6(7)
C(17)-C(16)-Nd(1)	74.6(4)	C(34)-C(35)-C(36)	104.9(6)
C(15)-C(16)-Nd(1)	74.3(4)	O(1)-C(36)-C(35)	105.9(6)
C(16)-C(17)-C(18)	135.4(8)	C(33)-O(1)-C(36)	109.3(6)
C(16)-C(17)-Nd(1)	75.8(4)	C(33)-O(1)-Li(1)	125.3(6)
C(18)-C(17)-Nd(1)	74.5(4)	C(36)-O(1)-Li(1)	123.2(6)
C(19)-C(18)-C(17)	135.5(8)	C(73)-O(2)-C(76)	109.2(6)
C(19)-C(18)-Nd(1)	75.4(4)	C(73)-O(2)-Li(2)	128.8(6)
C(17)-C(18)-Nd(1)	75.1(3)	C(76)-O(2)-Li(2)	119.6(6)
C(18)-C(19)-C(20)	135.6(8)	O(2)-Li(2)-N(7)	124.2(6)
C(18)-C(19)-Nd(1)	75.4(4)	O(2)-Li(2)-N(5)	126.5(6)
C(20)-C(19)-Nd(1)	75.8(4)	N(7)-Li(2)-N(5)	103.5(5)
C(19)-C(20)-C(13)	134.0(9)	O(2)-Li(2)-N(6)	111.9(5)
C(19)-C(20)-Nd(1)	74.4(4)	N(7)-Li(2)-N(6)	111.4(5)
C(13)-C(20)-Nd(1)	75.0(4)	N(5)-Li(2)-N(6)	64.0(4)
N(3)-C(21)-N(4)	116.1(6)	O(2)-Li(2)-C(41)	113.2(5)
N(3)-C(21)-C(22)	122.5(6)	N(7)-Li(2)-C(41)	122.4(5)
N(4)-C(21)-C(22)	121.5(6)	N(5)-Li(2)-C(41)	33.9(2)
N(3)-C(21)-Li(1)	63.7(5)	N(6)-Li(2)-C(41)	33.9(2)
N(4)-C(21)-Li(1)	62.6(4)	O(2)-Li(2)-Nd(2)	163.5(5)
C(22)-C(21)-Li(1)	148.6(5)	N(7)-Li(2)-Nd(2)	58.7(3)
N(3)-C(21)-Nd(1)	59.9(3)	N(5)-Li(2)-Nd(2)	62.1(3)
N(4)-C(21)-Nd(1)	69.5(3)	N(6)-Li(2)-Nd(2)	56.8(3)
C(22)-C(21)-Nd(1)	143.4(4)	C(41)-Li(2)-Nd(2)	65.1(3)
Li(1)-C(21)-Nd(1)	67.9(3)	O(1)-Li(1)-N(1)	121.1(7)
C(23)-C(22)-C(21)	176.2(7)	O(1)-Li(1)-N(4)	130.6(7)
C(22)-C(23)-C(24)	175.8(7)	N(1)-Li(1)-N(4)	103.4(6)
C(23)-C(24)-C(25)	117.1(7)	O(1)-Li(1)-N(3)	114.0(6)
C(23)-C(24)-C(26)	116.4(7)	N(1)-Li(1)-N(3)	110.4(5)
C(25)-C(24)-C(26)	59.6(5)	N(4)-Li(1)-N(3)	62.6(4)
C(26)-C(25)-C(24)	60.3(5)	O(1)-Li(1)-C(21)	117.2(6)
C(25)-C(26)-C(24)	60.1(5)	N(1)-Li(1)-C(21)	121.2(6)
N(3)-C(27)-C(28)	109.8(6)	N(4)-Li(1)-C(21)	33.4(3)
N(3)-C(27)-C(29)	111.0(6)	N(3)-Li(1)-C(21)	32.8(3)
C(28)-C(27)-C(29)	110.5(6)	O(1)-Li(1)-Nd(1)	161.1(7)

N(1)-Li(1)-Nd(1)	58.1(3)	N(3)-Li(1)-Nd(1)	56.0(3)
N(4)-Li(1)-Nd(1)	62.2(3)	C(21)-Li(1)-Nd(1)	64.5(3)

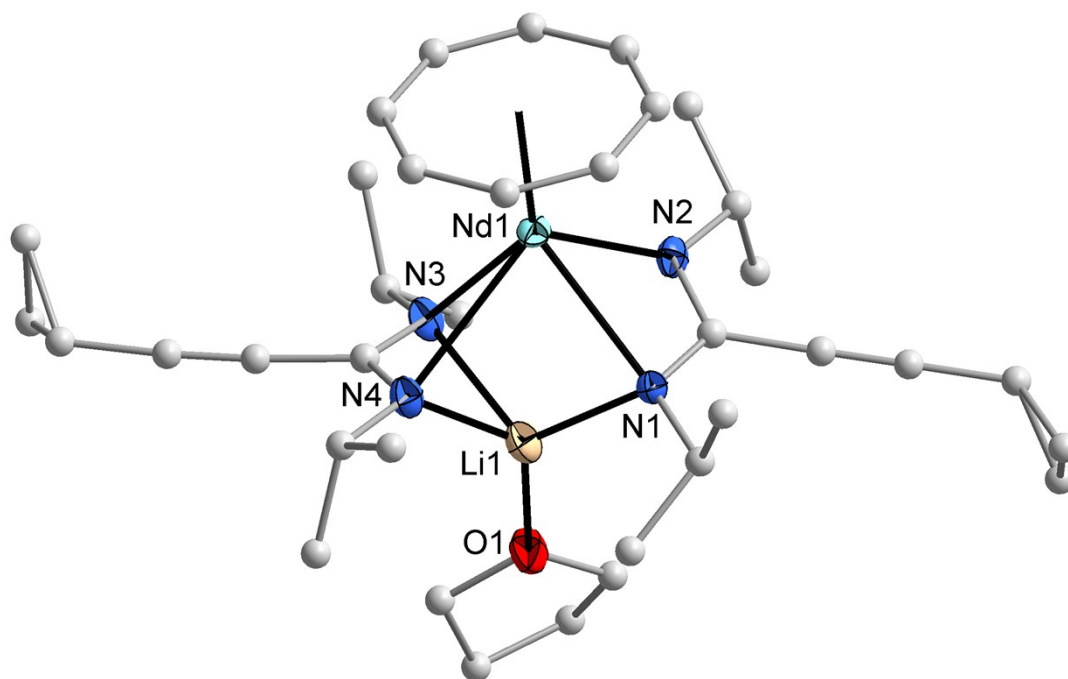


Figure S3. Molecular structure of (COT)Nd[μ -*c*-C₃H₅-C $\equiv$ C-C(N^{*i*}Pr)₂]₂Li(THF) (**3**) in the crystal (molecule 1 of 2 in the asymmetric unit). Ellipsoids of the heavier atoms and Li with 50% probability, H atoms omitted for clarity.

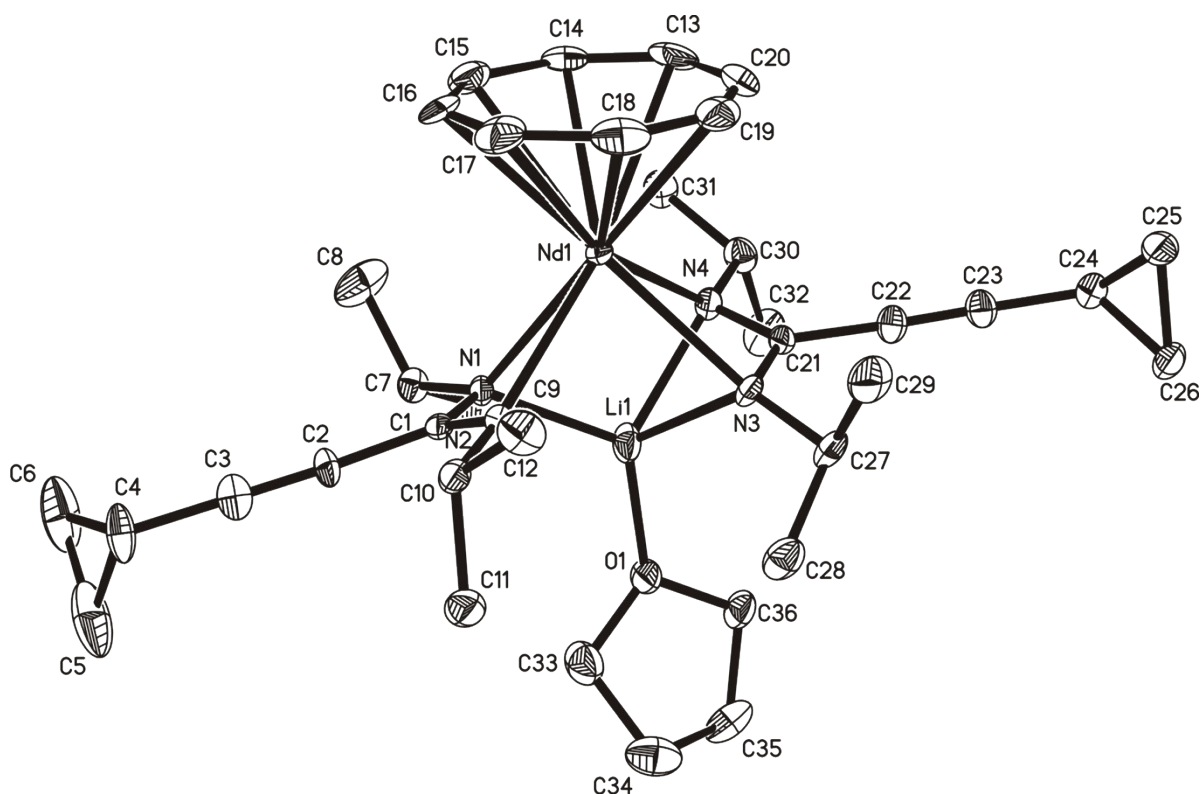


Figure S4. ORTEP drawing of (COT)Nd[μ -*c*-C₃H₅-C $\equiv$ C-C(N^{*i*}Pr)₂]₂Li(THF) (**3**).

Table S5. Crystal data and structure refinement (7).

Identification code	ip447	
Empirical formula	C ₅₆ H ₈₄ Ce ₂ N ₈	
Formula weight	1149.55	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.938(4) Å	α = 90°
	b = 17.320(4) Å	β = 112.97(3)°
	c = 16.644(3) Å	γ = 90°
Volume	5823(2) Å ³	
Z	4	
Density (calculated)	1.311 Mg/m ³	
Absorption coefficient	1.584 mm ⁻¹	
F(000)	2368	
Crystal size	0.57 x 0.18 x 0.17 mm ³	
Theta range for data collection	2.28 to 29.23°	
Index ranges	-29 ≤ h ≤ 30, -23 ≤ k ≤ 23, -21 ≤ l ≤ 22	
Reflections collected	35080	
Independent reflections	7841 [R(int) = 0.0551]	
Completeness to theta = 29.23°	99.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7841 / 0 / 299	
Goodness-of-fit on F ²	1.155	
Final R indices [I > 2σ(I)]	R1 = 0.0333, wR2 = 0.0806	
R indices (all data)	R1 = 0.0367, wR2 = 0.0821	
Largest diff. peak and hole	1.347 and -1.886 e.Å ⁻³	

Table S6. Bond lengths [Å] and angles [°] (7).

Ce(1)-N(2)#1	2.478(2)	N(3)-C(19)	1.460(3)
Ce(1)-N(2)	2.478(2)	N(4)-C(13)#1	1.331(4)
Ce(1)-N(1)#1	2.521(2)	N(4)-C(22)	1.457(4)
Ce(1)-N(1)	2.521(2)	C(1)-C(2)	1.458(4)
Ce(1)-C(28)	2.862(3)	C(2)-C(3)	1.183(5)
Ce(1)-C(28)#1	2.862(3)	C(3)-C(4)	1.457(5)
Ce(1)-C(27)	2.873(3)	C(4)-C(5)	1.422(9)
Ce(1)-C(27)#1	2.873(3)	C(4)-C(6)	1.449(6)
Ce(1)-C(25)#1	2.884(3)	C(5)-C(6)	1.480(8)
Ce(1)-C(25)	2.884(3)	C(7)-C(9)	1.516(5)
Ce(1)-C(1)#1	2.888(3)	C(7)-C(8)	1.518(5)
Ce(1)-C(1)	2.888(3)	C(10)-C(12)	1.516(5)
Ce(2)-N(4)	2.453(2)	C(10)-C(11)	1.529(5)
Ce(2)-N(4)#1	2.453(2)	C(13)-N(4)#1	1.331(4)
Ce(2)-N(3)#1	2.530(2)	C(13)-C(14)	1.455(4)
Ce(2)-N(3)	2.530(2)	C(14)-C(15)	1.191(4)
Ce(2)-C(26)#1	2.882(3)	C(15)-C(16)	1.444(4)
Ce(2)-C(26)	2.882(3)	C(16)-C(17)	1.504(4)
Ce(2)-C(27)#1	2.890(3)	C(16)-C(18)	1.506(5)
Ce(2)-C(27)	2.890(3)	C(17)-C(18)	1.490(5)
Ce(2)-C(13)#1	2.904(3)	C(19)-C(20)	1.519(4)
Ce(2)-C(13)	2.904(3)	C(19)-C(21)	1.523(4)
Ce(2)-C(25)	2.905(3)	C(22)-C(24)	1.521(5)
Ce(2)-C(25)#1	2.905(3)	C(22)-C(23)	1.523(5)
N(1)-C(1)	1.327(4)	C(25)-C(28)#1	1.398(5)
N(1)-C(7)	1.458(4)	C(25)-C(26)	1.402(5)
N(2)-C(1)	1.331(4)	C(26)-C(27)	1.409(5)
N(2)-C(10)	1.462(4)	C(27)-C(28)	1.399(5)
N(3)-C(13)	1.331(4)	C(28)-C(25)#1	1.398(5)
N(2)#1-Ce(1)-N(2)	101.04(12)	N(2)-Ce(1)-C(28)	141.01(9)
N(2)#1-Ce(1)-N(1)#1	54.03(8)	N(1)#1-Ce(1)-C(28)	127.10(9)
N(2)-Ce(1)-N(1)#1	91.87(8)	N(1)-Ce(1)-C(28)	93.89(9)
N(2)#1-Ce(1)-N(1)	91.87(8)	N(2)#1-Ce(1)-C(28)#1	141.01(9)
N(2)-Ce(1)-N(1)	54.03(8)	N(2)-Ce(1)-C(28)#1	101.59(9)
N(1)#1-Ce(1)-N(1)	128.28(11)	N(1)#1-Ce(1)-C(28)#1	93.89(9)
N(2)#1-Ce(1)-C(28)	101.59(9)	N(1)-Ce(1)-C(28)#1	127.10(9)

C(28)-Ce(1)-C(28)#1	79.45(11)	C(25)#1-Ce(1)-C(1)#1	99.88(8)
N(2)#1-Ce(1)-C(27)	124.79(9)	C(25)-Ce(1)-C(1)#1	147.49(9)
N(2)-Ce(1)-C(27)	114.37(9)	N(2)#1-Ce(1)-C(1)	92.81(8)
N(1)#1-Ce(1)-C(27)	151.93(8)	N(2)-Ce(1)-C(1)	27.38(8)
N(1)-Ce(1)-C(27)	78.00(8)	N(1)#1-Ce(1)-C(1)	108.23(8)
C(28)-Ce(1)-C(27)	28.23(9)	N(1)-Ce(1)-C(1)	27.33(8)
C(28)#1-Ce(1)-C(27)	72.05(8)	C(28)-Ce(1)-C(1)	120.28(9)
N(2)#1-Ce(1)-C(27)#1	114.37(9)	C(28)#1-Ce(1)-C(1)	120.70(9)
N(2)-Ce(1)-C(27)#1	124.79(9)	C(27)-Ce(1)-C(1)	99.82(8)
N(1)#1-Ce(1)-C(27)#1	78.00(8)	C(27)#1-Ce(1)-C(1)	148.16(9)
N(1)-Ce(1)-C(27)#1	151.93(8)	C(25)#1-Ce(1)-C(1)	147.49(9)
C(28)-Ce(1)-C(27)#1	72.05(8)	C(25)-Ce(1)-C(1)	99.88(8)
C(28)#1-Ce(1)-C(27)#1	28.23(9)	C(1)#1-Ce(1)-C(1)	97.45(11)
C(27)-Ce(1)-C(27)#1	78.73(11)	N(4)-Ce(2)-N(4)#1	102.87(12)
N(2)#1-Ce(1)-C(25)#1	90.16(8)	N(4)-Ce(2)-N(3)#1	54.25(8)
N(2)-Ce(1)-C(25)#1	167.29(9)	N(4)#1-Ce(2)-N(3)#1	92.22(8)
N(1)#1-Ce(1)-C(25)#1	99.63(9)	N(4)-Ce(2)-N(3)	92.22(8)
N(1)-Ce(1)-C(25)#1	120.25(9)	N(4)#1-Ce(2)-N(3)	54.25(8)
C(28)-Ce(1)-C(25)#1	28.16(10)	N(3)#1-Ce(2)-N(3)	128.10(11)
C(28)#1-Ce(1)-C(25)#1	72.44(8)	N(4)-Ce(2)-C(26)#1	102.02(9)
C(27)-Ce(1)-C(25)#1	53.40(9)	N(4)#1-Ce(2)-C(26)#1	138.95(9)
C(27)#1-Ce(1)-C(25)#1	53.61(9)	N(3)#1-Ce(2)-C(26)#1	128.83(9)
N(2)#1-Ce(1)-C(25)	167.29(9)	N(3)-Ce(2)-C(26)#1	92.78(8)
N(2)-Ce(1)-C(25)	90.16(8)	N(4)-Ce(2)-C(26)	138.95(9)
N(1)#1-Ce(1)-C(25)	120.25(9)	N(4)#1-Ce(2)-C(26)	102.02(9)
N(1)-Ce(1)-C(25)	99.63(9)	N(3)#1-Ce(2)-C(26)	92.78(8)
C(28)-Ce(1)-C(25)	72.44(8)	N(3)-Ce(2)-C(26)	128.83(9)
C(28)#1-Ce(1)-C(25)	28.16(10)	C(26)#1-Ce(2)-C(26)	78.94(11)
C(27)-Ce(1)-C(25)	53.61(9)	N(4)-Ce(2)-C(27)#1	125.92(9)
C(27)#1-Ce(1)-C(25)	53.40(9)	N(4)#1-Ce(2)-C(27)#1	112.40(9)
C(25)#1-Ce(1)-C(25)	79.42(11)	N(3)#1-Ce(2)-C(27)#1	152.77(8)
N(2)#1-Ce(1)-C(1)#1	27.38(8)	N(3)-Ce(2)-C(27)#1	77.89(8)
N(2)-Ce(1)-C(1)#1	92.81(8)	C(26)#1-Ce(2)-C(27)#1	28.25(9)
N(1)#1-Ce(1)-C(1)#1	27.33(8)	C(26)-Ce(2)-C(27)#1	71.49(8)
N(1)-Ce(1)-C(1)#1	108.23(8)	N(4)-Ce(2)-C(27)	112.40(9)
C(28)-Ce(1)-C(1)#1	120.70(9)	N(4)#1-Ce(2)-C(27)	125.92(9)
C(28)#1-Ce(1)-C(1)#1	120.28(9)	N(3)#1-Ce(2)-C(27)	77.89(8)
C(27)-Ce(1)-C(1)#1	148.16(9)	N(3)-Ce(2)-C(27)	152.77(8)
C(27)#1-Ce(1)-C(1)#1	99.82(8)	C(26)#1-Ce(2)-C(27)	71.49(8)

C(26)-Ce(2)-C(27)	28.25(9)	C(25)-Ce(2)-C(25)#1	78.72(11)
C(27)#1-Ce(2)-C(27)	78.18(11)	C(1)-N(1)-C(7)	118.7(3)
N(4)-Ce(2)-C(13)#1	27.14(8)	C(1)-N(1)-Ce(1)	91.93(17)
N(4)#1-Ce(2)-C(13)#1	96.41(8)	C(7)-N(1)-Ce(1)	147.8(2)
N(3)#1-Ce(2)-C(13)#1	27.26(8)	C(1)-N(2)-C(10)	120.2(3)
N(3)-Ce(2)-C(13)#1	110.04(8)	C(1)-N(2)-Ce(1)	93.74(17)
C(26)#1-Ce(2)-C(13)#1	119.74(9)	C(10)-N(2)-Ce(1)	141.1(2)
C(26)-Ce(2)-C(13)#1	117.88(9)	C(13)-N(3)-C(19)	119.1(2)
C(27)#1-Ce(2)-C(13)#1	147.63(9)	C(13)-N(3)-Ce(2)	92.20(16)
C(27)-Ce(2)-C(13)#1	97.14(8)	C(19)-N(3)-Ce(2)	148.71(18)
N(4)-Ce(2)-C(13)	96.41(8)	C(13)#1-N(4)-C(22)	121.1(2)
N(4)#1-Ce(2)-C(13)	27.14(8)	C(13)#1-N(4)-Ce(2)	95.64(17)
N(3)#1-Ce(2)-C(13)	110.04(8)	C(22)-N(4)-Ce(2)	141.92(18)
N(3)-Ce(2)-C(13)	27.26(8)	N(1)-C(1)-N(2)	117.4(2)
C(26)#1-Ce(2)-C(13)	117.88(9)	N(1)-C(1)-C(2)	122.1(3)
C(26)-Ce(2)-C(13)	119.74(9)	N(2)-C(1)-C(2)	120.4(3)
C(27)#1-Ce(2)-C(13)	97.14(8)	N(1)-C(1)-Ce(1)	60.74(14)
C(27)-Ce(2)-C(13)	147.63(9)	N(2)-C(1)-Ce(1)	58.88(15)
C(13)#1-Ce(2)-C(13)	102.75(11)	C(2)-C(1)-Ce(1)	162.8(2)
N(4)-Ce(2)-C(25)	165.31(8)	C(3)-C(2)-C(1)	174.8(4)
N(4)#1-Ce(2)-C(25)	89.81(8)	C(2)-C(3)-C(4)	178.1(5)
N(3)#1-Ce(2)-C(25)	118.74(9)	C(5)-C(4)-C(6)	62.1(4)
N(3)-Ce(2)-C(25)	101.30(8)	C(5)-C(4)-C(3)	118.3(5)
C(26)#1-Ce(2)-C(25)	71.87(8)	C(6)-C(4)-C(3)	119.3(4)
C(26)-Ce(2)-C(25)	28.04(9)	C(4)-C(5)-C(6)	59.9(4)
C(27)#1-Ce(2)-C(25)	53.02(9)	C(4)-C(6)-C(5)	58.1(4)
C(27)-Ce(2)-C(25)	53.22(9)	N(1)-C(7)-C(9)	110.4(3)
C(13)#1-Ce(2)-C(25)	145.28(9)	N(1)-C(7)-C(8)	110.5(3)
C(13)-Ce(2)-C(25)	98.24(8)	C(9)-C(7)-C(8)	109.7(3)
N(4)-Ce(2)-C(25)#1	89.81(8)	N(2)-C(10)-C(12)	109.1(3)
N(4)#1-Ce(2)-C(25)#1	165.32(8)	N(2)-C(10)-C(11)	110.7(3)
N(3)#1-Ce(2)-C(25)#1	101.30(8)	C(12)-C(10)-C(11)	113.0(3)
N(3)-Ce(2)-C(25)#1	118.74(9)	N(3)-C(13)-N(4)#1	117.3(2)
C(26)#1-Ce(2)-C(25)#1	28.04(9)	N(3)-C(13)-C(14)	122.1(3)
C(26)-Ce(2)-C(25)#1	71.87(8)	N(4)#1-C(13)-C(14)	120.6(3)
C(27)#1-Ce(2)-C(25)#1	53.22(9)	N(3)-C(13)-Ce(2)	60.54(13)
C(27)-Ce(2)-C(25)#1	53.02(9)	N(4)#1-C(13)-Ce(2)	57.22(14)
C(13)#1-Ce(2)-C(25)#1	98.24(8)	C(14)-C(13)-Ce(2)	171.9(2)
C(13)-Ce(2)-C(25)#1	145.28(9)	C(15)-C(14)-C(13)	177.8(3)

C(14)-C(15)-C(16)	178.5(3)
C(15)-C(16)-C(17)	119.0(3)
C(15)-C(16)-C(18)	118.3(3)
C(17)-C(16)-C(18)	59.3(2)
C(18)-C(17)-C(16)	60.4(2)
C(17)-C(18)-C(16)	60.3(2)
N(3)-C(19)-C(20)	109.8(2)
N(3)-C(19)-C(21)	111.1(2)
C(20)-C(19)-C(21)	110.4(3)
Symmetry: C(19), C(20), C(21) #1 -x+1, -y, -z+3/2	
N(4)-C(22)-C(24)	111.2(3)
N(4)-C(22)-C(23)	108.5(3)
C(24)-C(22)-C(23)	112.5(3)
C(28)#1-C(25)-C(26)	134.3(3)
C(28)#1-C(25)-Ce(1)	75.06(15)
C(26)-C(25)-Ce(1)	76.35(16)
C(28)#1-C(25)-Ce(2)	76.28(16)
C(26)-C(25)-Ce(2)	75.07(15)
Ce(1)-C(25)-Ce(2)	100.93(9)
C(25)-C(26)-C(27)	134.9(3)
C(25)-C(26)-Ce(2)	76.89(16)
C(27)-C(26)-Ce(2)	76.19(16)
C(25)-C(26)-Ce(1)	75.56(16)
C(27)-C(26)-Ce(1)	75.06(16)
Ce(2)-C(26)-Ce(1)	101.24(9)
C(28)-C(27)-C(26)	135.4(3)
C(28)-C(27)-Ce(1)	75.45(15)
C(26)-C(27)-Ce(1)	76.67(15)
C(28)-C(27)-Ce(2)	76.84(16)
C(26)-C(27)-Ce(2)	75.56(16)
Ce(1)-C(27)-Ce(2)	101.55(9)
C(25)#1-C(28)-C(27)	135.3(3)
C(25)#1-C(28)-Ce(1)	76.77(15)
C(27)-C(28)-Ce(1)	76.33(15)
C(25)#1-C(28)-Ce(2)	75.89(15)
C(27)-C(28)-Ce(2)	75.26(15)
Ce(1)-C(28)-Ce(2)	101.33(8)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, y, -z+3/2$

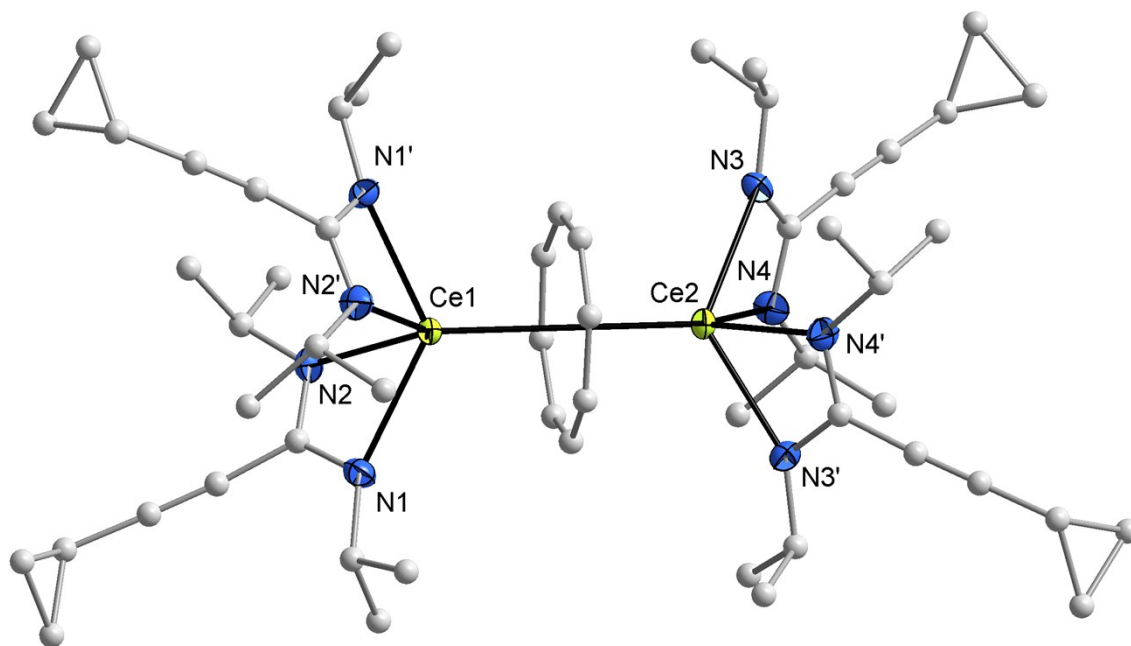


Figure S5. Molecular structure of $(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})[\text{Ce}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)_2]_2$ (**7**) in the crystal. Ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

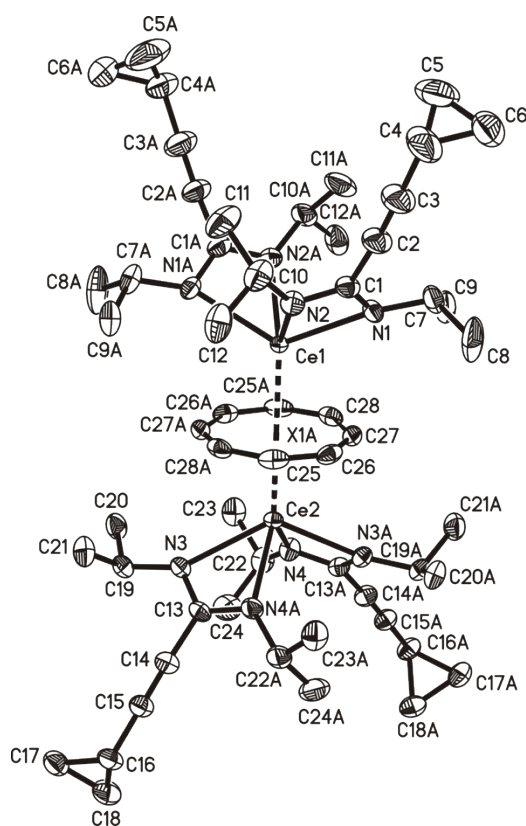


Figure S6. ORTEP drawing of $(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})[\text{Ce}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)_2]_2$ (**7**).

