Supporting Information

Metal Versus Ligand Reduction in Ln^{3+} Complexes of a Mesitylene-Anchored Tris(Aryloxide) Ligand

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Table S1. Crystal data and structure refinement for [((^{Ad,Me}ArO)$_3$mes)Ln] (Ln = La, Pr, Sm, Yb), **1-Ln**.

	1-La	**1-Pr**	**1-Sm**	**1-Yb**
Empirical formula	$C_{63}H_{75}O_3La$	$C_{63}H_{75}O_3Pr$	$C_{63}H_{75}O_3Sm$	$C_{63}H_{75}O_3Yb$•½($C_4H_{10}O$)•¼(C_6H_{14})
Formula weight	1019.14	1021.14	1030.59	1111.87
Temperature (K)	133(2)	133(2)	133(2)	88(2)
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	P-1
a (Å)	11.4819(4)	11.4697(17)	12.793(2)	15.585(2)
b (Å)	36.867(2)	36.682(6)	15.689(2)	15.766(2)
c (Å)	11.9433(5)	11.9101(18)	29.928(4)	28.332(4)
α (°)	90	90	90	105.3887(18)
β (°)	106.7174	106.757(2).	95.944(2)	105.3887(18)
γ (°)	90	90	90	113.4791(17)
Volume (Å^3)	4842.0(3)	4798.2(13)	5974.7(14)	6049.9(15)
Z	4	4	4	4
ρ_{calcd} (g/cm^3)	1.398	1.414	1.146	1.221
μ (mm^{-1})	0.931	1.064	1.022	1.589
$R1^a$	0.0315	0.0414	0.0286	0.0414
$wR2^b$	0.0726	0.0986	0.0658	0.0986

Definitions: ^{a}R1 = $\sum||Fo| - |Fc||/\sum|Fo|$; ^{b}wR2 = $[\sum[w(Fo^2 - Fc^2)^2]/\sum[w(Fo^2)^2]\ ]^{1/2}$.

X-ray Data Collection, Structure Solution and Refinement for [((^{Ad,Me}ArO)$_3$mes)La], **1-La**.

A colorless crystal of approximate dimensions 0.175 x 0.162 x 0.060 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (90 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/c$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis.
Hydrogen atoms were included using a riding model.

At convergence, wR2 = 0.0726 and Goof = 1.039 for 610 variables refined against 11962 data (0.75 Å), R1 = 0.0315 for those 10110 data with I > 2.0σ(I).

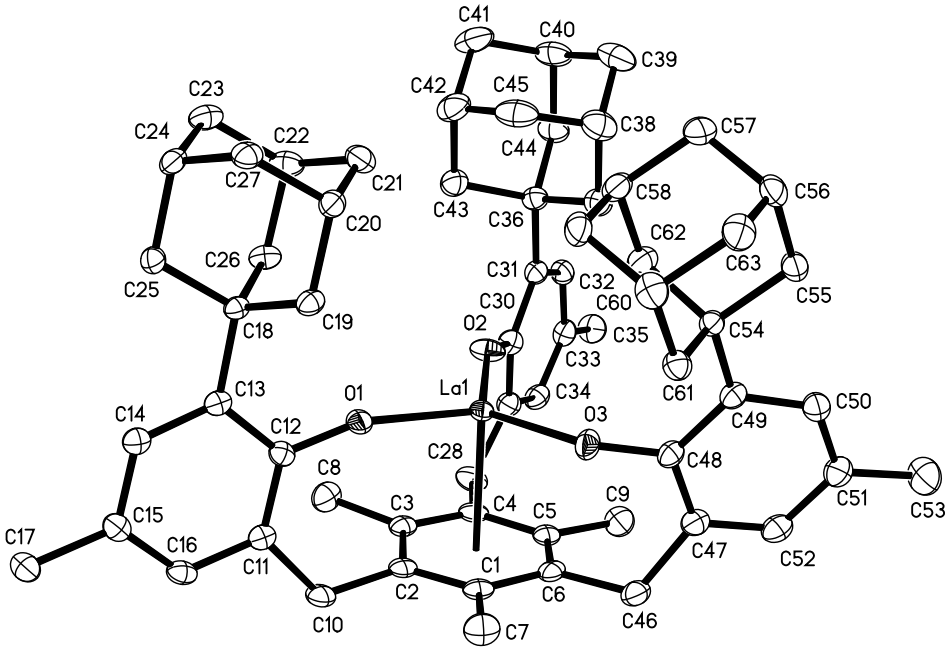

Figure S1. Molecular structure of [((^{Ad,Me}ArO)$_3$mes)La], **1-La**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [((^{Ad,Me}ArO)$_3$mes)Pr], **1-Pr**.

A yellow crystal of approximate dimensions 0.100 x 0.137 x 0.337 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (90 sec/frame scan time for a hemisphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/c$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

Least-squares analysis yielded wR2 = 0.1265 and Goof = 1.015 for 610 variables refined against 10621 data (0.78Å), R1 = 0.0523 for those 7114 data with I > 2.0σ(I).