Table S7. Crystal data and structure refinement (8).

Identification code	ip448	
Empirical formula	C ₈₀ H ₁₁₆ Ce ₂ N ₈	
Formula weight	1470.05	
Temperature	143(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Pn	
Unit cell dimensions	a = 21.084(4) Å	α = 90°
	b = 13.758(3) Å	β = 102.71(3)°
	c = 26.383(5) Å	γ = 90°
Volume	7465(3) Å ³	
Z	4	
Density (calculated)	1.308 Mg/m ³	
Absorption coefficient	1.251 mm ⁻¹	
F(000)	3072	
Crystal size	0.48 x 0.34 x 0.33 mm ³	
Theta range for data collection	2.04 to 25.68°	
Index ranges	-25 ≤ h ≤ 25, -14 ≤ k ≤ 16, -32 ≤ l ≤ 32	
Reflections collected	42721	
Independent reflections	23075 [R(int) = 0.0356]	
Completeness to theta = 25.68°	94.8 %	
Absorption correction	Sphere	
Max. and min. transmission	0.4303 and 0.4186	
Refinement method	Full-matrix-block least-squares on F ²	
Data / restraints / parameters	23075 / 2 / 1622	
Goodness-of-fit on F ²	0.972	
Final R indices [I > 2σ(I)]	R1 = 0.0268, wR2 = 0.0604	
R indices (all data)	R1 = 0.0324, wR2 = 0.0624	
Absolute structure parameter	0.530(7)	
Largest diff. peak and hole	0.845 and -0.748 e.Å ⁻³	

Table S8. Bond lengths [Å] and angles [°] (**8**).

Ce(1)-N(4)	2.438(4)	Ce(3)-C(175)	2.926(4)
Ce(1)-N(2)	2.470(4)	Ce(4)-N(16)	2.476(4)
Ce(1)-N(1)	2.504(4)	Ce(4)-N(18)	2.486(4)
Ce(1)-N(3)	2.528(4)	Ce(4)-N(17)	2.510(4)
Ce(1)-C(80)	2.872(4)	Ce(4)-N(15)	2.525(3)
Ce(1)-C(74)	2.873(4)	Ce(4)-C(175)	2.885(4)
Ce(1)-C(73)	2.879(4)	Ce(4)-C(173)	2.887(5)
Ce(1)-C(19)	2.886(4)	Ce(4)-C(174)	2.890(4)
Ce(1)-C(1)	2.890(5)	Ce(4)-C(177)	2.893(4)
Ce(1)-C(79)	2.894(4)	Ce(4)-C(180)	2.896(5)
Ce(1)-C(75)	2.901(4)	Ce(4)-C(176)	2.900(4)
Ce(1)-C(78)	2.908(4)	Ce(4)-C(137)	2.905(4)
Ce(2)-N(5)	2.484(3)	Ce(4)-C(179)	2.910(4)
Ce(2)-N(8)	2.502(4)	N(1)-C(1)	1.290(6)
Ce(2)-N(7)	2.504(4)	N(1)-C(7)	1.476(6)
Ce(2)-N(6)	2.527(4)	N(2)-C(1)	1.336(6)
Ce(2)-C(73)	2.852(4)	N(2)-C(13)	1.456(6)
Ce(2)-C(79)	2.874(4)	N(3)-C(19)	1.333(6)
Ce(2)-C(75)	2.877(4)	N(3)-C(25)	1.448(5)
Ce(2)-C(80)	2.881(4)	N(4)-C(19)	1.323(6)
Ce(2)-C(74)	2.887(4)	N(4)-C(31)	1.450(5)
Ce(2)-C(55)	2.899(4)	N(5)-C(37)	1.329(5)
Ce(2)-C(77)	2.904(4)	N(5)-C(43)	1.461(5)
Ce(2)-C(76)	2.904(4)	N(6)-C(37)	1.324(5)
Ce(3)-N(11)	2.479(3)	N(6)-C(49)	1.458(5)
Ce(3)-N(14)	2.497(3)	N(7)-C(55)	1.331(6)
Ce(3)-N(12)	2.498(3)	N(7)-C(67)	1.477(5)
Ce(3)-N(13)	2.526(4)	N(8)-C(55)	1.334(6)
Ce(3)-C(180)	2.883(4)	N(8)-C(61)	1.469(5)
Ce(3)-C(119)	2.883(4)	N(11)-C(101)	1.334(4)
Ce(3)-C(174)	2.894(4)	N(11)-C(107)	1.462(4)
Ce(3)-C(178)	2.897(4)	N(12)-C(101)	1.335(4)
Ce(3)-C(179)	2.901(4)	N(12)-C(113)	1.467(4)
Ce(3)-C(101)	2.904(4)	N(13)-C(119)	1.328(4)
Ce(3)-C(173)	2.905(4)	N(13)-C(125)	1.481(4)

N(14)-C(119)	1.323(4)	C(29)-C(30)	1.534(7)
N(14)-C(131)	1.463(4)	C(31)-C(36)	1.515(6)
N(15)-C(137)	1.324(4)	C(31)-C(32)	1.535(5)
N(15)-C(143)	1.460(4)	C(32)-C(33)	1.525(6)
N(16)-C(137)	1.335(4)	C(33)-C(34)	1.536(6)
N(16)-C(149)	1.463(4)	C(34)-C(35)	1.513(6)
N(17)-C(155)	1.323(4)	C(35)-C(36)	1.524(6)
N(17)-C(167)	1.471(5)	C(37)-C(38)	1.449(6)
N(18)-C(155)	1.336(4)	C(38)-C(39)	1.200(6)
N(18)-C(161)	1.468(4)	C(39)-C(40)	1.423(6)
C(1)-C(2)	1.468(6)	C(40)-C(42)	1.501(7)
C(2)-C(3)	1.188(6)	C(40)-C(41)	1.503(7)
C(3)-C(4)	1.437(6)	C(41)-C(42)	1.472(9)
C(4)-C(6)	1.507(6)	C(43)-C(44)	1.523(6)
C(4)-C(5)	1.514(6)	C(43)-C(48)	1.528(5)
C(5)-C(6)	1.481(6)	C(44)-C(45)	1.524(6)
C(7)-C(8)	1.462(7)	C(45)-C(46)	1.518(7)
C(7)-C(12)	1.524(6)	C(46)-C(47)	1.518(7)
C(8)-C(9)	1.569(8)	C(47)-C(48)	1.521(6)
C(9)-C(10)	1.538(8)	C(49)-C(50)	1.520(5)
C(10)-C(11)	1.496(8)	C(49)-C(54)	1.521(6)
C(11)-C(12)	1.536(7)	C(50)-C(51)	1.533(6)
C(13)-C(18)	1.488(6)	C(51)-C(52)	1.523(6)
C(13)-C(14)	1.527(6)	C(52)-C(53)	1.530(6)
C(14)-C(15)	1.511(7)	C(53)-C(54)	1.541(6)
C(15)-C(16)	1.505(8)	C(55)-C(56)	1.440(6)
C(16)-C(17)	1.521(7)	C(56)-C(57)	1.201(6)
C(17)-C(18)	1.533(7)	C(57)-C(58)	1.423(7)
C(19)-C(20)	1.466(6)	C(58)-C(60)	1.479(7)
C(20)-C(21)	1.178(6)	C(58)-C(59)	1.484(8)
C(21)-C(22)	1.442(6)	C(59)-C(60)	1.462(9)
C(22)-C(24)	1.470(7)	C(61)-C(62)	1.527(5)
C(22)-C(23)	1.485(6)	C(61)-C(66)	1.529(6)
C(23)-C(24)	1.454(7)	C(62)-C(63)	1.531(7)
C(25)-C(26)	1.515(6)	C(63)-C(64)	1.510(7)
C(25)-C(30)	1.538(6)	C(64)-C(65)	1.505(6)
C(26)-C(27)	1.525(7)	C(65)-C(66)	1.521(6)
C(27)-C(28)	1.538(8)	C(67)-C(72)	1.519(5)
C(28)-C(29)	1.507(8)	C(67)-C(68)	1.524(6)

C(68)-C(69)	1.522(6)	C(127)-C(128)	1.497(8)
C(69)-C(70)	1.527(7)	C(128)-C(129)	1.489(7)
C(70)-C(71)	1.522(7)	C(129)-C(130)	1.527(6)
C(71)-C(72)	1.525(6)	C(131)-C(136)	1.522(6)
C(73)-C(80)	1.402(7)	C(131)-C(132)	1.527(5)
C(73)-C(74)	1.401(7)	C(132)-C(133)	1.530(6)
C(74)-C(75)	1.406(7)	C(133)-C(134)	1.518(7)
C(75)-C(76)	1.394(7)	C(134)-C(135)	1.520(6)
C(76)-C(77)	1.393(7)	C(135)-C(136)	1.528(6)
C(77)-C(78)	1.416(7)	C(137)-C(138)	1.454(6)
C(78)-C(79)	1.405(7)	C(138)-C(139)	1.186(6)
C(79)-C(80)	1.402(7)	C(139)-C(140)	1.435(6)
C(101)-C(102)	1.457(5)	C(140)-C(141)	1.514(7)
C(102)-C(103)	1.177(5)	C(140)-C(142)	1.521(7)
C(103)-C(104)	1.439(5)	C(141)-C(142)	1.479(7)
C(104)-C(105)	1.501(6)	C(143)-C(148)	1.517(6)
C(104)-C(106)	1.510(6)	C(143)-C(144)	1.530(6)
C(105)-C(106)	1.468(7)	C(144)-C(145)	1.520(7)
C(107)-C(112)	1.525(5)	C(145)-C(146)	1.518(8)
C(107)-C(108)	1.531(5)	C(146)-C(147)	1.511(7)
C(108)-C(109)	1.526(6)	C(147)-C(148)	1.519(7)
C(109)-C(110)	1.519(7)	C(149)-C(154)	1.530(5)
C(110)-C(111)	1.531(6)	C(149)-C(150)	1.532(5)
C(111)-C(112)	1.537(6)	C(150)-C(151)	1.525(6)
C(113)-C(118)	1.521(5)	C(151)-C(152)	1.521(6)
C(113)-C(114)	1.531(5)	C(152)-C(153)	1.515(6)
C(114)-C(115)	1.531(6)	C(153)-C(154)	1.522(6)
C(115)-C(116)	1.503(6)	C(155)-C(156)	1.457(6)
C(116)-C(117)	1.518(6)	C(156)-C(157)	1.195(6)
C(117)-C(118)	1.520(6)	C(157)-C(158)	1.432(6)
C(119)-C(120)	1.458(6)	C(158)-C(160)	1.486(6)
C(120)-C(121)	1.203(6)	C(158)-C(159)	1.494(6)
C(121)-C(122)	1.427(6)	C(159)-C(160)	1.486(6)
C(122)-C(124)	1.501(7)	C(161)-C(162)	1.516(5)
C(122)-C(123)	1.503(7)	C(161)-C(166)	1.539(6)
C(123)-C(124)	1.475(7)	C(162)-C(163)	1.538(6)
C(125)-C(130)	1.511(6)	C(163)-C(164)	1.529(7)
C(125)-C(126)	1.511(6)	C(164)-C(165)	1.507(6)
C(126)-C(127)	1.533(6)	C(165)-C(166)	1.519(6)

C(167)-C(172)	1.401(8)	N(1)-Ce(1)-C(19)	112.12(12)
C(167)-C(168)	1.491(6)	N(3)-Ce(1)-C(19)	27.50(12)
C(168)-C(169)	1.502(8)	C(80)-Ce(1)-C(19)	161.74(13)
C(169)-C(170)	1.391(10)	C(74)-Ce(1)-C(19)	118.14(13)
C(170)-C(171)	1.591(11)	C(73)-Ce(1)-C(19)	146.33(13)
C(171)-C(172)	1.516(8)	N(4)-Ce(1)-C(1)	102.74(13)
C(173)-C(180)	1.408(7)	N(2)-Ce(1)-C(1)	27.45(13)
C(173)-C(174)	1.411(7)	N(1)-Ce(1)-C(1)	26.44(13)
C(174)-C(175)	1.393(7)	N(3)-Ce(1)-C(1)	112.95(13)
C(175)-C(176)	1.425(7)	C(80)-Ce(1)-C(1)	86.02(12)
C(176)-C(177)	1.377(6)	C(74)-Ce(1)-C(1)	106.40(14)
C(177)-C(178)	1.392(7)	C(73)-Ce(1)-C(1)	88.64(13)
C(178)-C(179)	1.415(6)	C(19)-Ce(1)-C(1)	112.21(12)
C(179)-C(180)	1.385(7)	N(4)-Ce(1)-C(79)	155.95(13)
		N(2)-Ce(1)-C(79)	90.27(13)
		N(1)-Ce(1)-C(79)	108.65(13)
N(4)-Ce(1)-N(2)	112.17(13)	N(3)-Ce(1)-C(79)	116.60(13)
N(4)-Ce(1)-N(1)	92.22(13)	C(80)-Ce(1)-C(79)	28.14(13)
N(2)-Ce(1)-N(1)	53.88(12)	C(74)-Ce(1)-C(79)	71.78(13)
N(4)-Ce(1)-N(3)	54.48(12)	C(73)-Ce(1)-C(79)	53.13(13)
N(2)-Ce(1)-N(3)	96.68(13)	C(19)-Ce(1)-C(79)	138.69(13)
N(1)-Ce(1)-N(3)	125.81(12)	C(1)-Ce(1)-C(79)	101.23(13)
N(4)-Ce(1)-C(80)	153.05(13)	N(4)-Ce(1)-C(75)	84.17(12)
N(2)-Ce(1)-C(80)	87.38(13)	N(2)-Ce(1)-C(75)	154.87(13)
N(1)-Ce(1)-C(80)	84.50(13)	N(1)-Ce(1)-C(75)	108.76(14)
N(3)-Ce(1)-C(80)	144.73(13)	N(3)-Ce(1)-C(75)	108.43(13)
N(4)-Ce(1)-C(74)	99.36(13)	C(80)-Ce(1)-C(75)	71.74(13)
N(2)-Ce(1)-C(74)	126.90(13)	C(74)-Ce(1)-C(75)	28.19(14)
N(1)-Ce(1)-C(74)	84.51(13)	C(73)-Ce(1)-C(75)	53.12(13)
N(3)-Ce(1)-C(74)	136.26(14)	C(19)-Ce(1)-C(75)	94.88(12)
C(80)-Ce(1)-C(74)	53.72(14)	C(1)-Ce(1)-C(75)	133.31(14)
N(4)-Ce(1)-C(73)	125.41(13)	C(79)-Ce(1)-C(75)	77.98(12)
N(2)-Ce(1)-C(73)	102.13(13)	N(4)-Ce(1)-C(78)	129.69(14)
N(1)-Ce(1)-C(73)	74.90(12)	N(2)-Ce(1)-C(78)	108.00(13)
N(3)-Ce(1)-C(73)	158.26(13)	N(1)-Ce(1)-C(78)	136.64(13)
C(80)-Ce(1)-C(73)	28.21(14)	N(3)-Ce(1)-C(78)	92.43(12)
C(74)-Ce(1)-C(73)	28.19(14)	C(80)-Ce(1)-C(78)	53.44(13)
N(4)-Ce(1)-C(19)	27.15(12)	C(74)-Ce(1)-C(78)	78.75(12)
N(2)-Ce(1)-C(19)	108.29(12)	C(73)-Ce(1)-C(78)	71.54(12)

C(19)-Ce(1)-C(78)	111.07(13)	C(80)-Ce(2)-C(74)	53.49(14)
C(1)-Ce(1)-C(78)	126.31(13)	N(5)-Ce(2)-C(55)	113.47(12)
C(79)-Ce(1)-C(78)	28.02(13)	N(8)-Ce(2)-C(55)	27.36(12)
C(75)-Ce(1)-C(78)	70.95(13)	N(7)-Ce(2)-C(55)	27.28(12)
N(5)-Ce(2)-N(8)	121.32(13)	N(6)-Ce(2)-C(55)	115.20(11)
N(5)-Ce(2)-N(7)	94.64(13)	C(73)-Ce(2)-C(55)	102.72(12)
N(8)-Ce(2)-N(7)	53.97(13)	C(79)-Ce(2)-C(55)	155.18(12)
N(5)-Ce(2)-N(6)	53.90(12)	C(75)-Ce(2)-C(55)	80.45(12)
N(8)-Ce(2)-N(6)	97.55(13)	C(80)-Ce(2)-C(55)	130.30(13)
N(7)-Ce(2)-N(6)	120.96(12)	C(74)-Ce(2)-C(55)	83.41(12)
N(5)-Ce(2)-C(73)	142.67(13)	N(5)-Ce(2)-C(77)	89.48(13)
N(8)-Ce(2)-C(73)	87.36(13)	N(8)-Ce(2)-C(77)	140.14(14)
N(7)-Ce(2)-C(73)	122.52(13)	N(7)-Ce(2)-C(77)	103.15(13)
N(6)-Ce(2)-C(73)	102.85(13)	N(6)-Ce(2)-C(77)	121.96(13)
N(5)-Ce(2)-C(79)	91.21(13)	C(73)-Ce(2)-C(77)	79.38(12)
N(8)-Ce(2)-C(79)	138.67(13)	C(79)-Ce(2)-C(77)	53.63(13)
N(7)-Ce(2)-C(79)	156.05(12)	C(75)-Ce(2)-C(77)	53.06(14)
N(6)-Ce(2)-C(79)	80.91(12)	C(80)-Ce(2)-C(77)	72.27(12)
C(73)-Ce(2)-C(79)	53.59(13)	C(74)-Ce(2)-C(77)	71.89(13)
N(5)-Ce(2)-C(75)	139.61(13)	C(55)-Ce(2)-C(77)	120.77(13)
N(8)-Ce(2)-C(75)	88.94(14)	N(5)-Ce(2)-C(76)	111.84(12)
N(7)-Ce(2)-C(75)	81.87(12)	N(8)-Ce(2)-C(76)	112.39(13)
N(6)-Ce(2)-C(75)	155.46(12)	N(7)-Ce(2)-C(76)	84.86(12)
C(73)-Ce(2)-C(75)	53.62(13)	N(6)-Ce(2)-C(76)	149.00(13)
C(79)-Ce(2)-C(75)	78.69(12)	C(73)-Ce(2)-C(76)	71.86(13)
N(5)-Ce(2)-C(80)	114.39(13)	C(79)-Ce(2)-C(76)	71.43(12)
N(8)-Ce(2)-C(80)	110.49(13)	C(75)-Ce(2)-C(76)	27.90(13)
N(7)-Ce(2)-C(80)	150.26(13)	C(80)-Ce(2)-C(76)	78.64(12)
N(6)-Ce(2)-C(80)	83.62(12)	C(74)-Ce(2)-C(76)	53.20(13)
C(73)-Ce(2)-C(80)	28.30(14)	C(55)-Ce(2)-C(76)	95.60(12)
C(79)-Ce(2)-C(80)	28.20(13)	C(77)-Ce(2)-C(76)	27.75(13)
C(75)-Ce(2)-C(80)	71.96(13)	N(11)-Ce(3)-N(14)	119.42(13)
N(5)-Ce(2)-C(74)	159.90(12)	N(11)-Ce(3)-N(12)	54.46(12)
N(8)-Ce(2)-C(74)	78.71(13)	N(14)-Ce(3)-N(12)	95.25(12)
N(7)-Ce(2)-C(74)	96.87(13)	N(11)-Ce(3)-N(13)	93.02(12)
N(6)-Ce(2)-C(74)	130.32(13)	N(14)-Ce(3)-N(13)	54.09(13)
C(73)-Ce(2)-C(74)	28.24(14)	N(12)-Ce(3)-N(13)	119.00(12)
C(79)-Ce(2)-C(74)	71.85(13)	N(11)-Ce(3)-C(180)	141.50(10)
C(75)-Ce(2)-C(74)	28.24(14)	N(14)-Ce(3)-C(180)	90.22(9)

N(12)-Ce(3)-C(180)	153.42(10)	N(12)-Ce(3)-C(173)	150.89(10)
N(13)-Ce(3)-C(180)	85.06(10)	N(13)-Ce(3)-C(173)	85.65(10)
N(11)-Ce(3)-C(119)	111.42(9)	C(180)-Ce(3)-C(173)	28.16(13)
N(14)-Ce(3)-C(119)	27.28(9)	C(119)-Ce(3)-C(173)	96.41(12)
N(12)-Ce(3)-C(119)	112.57(9)	C(174)-Ce(3)-C(173)	28.17(14)
N(13)-Ce(3)-C(119)	27.41(9)	C(178)-Ce(3)-C(173)	71.54(12)
C(180)-Ce(3)-C(119)	83.18(11)	C(179)-Ce(3)-C(173)	53.01(13)
N(11)-Ce(3)-C(174)	90.23(10)	C(101)-Ce(3)-C(173)	136.67(12)
N(14)-Ce(3)-C(174)	140.73(11)	N(11)-Ce(3)-C(175)	80.99(8)
N(12)-Ce(3)-C(174)	123.78(11)	N(14)-Ce(3)-C(175)	159.58(9)
N(13)-Ce(3)-C(174)	103.12(10)	N(12)-Ce(3)-C(175)	98.02(9)
C(180)-Ce(3)-C(174)	53.30(14)	N(13)-Ce(3)-C(175)	129.32(10)
C(119)-Ce(3)-C(174)	121.31(13)	C(180)-Ce(3)-C(175)	71.12(12)
N(11)-Ce(3)-C(178)	139.59(10)	C(119)-Ce(3)-C(175)	148.80(12)
N(14)-Ce(3)-C(178)	91.45(10)	C(174)-Ce(3)-C(175)	27.69(14)
N(12)-Ce(3)-C(178)	100.72(9)	C(178)-Ce(3)-C(175)	70.89(13)
N(13)-Ce(3)-C(178)	127.22(10)	C(179)-Ce(3)-C(175)	77.89(11)
C(180)-Ce(3)-C(178)	53.06(13)	C(101)-Ce(3)-C(175)	91.05(11)
C(119)-Ce(3)-C(178)	107.57(13)	C(173)-Ce(3)-C(175)	52.88(13)
C(174)-Ce(3)-C(178)	78.25(12)	N(16)-Ce(4)-N(18)	112.39(12)
N(11)-Ce(3)-C(179)	158.86(8)	N(16)-Ce(4)-N(17)	94.99(13)
N(14)-Ce(3)-C(179)	81.71(9)	N(18)-Ce(4)-N(17)	54.05(13)
N(12)-Ce(3)-C(179)	127.81(9)	N(16)-Ce(4)-N(15)	54.34(12)
N(13)-Ce(3)-C(179)	101.07(9)	N(18)-Ce(4)-N(15)	94.36(12)
C(180)-Ce(3)-C(179)	27.71(13)	N(17)-Ce(4)-N(15)	126.19(12)
C(119)-Ce(3)-C(179)	87.61(11)	N(16)-Ce(4)-C(175)	125.05(10)
C(174)-Ce(3)-C(179)	71.36(12)	N(18)-Ce(4)-C(175)	108.36(10)
C(178)-Ce(3)-C(179)	28.24(13)	N(17)-Ce(4)-C(175)	139.28(10)
N(11)-Ce(3)-C(101)	27.25(8)	N(15)-Ce(4)-C(175)	87.90(9)
N(14)-Ce(3)-C(101)	107.63(9)	N(16)-Ce(4)-C(173)	82.59(9)
N(12)-Ce(3)-C(101)	27.30(8)	N(18)-Ce(4)-C(173)	161.82(9)
N(13)-Ce(3)-C(101)	106.10(9)	N(17)-Ce(4)-C(173)	137.85(10)
C(180)-Ce(3)-C(101)	162.11(11)	N(15)-Ce(4)-C(173)	86.11(9)
C(119)-Ce(3)-C(101)	113.21(10)	C(175)-Ce(4)-C(173)	53.47(14)
C(174)-Ce(3)-C(101)	109.65(13)	N(16)-Ce(4)-C(174)	99.19(10)
C(178)-Ce(3)-C(101)	123.34(12)	N(18)-Ce(4)-C(174)	134.33(11)
C(179)-Ce(3)-C(101)	151.56(12)	N(17)-Ce(4)-C(174)	156.04(9)
N(11)-Ce(3)-C(173)	113.34(10)	N(15)-Ce(4)-C(174)	77.69(8)
N(14)-Ce(3)-C(173)	112.64(10)	C(175)-Ce(4)-C(174)	27.91(14)

C(173)-Ce(4)-C(174)	28.27(14)	C(175)-Ce(4)-C(179)	78.42(11)
N(16)-Ce(4)-C(177)	154.72(9)	C(173)-Ce(4)-C(179)	53.10(13)
N(18)-Ce(4)-C(177)	89.63(9)	C(174)-Ce(4)-C(179)	71.30(13)
N(17)-Ce(4)-C(177)	87.96(9)	C(177)-Ce(4)-C(179)	52.99(12)
N(15)-Ce(4)-C(177)	139.54(9)	C(180)-Ce(4)-C(179)	27.61(13)
C(175)-Ce(4)-C(177)	52.98(12)	C(176)-Ce(4)-C(179)	71.37(12)
C(173)-Ce(4)-C(177)	78.52(11)	C(137)-Ce(4)-C(179)	121.55(12)
C(174)-Ce(4)-C(177)	71.10(12)	C(1)-N(1)-C(7)	123.8(4)
N(16)-Ce(4)-C(180)	84.41(9)	C(1)-N(1)-Ce(1)	93.7(3)
N(18)-Ce(4)-C(180)	156.07(10)	C(7)-N(1)-Ce(1)	142.4(3)
N(17)-Ce(4)-C(180)	109.68(10)	C(1)-N(2)-C(13)	122.6(4)
N(15)-Ce(4)-C(180)	109.47(10)	C(1)-N(2)-Ce(1)	94.1(3)
C(175)-Ce(4)-C(180)	71.54(13)	C(13)-N(2)-Ce(1)	143.1(3)
C(173)-Ce(4)-C(180)	28.19(13)	C(19)-N(3)-C(25)	119.2(4)
C(174)-Ce(4)-C(180)	53.21(14)	C(19)-N(3)-Ce(1)	91.4(3)
C(177)-Ce(4)-C(180)	71.02(12)	C(25)-N(3)-Ce(1)	149.0(3)
N(16)-Ce(4)-C(176)	152.64(9)	C(19)-N(4)-C(31)	120.7(4)
N(18)-Ce(4)-C(176)	90.91(9)	C(19)-N(4)-Ce(1)	95.6(3)
N(17)-Ce(4)-C(176)	110.76(9)	C(31)-N(4)-Ce(1)	143.6(3)
N(15)-Ce(4)-C(176)	112.07(10)	C(37)-N(5)-C(43)	119.4(3)
C(175)-Ce(4)-C(176)	28.52(13)	C(37)-N(5)-Ce(2)	94.8(2)
C(173)-Ce(4)-C(176)	72.21(12)	C(43)-N(5)-Ce(2)	144.7(3)
C(174)-Ce(4)-C(176)	53.45(12)	C(37)-N(6)-C(49)	118.9(3)
C(177)-Ce(4)-C(176)	27.51(12)	C(37)-N(6)-Ce(2)	93.0(2)
C(180)-Ce(4)-C(176)	78.44(11)	C(49)-N(6)-Ce(2)	148.0(3)
N(16)-Ce(4)-C(137)	27.26(9)	C(55)-N(7)-C(67)	116.7(4)
N(18)-Ce(4)-C(137)	105.37(9)	C(55)-N(7)-Ce(2)	93.1(3)
N(17)-Ce(4)-C(137)	112.87(9)	C(67)-N(7)-Ce(2)	147.5(3)
N(15)-Ce(4)-C(137)	27.09(8)	C(55)-N(8)-C(61)	117.1(4)
C(175)-Ce(4)-C(137)	107.14(13)	C(55)-N(8)-Ce(2)	93.1(3)
C(173)-Ce(4)-C(137)	83.11(11)	C(61)-N(8)-Ce(2)	147.6(3)
C(174)-Ce(4)-C(137)	87.74(12)	C(101)-N(11)-C(107)	119.2(2)
C(177)-Ce(4)-C(137)	158.83(11)	C(101)-N(11)-Ce(3)	94.44(17)
C(180)-Ce(4)-C(137)	97.18(12)	C(107)-N(11)-Ce(3)	146.0(2)
C(176)-Ce(4)-C(137)	134.86(13)	C(101)-N(12)-C(113)	118.2(2)
N(16)-Ce(4)-C(179)	102.01(9)	C(101)-N(12)-Ce(3)	93.57(17)
N(18)-Ce(4)-C(179)	128.56(10)	C(113)-N(12)-Ce(3)	148.1(2)
N(17)-Ce(4)-C(179)	86.96(9)	C(119)-N(13)-C(125)	115.8(3)
N(15)-Ce(4)-C(179)	137.07(9)	C(119)-N(13)-Ce(3)	91.45(17)

C(125)-N(13)-Ce(3)	149.5(2)	C(18)-C(13)-C(14)	110.7(4)
C(119)-N(14)-C(131)	117.8(3)	C(15)-C(14)-C(13)	111.5(4)
C(119)-N(14)-Ce(3)	92.85(18)	C(16)-C(15)-C(14)	112.6(4)
C(131)-N(14)-Ce(3)	147.1(2)	C(15)-C(16)-C(17)	110.2(4)
C(137)-N(15)-C(143)	118.8(2)	C(16)-C(17)-C(18)	110.0(4)
C(137)-N(15)-Ce(4)	92.66(17)	C(13)-C(18)-C(17)	112.6(4)
C(143)-N(15)-Ce(4)	148.5(2)	N(4)-C(19)-N(3)	117.8(4)
C(137)-N(16)-C(149)	119.8(3)	N(4)-C(19)-C(20)	120.5(4)
C(137)-N(16)-Ce(4)	94.55(18)	N(3)-C(19)-C(20)	121.7(4)
C(149)-N(16)-Ce(4)	145.6(2)	N(4)-C(19)-Ce(1)	57.2(2)
C(155)-N(17)-C(167)	119.7(3)	N(3)-C(19)-Ce(1)	61.1(2)
C(155)-N(17)-Ce(4)	93.9(2)	C(20)-C(19)-Ce(1)	170.9(3)
C(167)-N(17)-Ce(4)	146.2(3)	C(21)-C(20)-C(19)	175.0(5)
C(155)-N(18)-C(161)	118.2(3)	C(20)-C(21)-C(22)	179.4(5)
C(155)-N(18)-Ce(4)	94.68(19)	C(21)-C(22)-C(24)	119.3(5)
C(161)-N(18)-Ce(4)	146.9(2)	C(21)-C(22)-C(23)	118.8(4)
N(1)-C(1)-N(2)	118.3(4)	C(24)-C(22)-C(23)	59.0(3)
N(1)-C(1)-C(2)	123.0(4)	C(24)-C(23)-C(22)	60.0(3)
N(2)-C(1)-C(2)	118.7(4)	C(23)-C(24)-C(22)	61.0(3)
N(1)-C(1)-Ce(1)	59.9(2)	N(3)-C(25)-C(26)	110.4(4)
N(2)-C(1)-Ce(1)	58.5(2)	N(3)-C(25)-C(30)	111.3(4)
C(2)-C(1)-Ce(1)	177.1(3)	C(26)-C(25)-C(30)	110.5(4)
C(3)-C(2)-C(1)	175.5(5)	C(25)-C(26)-C(27)	112.3(4)
C(2)-C(3)-C(4)	175.5(5)	C(26)-C(27)-C(28)	110.6(4)
C(3)-C(4)-C(6)	117.0(4)	C(29)-C(28)-C(27)	110.4(4)
C(3)-C(4)-C(5)	117.6(4)	C(28)-C(29)-C(30)	111.1(5)
C(6)-C(4)-C(5)	58.7(3)	C(29)-C(30)-C(25)	110.6(4)
C(6)-C(5)-C(4)	60.4(3)	N(4)-C(31)-C(36)	110.8(3)
C(5)-C(6)-C(4)	60.9(3)	N(4)-C(31)-C(32)	109.1(3)
C(8)-C(7)-N(1)	116.0(4)	C(36)-C(31)-C(32)	110.6(3)
C(8)-C(7)-C(12)	115.9(4)	C(33)-C(32)-C(31)	111.2(3)
N(1)-C(7)-C(12)	113.7(4)	C(32)-C(33)-C(34)	110.4(3)
C(7)-C(8)-C(9)	107.7(5)	C(35)-C(34)-C(33)	110.3(4)
C(10)-C(9)-C(8)	110.3(5)	C(34)-C(35)-C(36)	111.8(3)
C(11)-C(10)-C(9)	109.9(5)	C(31)-C(36)-C(35)	112.9(3)
C(10)-C(11)-C(12)	113.7(5)	N(6)-C(37)-N(5)	117.8(4)
C(7)-C(12)-C(11)	110.8(4)	N(6)-C(37)-C(38)	122.2(4)
N(2)-C(13)-C(18)	110.7(3)	N(5)-C(37)-C(38)	119.9(4)
N(2)-C(13)-C(14)	112.0(4)	N(6)-C(37)-Ce(2)	60.0(2)

N(5)-C(37)-Ce(2)	58.2(2)	N(8)-C(61)-C(66)	111.8(3)
C(38)-C(37)-Ce(2)	171.1(3)	C(62)-C(61)-C(66)	109.2(3)
C(39)-C(38)-C(37)	170.3(4)	C(61)-C(62)-C(63)	111.1(4)
C(38)-C(39)-C(40)	175.3(5)	C(64)-C(63)-C(62)	111.3(4)
C(39)-C(40)-C(42)	117.6(4)	C(65)-C(64)-C(63)	110.5(4)
C(39)-C(40)-C(41)	118.6(4)	C(64)-C(65)-C(66)	112.6(4)
C(42)-C(40)-C(41)	58.7(4)	C(65)-C(66)-C(61)	109.5(4)
C(42)-C(41)-C(40)	60.6(3)	N(7)-C(67)-C(72)	110.3(3)
C(41)-C(42)-C(40)	60.7(4)	N(7)-C(67)-C(68)	111.0(3)
N(5)-C(43)-C(44)	111.2(3)	C(72)-C(67)-C(68)	110.3(3)
N(5)-C(43)-C(48)	110.8(3)	C(69)-C(68)-C(67)	112.1(4)
C(44)-C(43)-C(48)	111.0(3)	C(68)-C(69)-C(70)	112.0(4)
C(43)-C(44)-C(45)	112.6(4)	C(71)-C(70)-C(69)	110.5(4)
C(46)-C(45)-C(44)	111.3(4)	C(70)-C(71)-C(72)	110.7(4)
C(47)-C(46)-C(45)	111.4(4)	C(67)-C(72)-C(71)	112.0(4)
C(46)-C(47)-C(48)	111.0(4)	C(80)-C(73)-C(74)	135.7(4)
C(47)-C(48)-C(43)	111.2(3)	C(80)-C(73)-Ce(2)	77.0(3)
N(6)-C(49)-C(50)	112.5(3)	C(74)-C(73)-Ce(2)	77.3(3)
N(6)-C(49)-C(54)	109.9(3)	C(80)-C(73)-Ce(1)	75.6(2)
C(50)-C(49)-C(54)	110.2(3)	C(74)-C(73)-Ce(1)	75.7(3)
C(49)-C(50)-C(51)	111.5(3)	Ce(2)-C(73)-Ce(1)	102.70(14)
C(52)-C(51)-C(50)	111.6(3)	C(73)-C(74)-C(75)	134.0(4)
C(51)-C(52)-C(53)	111.3(3)	C(73)-C(74)-Ce(1)	76.1(2)
C(52)-C(53)-C(54)	110.6(3)	C(75)-C(74)-Ce(1)	77.0(3)
C(49)-C(54)-C(53)	111.5(3)	C(73)-C(74)-Ce(2)	74.5(2)
N(7)-C(55)-N(8)	117.0(4)	C(75)-C(74)-Ce(2)	75.5(2)
N(7)-C(55)-C(56)	122.2(4)	Ce(1)-C(74)-Ce(2)	101.97(13)
N(8)-C(55)-C(56)	120.8(4)	C(76)-C(75)-C(74)	135.6(4)
N(7)-C(55)-Ce(2)	59.6(2)	C(76)-C(75)-Ce(2)	77.1(2)
N(8)-C(55)-Ce(2)	59.6(2)	C(74)-C(75)-Ce(2)	76.3(2)
C(56)-C(55)-Ce(2)	163.8(3)	C(76)-C(75)-Ce(1)	76.6(2)
C(57)-C(56)-C(55)	177.4(5)	C(74)-C(75)-Ce(1)	74.8(2)
C(56)-C(57)-C(58)	179.0(5)	Ce(2)-C(75)-Ce(1)	101.51(13)
C(57)-C(58)-C(60)	120.8(5)	C(77)-C(76)-C(75)	135.8(4)
C(57)-C(58)-C(59)	119.2(5)	C(77)-C(76)-Ce(2)	76.1(2)
C(60)-C(58)-C(59)	59.1(4)	C(75)-C(76)-Ce(2)	75.0(2)
C(60)-C(59)-C(58)	60.2(4)	C(77)-C(76)-Ce(1)	77.7(2)
C(59)-C(60)-C(58)	60.6(4)	C(75)-C(76)-Ce(1)	75.7(2)
N(8)-C(61)-C(62)	110.2(3)	Ce(2)-C(76)-Ce(1)	100.58(13)

C(76)-C(77)-C(78)	133.7(4)	C(112)-C(107)-C(108)	111.1(3)
C(76)-C(77)-Ce(2)	76.1(2)	C(109)-C(108)-C(107)	111.2(4)
C(78)-C(77)-Ce(2)	75.9(2)	C(110)-C(109)-C(108)	111.2(4)
C(76)-C(77)-Ce(1)	74.8(2)	C(109)-C(110)-C(111)	109.7(4)
C(78)-C(77)-Ce(1)	74.4(2)	C(110)-C(111)-C(112)	110.7(4)
Ce(2)-C(77)-Ce(1)	99.74(14)	C(107)-C(112)-C(111)	111.4(3)
C(79)-C(78)-C(77)	135.1(4)	N(12)-C(113)-C(118)	109.7(3)
C(79)-C(78)-Ce(2)	74.7(2)	N(12)-C(113)-C(114)	112.6(3)
C(77)-C(78)-Ce(2)	75.8(2)	C(118)-C(113)-C(114)	109.9(3)
C(79)-C(78)-Ce(1)	75.4(2)	C(115)-C(114)-C(113)	111.0(3)
C(77)-C(78)-Ce(1)	77.7(2)	C(116)-C(115)-C(114)	111.9(3)
Ce(2)-C(78)-Ce(1)	100.69(12)	C(115)-C(116)-C(117)	111.3(4)
C(80)-C(79)-C(78)	135.7(4)	C(116)-C(117)-C(118)	112.1(4)
C(80)-C(79)-Ce(2)	76.2(3)	C(117)-C(118)-C(113)	111.4(3)
C(78)-C(79)-Ce(2)	77.2(3)	N(14)-C(119)-N(13)	119.0(3)
C(80)-C(79)-Ce(1)	75.1(2)	N(14)-C(119)-C(120)	119.9(3)
C(78)-C(79)-Ce(1)	76.6(2)	N(13)-C(119)-C(120)	121.0(3)
Ce(2)-C(79)-Ce(1)	101.78(14)	N(14)-C(119)-Ce(3)	59.86(15)
C(73)-C(80)-C(79)	134.0(4)	N(13)-C(119)-Ce(3)	61.14(15)
C(73)-C(80)-Ce(1)	76.1(2)	C(120)-C(119)-Ce(3)	161.8(3)
C(79)-C(80)-Ce(1)	76.8(2)	C(121)-C(120)-C(119)	175.5(4)
C(73)-C(80)-Ce(2)	74.7(3)	C(120)-C(121)-C(122)	177.9(5)
C(79)-C(80)-Ce(2)	75.6(3)	C(121)-C(122)-C(124)	119.7(4)
Ce(1)-C(80)-Ce(2)	102.13(14)	C(121)-C(122)-C(123)	119.0(4)
N(11)-C(101)-N(12)	117.1(3)	C(124)-C(122)-C(123)	58.8(3)
N(11)-C(101)-C(102)	120.4(3)	C(124)-C(123)-C(122)	60.5(3)
N(12)-C(101)-C(102)	122.5(3)	C(123)-C(124)-C(122)	60.7(3)
N(11)-C(101)-Ce(3)	58.31(14)	N(13)-C(125)-C(130)	110.4(3)
N(12)-C(101)-Ce(3)	59.12(15)	N(13)-C(125)-C(126)	111.6(3)
C(102)-C(101)-Ce(3)	172.1(3)	C(130)-C(125)-C(126)	110.1(4)
C(103)-C(102)-C(101)	172.9(4)	C(125)-C(126)-C(127)	110.7(4)
C(102)-C(103)-C(104)	174.2(4)	C(128)-C(127)-C(126)	110.9(5)
C(103)-C(104)-C(105)	118.5(4)	C(129)-C(128)-C(127)	111.8(4)
C(103)-C(104)-C(106)	116.9(4)	C(128)-C(129)-C(130)	111.6(4)
C(105)-C(104)-C(106)	58.4(3)	C(125)-C(130)-C(129)	110.0(4)
C(106)-C(105)-C(104)	61.1(3)	N(14)-C(131)-C(136)	111.7(3)
C(105)-C(106)-C(104)	60.5(3)	N(14)-C(131)-C(132)	111.0(3)
N(11)-C(107)-C(112)	108.4(3)	C(136)-C(131)-C(132)	110.6(3)
N(11)-C(107)-C(108)	111.5(3)	C(131)-C(132)-C(133)	110.2(4)

C(134)-C(133)-C(132)	111.6(4)	C(157)-C(156)-C(155)	177.2(5)
C(133)-C(134)-C(135)	111.4(4)	C(156)-C(157)-C(158)	175.3(5)
C(134)-C(135)-C(136)	111.8(4)	C(157)-C(158)-C(160)	117.4(4)
C(131)-C(136)-C(135)	109.9(3)	C(157)-C(158)-C(159)	118.1(4)
N(15)-C(137)-N(16)	118.4(3)	C(160)-C(158)-C(159)	59.8(3)
N(15)-C(137)-C(138)	121.0(3)	C(160)-C(159)-C(158)	59.8(3)
N(16)-C(137)-C(138)	120.6(3)	C(159)-C(160)-C(158)	60.4(3)
N(15)-C(137)-Ce(4)	60.25(15)	N(18)-C(161)-C(162)	113.4(3)
N(16)-C(137)-Ce(4)	58.19(15)	N(18)-C(161)-C(166)	108.7(3)
C(138)-C(137)-Ce(4)	177.4(3)	C(162)-C(161)-C(166)	110.3(4)
C(139)-C(138)-C(137)	179.5(5)	C(161)-C(162)-C(163)	110.0(4)
C(138)-C(139)-C(140)	178.6(5)	C(164)-C(163)-C(162)	111.2(4)
C(139)-C(140)-C(141)	117.9(4)	C(165)-C(164)-C(163)	110.4(4)
C(139)-C(140)-C(142)	118.1(4)	C(164)-C(165)-C(166)	111.7(4)
C(141)-C(140)-C(142)	58.3(3)	C(165)-C(166)-C(161)	111.2(4)
C(142)-C(141)-C(140)	61.1(3)	C(172)-C(167)-N(17)	115.9(4)
C(141)-C(142)-C(140)	60.6(3)	C(172)-C(167)-C(168)	116.0(5)
N(15)-C(143)-C(148)	111.6(3)	N(17)-C(167)-C(168)	114.1(4)
N(15)-C(143)-C(144)	109.9(3)	C(167)-C(168)-C(169)	114.0(5)
C(148)-C(143)-C(144)	110.2(4)	C(170)-C(169)-C(168)	116.1(6)
C(145)-C(144)-C(143)	111.9(4)	C(169)-C(170)-C(171)	110.3(6)
C(146)-C(145)-C(144)	110.6(4)	C(172)-C(171)-C(170)	106.4(6)
C(147)-C(146)-C(145)	111.4(4)	C(167)-C(172)-C(171)	115.2(6)
C(146)-C(147)-C(148)	111.3(4)	C(180)-C(173)-C(174)	133.6(4)
C(143)-C(148)-C(147)	112.2(4)	C(180)-C(173)-Ce(4)	76.2(3)
N(16)-C(149)-C(154)	110.7(3)	C(174)-C(173)-Ce(4)	76.0(3)
N(16)-C(149)-C(150)	108.8(3)	C(180)-C(173)-Ce(3)	75.1(2)
C(154)-C(149)-C(150)	110.3(3)	C(174)-C(173)-Ce(3)	75.5(2)
C(151)-C(150)-C(149)	112.4(3)	Ce(4)-C(173)-Ce(3)	102.29(14)
C(152)-C(151)-C(150)	111.7(4)	C(175)-C(174)-C(173)	135.6(4)
C(153)-C(152)-C(151)	110.5(4)	C(175)-C(174)-Ce(4)	75.8(3)
C(152)-C(153)-C(154)	110.8(3)	C(173)-C(174)-Ce(4)	75.7(3)
C(153)-C(154)-C(149)	111.1(3)	C(175)-C(174)-Ce(3)	77.4(2)
N(17)-C(155)-N(18)	117.3(3)	C(173)-C(174)-Ce(3)	76.4(2)
N(17)-C(155)-C(156)	122.1(4)	Ce(4)-C(174)-Ce(3)	102.49(14)
N(18)-C(155)-C(156)	120.6(4)	C(174)-C(175)-C(176)	135.0(4)
N(17)-C(155)-Ce(4)	59.15(17)	C(174)-C(175)-Ce(4)	76.3(2)
N(18)-C(155)-Ce(4)	58.16(15)	C(176)-C(175)-Ce(4)	76.3(2)
C(156)-C(155)-Ce(4)	177.5(3)	C(174)-C(175)-Ce(3)	74.9(2)

C(176)-C(175)-Ce(3)	76.7(2)
Ce(4)-C(175)-Ce(3)	101.84(12)
C(177)-C(176)-C(175)	133.7(4)
C(177)-C(176)-Ce(4)	76.0(2)
C(175)-C(176)-Ce(4)	75.1(2)
C(177)-C(176)-Ce(3)	75.8(2)
C(175)-C(176)-Ce(3)	75.2(2)
Ce(4)-C(176)-Ce(3)	101.00(13)
C(176)-C(177)-C(178)	136.7(4)
C(176)-C(177)-Ce(4)	76.5(2)
C(178)-C(177)-Ce(4)	77.6(2)
C(176)-C(177)-Ce(3)	77.1(2)
C(178)-C(177)-Ce(3)	74.9(2)
Ce(4)-C(177)-Ce(3)	101.55(13)
C(177)-C(178)-C(179)	134.5(4)
C(177)-C(178)-Ce(3)	77.5(2)
C(179)-C(178)-Ce(3)	76.0(2)
C(177)-C(178)-Ce(4)	74.7(2)
C(179)-C(178)-Ce(4)	75.2(2)
Ce(3)-C(178)-Ce(4)	101.46(14)
C(180)-C(179)-C(178)	134.5(4)
C(180)-C(179)-Ce(3)	75.4(2)
C(178)-C(179)-Ce(3)	75.7(2)
C(180)-C(179)-Ce(4)	75.6(2)
C(178)-C(179)-Ce(4)	76.8(2)
Ce(3)-C(179)-Ce(4)	101.84(12)
C(179)-C(180)-C(173)	136.1(4)
C(179)-C(180)-Ce(3)	76.9(2)
C(173)-C(180)-Ce(3)	76.8(2)
C(179)-C(180)-Ce(4)	76.8(3)
C(173)-C(180)-Ce(4)	75.6(3)
Ce(3)-C(180)-Ce(4)	102.62(14)

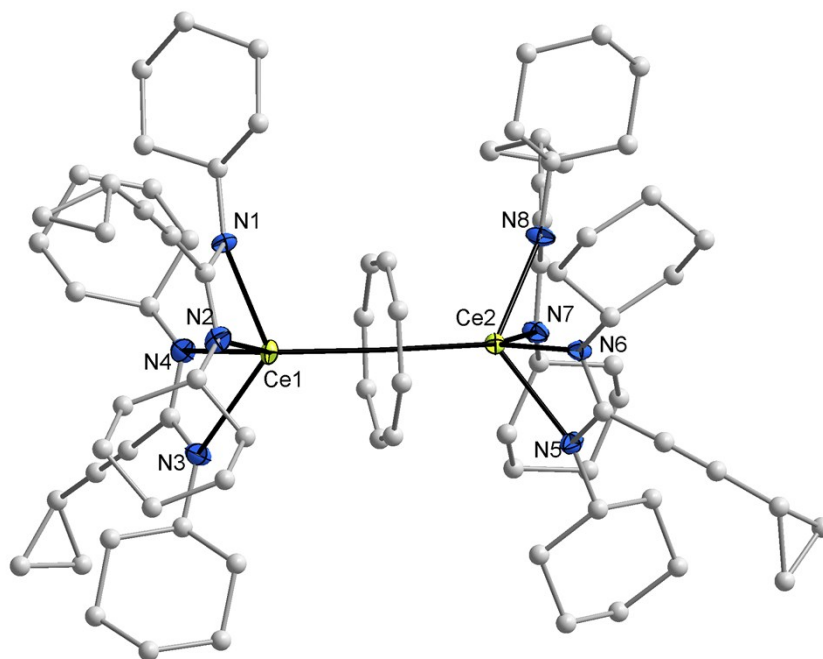


Figure S7. Molecular structure of $(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})[\text{Ce}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{NCy})_2)_2]_2$ (**8**) in the crystal (molecule 1 of 2 in the asymmetric unit). Ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

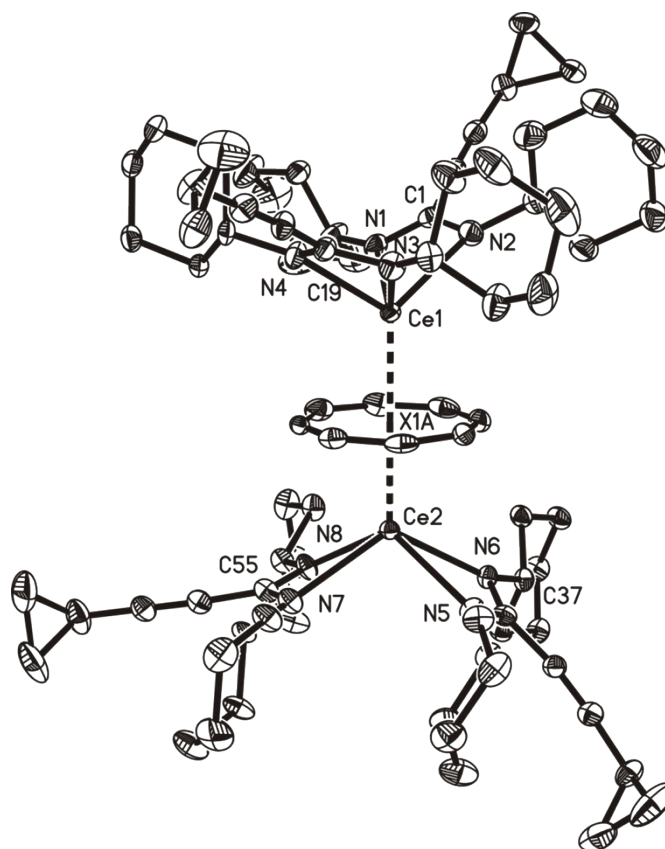


Figure S8. ORTEP drawing of $(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})[\text{Ce}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{NCy})_2)_2]_2$ (**8**).

NMR spectra (toluene-*d*₈, 25 °C) of **(9)**

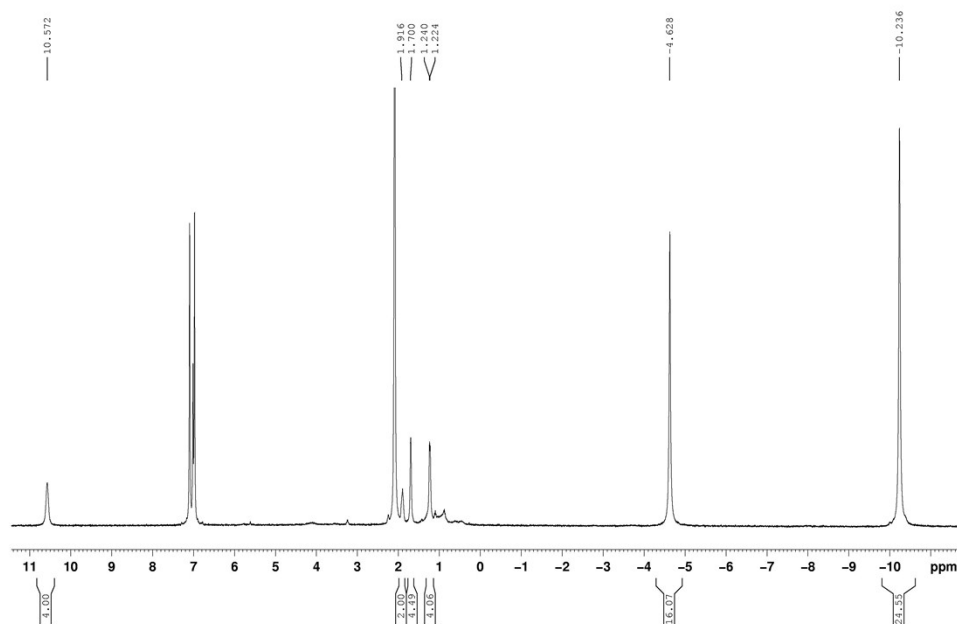


Figure S9. ¹H NMR spectrum (toluene-*d*₈, 25°C) of [(COT)Pr(*μ*-*c*-C₃H₅-C≡C-C(N^{*i*}Pr)₂)]₂ (**9**).

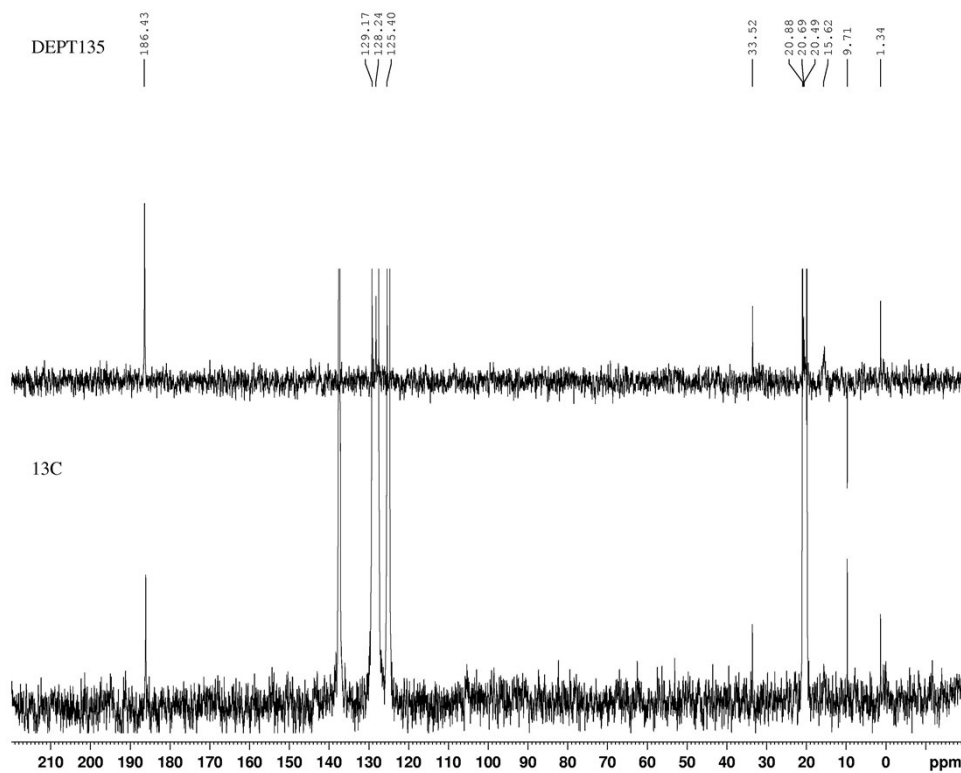


Figure S10. ¹³C NMR and dept spectrum (toluene-*d*₈, 25°C) of [(COT)Pr(*μ*-*c*-C₃H₅-C≡C-C(N^{*i*}Pr)₂)]₂ (**9**).

(^1H - ^{13}C) HSQC experiment of (**9**)

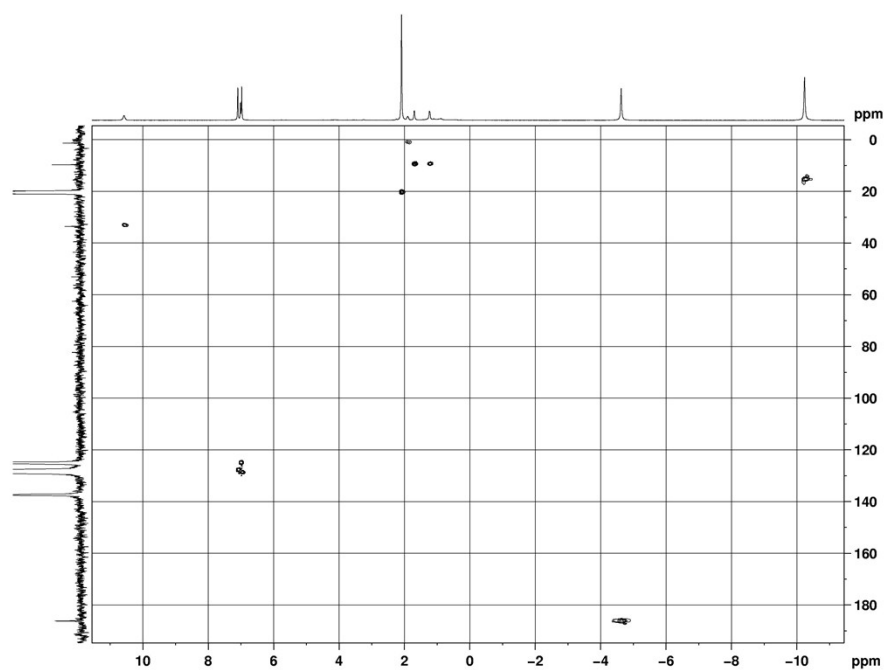


Figure S11. HSQC (^1H , ^{13}C - correlation via 1J (^{13}C , ^1H)) spectrum (toluene- d_8 , 25°C) of $[(\text{COT})\text{Pr}(\mu\text{-}i\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)]_2$ (**9**)

Table S9. Crystal data and structure refinement (10).

Identification code	magd126	
Empirical formula	C ₄₀ H ₅₄ Ce ₂ N ₄	
Formula weight	871.11	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 19.23876(16) Å	α = 90°
	b = 19.87633(16) Å	β = 99.8124(9)°
	c = 9.97581(10) Å	γ = 90°
Volume	3758.90(6) Å ³	
Z	4	
Density (calculated)	1.539 Mg/m ³	
Absorption coefficient	18.699 mm ⁻¹	
F(000)	1752	
Crystal size	0.28 x 0.08 x 0.06 mm ³	
Theta range for data collection	3.22 to 75.90°	
Index ranges	-24 ≤ h ≤ 24, -24 ≤ k ≤ 24, -12 ≤ l ≤ 10	
Reflections collected	157545	
Independent reflections	7809 [R(int) = 0.0744]	
Completeness to theta = 75.90°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4000 and 0.0775	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7809 / 54 / 441	
Goodness-of-fit on F ²	1.130	
Final R indices [I > 2σ(I)]	R1 = 0.0442, wR2 = 0.1077	
R indices (all data)	R1 = 0.0462, wR2 = 0.1091	
Largest diff. peak and hole	1.229 and -1.555 e.Å ⁻³	

Table S10. Bond lengths [Å] and angles [°] (**10**).

Ce(1)-N(2)#1	2.625(5)	N(4)-Ce(2)#2	2.754(4)
Ce(1)-N(1)#1	2.634(4)	C(1)-C(2)	1.452(7)
Ce(1)-N(1)	2.664(4)	C(1)-Ce(1)#1	3.000(5)
Ce(1)-C(18)	2.694(7)	C(2)-C(3)	1.194(8)
Ce(1)-C(19)	2.694(7)	C(3)-C(4)	1.443(7)
Ce(1)-C(13)	2.702(5)	C(4)-C(6)	1.501(8)
Ce(1)-C(17)	2.705(6)	C(4)-C(5)	1.505(8)
Ce(1)-C(14)	2.706(6)	C(5)-C(6)	1.488(10)
Ce(1)-C(16)	2.712(6)	C(7)-C(9)	1.516(8)
Ce(1)-C(20)	2.712(6)	C(7)-C(8)	1.526(8)
Ce(1)-C(15)	2.713(6)	C(10)-C(12)	1.512(13)
Ce(1)-C(1)#1	3.000(5)	C(10)-C(11)	1.558(13)
Ce(2)-N(4)	2.683(4)	C(10')-C(11')	1.29(4)
Ce(2)-N(3)	2.685(5)	C(10')-C(12')	1.57(4)
Ce(2)-C(40)	2.689(8)	C(13)-C(20)	1.376(10)
Ce(2)-C(38)	2.691(8)	C(13)-C(14)	1.399(9)
Ce(2)-C(37)	2.691(7)	C(14)-C(15)	1.403(8)
Ce(2)-N(3)#2	2.694(5)	C(15)-C(16)	1.400(10)
Ce(2)-C(39)	2.695(8)	C(16)-C(17)	1.381(11)
Ce(2)-C(36)	2.696(6)	C(17)-C(18)	1.414(11)
Ce(2)-C(35)	2.701(6)	C(18)-C(19)	1.430(11)
Ce(2)-C(34)	2.705(7)	C(19)-C(20)	1.402(10)
Ce(2)-C(33)	2.714(8)	C(21)-C(22)	1.443(7)
Ce(2)-N(4)#2	2.754(4)	C(21)-Ce(2)#2	2.942(5)
N(1)-C(1)	1.350(8)	C(22)-C(23)	1.201(8)
N(1)-C(7)	1.487(7)	C(23)-C(24)	1.433(7)
N(1)-Ce(1)#1	2.635(4)	C(24)-C(25)	1.502(7)
N(2)-C(1)	1.321(9)	C(24)-C(26)	1.506(7)
N(2)-C(10')	1.41(3)	C(25)-C(26)	1.472(9)
N(2)-C(10)	1.611(11)	C(27)-C(29)	1.513(12)
N(2)-Ce(1)#1	2.625(5)	C(27)-C(28)	1.512(13)
N(3)-C(21)	1.342(7)	C(27')-C(28')	1.45(3)
N(3)-C(27')	1.503(15)	C(27')-C(29')	1.47(2)
N(3)-C(27)	1.552(9)	C(30)-C(31)	1.505(8)
N(3)-Ce(2)#2	2.694(5)	C(30)-C(32)	1.529(7)
N(4)-C(21)	1.342(6)	C(33)-C(40)	1.336(16)
N(4)-C(30)	1.486(6)	C(33)-C(34)	1.391(12)

C(34)-C(35)	1.399(9)	C(37)-C(38)	1.465(15)
C(35)-C(36)	1.393(9)	C(38)-C(39)	1.459(17)
C(36)-C(37)	1.394(10)	C(39)-C(40)	1.302(17)
N(2)#1-Ce(1)-N(1)#1	51.08(19)	C(14)-Ce(1)-C(16)	56.9(2)
N(2)#1-Ce(1)-N(1)	81.40(18)	N(2)#1-Ce(1)-C(20)	115.8(2)
N(1)#1-Ce(1)-N(1)	89.93(14)	N(1)#1-Ce(1)-C(20)	166.0(2)
N(2)#1-Ce(1)-C(18)	94.1(3)	N(1)-Ce(1)-C(20)	92.62(17)
N(1)#1-Ce(1)-C(18)	114.1(2)	C(18)-Ce(1)-C(20)	58.1(2)
N(1)-Ce(1)-C(18)	145.1(2)	C(19)-Ce(1)-C(20)	30.1(2)
N(2)#1-Ce(1)-C(19)	98.3(3)	C(13)-Ce(1)-C(20)	29.4(2)
N(1)#1-Ce(1)-C(19)	138.4(2)	C(17)-Ce(1)-C(20)	78.33(19)
N(1)-Ce(1)-C(19)	115.3(2)	C(14)-Ce(1)-C(20)	56.6(2)
C(18)-Ce(1)-C(19)	30.8(2)	C(16)-Ce(1)-C(20)	85.4(2)
N(2)#1-Ce(1)-C(13)	141.51(19)	N(2)#1-Ce(1)-C(15)	157.70(18)
N(1)#1-Ce(1)-C(13)	164.44(17)	N(1)#1-Ce(1)-C(15)	113.47(17)
N(1)-Ce(1)-C(13)	84.63(15)	N(1)-Ce(1)-C(15)	117.31(19)
C(18)-Ce(1)-C(13)	77.6(2)	C(18)-Ce(1)-C(15)	77.4(3)
C(19)-Ce(1)-C(13)	56.5(2)	C(19)-Ce(1)-C(15)	84.9(3)
N(2)#1-Ce(1)-C(17)	106.4(2)	C(13)-Ce(1)-C(15)	57.34(18)
N(1)#1-Ce(1)-C(17)	99.91(17)	C(17)-Ce(1)-C(15)	56.8(2)
N(1)-Ce(1)-C(17)	169.94(17)	C(14)-Ce(1)-C(15)	30.01(18)
C(18)-Ce(1)-C(17)	30.4(2)	C(16)-Ce(1)-C(15)	29.9(2)
C(19)-Ce(1)-C(17)	58.0(2)	C(20)-Ce(1)-C(15)	77.4(2)
C(13)-Ce(1)-C(17)	85.32(19)	N(2)#1-Ce(1)-C(1)#1	26.09(17)
N(2)#1-Ce(1)-C(14)	171.39(18)	N(1)#1-Ce(1)-C(1)#1	26.74(16)
N(1)#1-Ce(1)-C(14)	136.88(18)	N(1)-Ce(1)-C(1)#1	92.02(13)
N(1)-Ce(1)-C(14)	94.51(17)	C(18)-Ce(1)-C(1)#1	98.9(2)
C(18)-Ce(1)-C(14)	84.9(3)	C(19)-Ce(1)-C(1)#1	115.1(2)
C(19)-Ce(1)-C(14)	76.5(3)	C(13)-Ce(1)-C(1)#1	167.50(18)
C(13)-Ce(1)-C(14)	29.98(19)	C(17)-Ce(1)-C(1)#1	97.71(18)
C(17)-Ce(1)-C(14)	76.9(2)	C(14)-Ce(1)-C(1)#1	162.48(18)
N(2)#1-Ce(1)-C(16)	129.2(2)	C(16)-Ce(1)-C(1)#1	110.98(17)
N(1)#1-Ce(1)-C(16)	99.90(16)	C(20)-Ce(1)-C(1)#1	139.3(2)
N(1)-Ce(1)-C(16)	146.60(19)	C(15)-Ce(1)-C(1)#1	134.06(17)
C(18)-Ce(1)-C(16)	57.0(3)	N(4)-Ce(2)-N(3)	49.61(13)
C(19)-Ce(1)-C(16)	77.4(2)	N(4)-Ce(2)-C(40)	98.2(2)
C(13)-Ce(1)-C(16)	77.42(18)	N(3)-Ce(2)-C(40)	133.6(3)
C(17)-Ce(1)-C(16)	29.5(2)	N(4)-Ce(2)-C(38)	106.4(2)

N(3)-Ce(2)-C(38)	96.6(3)	C(36)-Ce(2)-C(34)	56.9(2)
C(40)-Ce(2)-C(38)	56.9(4)	C(35)-Ce(2)-C(34)	29.98(19)
N(4)-Ce(2)-C(37)	130.14(18)	N(4)-Ce(2)-C(33)	115.4(2)
N(3)-Ce(2)-C(37)	97.6(2)	N(3)-Ce(2)-C(33)	161.3(2)
C(40)-Ce(2)-C(37)	78.5(3)	C(40)-Ce(2)-C(33)	28.6(3)
C(38)-Ce(2)-C(37)	31.6(3)	C(38)-Ce(2)-C(33)	75.8(4)
N(4)-Ce(2)-N(3)#2	76.33(14)	C(37)-Ce(2)-C(33)	84.9(3)
N(3)-Ce(2)-N(3)#2	95.26(13)	N(3)#2-Ce(2)-C(33)	90.7(2)
C(40)-Ce(2)-N(3)#2	109.5(3)	C(39)-Ce(2)-C(33)	53.9(4)
C(38)-Ce(2)-N(3)#2	166.2(3)	C(36)-Ce(2)-C(33)	77.1(2)
C(37)-Ce(2)-N(3)#2	152.1(2)	C(35)-Ce(2)-C(33)	57.1(2)
N(4)-Ce(2)-C(39)	94.77(19)	C(34)-Ce(2)-C(33)	29.7(3)
N(3)-Ce(2)-C(39)	111.6(3)	N(4)-Ce(2)-N(4)#2	96.39(11)
C(40)-Ce(2)-C(39)	28.0(4)	N(3)-Ce(2)-N(4)#2	75.29(13)
C(38)-Ce(2)-C(39)	31.4(4)	C(40)-Ce(2)-N(4)#2	149.4(3)
C(37)-Ce(2)-C(39)	59.8(3)	C(38)-Ce(2)-N(4)#2	142.0(3)
N(3)#2-Ce(2)-C(39)	135.9(3)	C(37)-Ce(2)-N(4)#2	111.5(3)
N(4)-Ce(2)-C(36)	158.71(17)	N(3)#2-Ce(2)-N(4)#2	48.82(12)
N(3)-Ce(2)-C(36)	113.82(18)	C(39)-Ce(2)-N(4)#2	168.80(18)
C(40)-Ce(2)-C(36)	85.5(2)	C(36)-Ce(2)-N(4)#2	90.52(19)
C(38)-Ce(2)-C(36)	58.3(3)	C(35)-Ce(2)-N(4)#2	84.56(14)
C(37)-Ce(2)-C(36)	30.0(2)	C(34)-Ce(2)-N(4)#2	97.01(17)
N(3)#2-Ce(2)-C(36)	122.33(19)	C(33)-Ce(2)-N(4)#2	121.2(3)
C(39)-Ce(2)-C(36)	78.7(2)	C(1)-N(1)-C(7)	117.2(4)
N(4)-Ce(2)-C(35)	170.82(16)	C(1)-N(1)-Ce(1)#1	91.9(3)
N(3)-Ce(2)-C(35)	138.92(16)	C(7)-N(1)-Ce(1)#1	132.1(3)
C(40)-Ce(2)-C(35)	77.0(3)	C(1)-N(1)-Ce(1)	94.6(3)
C(38)-Ce(2)-C(35)	77.7(2)	C(7)-N(1)-Ce(1)	121.6(3)
C(37)-Ce(2)-C(35)	57.1(2)	Ce(1)#1-N(1)-Ce(1)	90.07(14)
N(3)#2-Ce(2)-C(35)	97.75(17)	C(1)-N(2)-C(10')	110.7(12)
C(39)-Ce(2)-C(35)	84.6(2)	C(1)-N(2)-C(10)	118.4(5)
C(36)-Ce(2)-C(35)	29.91(19)	C(10')-N(2)-C(10)	32.4(11)
N(4)-Ce(2)-C(34)	141.19(17)	C(1)-N(2)-Ce(1)#1	93.0(3)
N(3)-Ce(2)-C(34)	168.45(18)	C(10')-N(2)-Ce(1)#1	155.8(12)
C(40)-Ce(2)-C(34)	55.9(3)	C(10)-N(2)-Ce(1)#1	130.6(5)
C(38)-Ce(2)-C(34)	84.1(3)	C(21)-N(3)-C(27')	129.6(7)
C(37)-Ce(2)-C(34)	76.9(2)	C(21)-N(3)-C(27)	110.2(5)
N(3)#2-Ce(2)-C(34)	85.66(18)	C(27')-N(3)-C(27)	31.1(6)
C(39)-Ce(2)-C(34)	74.7(3)	C(21)-N(3)-Ce(2)	92.1(3)

C(27')-N(3)-Ce(2)	113.3(7)	C(20)-C(13)-Ce(1)	75.7(4)
C(27)-N(3)-Ce(2)	144.2(5)	C(14)-C(13)-Ce(1)	75.2(3)
C(21)-N(3)-Ce(2)#2	86.8(3)	C(13)-C(14)-C(15)	136.0(7)
C(27')-N(3)-Ce(2)#2	135.8(6)	C(13)-C(14)-Ce(1)	74.9(3)
C(27)-N(3)-Ce(2)#2	122.8(4)	C(15)-C(14)-Ce(1)	75.3(3)
Ce(2)-N(3)-Ce(2)#2	84.74(13)	C(16)-C(15)-C(14)	134.2(7)
C(21)-N(4)-C(30)	115.3(4)	C(16)-C(15)-Ce(1)	75.0(4)
C(21)-N(4)-Ce(2)	92.2(3)	C(14)-C(15)-Ce(1)	74.7(3)
C(30)-N(4)-Ce(2)	137.0(3)	C(17)-C(16)-C(15)	135.6(6)
C(21)-N(4)-Ce(2)#2	84.3(3)	C(17)-C(16)-Ce(1)	75.0(4)
C(30)-N(4)-Ce(2)#2	129.0(3)	C(15)-C(16)-Ce(1)	75.1(3)
Ce(2)-N(4)-Ce(2)#2	83.61(11)	C(16)-C(17)-C(18)	134.9(6)
N(2)-C(1)-N(1)	116.2(5)	C(16)-C(17)-Ce(1)	75.5(3)
N(2)-C(1)-C(2)	122.5(6)	C(18)-C(17)-Ce(1)	74.4(4)
N(1)-C(1)-C(2)	121.3(6)	C(17)-C(18)-C(19)	133.9(7)
N(2)-C(1)-Ce(1)#1	60.9(3)	C(17)-C(18)-Ce(1)	75.3(4)
N(1)-C(1)-Ce(1)#1	61.4(3)	C(19)-C(18)-Ce(1)	74.6(4)
C(2)-C(1)-Ce(1)#1	157.4(4)	C(20)-C(19)-C(18)	136.1(7)
N(2)-C(1)-Ce(1)	82.4(4)	C(20)-C(19)-Ce(1)	75.7(4)
N(1)-C(1)-Ce(1)	59.5(3)	C(18)-C(19)-Ce(1)	74.6(4)
C(2)-C(1)-Ce(1)	125.7(4)	C(13)-C(20)-C(19)	133.6(6)
Ce(1)#1-C(1)-Ce(1)	76.10(12)	C(13)-C(20)-Ce(1)	74.9(3)
C(3)-C(2)-C(1)	171.4(6)	C(19)-C(20)-Ce(1)	74.3(4)
C(2)-C(3)-C(4)	179.0(7)	N(4)-C(21)-N(3)	114.1(4)
C(3)-C(4)-C(6)	119.8(5)	N(4)-C(21)-C(22)	122.2(5)
C(3)-C(4)-C(5)	118.6(5)	N(3)-C(21)-C(22)	123.6(5)
C(6)-C(4)-C(5)	59.3(5)	N(4)-C(21)-Ce(2)#2	68.7(3)
C(6)-C(5)-C(4)	60.2(4)	N(3)-C(21)-Ce(2)#2	66.1(3)
C(5)-C(6)-C(4)	60.5(4)	C(22)-C(21)-Ce(2)#2	131.6(4)
N(1)-C(7)-C(9)	108.6(5)	N(4)-C(21)-Ce(2)	61.7(3)
N(1)-C(7)-C(8)	111.0(4)	N(3)-C(21)-Ce(2)	61.7(3)
C(9)-C(7)-C(8)	110.6(5)	C(22)-C(21)-Ce(2)	153.9(4)
C(12)-C(10)-C(11)	113.4(8)	Ce(2)#2-C(21)-Ce(2)	74.49(11)
C(12)-C(10)-N(2)	114.6(7)	C(23)-C(22)-C(21)	176.5(6)
C(11)-C(10)-N(2)	103.9(8)	C(22)-C(23)-C(24)	179.5(5)
C(11')-C(10')-N(2)	121(3)	C(23)-C(24)-C(25)	118.6(5)
C(11')-C(10')-C(12')	116(3)	C(23)-C(24)-C(26)	119.4(5)
N(2)-C(10')-C(12')	94.7(19)	C(25)-C(24)-C(26)	58.6(4)
C(20)-C(13)-C(14)	135.7(6)	C(26)-C(25)-C(24)	60.8(4)

C(25)-C(26)-C(24)	60.6(4)
C(29)-C(27)-C(28)	111.0(7)
C(29)-C(27)-N(3)	109.0(6)
C(28)-C(27)-N(3)	109.4(7)
C(28')-C(27')-C(29')	119.7(15)
C(28')-C(27')-N(3)	117.9(14)
C(29')-C(27')-N(3)	105.1(12)
N(4)-C(30)-C(31)	110.5(4)
N(4)-C(30)-C(32)	110.7(4)
C(31)-C(30)-C(32)	110.7(5)
C(40)-C(33)-C(34)	135.8(9)
C(40)-C(33)-Ce(2)	74.6(6)
C(34)-C(33)-Ce(2)	74.8(4)
C(33)-C(34)-C(35)	136.0(8)
C(33)-C(34)-Ce(2)	75.5(5)
C(35)-C(34)-Ce(2)	74.8(4)
C(36)-C(35)-C(34)	134.3(6)
C(36)-C(35)-Ce(2)	74.8(3)
C(34)-C(35)-Ce(2)	75.2(4)
C(35)-C(36)-C(37)	135.1(7)
C(35)-C(36)-Ce(2)	75.2(4)
C(37)-C(36)-Ce(2)	74.8(4)
C(36)-C(37)-C(38)	133.1(8)
C(36)-C(37)-Ce(2)	75.2(4)
C(38)-C(37)-Ce(2)	74.2(4)
C(39)-C(38)-C(37)	133.2(8)
C(39)-C(38)-Ce(2)	74.4(4)
C(37)-C(38)-Ce(2)	74.2(4)
C(40)-C(39)-C(38)	136.0(8)
C(40)-C(39)-Ce(2)	75.7(5)
C(38)-C(39)-Ce(2)	74.1(5)
C(39)-C(40)-C(33)	136.3(9)
C(39)-C(40)-Ce(2)	76.3(6)
C(33)-C(40)-Ce(2)	76.7(5)

Symmetry transformations used to generate equivalent atoms:

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

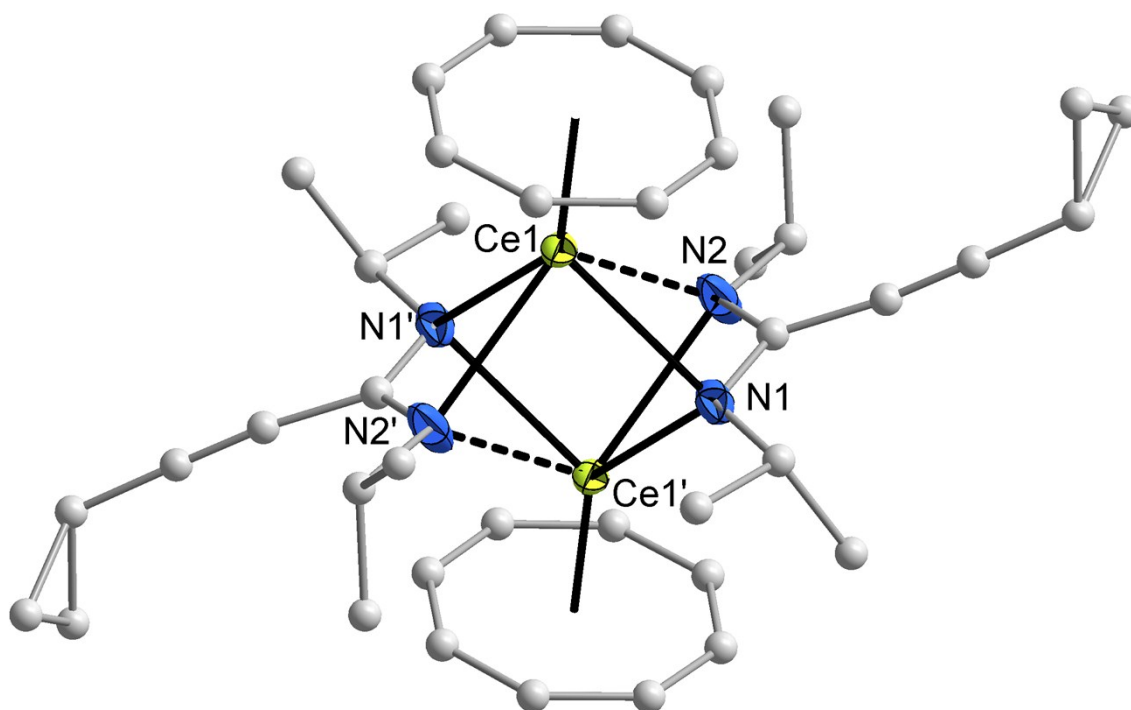


Figure S12. Molecular structure of $[(\text{COT})\text{Ce}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}'\text{Pr})_2)]_2$ (**10**) in the crystal (molecule 1 of 2 in the asymmetric unit). Ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

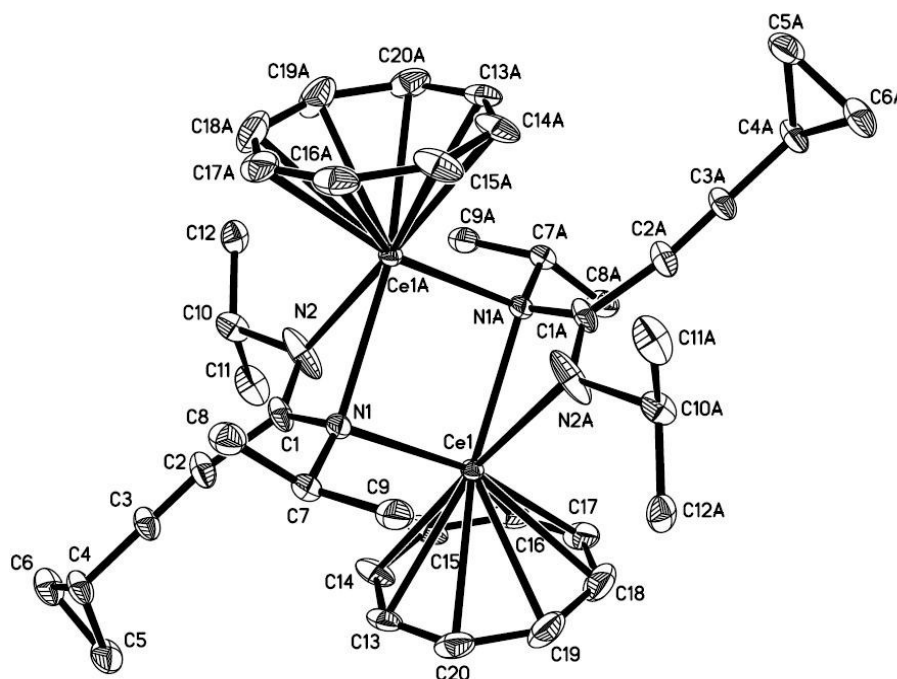


Figure S13. ORTEP drawing of $[(\text{COT})\text{Ce}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}'\text{Pr})_2)]_2$ (**10**).

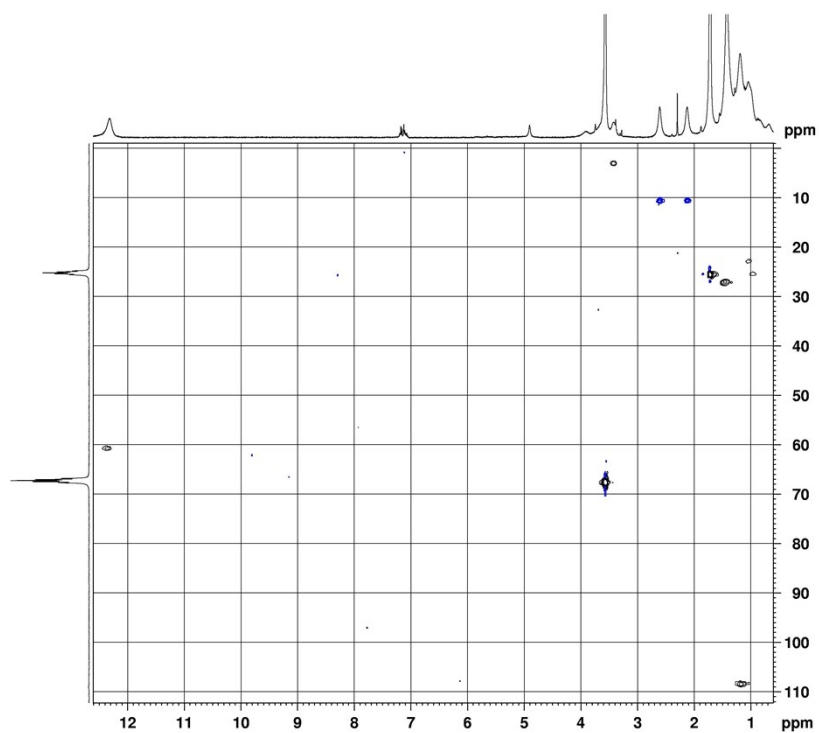


Figure S14. HSQC (H, C- correlation via 1J (C, H)) spectrum in (THF- d_8 , 25°C) of $[(\text{COT})\text{Ce}(\mu\text{-}i\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)]_2$ (**10**).

Table S11. Crystal data and structure refinement of (11).

Identification code	magd100	
Empirical formula	C ₅₂ H ₇₀ Ce ₂ N ₄	
Formula weight	1031.36	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 14.87097(10) Å	α = 90°
	b = 20.01756(14) Å	β = 93.5556(6)°
	c = 15.58600(8) Å	γ = 90°
Volume	4630.72(5) Å ³	
Z	4	
Density (calculated)	1.479 Mg/m ³	
Absorption coefficient	15.273 mm ⁻¹	
F(000)	2104	
Crystal size	0.14 x 0.11 x 0.03 mm ³	
Theta range for data collection	3.60 to 75.86°	
Index ranges	-18 ≤ h ≤ 18, -23 ≤ k ≤ 25, -19 ≤ l ≤ 19	
Reflections collected	214859	
Independent reflections	9629 [R(int) = 0.0566]	
Completeness to theta = 75.86°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6572 and 0.2236	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9629 / 38 / 599	
Goodness-of-fit on F ²	1.100	
Final R indices [I > 2σ(I)]	R1 = 0.0379, wR2 = 0.0921	
R indices (all data)	R1 = 0.0407, wR2 = 0.0939	
Largest diff. peak and hole	1.097 and -1.122 e.Å ⁻³	

Table S12. Bond lengths [Å] and angles [°] of (11).

Ce(1)-N(4)	2.648(3)	C(4)-C(6)	1.501(7)
Ce(1)-C(45)	2.693(4)	C(5)-C(6)	1.505(8)
Ce(1)-C(44)	2.697(4)	C(7)-C(8)	1.507(7)
Ce(1)-C(48)	2.699(4)	C(7)-C(12)	1.537(6)
Ce(1)-C(47)	2.699(4)	C(8)-C(9)	1.528(8)
Ce(1)-N(3)	2.700(3)	C(9)-C(10)	1.535(9)
Ce(1)-C(46)	2.704(4)	C(10)-C(11)	1.515(10)
Ce(1)-C(41)	2.706(4)	C(11)-C(12)	1.526(7)
Ce(1)-C(43)	2.718(4)	C(13)-C(14)	1.496(6)
Ce(1)-C(42)	2.721(4)	C(13)-C(18)	1.526(5)
Ce(1)-N(1)	2.731(3)	C(14)-C(15)	1.515(6)
Ce(1)-N(2)	2.767(3)	C(15)-C(16)	1.510(6)
Ce(2)-N(1)	2.642(3)	C(16)-C(17)	1.484(7)
Ce(2)-N(2)	2.666(3)	C(17)-C(18)	1.542(6)
Ce(2)-C(53)	2.686(5)	C(21)-C(22)	1.442(7)
Ce(2)-C(54)	2.691(5)	C(21)-C(22')	1.494(11)
Ce(2)-C(52)	2.692(5)	C(22)-C(23)	1.181(8)
Ce(2)-C(56)	2.693(5)	C(23)-C(24)	1.446(8)
Ce(2)-C(57)	2.696(5)	C(24)-C(26)	1.438(11)
Ce(2)-C(51)	2.696(5)	C(24)-C(25)	1.456(10)
Ce(2)-N(4)	2.704(3)	C(25)-C(26)	1.428(13)
Ce(2)-C(55)	2.706(5)	C(22')-C(23')	1.205(13)
Ce(2)-C(58)	2.715(5)	C(23')-C(24')	1.459(16)
Ce(2)-N(3)	2.817(4)	C(24')-C(25')	1.402(18)
N(1)-C(1)	1.349(5)	C(24')-C(26')	1.478(17)
N(1)-C(7)	1.483(5)	C(25')-C(26')	1.368(19)
N(2)-C(1)	1.334(5)	C(27)-C(32)	1.497(11)
N(2)-C(13)	1.487(5)	C(27)-C(28)	1.530(9)
N(3)-C(21)	1.332(5)	C(28)-C(29)	1.541(9)
N(3)-C(27)	1.487(10)	C(29)-C(30)	1.459(15)
N(3)-C(27')	1.586(18)	C(30)-C(31)	1.534(13)
N(4)-C(21)	1.348(5)	C(31)-C(32)	1.538(9)
N(4)-C(33)	1.482(5)	C(27')-C(28')	1.524(19)
C(1)-C(2)	1.446(6)	C(27')-C(32')	1.539(19)
C(2)-C(3)	1.208(6)	C(28')-C(29')	1.535(19)
C(3)-C(4)	1.454(6)	C(29')-C(30')	1.52(2)
C(4)-C(5)	1.485(6)	C(30')-C(31')	1.54(2)

C(31')-C(32')	1.538(16)	C(45)-C(46)	1.409(7)
C(33)-C(38)	1.518(5)	C(46)-C(47)	1.415(7)
C(33)-C(34)	1.521(5)	C(47)-C(48)	1.389(7)
C(34)-C(35)	1.532(6)	C(51)-C(58)	1.448(10)
C(35)-C(36)	1.520(7)	C(51)-C(52)	1.473(11)
C(36)-C(37)	1.521(6)	C(52)-C(53)	1.453(11)
C(37)-C(38)	1.527(6)	C(53)-C(54)	1.372(10)
C(41)-C(42)	1.400(7)	C(54)-C(55)	1.331(9)
C(41)-C(48)	1.409(7)	C(55)-C(56)	1.329(9)
C(42)-C(43)	1.402(7)	C(56)-C(57)	1.368(9)
C(43)-C(44)	1.398(8)	C(57)-C(58)	1.390(9)
C(44)-C(45)	1.403(7)		
N(4)-Ce(1)-C(45)	111.97(12)	N(3)-Ce(1)-C(41)	98.13(13)
N(4)-Ce(1)-C(44)	98.80(12)	C(46)-Ce(1)-C(41)	77.00(15)
C(45)-Ce(1)-C(44)	30.19(16)	N(4)-Ce(1)-C(43)	100.53(12)
N(4)-Ce(1)-C(48)	167.45(13)	C(45)-Ce(1)-C(43)	57.08(17)
C(45)-Ce(1)-C(48)	77.90(14)	C(44)-Ce(1)-C(43)	29.93(16)
C(44)-Ce(1)-C(48)	86.09(13)	C(48)-Ce(1)-C(43)	77.97(14)
N(4)-Ce(1)-C(47)	162.56(13)	C(47)-Ce(1)-C(43)	85.80(14)
C(45)-Ce(1)-C(47)	57.99(16)	N(3)-Ce(1)-C(43)	101.56(15)
C(44)-Ce(1)-C(47)	78.53(15)	C(46)-Ce(1)-C(43)	77.30(16)
C(48)-Ce(1)-C(47)	29.83(15)	C(41)-Ce(1)-C(43)	57.19(15)
N(4)-Ce(1)-N(3)	50.04(10)	N(4)-Ce(1)-C(42)	115.99(13)
C(45)-Ce(1)-N(3)	152.14(14)	C(45)-Ce(1)-C(42)	76.87(16)
C(44)-Ce(1)-N(3)	123.40(14)	C(44)-Ce(1)-C(42)	56.91(17)
C(48)-Ce(1)-N(3)	117.75(13)	C(48)-Ce(1)-C(42)	57.31(15)
C(47)-Ce(1)-N(3)	144.94(14)	C(47)-Ce(1)-C(42)	77.25(15)
N(4)-Ce(1)-C(46)	135.04(13)	N(3)-Ce(1)-C(42)	92.16(14)
C(45)-Ce(1)-C(46)	30.26(16)	C(46)-Ce(1)-C(42)	84.41(15)
C(44)-Ce(1)-C(46)	57.56(16)	C(41)-Ce(1)-C(42)	29.90(15)
C(48)-Ce(1)-C(46)	57.13(15)	C(43)-Ce(1)-C(42)	29.87(16)
C(47)-Ce(1)-C(46)	30.36(15)	N(4)-Ce(1)-N(1)	94.44(9)
N(3)-Ce(1)-C(46)	174.86(13)	C(45)-Ce(1)-N(1)	127.14(14)
N(4)-Ce(1)-C(41)	139.62(13)	C(44)-Ce(1)-N(1)	157.25(14)
C(45)-Ce(1)-C(41)	85.09(14)	C(48)-Ce(1)-N(1)	84.86(11)
C(44)-Ce(1)-C(41)	77.56(15)	C(47)-Ce(1)-N(1)	83.28(12)
C(48)-Ce(1)-C(41)	30.23(15)	N(3)-Ce(1)-N(1)	79.18(11)
C(47)-Ce(1)-C(41)	57.09(15)	C(46)-Ce(1)-N(1)	100.23(14)

C(41)-Ce(1)-N(1)	103.81(13)	C(52)-Ce(2)-C(51)	31.7(2)
C(43)-Ce(1)-N(1)	160.99(13)	C(56)-Ce(2)-C(51)	77.79(19)
C(42)-Ce(1)-N(1)	131.62(14)	C(57)-Ce(2)-C(51)	57.9(2)
N(4)-Ce(1)-N(2)	72.66(9)	N(1)-Ce(2)-N(4)	95.22(9)
C(45)-Ce(1)-N(2)	95.94(12)	N(2)-Ce(2)-N(4)	73.41(9)
C(44)-Ce(1)-N(2)	119.00(13)	C(53)-Ce(2)-N(4)	94.30(16)
C(48)-Ce(1)-N(2)	115.10(12)	C(54)-Ce(2)-N(4)	82.87(13)
C(47)-Ce(1)-N(2)	93.38(12)	C(52)-Ce(2)-N(4)	119.7(2)
N(3)-Ce(1)-N(2)	97.16(10)	C(56)-Ce(2)-N(4)	108.93(16)
C(46)-Ce(1)-N(2)	86.09(12)	C(57)-Ce(2)-N(4)	137.05(17)
C(41)-Ce(1)-N(2)	144.32(13)	C(51)-Ce(2)-N(4)	151.4(2)
C(43)-Ce(1)-N(2)	148.32(14)	N(1)-Ce(2)-C(55)	158.39(16)
C(42)-Ce(1)-N(2)	170.24(13)	N(2)-Ce(2)-C(55)	111.78(15)
N(1)-Ce(1)-N(2)	48.32(10)	C(53)-Ce(2)-C(55)	55.5(2)
N(1)-Ce(2)-N(2)	50.18(10)	C(54)-Ce(2)-C(55)	28.56(19)
N(1)-Ce(2)-C(53)	144.67(19)	C(52)-Ce(2)-C(55)	77.2(2)
N(2)-Ce(2)-C(53)	163.2(2)	C(56)-Ce(2)-C(55)	28.50(18)
N(1)-Ce(2)-C(54)	173.02(17)	C(57)-Ce(2)-C(55)	55.2(2)
N(2)-Ce(2)-C(54)	134.75(17)	C(51)-Ce(2)-C(55)	85.31(17)
C(53)-Ce(2)-C(54)	29.6(2)	N(4)-Ce(2)-C(55)	89.09(15)
N(1)-Ce(2)-C(52)	118.0(2)	N(1)-Ce(2)-C(58)	97.97(13)
N(2)-Ce(2)-C(52)	165.1(2)	N(2)-Ce(2)-C(58)	110.07(15)
C(53)-Ce(2)-C(52)	31.4(2)	C(53)-Ce(2)-C(58)	78.97(18)
C(54)-Ce(2)-C(52)	58.1(2)	C(54)-Ce(2)-C(58)	84.85(16)
N(1)-Ce(2)-C(56)	132.08(16)	C(52)-Ce(2)-C(58)	59.3(2)
N(2)-Ce(2)-C(56)	97.37(14)	C(56)-Ce(2)-C(58)	56.5(2)
C(53)-Ce(2)-C(56)	75.47(18)	C(57)-Ce(2)-C(58)	29.8(2)
C(54)-Ce(2)-C(56)	54.7(2)	C(51)-Ce(2)-C(58)	31.0(2)
C(52)-Ce(2)-C(56)	85.29(16)	N(4)-Ce(2)-C(58)	165.00(15)
N(1)-Ce(2)-C(57)	110.23(15)	C(55)-Ce(2)-C(58)	76.03(18)
N(2)-Ce(2)-C(57)	96.60(13)	N(1)-Ce(2)-N(3)	78.63(10)
C(53)-Ce(2)-C(57)	84.56(16)	N(2)-Ce(2)-N(3)	96.76(9)
C(54)-Ce(2)-C(57)	75.28(18)	C(53)-Ce(2)-N(3)	82.66(13)
C(52)-Ce(2)-C(57)	78.50(18)	C(54)-Ce(2)-N(3)	95.20(15)
C(56)-Ce(2)-C(57)	29.41(19)	C(52)-Ce(2)-N(3)	88.54(16)
N(1)-Ce(2)-C(51)	100.27(15)	C(56)-Ce(2)-N(3)	147.28(17)
N(2)-Ce(2)-C(51)	134.5(2)	C(57)-Ce(2)-N(3)	166.64(14)
C(53)-Ce(2)-C(51)	59.6(2)	C(51)-Ce(2)-N(3)	111.59(19)
C(54)-Ce(2)-C(51)	78.84(19)	N(4)-Ce(2)-N(3)	48.33(10)

C(55)-Ce(2)-N(3)	118.95(16)	Ce(1)-C(1)-Ce(2)	74.69(9)
C(58)-Ce(2)-N(3)	141.97(18)	C(3)-C(2)-C(1)	174.5(4)
C(1)-N(1)-C(7)	116.0(4)	C(2)-C(3)-C(4)	177.6(5)
C(1)-N(1)-Ce(2)	92.6(2)	C(3)-C(4)-C(5)	119.4(4)
C(7)-N(1)-Ce(2)	134.6(2)	C(3)-C(4)-C(6)	117.5(5)
C(1)-N(1)-Ce(1)	85.8(2)	C(5)-C(4)-C(6)	60.5(4)
C(7)-N(1)-Ce(1)	129.0(2)	C(4)-C(5)-C(6)	60.2(3)
Ce(2)-N(1)-Ce(1)	84.85(10)	C(4)-C(6)-C(5)	59.2(3)
C(1)-N(2)-C(13)	122.5(3)	N(1)-C(7)-C(8)	110.2(4)
C(1)-N(2)-Ce(2)	91.9(2)	N(1)-C(7)-C(12)	111.2(3)
C(13)-N(2)-Ce(2)	127.4(2)	C(8)-C(7)-C(12)	110.2(4)
C(1)-N(2)-Ce(1)	84.5(2)	C(7)-C(8)-C(9)	111.8(5)
C(13)-N(2)-Ce(1)	132.9(2)	C(8)-C(9)-C(10)	111.0(4)
Ce(2)-N(2)-Ce(1)	83.69(9)	C(11)-C(10)-C(9)	111.4(5)
C(21)-N(3)-C(27)	119.1(5)	C(10)-C(11)-C(12)	111.7(6)
C(21)-N(3)-C(27')	110.7(6)	C(11)-C(12)-C(7)	110.0(4)
C(27)-N(3)-C(27')	21.5(5)	N(2)-C(13)-C(14)	115.1(4)
C(21)-N(3)-Ce(1)	91.0(2)	N(2)-C(13)-C(18)	113.7(3)
C(27)-N(3)-Ce(1)	139.8(4)	C(14)-C(13)-C(18)	112.0(4)
C(27')-N(3)-Ce(1)	126.7(6)	C(13)-C(14)-C(15)	112.1(4)
C(21)-N(3)-Ce(2)	82.8(2)	C(16)-C(15)-C(14)	112.0(4)
C(27)-N(3)-Ce(2)	124.7(4)	C(17)-C(16)-C(15)	113.1(4)
C(27')-N(3)-Ce(2)	146.1(7)	C(16)-C(17)-C(18)	111.7(4)
Ce(1)-N(3)-Ce(2)	82.13(10)	C(13)-C(18)-C(17)	110.0(4)
C(21)-N(4)-C(33)	117.4(3)	N(3)-C(21)-N(4)	115.1(3)
C(21)-N(4)-Ce(1)	92.9(2)	N(3)-C(21)-C(22)	121.6(4)
C(33)-N(4)-Ce(1)	135.2(2)	N(4)-C(21)-C(22)	122.4(4)
C(21)-N(4)-Ce(2)	87.2(2)	N(3)-C(21)-C(22')	127.7(7)
C(33)-N(4)-Ce(2)	125.6(2)	N(4)-C(21)-C(22')	116.3(7)
Ce(1)-N(4)-Ce(2)	85.28(9)	C(22)-C(21)-C(22')	17.9(5)
N(2)-C(1)-N(1)	114.1(3)	N(3)-C(21)-Ce(2)	70.7(2)
N(2)-C(1)-C(2)	123.5(4)	N(4)-C(21)-Ce(2)	65.8(2)
N(1)-C(1)-C(2)	122.3(4)	C(22)-C(21)-Ce(2)	125.1(4)
N(2)-C(1)-Ce(1)	68.78(19)	C(22')-C(21)-Ce(2)	141.1(6)
N(1)-C(1)-Ce(1)	67.2(2)	N(3)-C(21)-Ce(1)	62.9(2)
C(2)-C(1)-Ce(1)	130.7(2)	N(4)-C(21)-Ce(1)	60.69(18)
N(2)-C(1)-Ce(2)	61.9(2)	C(22)-C(21)-Ce(1)	160.4(4)
N(1)-C(1)-Ce(2)	60.9(2)	C(22')-C(21)-Ce(1)	142.9(7)
C(2)-C(1)-Ce(2)	154.6(3)	Ce(2)-C(21)-Ce(1)	74.43(9)

C(23)-C(22)-C(21)	171.6(7)	C(42)-C(41)-Ce(1)	75.6(3)
C(22)-C(23)-C(24)	178.0(8)	C(48)-C(41)-Ce(1)	74.6(2)
C(26)-C(24)-C(23)	122.4(8)	C(41)-C(42)-C(43)	135.8(5)
C(26)-C(24)-C(25)	59.1(6)	C(41)-C(42)-Ce(1)	74.5(3)
C(23)-C(24)-C(25)	119.3(7)	C(43)-C(42)-Ce(1)	74.9(3)
C(26)-C(25)-C(24)	59.8(5)	C(44)-C(43)-C(42)	134.4(5)
C(25)-C(26)-C(24)	61.1(5)	C(44)-C(43)-Ce(1)	74.2(2)
C(23')-C(22')-C(21)	171.3(15)	C(42)-C(43)-Ce(1)	75.2(3)
C(22')-C(23')-C(24')	162.8(18)	C(43)-C(44)-C(45)	134.7(4)
C(25')-C(24')-C(23')	122(2)	C(43)-C(44)-Ce(1)	75.9(3)
C(25')-C(24')-C(26')	56.6(10)	C(45)-C(44)-Ce(1)	74.8(2)
C(23')-C(24')-C(26')	123.4(19)	C(44)-C(45)-C(46)	135.2(5)
C(26')-C(25')-C(24')	64.5(9)	C(44)-C(45)-Ce(1)	75.0(3)
C(25')-C(26')-C(24')	58.9(8)	C(46)-C(45)-Ce(1)	75.3(3)
N(3)-C(27)-C(32)	112.6(7)	C(45)-C(46)-C(47)	135.5(5)
N(3)-C(27)-C(28)	106.4(6)	C(45)-C(46)-Ce(1)	74.4(3)
C(32)-C(27)-C(28)	109.4(7)	C(47)-C(46)-Ce(1)	74.6(2)
C(27)-C(28)-C(29)	110.4(6)	C(48)-C(47)-C(46)	134.2(4)
C(30)-C(29)-C(28)	113.2(8)	C(48)-C(47)-Ce(1)	75.1(2)
C(29)-C(30)-C(31)	110.5(8)	C(46)-C(47)-Ce(1)	75.0(2)
C(30)-C(31)-C(32)	111.4(7)	C(47)-C(48)-C(41)	134.7(4)
C(27)-C(32)-C(31)	111.8(7)	C(47)-C(48)-Ce(1)	75.1(2)
C(28')-C(27')-C(32')	111.4(13)	C(41)-C(48)-Ce(1)	75.2(2)
C(28')-C(27')-N(3)	115.8(11)	C(58)-C(51)-C(52)	132.7(6)
C(32')-C(27')-N(3)	100.0(11)	C(58)-C(51)-Ce(2)	75.2(3)
C(27')-C(28')-C(29')	111.0(11)	C(52)-C(51)-Ce(2)	74.0(3)
C(30')-C(29')-C(28')	109.9(14)	C(53)-C(52)-C(51)	132.4(5)
C(29')-C(30')-C(31')	109.8(14)	C(53)-C(52)-Ce(2)	74.1(3)
C(30')-C(31')-C(32')	110.4(12)	C(51)-C(52)-Ce(2)	74.3(3)
C(31')-C(32')-C(27')	110.0(11)	C(54)-C(53)-C(52)	135.2(6)
N(4)-C(33)-C(38)	110.4(3)	C(54)-C(53)-Ce(2)	75.4(3)
N(4)-C(33)-C(34)	112.4(3)	C(52)-C(53)-Ce(2)	74.5(3)
C(38)-C(33)-C(34)	109.5(3)	C(55)-C(54)-C(53)	136.4(6)
C(33)-C(34)-C(35)	110.5(3)	C(55)-C(54)-Ce(2)	76.4(3)
C(36)-C(35)-C(34)	112.2(4)	C(53)-C(54)-Ce(2)	75.0(3)
C(35)-C(36)-C(37)	111.0(4)	C(56)-C(55)-C(54)	136.7(6)
C(36)-C(37)-C(38)	111.1(3)	C(56)-C(55)-Ce(2)	75.2(3)
C(33)-C(38)-C(37)	110.9(3)	C(54)-C(55)-Ce(2)	75.1(3)
C(42)-C(41)-C(48)	135.4(5)	C(55)-C(56)-C(57)	136.4(6)

C(55)-C(56)-Ce(2)	76.3(3)
C(57)-C(56)-Ce(2)	75.4(3)
C(56)-C(57)-C(58)	136.4(5)
C(56)-C(57)-Ce(2)	75.2(3)
C(58)-C(57)-Ce(2)	75.9(3)
C(57)-C(58)-C(51)	133.7(5)
C(57)-C(58)-Ce(2)	74.4(3)
C(51)-C(58)-Ce(2)	73.8(3)

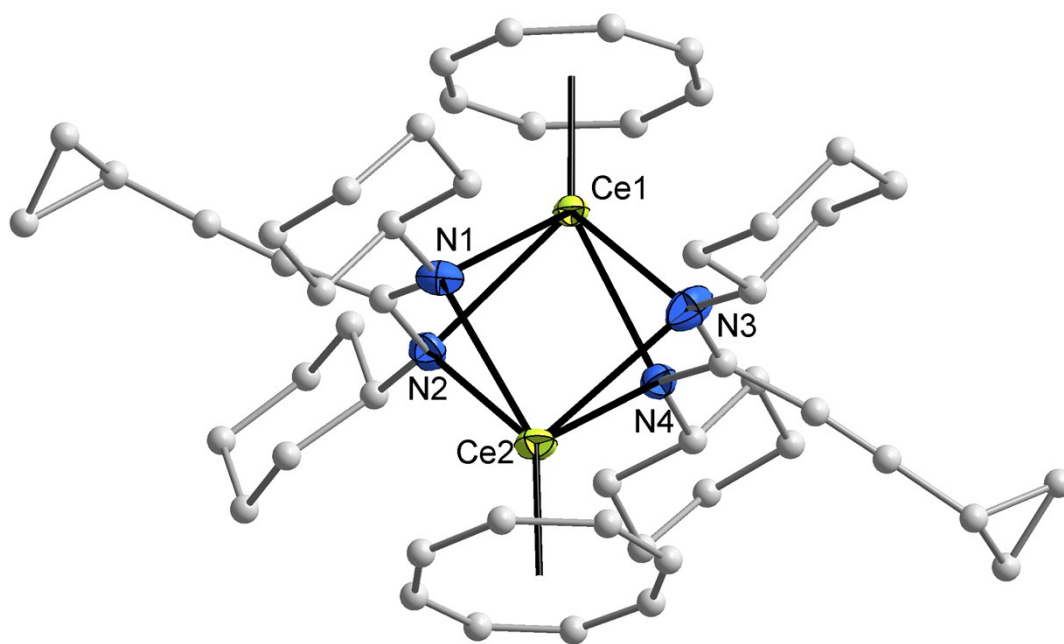


Figure S15. Molecular structure of $[(\text{COT})\text{Ce}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{NCy})_2)]_2$ (**11**) in the crystal. Ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

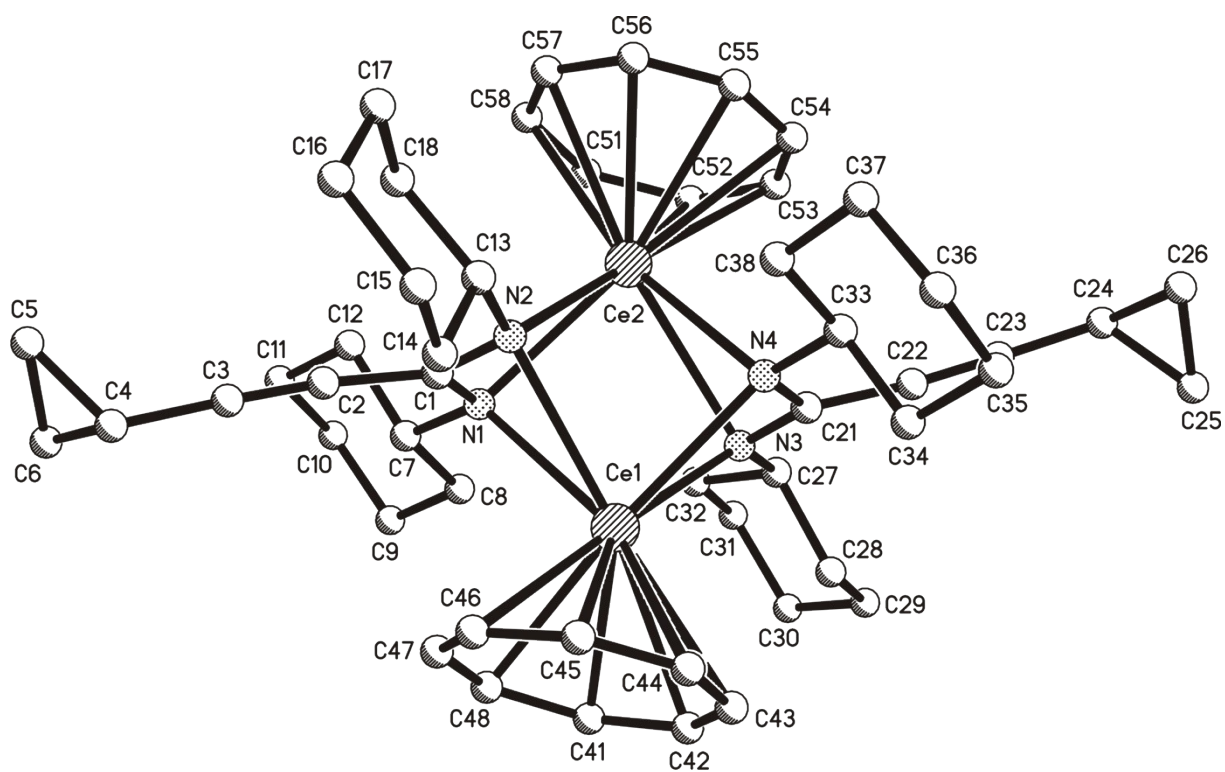


Figure S16. ORTEP drawing of $[(\text{COT})\text{Ce}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{NCy})_2)]_2$ (**11**).

Table S13. Crystal data and structure refinement (12).

Identification code	magd125	
Empirical formula	C ₄₀ H ₅₄ N ₄ Nd ₂	
Formula weight	879.35	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 19.11720(10) Å	α = 90°
	b = 19.80540(10) Å	β = 99.5500(10)°
	c = 9.95780(10) Å	γ = 90°
Volume	3718.01(5) Å ³	
Z	4	
Density (calculated)	1.571 Mg/m ³	
Absorption coefficient	21.293 mm ⁻¹	
F(000)	1768	
Crystal size	0.12 x 0.10 x 0.06 mm ³	
Theta range for data collection	3.24 to 75.80°	
Index ranges	-24 ≤ h ≤ 24, -24 ≤ k ≤ 24, -10 ≤ l ≤ 12	
Reflections collected	283708	
Independent reflections	7724 [R(int) = 0.0652]	
Completeness to theta = 75.80°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3615 and 0.1843	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7724 / 48 / 443	
Goodness-of-fit on F ²	1.113	
Final R indices [I > 2σ(I)]	R1 = 0.0395, wR2 = 0.0960	
R indices (all data)	R1 = 0.0398, wR2 = 0.0962	
Largest diff. peak and hole	2.307 and -2.782 e.Å ⁻³	

Table S14. Bond lengths [Å] and angles [°] (**12**).

Nd(1)-N(2)#1	2.570(4)	C(4)-C(5)	1.504(8)
Nd(1)-N(1)#1	2.581(4)	C(4)-C(6)	1.506(7)
Nd(1)-N(1)	2.610(4)	C(5)-C(6)	1.479(10)
Nd(1)-C(18)	2.658(5)	C(7)-C(9)	1.518(6)
Nd(1)-C(19)	2.659(5)	C(7)-C(8)	1.526(7)
Nd(1)-C(13)	2.671(5)	C(10)-C(12)	1.521(7)
Nd(1)-C(17)	2.673(5)	C(10)-C(11)	1.526(7)
Nd(1)-C(15)	2.674(4)	C(13)-C(20)	1.398(8)
Nd(1)-C(16)	2.675(5)	C(13)-C(14)	1.404(7)
Nd(1)-C(20)	2.677(5)	C(14)-C(15)	1.400(7)
Nd(1)-C(14)	2.679(5)	C(15)-C(16)	1.418(7)
Nd(1)-C(1)#1	2.944(4)	C(16)-C(17)	1.404(8)
Nd(2)-N(3)	2.634(6)	C(17)-C(18)	1.413(8)
Nd(2)-N(4)	2.652(4)	C(18)-C(19)	1.416(8)
Nd(2)-C(39)	2.652(7)	C(19)-C(20)	1.410(8)
Nd(2)-N(3)#2	2.656(4)	C(21)-N(3)	1.346(7)
Nd(2)-C(38)	2.655(7)	C(21)-C(22)	1.434(7)
Nd(2)-C(37)	2.658(6)	C(21)-Nd(2)#2	2.919(4)
Nd(2)-C(36)	2.667(5)	C(22)-C(23)	1.201(8)
Nd(2)-C(35)	2.668(5)	C(23)-C(24)	1.433(7)
Nd(2)-C(34)	2.671(7)	C(24)-C(25)	1.508(7)
Nd(2)-C(40)	2.682(10)	C(24)-C(26)	1.519(7)
Nd(2)-C(33)	2.682(9)	C(25)-C(26)	1.480(8)
Nd(2)-N(4)#2	2.761(4)	N(3)-C(27')	1.453(10)
N(1)-C(1)	1.361(6)	N(3)-C(27)	1.624(10)
N(1)-C(7)	1.496(6)	N(3)-Nd(2)#2	2.656(4)
N(1)-Nd(1)#1	2.581(4)	C(29)-C(27)	1.502(13)
N(2)-C(1)	1.329(6)	C(28)-C(27)	1.530(14)
N(2)-C(10)	1.490(6)	C(29')-C(27')	1.518(14)
N(2)-Nd(1)#1	2.571(4)	C(28')-C(27')	1.501(18)
N(4)-C(21)	1.343(6)	C(30)-C(31)	1.507(6)
N(4)-C(30)	1.482(5)	C(30)-C(32)	1.532(6)
N(4)-Nd(2)#2	2.761(4)	C(33)-C(40)	1.249(17)
C(1)-C(2)	1.450(6)	C(33)-C(34)	1.372(12)
C(1)-Nd(1)#1	2.944(4)	C(34)-C(35)	1.408(9)
C(2)-C(3)	1.203(7)	C(35)-C(36)	1.385(8)
C(3)-C(4)	1.439(6)	C(36)-C(37)	1.396(9)

C(37)-C(38)	1.490(14)	C(39)-C(40)	1.290(17)
C(38)-C(39)	1.558(18)		
N(2)#1-Nd(1)-N(1)#1	52.85(12)	N(1)#1-Nd(1)-C(20)	168.03(15)
N(2)#1-Nd(1)-N(1)	85.93(12)	N(1)-Nd(1)-C(20)	96.18(14)
N(1)#1-Nd(1)-N(1)	85.33(12)	C(18)-Nd(1)-C(20)	58.69(17)
N(2)#1-Nd(1)-C(18)	91.91(16)	C(19)-Nd(1)-C(20)	30.64(17)
N(1)#1-Nd(1)-C(18)	116.15(15)	C(13)-Nd(1)-C(20)	30.32(16)
N(1)-Nd(1)-C(18)	150.87(15)	C(17)-Nd(1)-C(20)	79.34(16)
N(2)#1-Nd(1)-C(19)	96.56(15)	C(15)-Nd(1)-C(20)	78.53(16)
N(1)#1-Nd(1)-C(19)	140.48(15)	C(16)-Nd(1)-C(20)	86.83(15)
N(1)-Nd(1)-C(19)	120.50(15)	N(2)#1-Nd(1)-C(14)	172.26(14)
C(18)-Nd(1)-C(19)	30.90(17)	N(1)#1-Nd(1)-C(14)	134.06(13)
N(2)#1-Nd(1)-C(13)	141.93(14)	N(1)-Nd(1)-C(14)	91.07(14)
N(1)#1-Nd(1)-C(13)	160.99(14)	C(18)-Nd(1)-C(14)	87.24(17)
N(1)-Nd(1)-C(13)	84.53(13)	C(19)-Nd(1)-C(14)	78.82(16)
C(18)-Nd(1)-C(13)	79.38(17)	C(13)-Nd(1)-C(14)	30.44(15)
C(19)-Nd(1)-C(13)	58.21(17)	C(17)-Nd(1)-C(14)	79.12(16)
N(2)#1-Nd(1)-C(17)	103.91(15)	C(15)-Nd(1)-C(14)	30.32(15)
N(1)#1-Nd(1)-C(17)	100.88(14)	C(16)-Nd(1)-C(14)	58.24(16)
N(1)-Nd(1)-C(17)	170.16(15)	C(20)-Nd(1)-C(14)	57.88(16)
C(18)-Nd(1)-C(17)	30.75(17)	N(2)#1-Nd(1)-C(1)#1	26.81(12)
C(19)-Nd(1)-C(17)	58.66(17)	N(1)#1-Nd(1)-C(1)#1	27.53(12)
C(13)-Nd(1)-C(17)	87.33(16)	N(1)-Nd(1)-C(1)#1	91.69(11)
N(2)#1-Nd(1)-C(15)	156.64(14)	C(18)-Nd(1)-C(1)#1	99.37(15)
N(1)#1-Nd(1)-C(15)	111.95(14)	C(19)-Nd(1)-C(1)#1	115.72(15)
N(1)-Nd(1)-C(15)	112.24(14)	C(13)-Nd(1)-C(1)#1	168.66(14)
C(18)-Nd(1)-C(15)	79.22(16)	C(17)-Nd(1)-C(1)#1	97.33(15)
C(19)-Nd(1)-C(15)	86.89(16)	C(15)-Nd(1)-C(1)#1	133.10(14)
C(13)-Nd(1)-C(15)	57.98(15)	C(16)-Nd(1)-C(1)#1	110.13(14)
C(17)-Nd(1)-C(15)	58.43(16)	C(20)-Nd(1)-C(1)#1	140.52(15)
N(2)#1-Nd(1)-C(16)	127.33(14)	C(14)-Nd(1)-C(1)#1	160.75(14)
N(1)#1-Nd(1)-C(16)	99.42(13)	N(3)-Nd(2)-N(4)	50.33(13)
N(1)-Nd(1)-C(16)	141.40(14)	N(3)-Nd(2)-C(39)	113.8(3)
C(18)-Nd(1)-C(16)	58.29(17)	N(4)-Nd(2)-C(39)	94.37(16)
C(19)-Nd(1)-C(16)	78.99(16)	N(3)-Nd(2)-N(3)#2	94.52(15)
C(13)-Nd(1)-C(16)	78.96(15)	N(4)-Nd(2)-N(3)#2	76.10(15)
C(17)-Nd(1)-C(16)	30.45(17)	C(39)-Nd(2)-N(3)#2	134.0(3)
C(15)-Nd(1)-C(16)	30.75(15)	N(3)-Nd(2)-C(38)	95.4(3)
N(2)#1-Nd(1)-C(20)	115.32(15)	N(4)-Nd(2)-C(38)	104.9(2)

C(39)-Nd(2)-C(38)	34.2(4)	C(39)-Nd(2)-C(33)	52.1(4)
N(3)#2-Nd(2)-C(38)	167.7(3)	N(3)#2-Nd(2)-C(33)	91.4(3)
N(3)-Nd(2)-C(37)	95.6(2)	C(38)-Nd(2)-C(33)	77.1(4)
N(4)-Nd(2)-C(37)	128.95(17)	C(37)-Nd(2)-C(33)	86.5(3)
C(39)-Nd(2)-C(37)	62.7(3)	C(36)-Nd(2)-C(33)	78.1(2)
N(3)#2-Nd(2)-C(37)	152.7(2)	C(35)-Nd(2)-C(33)	57.7(2)
C(38)-Nd(2)-C(37)	32.6(3)	C(34)-Nd(2)-C(33)	29.7(3)
N(3)-Nd(2)-C(36)	111.94(17)	C(40)-Nd(2)-C(33)	26.9(4)
N(4)-Nd(2)-C(36)	157.75(15)	N(3)-Nd(2)-N(4)#2	74.62(12)
C(39)-Nd(2)-C(36)	80.6(2)	N(4)-Nd(2)-N(4)#2	96.91(10)
N(3)#2-Nd(2)-C(36)	122.71(17)	C(39)-Nd(2)-N(4)#2	168.69(17)
C(38)-Nd(2)-C(36)	59.5(2)	N(3)#2-Nd(2)-N(4)#2	48.99(12)
C(37)-Nd(2)-C(36)	30.41(19)	C(38)-Nd(2)-N(4)#2	141.4(3)
N(3)-Nd(2)-C(35)	137.10(16)	C(37)-Nd(2)-N(4)#2	110.1(2)
N(4)-Nd(2)-C(35)	171.84(15)	C(36)-Nd(2)-N(4)#2	89.28(16)
C(39)-Nd(2)-C(35)	85.04(19)	C(35)-Nd(2)-N(4)#2	83.67(13)
N(3)#2-Nd(2)-C(35)	98.46(18)	C(34)-Nd(2)-N(4)#2	96.75(18)
C(38)-Nd(2)-C(35)	79.1(2)	C(40)-Nd(2)-N(4)#2	147.4(4)
C(37)-Nd(2)-C(35)	57.8(2)	C(33)-Nd(2)-N(4)#2	121.0(3)
C(36)-Nd(2)-C(35)	30.09(18)	C(1)-N(1)-C(7)	116.2(4)
N(3)-Nd(2)-C(34)	167.19(19)	C(1)-N(1)-Nd(1)#1	91.2(3)
N(4)-Nd(2)-C(34)	141.67(17)	C(7)-N(1)-Nd(1)#1	130.9(3)
C(39)-Nd(2)-C(34)	73.6(3)	C(1)-N(1)-Nd(1)	102.6(3)
N(3)#2-Nd(2)-C(34)	86.5(2)	C(7)-N(1)-Nd(1)	115.7(3)
C(38)-Nd(2)-C(34)	85.5(3)	Nd(1)#1-N(1)-Nd(1)	94.67(12)
C(37)-Nd(2)-C(34)	78.3(2)	C(1)-N(2)-C(10)	117.9(4)
C(36)-Nd(2)-C(34)	57.7(2)	C(1)-N(2)-Nd(1)#1	92.5(3)
C(35)-Nd(2)-C(34)	30.58(19)	C(10)-N(2)-Nd(1)#1	140.6(3)
N(3)-Nd(2)-C(40)	136.2(4)	C(21)-N(4)-C(30)	116.2(4)
N(4)-Nd(2)-C(40)	98.7(3)	C(21)-N(4)-Nd(2)	92.0(3)
C(39)-Nd(2)-C(40)	28.0(4)	C(30)-N(4)-Nd(2)	137.3(3)
N(3)#2-Nd(2)-C(40)	108.0(3)	C(21)-N(4)-Nd(2)#2	83.0(2)
C(38)-Nd(2)-C(40)	59.7(4)	C(30)-N(4)-Nd(2)#2	129.1(3)
C(37)-Nd(2)-C(40)	81.4(3)	Nd(2)-N(4)-Nd(2)#2	83.09(10)
C(36)-Nd(2)-C(40)	87.0(3)	N(2)-C(1)-N(1)	116.9(4)
C(35)-Nd(2)-C(40)	77.1(3)	N(2)-C(1)-C(2)	122.4(4)
C(34)-Nd(2)-C(40)	54.5(4)	N(1)-C(1)-C(2)	120.7(4)
N(3)-Nd(2)-C(33)	162.5(3)	N(2)-C(1)-Nd(1)#1	60.7(2)
N(4)-Nd(2)-C(33)	115.8(2)	N(1)-C(1)-Nd(1)#1	61.2(2)

C(2)-C(1)-Nd(1)#1	158.9(3)	N(4)-C(21)-C(22)	121.9(4)
C(3)-C(2)-C(1)	173.1(5)	N(3)-C(21)-C(22)	124.5(5)
C(2)-C(3)-C(4)	178.8(5)	N(4)-C(21)-Nd(2)#2	69.8(2)
C(3)-C(4)-C(5)	118.8(4)	N(3)-C(21)-Nd(2)#2	65.3(2)
C(3)-C(4)-C(6)	119.8(5)	C(22)-C(21)-Nd(2)#2	131.1(3)
C(5)-C(4)-C(6)	58.9(4)	N(4)-C(21)-Nd(2)	61.5(3)
C(6)-C(5)-C(4)	60.6(4)	N(3)-C(21)-Nd(2)	60.8(3)
C(5)-C(6)-C(4)	60.5(4)	C(22)-C(21)-Nd(2)	154.4(3)
N(1)-C(7)-C(9)	108.8(4)	Nd(2)#2-C(21)-Nd(2)	74.45(11)
N(1)-C(7)-C(8)	112.0(4)	C(23)-C(22)-C(21)	175.5(6)
C(9)-C(7)-C(8)	109.8(4)	C(22)-C(23)-C(24)	179.1(5)
N(2)-C(10)-C(12)	109.9(4)	C(23)-C(24)-C(25)	118.6(4)
N(2)-C(10)-C(11)	111.2(4)	C(23)-C(24)-C(26)	119.7(5)
C(12)-C(10)-C(11)	110.4(4)	C(25)-C(24)-C(26)	58.5(4)
C(20)-C(13)-C(14)	135.3(5)	C(26)-C(25)-C(24)	61.1(3)
C(20)-C(13)-Nd(1)	75.1(3)	C(25)-C(26)-C(24)	60.4(3)
C(14)-C(13)-Nd(1)	75.1(3)	C(21)-N(3)-C(27')	130.5(6)
C(15)-C(14)-C(13)	135.0(5)	C(21)-N(3)-C(27)	107.3(5)
C(15)-C(14)-Nd(1)	74.6(3)	C(27')-N(3)-C(27)	34.3(5)
C(13)-C(14)-Nd(1)	74.4(3)	C(21)-N(3)-Nd(2)	92.7(3)
C(14)-C(15)-C(16)	135.2(5)	C(27')-N(3)-Nd(2)	113.1(5)
C(14)-C(15)-Nd(1)	75.0(3)	C(27)-N(3)-Nd(2)	146.9(5)
C(16)-C(15)-Nd(1)	74.7(3)	C(21)-N(3)-Nd(2)#2	87.2(3)
C(17)-C(16)-C(15)	135.2(5)	C(27')-N(3)-Nd(2)#2	134.0(5)
C(17)-C(16)-Nd(1)	74.7(3)	C(27)-N(3)-Nd(2)#2	120.8(4)
C(15)-C(16)-Nd(1)	74.6(3)	Nd(2)-N(3)-Nd(2)#2	85.48(15)
C(16)-C(17)-C(18)	134.4(5)	C(29)-C(27)-C(28)	110.1(8)
C(16)-C(17)-Nd(1)	74.9(3)	C(29)-C(27)-N(3)	107.6(7)
C(18)-C(17)-Nd(1)	74.0(3)	C(28)-C(27)-N(3)	109.3(8)
C(17)-C(18)-C(19)	134.8(5)	N(3)-C(27')-C(28')	115.4(9)
C(17)-C(18)-Nd(1)	75.2(3)	N(3)-C(27')-C(29')	104.6(8)
C(19)-C(18)-Nd(1)	74.6(3)	C(28')-C(27')-C(29')	112.6(10)
C(20)-C(19)-C(18)	135.4(5)	N(4)-C(30)-C(31)	110.5(4)
C(20)-C(19)-Nd(1)	75.4(3)	N(4)-C(30)-C(32)	111.2(4)
C(18)-C(19)-Nd(1)	74.5(3)	C(31)-C(30)-C(32)	110.4(4)
C(13)-C(20)-C(19)	134.8(5)	C(40)-C(33)-C(34)	138.7(11)
C(13)-C(20)-Nd(1)	74.6(3)	C(40)-C(33)-Nd(2)	76.5(7)
C(19)-C(20)-Nd(1)	74.0(3)	C(34)-C(33)-Nd(2)	74.7(4)
N(4)-C(21)-N(3)	113.4(4)	C(33)-C(34)-C(35)	136.4(9)

C(33)-C(34)-Nd(2)	75.6(5)
C(35)-C(34)-Nd(2)	74.6(4)
C(36)-C(35)-C(34)	134.4(6)
C(36)-C(35)-Nd(2)	74.9(3)
C(34)-C(35)-Nd(2)	74.8(4)
C(35)-C(36)-C(37)	135.4(6)
C(35)-C(36)-Nd(2)	75.0(3)
C(37)-C(36)-Nd(2)	74.5(3)
C(36)-C(37)-C(38)	132.4(9)
C(36)-C(37)-Nd(2)	75.1(3)
C(38)-C(37)-Nd(2)	73.6(4)
C(37)-C(38)-C(39)	130.1(8)
C(37)-C(38)-Nd(2)	73.8(4)
C(39)-C(38)-Nd(2)	72.8(4)
C(40)-C(39)-C(38)	137.7(8)
C(40)-C(39)-Nd(2)	77.3(5)
C(38)-C(39)-Nd(2)	73.0(4)
C(33)-C(40)-C(39)	134.8(11)
C(33)-C(40)-Nd(2)	76.5(6)
C(39)-C(40)-Nd(2)	74.7(6)

Symmetry transformations used to
generate equivalent atoms:

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

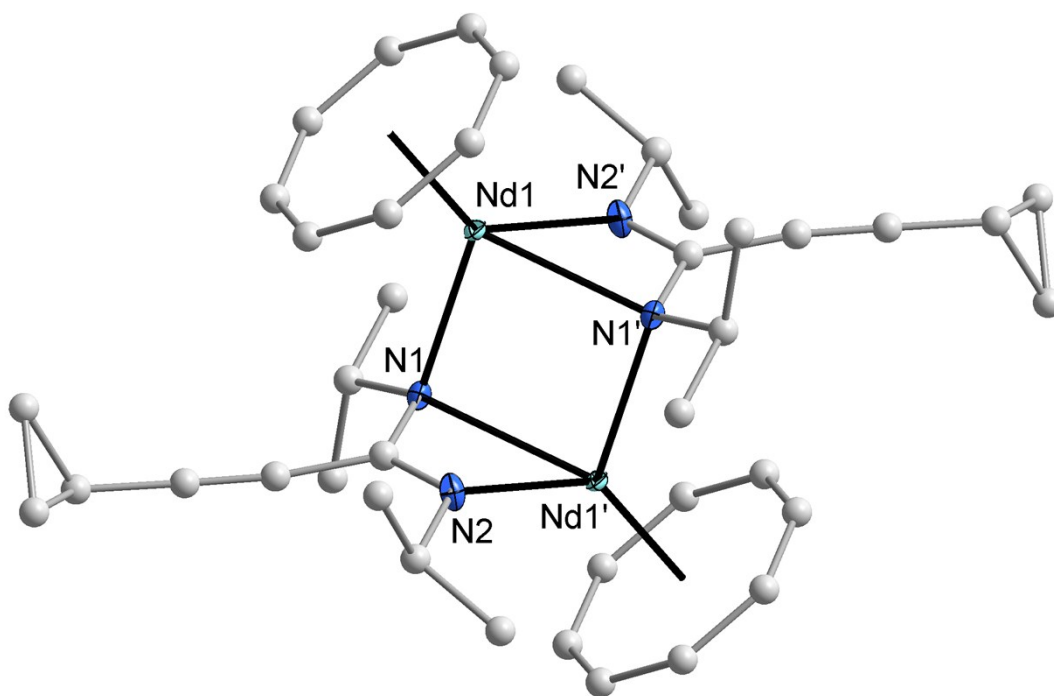


Figure S17. Molecular structure of $[(\text{COT})\text{Nd}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)]_2$ (**12**) in the crystal (molecule 1 of 2 in the asymmetric unit). Ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

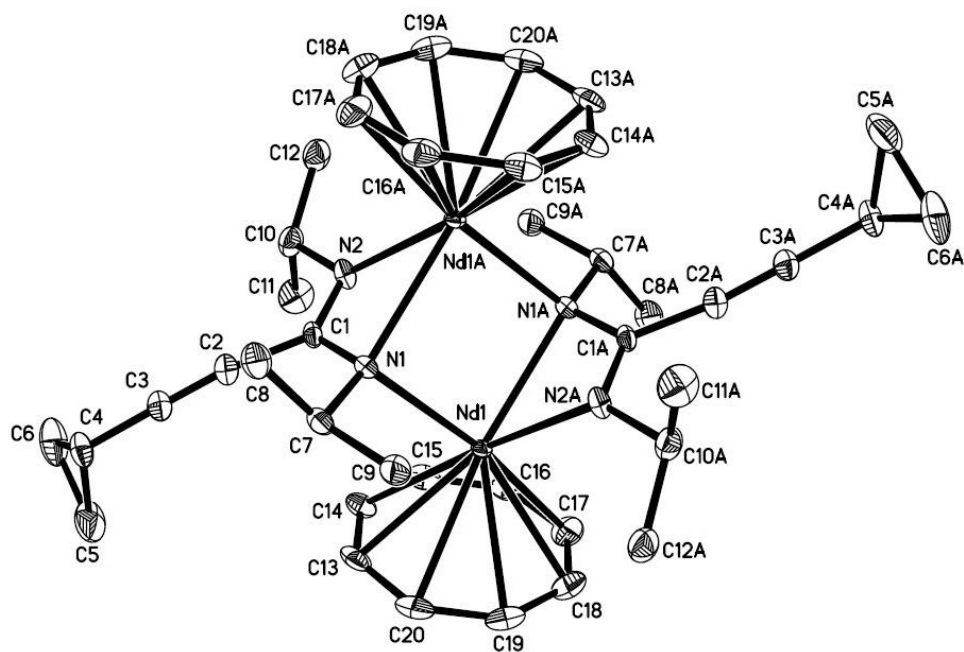


Figure S18. ORTEP drawing of $[(\text{COT})\text{Nd}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)]_2$ (**12**).

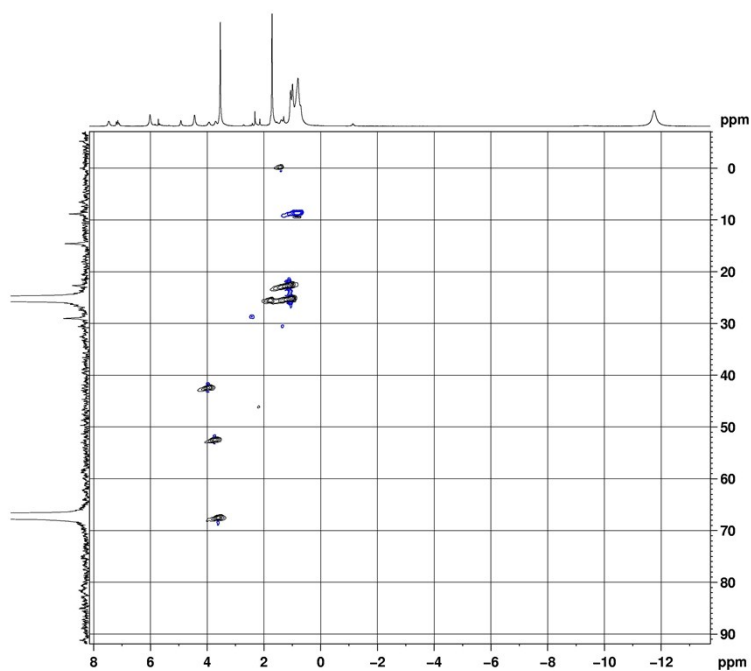


Figure S19. HSQC (H, C- correlation via 1J (C, H)) spectrum in (THF- d_8 , 25°C) of $[(\text{COT})\text{Nd}(\mu\text{-}c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)]_2$ (**12**).

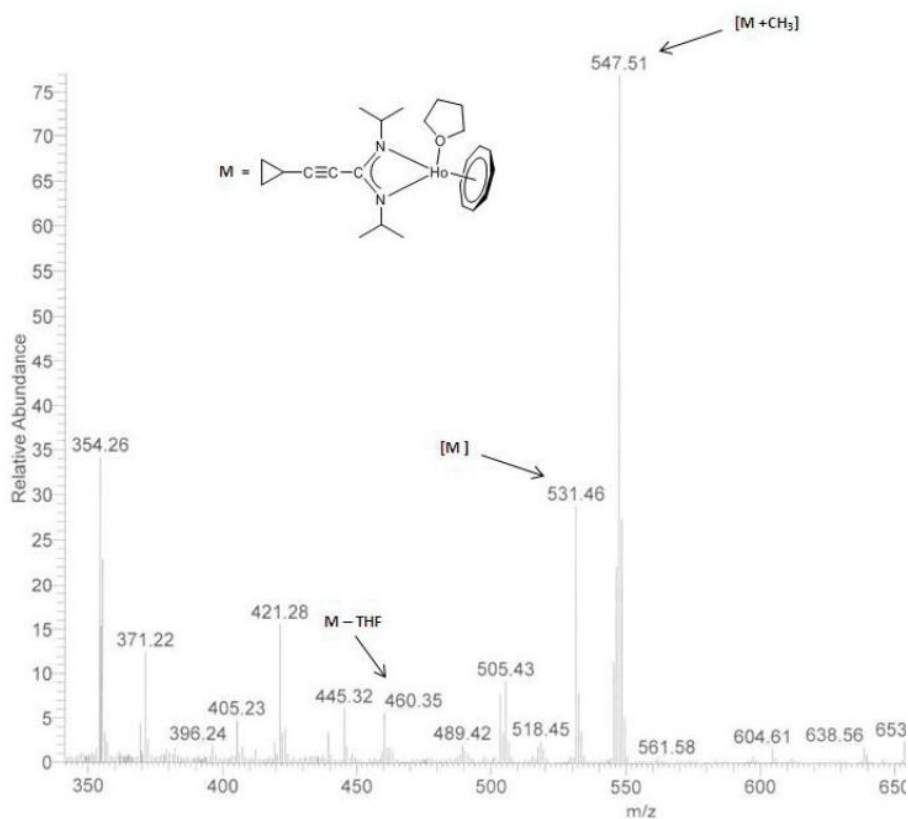


Figure S20. Mass Spectrum (EI) of $(\text{COT})\text{Ho}(c\text{-}\text{C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{N}^i\text{Pr})_2)(\text{THF})$ (**13**).

Table S15. Crystal data and structure refinement (14).

Identification code	ip455	
Empirical formula	C ₃₀ H ₄₃ HoN ₂ O	
Formula weight	612.59	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 12.872(3) Å	α = 90°
	b = 14.491(3) Å	β = 100.37(3)°
	c = 15.056(3) Å	γ = 90°
Volume	2762.4(10) Å ³	
Z	4	
Density (calculated)	1.473 Mg/m ³	
Absorption coefficient	2.888 mm ⁻¹	
F(000)	1248	
Crystal size	0.44 x 0.38 x 0.22 mm ³	
Theta range for data collection	1.92 to 29.24°	
Index ranges	-17 ≤ h ≤ 17, -19 ≤ k ≤ 19, -18 ≤ l ≤ 20	
Reflections collected	30635	
Independent reflections	7466 [R(int) = 0.0647]	
Completeness to theta = 29.24°	99.2 %	
Absorption correction	Sphere	
Max. and min. transmission	0.1886 and 0.1648	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7466 / 48 / 307	
Goodness-of-fit on F ²	1.036	
Final R indices [I > 2sigma(I)]	R1 = 0.0362, wR2 = 0.0843	
R indices (all data)	R1 = 0.0461, wR2 = 0.0881	
Largest diff. peak and hole	1.899 and -2.651 e.Å ⁻³	

Table S16. Bond lengths [Å] and angles [°] (**14**).

Ho-N(2)	2.342(3)	C(9)-C(10)	1.491(5)
Ho-N(1)	2.349(3)	C(10)-C(11)	1.500(6)
Ho-O	2.397(2)	C(11)-C(12)	1.522(5)
Ho-C(26)	2.552(5)	C(13)-N(2)	1.453(4)
Ho-C(23)	2.557(4)	C(13)-C(18)	1.521(5)
Ho-C(25)	2.557(4)	C(13)-C(14)	1.523(5)
Ho-C(24)	2.558(4)	C(14)-C(15)	1.523(6)
Ho-C(22)	2.569(4)	C(15)-C(16)	1.508(7)
Ho-C(19)	2.570(5)	C(16)-C(17)	1.512(8)
Ho-C(21)	2.588(4)	C(17)-C(18)	1.522(6)
Ho-C(20)	2.598(4)	C(19)-C(20)	1.417(10)
Ho-C(1)	2.767(3)	C(19)-C(26)	1.514(11)
C(1)-N(1)	1.324(4)	C(20)-C(21)	1.369(9)
C(1)-N(2)	1.329(4)	C(21)-C(22)	1.324(9)
C(1)-C(2)	1.453(4)	C(22)-C(23)	1.325(9)
C(2)-C(3)	1.197(4)	C(23)-C(24)	1.345(9)
C(3)-C(4)	1.437(4)	C(24)-C(25)	1.381(9)
C(4)-C(5)	1.502(4)	C(25)-C(26)	1.423(10)
C(4)-C(6)	1.506(5)	C(27)-O	1.453(5)
C(5)-C(6)	1.473(5)	C(27)-C(28)	1.469(6)
C(7)-N(1)	1.457(4)	C(28)-C(29)	1.497(6)
C(7)-C(12)	1.500(5)	C(29)-C(30)	1.481(5)
C(7)-C(8)	1.504(6)	C(30)-O	1.437(5)
C(8)-C(9)	1.530(5)		

N(2)-Ho-N(1)	57.15(9)	C(26)-Ho-C(21)	82.69(18)
N(2)-Ho-O	84.13(9)	C(23)-Ho-C(21)	57.2(2)
N(1)-Ho-O	84.63(10)	C(25)-Ho-C(21)	89.21(15)
N(2)-Ho-C(26)	132.71(19)	C(24)-Ho-C(21)	78.60(19)
N(1)-Ho-C(26)	95.80(13)	C(22)-Ho-C(21)	29.8(2)
O-Ho-C(26)	135.5(2)	C(19)-Ho-C(21)	60.0(2)
N(2)-Ho-C(23)	94.69(14)	N(2)-Ho-C(20)	163.22(17)
N(1)-Ho-C(23)	138.85(18)	N(1)-Ho-C(20)	135.78(18)
O-Ho-C(23)	125.03(17)	O-Ho-C(20)	86.65(13)
C(26)-Ho-C(23)	82.01(19)	C(26)-Ho-C(20)	62.4(2)
N(2)-Ho-C(25)	107.63(15)	C(23)-Ho-C(20)	79.2(2)
N(1)-Ho-C(25)	98.21(13)	C(25)-Ho-C(20)	82.88(17)
O-Ho-C(25)	167.56(17)	C(24)-Ho-C(20)	88.60(16)
C(26)-Ho-C(25)	32.4(2)	C(22)-Ho-C(20)	57.9(2)
C(23)-Ho-C(25)	59.4(2)	C(19)-Ho-C(20)	31.8(2)
N(2)-Ho-C(24)	93.96(13)	C(21)-Ho-C(20)	30.6(2)
N(1)-Ho-C(24)	114.91(16)	N(2)-Ho-C(1)	28.63(8)
O-Ho-C(24)	155.37(17)	N(1)-Ho-C(1)	28.52(9)
C(26)-Ho-C(24)	60.7(2)	O-Ho-C(1)	83.22(8)
C(23)-Ho-C(24)	30.5(2)	C(26)-Ho-C(1)	116.58(15)
C(25)-Ho-C(24)	31.3(2)	C(23)-Ho-C(1)	118.65(15)
N(2)-Ho-C(22)	109.95(16)	C(25)-Ho-C(1)	105.06(12)
N(1)-Ho-C(22)	166.14(18)	C(24)-Ho-C(1)	106.58(13)
O-Ho-C(22)	99.77(16)	C(22)-Ho-C(1)	138.44(17)
C(26)-Ho-C(22)	90.24(16)	C(19)-Ho-C(1)	138.60(17)
C(23)-Ho-C(22)	30.0(2)	C(21)-Ho-C(1)	160.33(16)
C(25)-Ho-C(22)	80.32(18)	C(20)-Ho-C(1)	162.13(15)
C(24)-Ho-C(22)	57.8(2)	N(1)-C(1)-N(2)	115.5(3)
N(2)-Ho-C(19)	165.0(2)	N(1)-C(1)-C(2)	121.4(3)
N(1)-Ho-C(19)	110.56(17)	N(2)-C(1)-C(2)	123.0(3)
O-Ho-C(19)	104.30(19)	N(1)-C(1)-Ho	57.90(16)
C(26)-Ho-C(19)	34.4(2)	N(2)-C(1)-Ho	57.64(16)
C(23)-Ho-C(19)	90.59(17)	C(2)-C(1)-Ho	177.36(19)
C(25)-Ho-C(19)	63.3(2)	C(3)-C(2)-C(1)	174.3(3)
C(24)-Ho-C(19)	83.50(19)	C(2)-C(3)-C(4)	178.4(3)
C(22)-Ho-C(19)	81.3(2)	C(3)-C(4)-C(5)	120.2(3)
N(2)-Ho-C(21)	134.11(18)	C(3)-C(4)-C(6)	119.4(3)
N(1)-Ho-C(21)	163.67(19)	C(5)-C(4)-C(6)	58.6(2)
O-Ho-C(21)	85.15(14)	C(6)-C(5)-C(4)	60.8(2)

C(5)-C(6)-C(4)	60.6(2)	C(25)-C(26)-Ho	74.0(3)
N(1)-C(7)-C(12)	110.3(3)	C(19)-C(26)-Ho	73.5(3)
N(1)-C(7)-C(8)	110.0(3)	O-C(27)-C(28)	107.7(4)
C(12)-C(7)-C(8)	110.7(3)	C(27)-C(28)-C(29)	104.2(4)
C(7)-C(8)-C(9)	111.8(3)	C(30)-C(29)-C(28)	105.9(4)
C(10)-C(9)-C(8)	111.5(3)	O-C(30)-C(29)	106.4(3)
C(9)-C(10)-C(11)	111.4(4)	C(1)-N(1)-C(7)	123.0(3)
C(10)-C(11)-C(12)	110.8(4)	C(1)-N(1)-Ho	93.58(18)
C(7)-C(12)-C(11)	112.7(3)	C(7)-N(1)-Ho	142.6(2)
N(2)-C(13)-C(18)	109.6(3)	C(1)-N(2)-C(13)	121.6(3)
N(2)-C(13)-C(14)	110.4(3)	C(1)-N(2)-Ho	93.72(19)
C(18)-C(13)-C(14)	110.3(3)	C(13)-N(2)-Ho	144.16(19)
C(13)-C(14)-C(15)	111.5(4)	C(30)-O-C(27)	109.1(3)
C(16)-C(15)-C(14)	111.2(4)	C(30)-O-Ho	127.2(2)
C(15)-C(16)-C(17)	110.4(4)	C(27)-O-Ho	123.5(3)
C(16)-C(17)-C(18)	111.0(4)		
C(13)-C(18)-C(17)	112.8(4)		
C(20)-C(19)-C(26)	131.0(5)		
C(20)-C(19)-Ho	75.1(3)		
C(26)-C(19)-Ho	72.1(3)		
C(21)-C(20)-C(19)	135.7(5)		
C(21)-C(20)-Ho	74.3(3)		
C(19)-C(20)-Ho	73.0(3)		
C(22)-C(21)-C(20)	136.6(5)		
C(22)-C(21)-Ho	74.3(3)		
C(20)-C(21)-Ho	75.1(3)		
C(21)-C(22)-C(23)	136.8(5)		
C(21)-C(22)-Ho	75.9(3)		
C(23)-C(22)-Ho	74.5(3)		
C(22)-C(23)-C(24)	136.1(6)		
C(22)-C(23)-Ho	75.5(3)		
C(24)-C(23)-Ho	74.8(3)		
C(23)-C(24)-C(25)	136.7(5)		
C(23)-C(24)-Ho	74.7(3)		
C(25)-C(24)-Ho	74.3(3)		
C(24)-C(25)-C(26)	134.0(5)		
C(24)-C(25)-Ho	74.4(3)		
C(26)-C(25)-Ho	73.6(3)		
C(25)-C(26)-C(19)	132.8(5)		

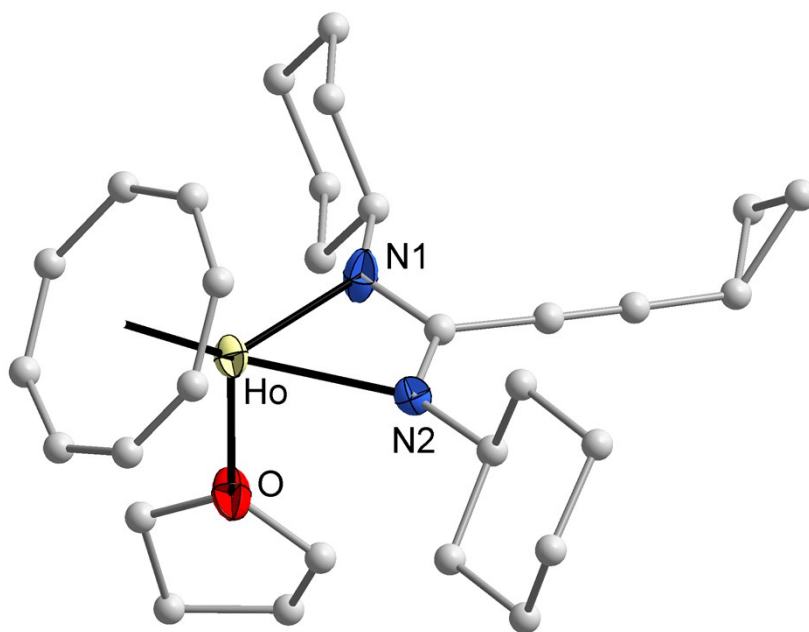


Figure S21. Molecular structure of (COT)Ho(*c*-C₃H₅-C≡C-C(NCy)₂)(THF) (**14**) in the crystal. Ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

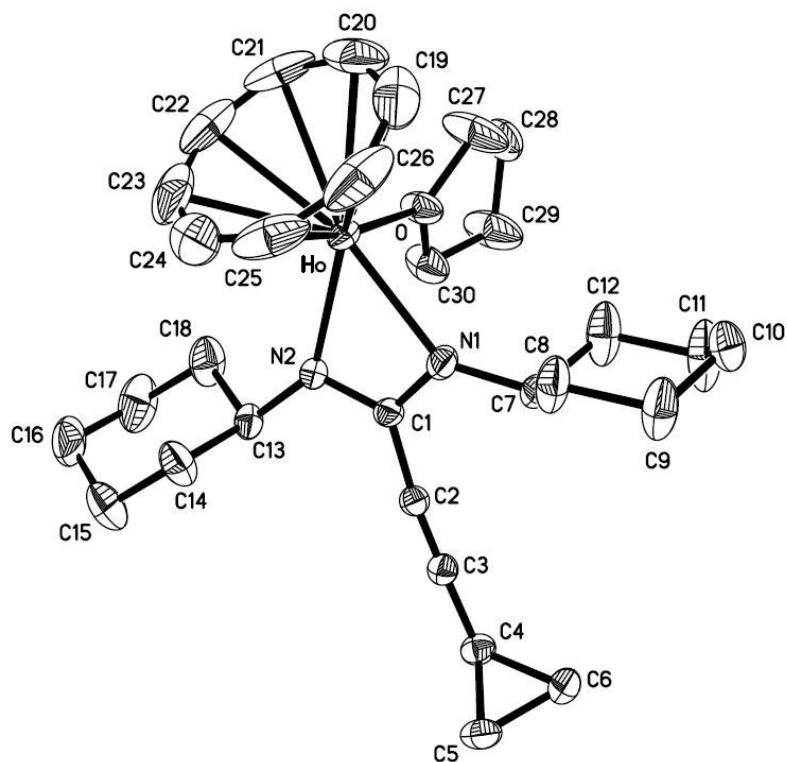


Figure S22. ORTEP drawing of [(COT)Ho(*c*-C₃H₅-C≡C-C(NCy)₂)(THF)] (**14**).

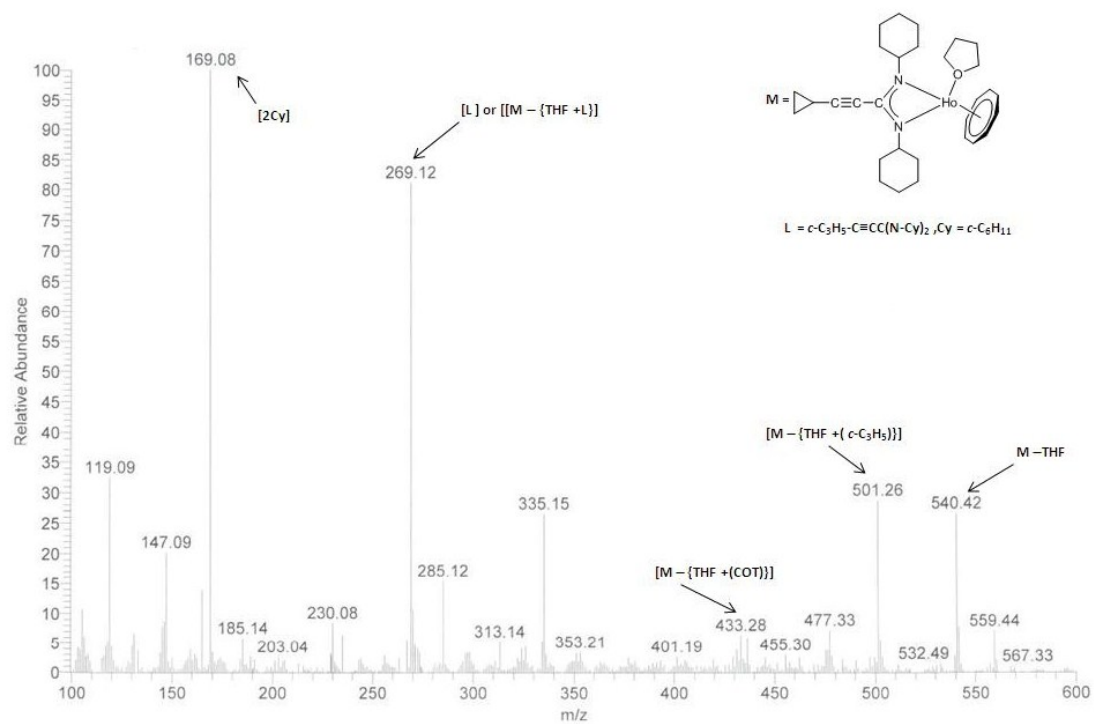


Figure S23. Mass Spectrum (EI) of (COT)Ho(*c*-C₃H₅-C≡C-C(NCy)₂)(THF) (**14**).

Table S17. Crystal data and structure refinement of **(15)**.

Identification code	magd112	
Empirical formula	C ₁₉₀ H ₂₆₄ Cl ₈ N ₁₆ Nd ₈ (6·C ₇ H ₈)	
Formula weight	4209.69 + 552.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 44.794(9) Å	α = 90°
	b = 21.617(4) Å	β = 125.03(3)°
	c = 32.326(7) Å	γ = 90°
Volume	25631(9) Å ³	
Z	4	
Density (calculated)	1.091 Mg/m ³	
Absorption coefficient	1.712 mm ⁻¹	
F(000)	8528	
Crystal size	0.18 x 0.12 x 0.11 mm ³	
Theta range for data collection	1.51 to 26.56°	
Index ranges	-55 ≤ h ≤ 56, -26 ≤ k ≤ 27, -40 ≤ l ≤ 40	
Reflections collected	451720	
Independent reflections	26581 [R(int) = 0.0925]	
Completeness to theta = 26.56°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.52253	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	26581 / 0 / 1001	
Goodness-of-fit on F ²	1.056	
Final R indices [I > 2σ(I)]	R1 = 0.0478, wR2 = 0.1160	
R indices (all data)	R1 = 0.0554, wR2 = 0.1205	
Largest diff. peak and hole	2.533 and -1.664 e.Å ⁻³	

Table S18. Bond lengths [Å] and angles [°] of **(15)**.

Nd(1)-N(2)	2.403(4)	Nd(4)-N(8)	2.418(4)
Nd(1)-N(1)	2.424(4)	Nd(4)-Cl(3)	2.7655(11)
Nd(1)-Cl(2)	2.7895(11)	Nd(4)-C(86)	2.812(5)
Nd(1)-C(22)	2.815(5)	Nd(4)-C(85)	2.817(5)
Nd(1)-C(19)#1	2.822(6)	Nd(4)-C(88)	2.836(5)
Nd(1)-C(21)	2.822(5)	Nd(4)-C(67)	2.838(4)
Nd(1)-C(21)#1	2.827(5)	Nd(4)-Cl(4)	2.8377(15)
Nd(1)-C(20)#1	2.829(5)	Nd(4)-C(87)	2.843(4)
Nd(1)-Cl(1)	2.8289(11)	Nd(4)-C(88)#1	2.847(5)
Nd(1)-C(1)	2.831(5)	Nd(4)-C(85)#1	2.848(5)
Nd(1)-C(20)	2.833(5)	Nd(4)-C(89)	2.858(4)
Nd(1)-C(22)#1	2.839(5)	N(1)-C(1)	1.331(6)
Nd(2)-N(4)	2.380(4)	N(1)-C(7)	1.466(6)
Nd(2)-N(3)	2.434(4)	N(2)-C(1)	1.341(6)
Nd(2)-Cl(1)	2.7684(12)	N(2)-C(13)	1.474(6)
Nd(2)-C(42)	2.819(5)	N(3)-C(23)	1.327(6)
Nd(2)-C(23)	2.821(4)	N(3)-C(29)	1.458(5)
Nd(2)-C(46)	2.824(5)	N(4)-C(23)	1.343(6)
Nd(2)-C(48)	2.831(5)	N(4)-C(35)	1.452(5)
Nd(2)-Cl(2)	2.8324(11)	N(5)-C(49)	1.339(6)
Nd(2)-C(47)	2.835(5)	N(5)-C(55)	1.455(6)
Nd(2)-C(43)	2.836(5)	N(6)-C(49)	1.335(6)
Nd(2)-C(44)	2.836(5)	N(6)-C(61)	1.476(5)
Nd(2)-C(45)	2.851(5)	N(7)-C(67)	1.328(6)
Nd(3)-N(6)	2.404(3)	N(7)-C(73)	1.476(5)
Nd(3)-N(5)	2.439(4)	N(8)-C(67)	1.331(6)
Nd(3)-Cl(4)	2.7771(11)	N(8)-C(79)	1.468(5)
Nd(3)-C(47)	2.804(5)	C(1)-C(2)	1.448(6)
Nd(3)-Cl(3)	2.8081(16)	C(2)-C(3)	1.214(7)
Nd(3)-C(45)	2.823(5)	C(3)-C(4)	1.421(7)
Nd(3)-C(48)	2.824(5)	C(4)-C(5)	1.476(7)
Nd(3)-C(41)	2.829(5)	C(4)-C(6)	1.547(9)
Nd(3)-C(46)	2.831(5)	C(5)-C(6)	1.450(11)
Nd(3)-C(49)	2.833(4)	C(7)-C(8)	1.524(7)
Nd(3)-C(42)	2.867(5)	C(7)-C(12)	1.530(6)
Nd(3)-C(44)	2.875(5)	C(8)-C(9)	1.526(6)
Nd(4)-N(7)	2.395(3)	C(9)-C(10)	1.519(8)

C(10)-C(11)	1.522(8)	C(44)-C(45)	1.423(10)
C(11)-C(12)	1.536(7)	C(45)-C(46)	1.416(10)
C(13)-C(14)	1.516(7)	C(46)-C(47)	1.385(10)
C(13)-C(18)	1.531(7)	C(47)-C(48)	1.400(10)
C(14)-C(15)	1.534(7)	C(49)-C(50)	1.456(6)
C(15)-C(16)	1.521(8)	C(50)-C(51)	1.195(7)
C(16)-C(17)	1.530(8)	C(51)-C(52)	1.447(7)
C(17)-C(18)	1.522(7)	C(52)-C(53)	1.489(9)
C(19)-C(19)#1	1.363(16)	C(52)-C(54)	1.492(10)
C(19)-C(20)	1.389(10)	C(53)-C(54)	1.485(12)
C(19)-Nd(1)#1	2.822(6)	C(55)-C(56)	1.523(6)
C(20)-C(21)	1.404(10)	C(55)-C(60)	1.525(6)
C(20)-Nd(1)#1	2.829(5)	C(56)-C(57)	1.531(7)
C(21)-C(22)	1.393(10)	C(57)-C(58)	1.528(8)
C(21)-Nd(1)#1	2.827(5)	C(58)-C(59)	1.538(8)
C(22)-C(22)#1	1.439(15)	C(59)-C(60)	1.519(7)
C(22)-Nd(1)#1	2.839(5)	C(61)-C(62)	1.528(7)
C(23)-C(24)	1.450(6)	C(61)-C(66)	1.534(6)
C(24)-C(25)	1.189(7)	C(62)-C(63)	1.524(6)
C(25)-C(26)	1.447(7)	C(63)-C(64)	1.526(8)
C(26)-C(27)	1.437(10)	C(64)-C(65)	1.537(8)
C(26)-C(28)	1.482(9)	C(65)-C(66)	1.520(6)
C(27)-C(28)	1.631(12)	C(67)-C(68)	1.446(6)
C(29)-C(30)	1.515(7)	C(68)-C(69)	1.201(7)
C(29)-C(34)	1.536(6)	C(69)-C(70)	1.436(7)
C(30)-C(31)	1.518(6)	C(70)-C(72)	1.485(9)
C(31)-C(32)	1.531(8)	C(70)-C(71)	1.501(11)
C(32)-C(33)	1.544(9)	C(71)-C(72)	1.453(15)
C(33)-C(34)	1.531(6)	C(73)-C(74)	1.513(6)
C(35)-C(40)	1.517(6)	C(73)-C(78)	1.525(7)
C(35)-C(36)	1.529(7)	C(74)-C(75)	1.533(7)
C(36)-C(37)	1.531(6)	C(75)-C(76)	1.520(8)
C(37)-C(38)	1.534(7)	C(76)-C(77)	1.529(7)
C(38)-C(39)	1.517(8)	C(77)-C(78)	1.517(6)
C(39)-C(40)	1.525(7)	C(79)-C(84)	1.530(7)
C(41)-C(42)	1.375(9)	C(79)-C(80)	1.533(7)
C(41)-C(48)	1.423(9)	C(80)-C(81)	1.519(7)
C(42)-C(43)	1.423(10)	C(81)-C(82)	1.522(10)
C(43)-C(44)	1.385(10)	C(82)-C(83)	1.539(10)

C(83)-C(84)	1.531(7)	C(88)-Nd(4)#1	2.847(5)
C(85)-C(86)	1.411(7)	C(89)-C(88)#1	1.414(5)
C(85)-C(88)#1	1.417(7)	C(89)-Nd(4)#1	2.858(4)
C(85)-Nd(4)#1	2.848(5)	C(101)-C(102)	1.381(9)
C(86)-C(87)	1.403(6)	C(101)-C(106)	1.381(11)
C(86)-Nd(4)#1	2.862(4)	C(101)-C(107)	1.479(11)
C(87)-C(86)#1	1.403(6)	C(102)-C(103)	1.393(12)
C(87)-Nd(4)#1	2.843(4)	C(103)-C(104)	1.363(14)
C(88)-C(89)	1.414(5)	C(104)-C(105)	1.399(15)
C(88)-C(85)#1	1.417(7)	C(105)-C(106)	1.400(14)
N(2)-Nd(1)-N(1)	56.05(12)	N(2)-Nd(1)-Cl(1)	84.97(9)
N(2)-Nd(1)-Cl(2)	112.87(10)	N(1)-Nd(1)-Cl(1)	126.44(10)
N(1)-Nd(1)-Cl(2)	86.89(10)	Cl(2)-Nd(1)-Cl(1)	75.44(3)
N(2)-Nd(1)-C(22)	159.91(18)	C(22)-Nd(1)-Cl(1)	87.68(14)
N(1)-Nd(1)-C(22)	140.46(18)	C(19)#1-Nd(1)-Cl(1)	128.55(16)
Cl(2)-Nd(1)-C(22)	83.13(12)	C(21)-Nd(1)-Cl(1)	114.32(16)
N(2)-Nd(1)-C(19)#1	89.26(16)	C(21)#1-Nd(1)-Cl(1)	78.11(13)
N(1)-Nd(1)-C(19)#1	89.67(16)	C(20)#1-Nd(1)-Cl(1)	100.22(17)
Cl(2)-Nd(1)-C(19)#1	150.11(16)	N(2)-Nd(1)-C(1)	28.21(13)
C(22)-Nd(1)-C(19)#1	80.78(16)	N(1)-Nd(1)-C(1)	28.00(13)
N(2)-Nd(1)-C(21)	159.25(18)	Cl(2)-Nd(1)-C(1)	98.94(10)
N(1)-Nd(1)-C(21)	111.99(18)	C(22)-Nd(1)-C(1)	166.98(17)
Cl(2)-Nd(1)-C(21)	80.92(11)	C(19)#1-Nd(1)-C(1)	91.58(15)
C(22)-Nd(1)-C(21)	28.6(2)	C(21)-Nd(1)-C(1)	138.75(18)
C(19)#1-Nd(1)-C(21)	72.91(18)	C(21)#1-Nd(1)-C(1)	127.80(18)
N(2)-Nd(1)-C(21)#1	105.04(17)	C(20)#1-Nd(1)-C(1)	104.09(17)
N(1)-Nd(1)-C(21)#1	141.44(18)	Cl(1)-Nd(1)-C(1)	105.31(10)
Cl(2)-Nd(1)-C(21)#1	130.90(16)	N(2)-Nd(1)-C(20)	130.7(2)
C(22)-Nd(1)-C(21)#1	55.1(2)	N(1)-Nd(1)-C(20)	89.08(16)
C(19)#1-Nd(1)-C(21)#1	54.3(2)	Cl(2)-Nd(1)-C(20)	96.65(16)
C(21)-Nd(1)-C(21)#1	73.4(2)	C(22)-Nd(1)-C(20)	54.5(2)
N(2)-Nd(1)-C(20)#1	89.00(15)	C(19)#1-Nd(1)-C(20)	53.6(2)
N(1)-Nd(1)-C(20)#1	112.75(19)	C(21)-Nd(1)-C(20)	28.7(2)
Cl(2)-Nd(1)-C(20)#1	156.87(14)	C(21)#1-Nd(1)-C(20)	80.20(16)
C(22)-Nd(1)-C(20)#1	73.94(18)	C(20)#1-Nd(1)-C(20)	72.6(2)
C(19)#1-Nd(1)-C(20)#1	28.5(2)	Cl(1)-Nd(1)-C(20)	142.19(16)
C(21)-Nd(1)-C(20)#1	80.36(15)	C(1)-Nd(1)-C(20)	112.47(18)
C(21)#1-Nd(1)-C(20)#1	28.7(2)	N(2)-Nd(1)-C(22)#1	130.65(18)

N(1)-Nd(1)-C(22)#1	160.54(14)	N(3)-Nd(2)-C(47)	103.02(17)
Cl(2)-Nd(1)-C(22)#1	103.37(15)	Cl(1)-Nd(2)-C(47)	167.56(11)
C(22)-Nd(1)-C(22)#1	29.5(3)	C(42)-Nd(2)-C(47)	73.11(17)
C(19)#1-Nd(1)-C(22)#1	73.14(18)	C(23)-Nd(2)-C(47)	96.29(15)
C(21)-Nd(1)-C(22)#1	54.8(2)	C(46)-Nd(2)-C(47)	28.3(2)
C(21)#1-Nd(1)-C(22)#1	28.5(2)	C(48)-Nd(2)-C(47)	28.6(2)
C(20)#1-Nd(1)-C(22)#1	54.3(2)	Cl(2)-Nd(2)-C(47)	107.90(15)
Cl(1)-Nd(1)-C(22)#1	72.66(11)	N(4)-Nd(2)-C(43)	162.05(16)
C(1)-Nd(1)-C(22)#1	156.11(18)	N(3)-Nd(2)-C(43)	118.26(19)
C(20)-Nd(1)-C(22)#1	73.49(17)	Cl(1)-Nd(2)-C(43)	87.01(11)
N(4)-Nd(2)-N(3)	56.19(12)	C(42)-Nd(2)-C(43)	29.2(2)
N(4)-Nd(2)-Cl(1)	108.01(9)	C(23)-Nd(2)-C(43)	144.84(19)
N(3)-Nd(2)-Cl(1)	83.05(10)	C(46)-Nd(2)-C(43)	73.72(17)
N(4)-Nd(2)-C(42)	150.40(18)	C(48)-Nd(2)-C(43)	73.64(17)
N(3)-Nd(2)-C(42)	146.97(17)	Cl(2)-Nd(2)-C(43)	108.25(17)
Cl(1)-Nd(2)-C(42)	95.83(13)	C(47)-Nd(2)-C(43)	80.55(15)
N(4)-Nd(2)-C(23)	28.33(13)	N(4)-Nd(2)-C(44)	136.58(19)
N(3)-Nd(2)-C(23)	28.03(13)	N(3)-Nd(2)-C(44)	92.61(16)
Cl(1)-Nd(2)-C(23)	94.02(9)	Cl(1)-Nd(2)-C(44)	95.50(13)
C(42)-Nd(2)-C(23)	167.70(14)	C(42)-Nd(2)-C(44)	54.5(2)
N(4)-Nd(2)-C(46)	88.39(15)	C(23)-Nd(2)-C(44)	117.16(18)
N(3)-Nd(2)-C(46)	82.25(15)	C(46)-Nd(2)-C(44)	55.2(2)
Cl(1)-Nd(2)-C(46)	146.29(16)	C(48)-Nd(2)-C(44)	80.85(14)
C(42)-Nd(2)-C(46)	80.76(15)	Cl(2)-Nd(2)-C(44)	136.49(16)
C(23)-Nd(2)-C(46)	86.95(13)	C(47)-Nd(2)-C(44)	73.58(17)
N(4)-Nd(2)-C(48)	97.22(16)	C(43)-Nd(2)-C(44)	28.3(2)
N(3)-Nd(2)-C(48)	131.07(18)	N(4)-Nd(2)-C(45)	108.74(18)
Cl(1)-Nd(2)-C(48)	145.63(15)	N(3)-Nd(2)-C(45)	78.22(14)
C(42)-Nd(2)-C(48)	54.3(2)	Cl(1)-Nd(2)-C(45)	117.96(16)
C(23)-Nd(2)-C(48)	118.20(17)	C(42)-Nd(2)-C(45)	73.23(18)
C(46)-Nd(2)-C(48)	54.3(2)	C(23)-Nd(2)-C(45)	95.62(16)
N(4)-Nd(2)-Cl(2)	85.51(9)	C(46)-Nd(2)-C(45)	28.9(2)
N(3)-Nd(2)-Cl(2)	127.29(9)	C(48)-Nd(2)-C(45)	73.09(17)
Cl(1)-Nd(2)-Cl(2)	75.72(4)	Cl(2)-Nd(2)-C(45)	153.81(11)
C(42)-Nd(2)-Cl(2)	83.60(14)	C(47)-Nd(2)-C(45)	54.1(2)
C(23)-Nd(2)-Cl(2)	106.02(9)	C(43)-Nd(2)-C(45)	54.2(2)
C(46)-Nd(2)-Cl(2)	136.23(16)	C(44)-Nd(2)-C(45)	29.0(2)
C(48)-Nd(2)-Cl(2)	83.60(13)	N(6)-Nd(3)-N(5)	55.96(12)
N(4)-Nd(2)-C(47)	84.29(14)	N(6)-Nd(3)-Cl(4)	110.35(9)

N(5)-Nd(3)-Cl(4)	83.19(9)	C(45)-Nd(3)-C(49)	118.52(18)
N(6)-Nd(3)-C(47)	90.47(15)	C(48)-Nd(3)-C(49)	100.82(15)
N(5)-Nd(3)-C(47)	86.84(15)	C(41)-Nd(3)-C(49)	122.77(16)
Cl(4)-Nd(3)-C(47)	145.66(15)	C(46)-Nd(3)-C(49)	98.28(15)
N(6)-Nd(3)-Cl(3)	83.48(9)	N(6)-Nd(3)-C(42)	124.64(18)
N(5)-Nd(3)-Cl(3)	124.63(9)	N(5)-Nd(3)-C(42)	159.56(14)
Cl(4)-Nd(3)-Cl(3)	77.36(3)	Cl(4)-Nd(3)-C(42)	112.38(15)
C(47)-Nd(3)-Cl(3)	133.72(15)	C(47)-Nd(3)-C(42)	72.83(17)
N(6)-Nd(3)-C(45)	136.91(19)	Cl(3)-Nd(3)-C(42)	73.45(11)
N(5)-Nd(3)-C(45)	93.78(16)	C(45)-Nd(3)-C(42)	72.92(17)
Cl(4)-Nd(3)-C(45)	93.21(14)	C(48)-Nd(3)-C(42)	53.82(19)
C(47)-Nd(3)-C(45)	54.7(2)	C(41)-Nd(3)-C(42)	27.92(19)
Cl(3)-Nd(3)-C(45)	138.14(16)	C(46)-Nd(3)-C(42)	79.81(15)
N(6)-Nd(3)-C(48)	86.78(14)	C(49)-Nd(3)-C(42)	150.18(18)
N(5)-Nd(3)-C(48)	108.12(17)	N(6)-Nd(3)-C(44)	163.72(15)
Cl(4)-Nd(3)-C(48)	162.85(11)	N(5)-Nd(3)-C(44)	119.03(18)
C(47)-Nd(3)-C(48)	28.8(2)	Cl(4)-Nd(3)-C(44)	82.93(10)
Cl(3)-Nd(3)-C(48)	104.93(15)	C(47)-Nd(3)-C(44)	73.45(17)
C(45)-Nd(3)-C(48)	73.61(17)	Cl(3)-Nd(3)-C(44)	109.32(16)
N(6)-Nd(3)-C(41)	100.19(15)	C(45)-Nd(3)-C(44)	28.9(2)
N(5)-Nd(3)-C(41)	136.70(17)	C(48)-Nd(3)-C(44)	80.30(14)
Cl(4)-Nd(3)-C(41)	139.74(15)	C(41)-Nd(3)-C(44)	72.94(16)
C(47)-Nd(3)-C(41)	55.11(19)	C(46)-Nd(3)-C(44)	54.7(2)
Cl(3)-Nd(3)-C(41)	80.84(12)	C(49)-Nd(3)-C(44)	146.22(19)
C(45)-Nd(3)-C(41)	81.03(15)	C(42)-Nd(3)-C(44)	53.6(2)
C(48)-Nd(3)-C(41)	29.15(19)	N(7)-Nd(4)-N(8)	55.57(13)
N(6)-Nd(3)-C(46)	109.47(17)	N(7)-Nd(4)-Cl(3)	108.71(10)
N(5)-Nd(3)-C(46)	81.22(14)	N(8)-Nd(4)-Cl(3)	84.46(10)
Cl(4)-Nd(3)-C(46)	117.26(16)	N(7)-Nd(4)-C(86)	150.81(14)
C(47)-Nd(3)-C(46)	28.4(2)	N(8)-Nd(4)-C(86)	100.51(14)
Cl(3)-Nd(3)-C(46)	153.00(11)	Cl(3)-Nd(4)-C(86)	82.31(10)
C(45)-Nd(3)-C(46)	29.0(2)	N(7)-Nd(4)-C(85)	122.69(14)
C(48)-Nd(3)-C(46)	54.3(2)	N(8)-Nd(4)-C(85)	82.07(14)
C(41)-Nd(3)-C(46)	73.70(16)	Cl(3)-Nd(4)-C(85)	102.64(11)
N(6)-Nd(3)-C(49)	28.03(13)	C(86)-Nd(4)-C(85)	29.03(15)
N(5)-Nd(3)-C(49)	28.18(12)	N(7)-Nd(4)-C(88)	98.16(13)
Cl(4)-Nd(3)-C(49)	95.09(9)	N(8)-Nd(4)-C(88)	124.28(14)
C(47)-Nd(3)-C(49)	91.26(14)	Cl(3)-Nd(4)-C(88)	149.12(10)
Cl(3)-Nd(3)-C(49)	103.02(10)	C(86)-Nd(4)-C(88)	81.41(13)

C(85)-Nd(4)-C(88)	73.81(14)	C(87)-Nd(4)-C(85)#1	54.39(12)
N(7)-Nd(4)-C(67)	27.80(13)	C(88)#1-Nd(4)-C(85)#1	73.18(14)
N(8)-Nd(4)-C(67)	27.92(13)	N(7)-Nd(4)-C(89)	91.11(13)
Cl(3)-Nd(4)-C(67)	95.43(9)	N(8)-Nd(4)-C(89)	97.45(11)
C(86)-Nd(4)-C(67)	127.46(14)	Cl(3)-Nd(4)-C(89)	156.64(8)
C(85)-Nd(4)-C(67)	104.58(14)	C(86)-Nd(4)-C(89)	74.44(13)
C(88)-Nd(4)-C(67)	115.29(13)	C(85)-Nd(4)-C(89)	54.98(12)
N(7)-Nd(4)-Cl(4)	86.48(10)	C(88)-Nd(4)-C(89)	28.76(10)
N(8)-Nd(4)-Cl(4)	129.28(10)	C(67)-Nd(4)-C(89)	96.92(12)
Cl(3)-Nd(4)-Cl(4)	77.05(3)	Cl(4)-Nd(4)-C(89)	117.52(3)
C(86)-Nd(4)-Cl(4)	122.65(11)	C(87)-Nd(4)-C(89)	81.42(13)
C(85)-Nd(4)-Cl(4)	147.82(10)	C(88)#1-Nd(4)-C(89)	28.70(10)
C(88)-Nd(4)-Cl(4)	90.02(10)	C(85)#1-Nd(4)-C(89)	54.66(12)
C(67)-Nd(4)-Cl(4)	107.50(10)	Nd(2)-Cl(1)-Nd(1)	104.02(4)
N(7)-Nd(4)-C(87)	172.03(13)	Nd(1)-Cl(2)-Nd(2)	103.38(4)
N(8)-Nd(4)-C(87)	127.96(9)	Nd(4)-Cl(3)-Nd(3)	103.01(3)
Cl(3)-Nd(4)-C(87)	79.19(9)	Nd(3)-Cl(4)-Nd(4)	101.96(3)
C(86)-Nd(4)-C(87)	28.73(11)	C(1)-N(1)-C(7)	120.0(4)
C(85)-Nd(4)-C(87)	54.71(12)	C(1)-N(1)-Nd(1)	93.2(3)
C(88)-Nd(4)-C(87)	73.93(13)	C(7)-N(1)-Nd(1)	146.1(3)
C(67)-Nd(4)-C(87)	155.72(9)	C(1)-N(2)-C(13)	120.1(4)
Cl(4)-Nd(4)-C(87)	94.46(6)	C(1)-N(2)-Nd(1)	93.9(3)
N(7)-Nd(4)-C(88)#1	100.93(13)	C(13)-N(2)-Nd(1)	144.9(3)
N(8)-Nd(4)-C(88)#1	81.09(14)	C(23)-N(3)-C(29)	120.0(4)
Cl(3)-Nd(4)-C(88)#1	130.87(10)	C(23)-N(3)-Nd(2)	92.4(3)
C(86)-Nd(4)-C(88)#1	55.08(14)	C(29)-N(3)-Nd(2)	146.5(3)
C(85)-Nd(4)-C(88)#1	28.97(14)	C(23)-N(4)-C(35)	120.3(4)
C(88)-Nd(4)-C(88)#1	54.39(18)	C(23)-N(4)-Nd(2)	94.4(3)
C(67)-Nd(4)-C(88)#1	93.10(13)	C(35)-N(4)-Nd(2)	143.5(3)
Cl(4)-Nd(4)-C(88)#1	144.21(10)	C(49)-N(5)-C(55)	119.8(4)
C(87)-Nd(4)-C(88)#1	73.77(12)	C(49)-N(5)-Nd(3)	92.5(3)
N(7)-Nd(4)-C(85)#1	118.72(14)	C(55)-N(5)-Nd(3)	147.3(3)
N(8)-Nd(4)-C(85)#1	152.10(14)	C(49)-N(6)-C(61)	120.1(4)
Cl(3)-Nd(4)-C(85)#1	120.64(11)	C(49)-N(6)-Nd(3)	94.1(3)
C(86)-Nd(4)-C(85)#1	73.52(14)	C(61)-N(6)-Nd(3)	144.1(3)
C(85)-Nd(4)-C(85)#1	80.60(15)	C(67)-N(7)-C(73)	120.5(4)
C(88)-Nd(4)-C(85)#1	28.87(14)	C(67)-N(7)-Nd(4)	95.0(3)
C(67)-Nd(4)-C(85)#1	141.93(14)	C(73)-N(7)-Nd(4)	143.0(3)
Cl(4)-Nd(4)-C(85)#1	72.62(10)	C(67)-N(8)-C(79)	119.9(4)

C(67)-N(8)-Nd(4)	93.8(3)	C(21)-C(20)-Nd(1)#1	75.6(3)
C(79)-N(8)-Nd(4)	146.1(3)	C(19)-C(20)-Nd(1)	76.2(3)
N(1)-C(1)-N(2)	116.2(4)	C(21)-C(20)-Nd(1)	75.2(3)
N(1)-C(1)-C(2)	122.4(4)	Nd(1)#1-C(20)-Nd(1)	99.55(18)
N(2)-C(1)-C(2)	121.4(4)	C(22)-C(21)-C(20)	135.4(5)
N(1)-C(1)-Nd(1)	58.8(2)	C(22)-C(21)-Nd(1)	75.4(3)
N(2)-C(1)-Nd(1)	57.9(2)	C(20)-C(21)-Nd(1)	76.1(3)
C(2)-C(1)-Nd(1)	172.2(3)	C(22)-C(21)-Nd(1)#1	76.3(3)
C(3)-C(2)-C(1)	174.4(5)	C(20)-C(21)-Nd(1)#1	75.7(3)
C(2)-C(3)-C(4)	175.7(5)	Nd(1)-C(21)-Nd(1)#1	99.86(16)
C(3)-C(4)-C(5)	120.7(5)	C(21)-C(22)-C(22)#1	134.1(3)
C(3)-C(4)-C(6)	117.5(5)	C(21)-C(22)-Nd(1)	76.0(3)
C(5)-C(4)-C(6)	57.3(5)	C(22)#1-C(22)-Nd(1)	76.2(3)
C(6)-C(5)-C(4)	63.8(5)	C(21)-C(22)-Nd(1)#1	75.3(3)
C(5)-C(6)-C(4)	58.9(4)	C(22)#1-C(22)-Nd(1)#1	74.3(4)
N(1)-C(7)-C(8)	109.1(3)	Nd(1)-C(22)-Nd(1)#1	99.74(16)
N(1)-C(7)-C(12)	111.1(4)	N(3)-C(23)-N(4)	116.3(4)
C(8)-C(7)-C(12)	109.8(4)	N(3)-C(23)-C(24)	123.3(4)
C(7)-C(8)-C(9)	112.2(4)	N(4)-C(23)-C(24)	120.4(4)
C(10)-C(9)-C(8)	111.2(5)	N(3)-C(23)-Nd(2)	59.6(2)
C(9)-C(10)-C(11)	110.6(4)	N(4)-C(23)-Nd(2)	57.3(2)
C(10)-C(11)-C(12)	111.1(4)	C(24)-C(23)-Nd(2)	172.8(3)
C(7)-C(12)-C(11)	111.0(4)	C(25)-C(24)-C(23)	174.2(5)
N(2)-C(13)-C(14)	108.2(4)	C(24)-C(25)-C(26)	176.9(6)
N(2)-C(13)-C(18)	112.0(4)	C(27)-C(26)-C(25)	116.9(6)
C(14)-C(13)-C(18)	111.2(4)	C(27)-C(26)-C(28)	67.9(6)
C(13)-C(14)-C(15)	111.5(4)	C(25)-C(26)-C(28)	119.5(6)
C(16)-C(15)-C(14)	111.2(4)	C(26)-C(27)-C(28)	57.4(5)
C(15)-C(16)-C(17)	111.7(5)	C(26)-C(28)-C(27)	54.7(5)
C(18)-C(17)-C(16)	111.3(4)	N(3)-C(29)-C(30)	110.3(4)
C(17)-C(18)-C(13)	111.1(4)	N(3)-C(29)-C(34)	111.0(4)
C(19)#1-C(19)-C(20)	135.7(4)	C(30)-C(29)-C(34)	110.0(4)
C(19)#1-C(19)-Nd(1)#1	77.0(4)	C(29)-C(30)-C(31)	112.5(4)
C(20)-C(19)-Nd(1)#1	76.1(3)	C(30)-C(31)-C(32)	111.2(4)
C(19)#1-C(19)-Nd(1)	75.2(4)	C(31)-C(32)-C(33)	110.8(5)
C(20)-C(19)-Nd(1)	75.4(3)	C(34)-C(33)-C(32)	110.7(5)
Nd(1)#1-C(19)-Nd(1)	99.49(17)	C(33)-C(34)-C(29)	111.0(4)
C(19)-C(20)-C(21)	134.8(5)	N(4)-C(35)-C(40)	112.0(4)
C(19)-C(20)-Nd(1)#1	75.5(3)	N(4)-C(35)-C(36)	109.8(4)

C(40)-C(35)-C(36)	110.1(4)	C(47)-C(46)-Nd(3)	74.7(3)
C(35)-C(36)-C(37)	111.0(4)	C(45)-C(46)-Nd(3)	75.2(3)
C(36)-C(37)-C(38)	111.0(4)	Nd(2)-C(46)-Nd(3)	100.09(16)
C(39)-C(38)-C(37)	111.7(4)	C(46)-C(47)-C(48)	135.7(5)
C(38)-C(39)-C(40)	112.1(4)	C(46)-C(47)-Nd(3)	76.9(3)
C(35)-C(40)-C(39)	110.8(4)	C(48)-C(47)-Nd(3)	76.4(3)
C(42)-C(41)-C(48)	134.1(5)	C(46)-C(47)-Nd(2)	75.4(3)
C(42)-C(41)-Nd(3)	77.6(3)	C(48)-C(47)-Nd(2)	75.5(3)
C(48)-C(41)-Nd(3)	75.2(3)	Nd(3)-C(47)-Nd(2)	100.49(17)
C(42)-C(41)-Nd(2)	74.3(3)	C(47)-C(48)-C(41)	134.8(5)
C(48)-C(41)-Nd(2)	74.4(3)	C(47)-C(48)-Nd(3)	74.8(3)
Nd(3)-C(41)-Nd(2)	99.28(15)	C(41)-C(48)-Nd(3)	75.6(3)
C(41)-C(42)-C(43)	136.4(5)	C(47)-C(48)-Nd(2)	75.9(3)
C(41)-C(42)-Nd(2)	77.6(3)	C(41)-C(48)-Nd(2)	76.6(3)
C(43)-C(42)-Nd(2)	76.1(3)	Nd(3)-C(48)-Nd(2)	100.09(16)
C(41)-C(42)-Nd(3)	74.5(3)	N(6)-C(49)-N(5)	116.4(4)
C(43)-C(42)-Nd(3)	76.1(3)	N(6)-C(49)-C(50)	121.4(4)
Nd(2)-C(42)-Nd(3)	99.33(17)	N(5)-C(49)-C(50)	122.2(4)
C(44)-C(43)-C(42)	134.6(5)	N(6)-C(49)-Nd(3)	57.8(2)
C(44)-C(43)-Nd(2)	75.9(3)	N(5)-C(49)-Nd(3)	59.3(2)
C(42)-C(43)-Nd(2)	74.7(3)	C(50)-C(49)-Nd(3)	169.4(3)
C(44)-C(43)-Nd(3)	75.9(3)	C(51)-C(50)-C(49)	173.0(5)
C(42)-C(43)-Nd(3)	75.2(3)	C(50)-C(51)-C(52)	176.0(6)
Nd(2)-C(43)-Nd(3)	98.64(16)	C(51)-C(52)-C(53)	118.2(6)
C(43)-C(44)-C(45)	134.5(5)	C(51)-C(52)-C(54)	117.4(6)
C(43)-C(44)-Nd(2)	75.9(3)	C(53)-C(52)-C(54)	59.7(6)
C(45)-C(44)-Nd(2)	76.1(3)	C(54)-C(53)-C(52)	60.2(5)
C(43)-C(44)-Nd(3)	76.3(3)	C(53)-C(54)-C(52)	60.0(5)
C(45)-C(44)-Nd(3)	73.5(3)	N(5)-C(55)-C(56)	110.7(4)
Nd(2)-C(44)-Nd(3)	98.75(16)	N(5)-C(55)-C(60)	110.3(4)
C(46)-C(45)-C(44)	134.9(5)	C(56)-C(55)-C(60)	110.0(4)
C(46)-C(45)-Nd(3)	75.8(3)	C(55)-C(56)-C(57)	110.4(4)
C(44)-C(45)-Nd(3)	77.6(3)	C(58)-C(57)-C(56)	111.9(4)
C(46)-C(45)-Nd(2)	74.5(3)	C(57)-C(58)-C(59)	111.0(4)
C(44)-C(45)-Nd(2)	74.9(3)	C(60)-C(59)-C(58)	110.4(4)
Nd(3)-C(45)-Nd(2)	99.63(17)	C(59)-C(60)-C(55)	112.2(4)
C(47)-C(46)-C(45)	134.7(5)	N(6)-C(61)-C(62)	108.2(3)
C(47)-C(46)-Nd(2)	76.3(3)	N(6)-C(61)-C(66)	112.5(4)
C(45)-C(46)-Nd(2)	76.6(3)	C(62)-C(61)-C(66)	110.5(4)

C(63)-C(62)-C(61)	111.0(4)	Nd(4)-C(85)-Nd(4)#1	99.40(15)
C(62)-C(63)-C(64)	110.5(4)	C(87)-C(86)-C(85)	135.1(5)
C(63)-C(64)-C(65)	111.0(5)	C(87)-C(86)-Nd(4)	76.8(2)
C(66)-C(65)-C(64)	111.0(4)	C(85)-C(86)-Nd(4)	75.7(3)
C(65)-C(66)-C(61)	110.5(4)	C(87)-C(86)-Nd(4)#1	75.0(2)
N(7)-C(67)-N(8)	115.0(4)	C(85)-C(86)-Nd(4)#1	75.2(3)
N(7)-C(67)-C(68)	122.6(4)	Nd(4)-C(86)-Nd(4)#1	99.21(14)
N(8)-C(67)-C(68)	122.4(4)	C(86)-C(87)-C(86)#1	134.6(6)
N(7)-C(67)-Nd(4)	57.2(2)	C(86)-C(87)-Nd(4)	74.4(3)
N(8)-C(67)-Nd(4)	58.3(2)	C(86)#1-C(87)-Nd(4)	76.5(3)
C(68)-C(67)-Nd(4)	174.6(3)	C(86)-C(87)-Nd(4)#1	76.5(3)
C(69)-C(68)-C(67)	177.3(6)	C(86)#1-C(87)-Nd(4)#1	74.4(3)
C(68)-C(69)-C(70)	177.9(6)	Nd(4)-C(87)-Nd(4)#1	98.92(19)
C(69)-C(70)-C(72)	119.6(5)	C(89)-C(88)-C(85)#1	135.4(5)
C(69)-C(70)-C(71)	117.6(6)	C(89)-C(88)-Nd(4)	76.5(2)
C(72)-C(70)-C(71)	58.2(7)	C(85)#1-C(88)-Nd(4)	76.1(3)
C(72)-C(71)-C(70)	60.3(6)	C(89)-C(88)-Nd(4)#1	76.1(2)
C(71)-C(72)-C(70)	61.4(5)	C(85)#1-C(88)-Nd(4)#1	74.4(3)
N(7)-C(73)-C(74)	108.8(4)	Nd(4)-C(88)-Nd(4)#1	99.01(14)
N(7)-C(73)-C(78)	111.8(3)	C(88)#1-C(89)-C(88)	133.4(6)
C(74)-C(73)-C(78)	110.6(4)	C(88)#1-C(89)-Nd(4)	75.2(3)
C(73)-C(74)-C(75)	112.6(4)	C(88)-C(89)-Nd(4)	74.8(3)
C(76)-C(75)-C(74)	110.5(4)	C(88)#1-C(89)-Nd(4)#1	74.8(3)
C(75)-C(76)-C(77)	111.1(4)	C(88)-C(89)-Nd(4)#1	75.2(3)
C(78)-C(77)-C(76)	111.1(4)	Nd(4)-C(89)-Nd(4)#1	98.24(19)
C(77)-C(78)-C(73)	110.9(4)	C(102)-C(101)-C(106)	117.6(8)
N(8)-C(79)-C(84)	110.6(4)	C(102)-C(101)-C(107)	121.5(7)
N(8)-C(79)-C(80)	108.9(4)	C(106)-C(101)-C(107)	120.9(7)
C(84)-C(79)-C(80)	109.8(4)	C(101)-C(102)-C(103)	121.8(8)
C(81)-C(80)-C(79)	112.2(4)	C(104)-C(103)-C(102)	120.6(9)
C(80)-C(81)-C(82)	112.0(5)	C(103)-C(104)-C(105)	118.7(10)
C(81)-C(82)-C(83)	110.5(5)	C(104)-C(105)-C(106)	120.1(9)
C(84)-C(83)-C(82)	110.7(5)	C(101)-C(106)-C(105)	121.1(8)
C(79)-C(84)-C(83)	111.9(5)		
C(86)-C(85)-C(88)#1	135.4(4)		
C(86)-C(85)-Nd(4)	75.3(3)		
C(88)#1-C(85)-Nd(4)	76.7(3)		
C(86)-C(85)-Nd(4)#1	76.2(3)		
C(88)#1-C(85)-Nd(4)#1	75.1(3)		

Symmetry transformations used to generate equivalent atoms:

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

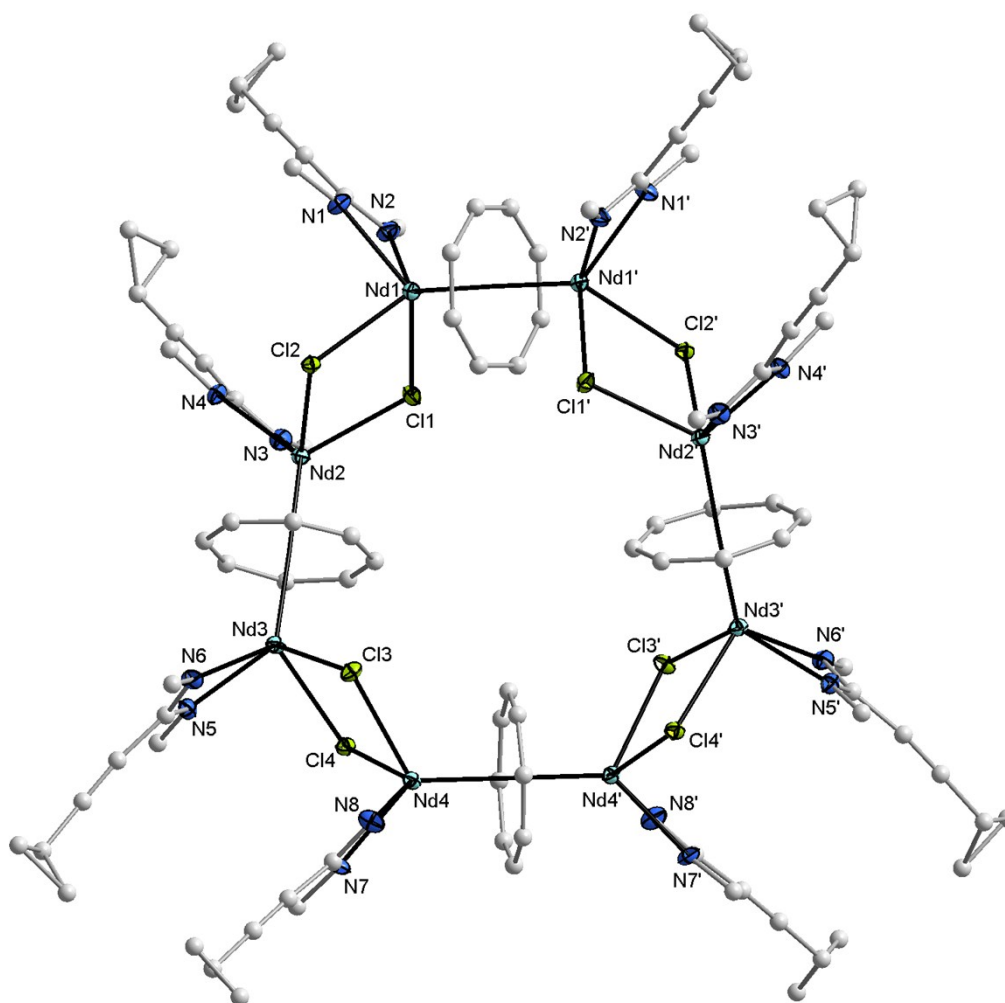


Figure S24. Molecular structure of $[(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})\{\text{Nd}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{CC}(\text{NR})_2)(\mu\text{-Cl})\}_2]_4$ (**15**) in the crystal. Ellipsoids of the heavier atoms with 50% probability, H atoms and peripheral C atoms of the cyclohexyl groups omitted for clarity.

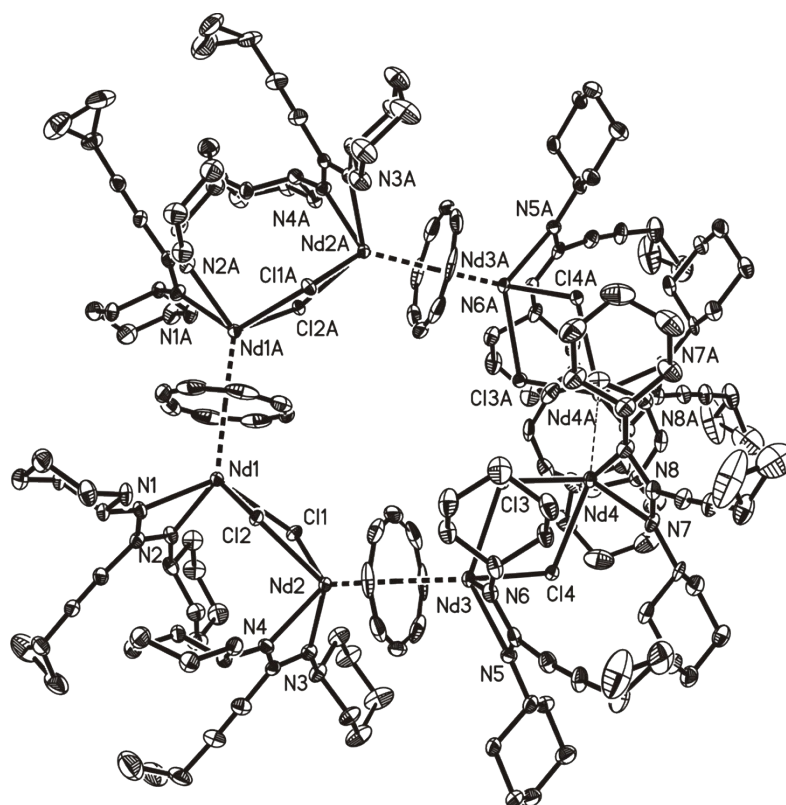


Figure S25. ORTEP drawing of $[(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})\{\text{Nd}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{NR})_2)(\mu\text{-Cl})\}_2]_4$ (**15**).

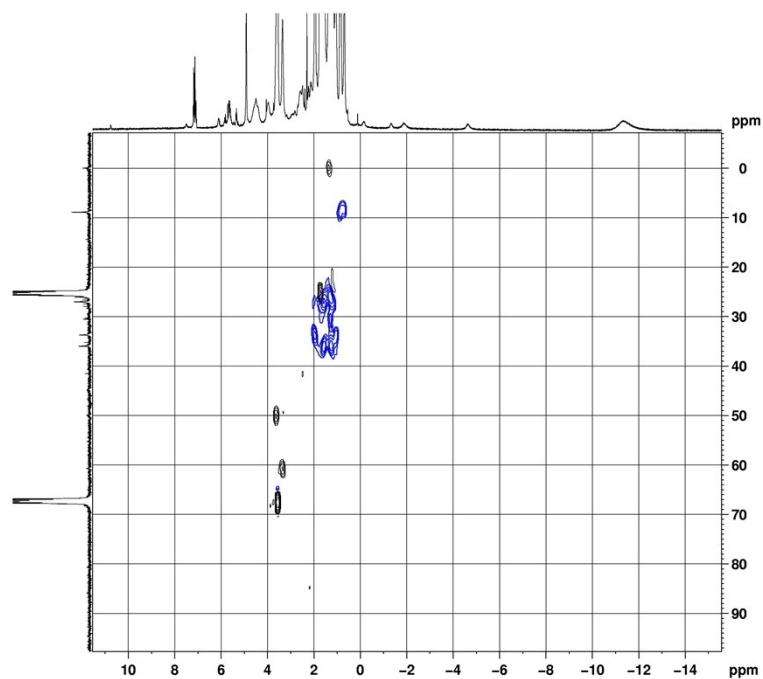


Figure S26. HSQC (H, C-correlation via $^1J(\text{C}, \text{H})$) spectrum in (toluene- d_8 , 25°C) of $[(\mu\text{-}\eta^8\text{:}\eta^8\text{-COT})\{\text{Nd}(c\text{-C}_3\text{H}_5\text{-C}\equiv\text{C-C}(\text{NR})_2)(\mu\text{-Cl})\}_2]_4$ (**15**).

References

- 1 Stoe & Cie, X-Area Program for X-ray Crystal Data collection (X-RED32 included in X-Area), **2002**.
- 2 Agilent Technologies, CrysAlisPro Program for X-ray Crystal Data collection, Vers. 1.171.36.28, **2013**.
- 3 G. M. Sheldrick, *SHELXS-97 Program for Crystal Structure Solution*, Universität Göttingen (Germany) 1997.
- 4 G. M. Sheldrick, *SHELXL-97 Program for Crystal Structure Refinement*, Universität Göttingen (Germany) 1997.