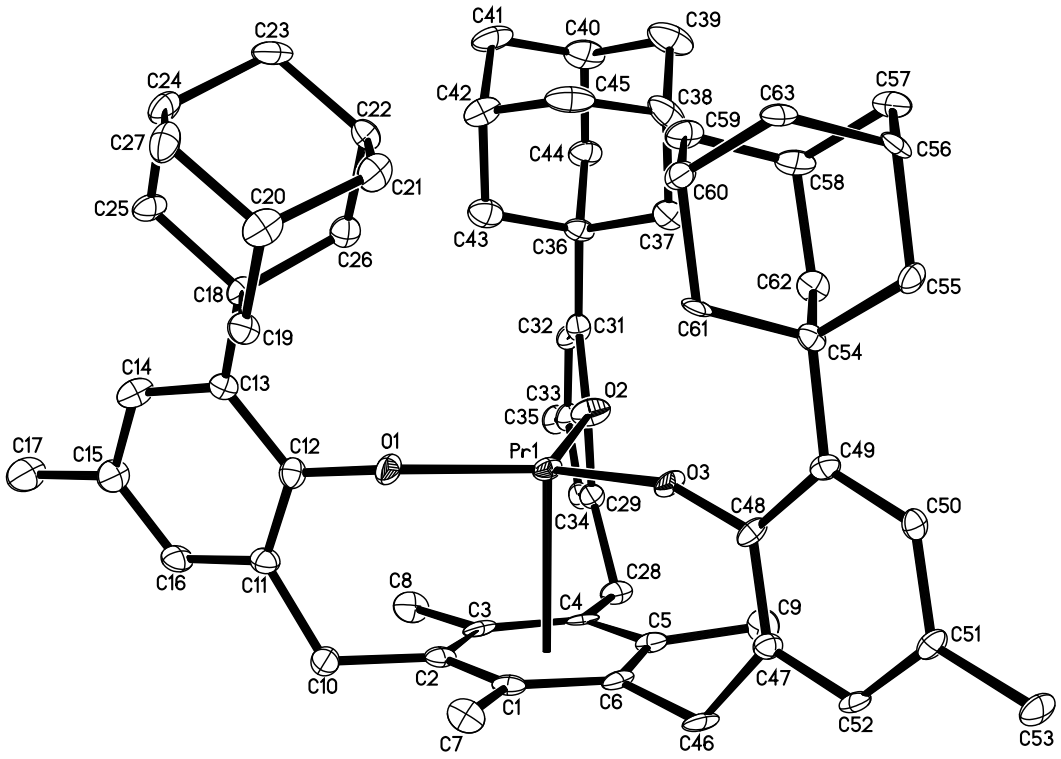

Figure S2. Molecular structure of [((^{Ad,Me}ArO)$_3$mes)Pr], **1-Pr**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [((^{Ad,Me}ArO)$_3$mes)Sm], **1-Sm**.

A yellow crystal of approximate dimensions 0.097 x 0.143 x 0.276 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/c$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

At convergence, wR2 = 0.0658 and Goof = 1.000 for 610 variables refined against 13192 data (0.78Å), R1 = 0.0286 for those 10480 data with $I > 2.0\sigma(I)$.

There were several high residuals present in the final difference-Fourier map. It was not possible to determine the nature of the residuals although it was probable that diethyether, tetrahydrofuran or hexane solvents were present. The SQUEEZE[6] routine in the PLATON[7] program package was used to account for the electrons in the solvent accessible voids.

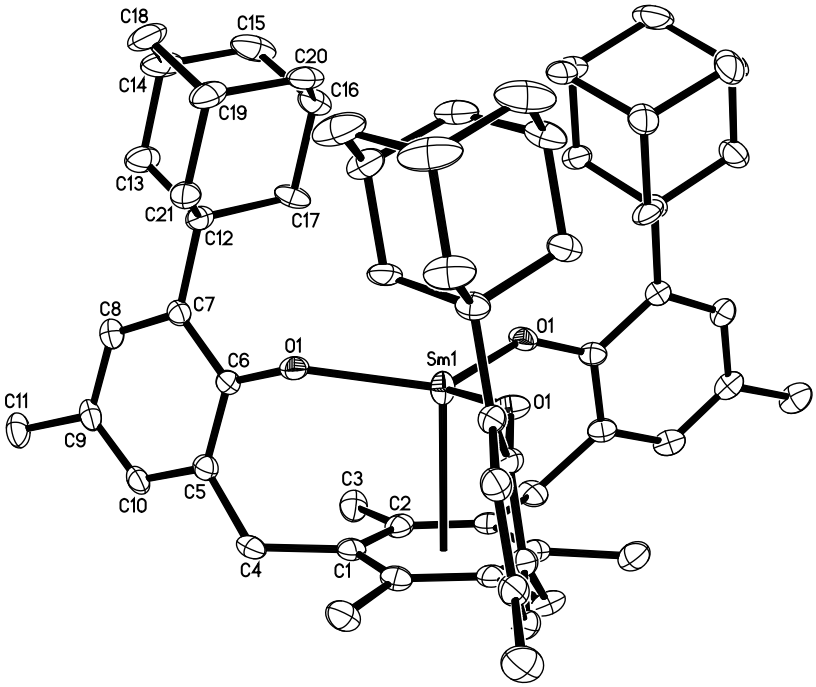

Figure S3. Molecular structure of [((^{Ad,Me}ArO)$_3$mes)Sm], **1-Sm**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [((^{Ad,Me}ArO)$_3$mes)Yb], **1-Yb**.

An orange crystal of approximate dimensions 0.118 x 0.200 x 0.254 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (60 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two molecules of the formula-unit present and one-half molecule of diethylether solvent and one-quarter molecule of hexane solvent. The hexane molecule was located about an inversion center.

At convergence, wR2 = 0.0986 and Goof = 1.021 for 1279 variables refined against 24713 data (0.80 Å), R1 = 0.0414 for those 17489 data with I > 2.0σ(I).

There were several high residuals present in the final difference-Fourier map. It was not possible to determine the nature of the residuals although it was probable that diethylether, hexane, toluene and tetrahydrofuran solvents were present. The SQUEEZE[6] routine in the PLATON[7] program package was used to account for the electrons in the solvent accessible voids.

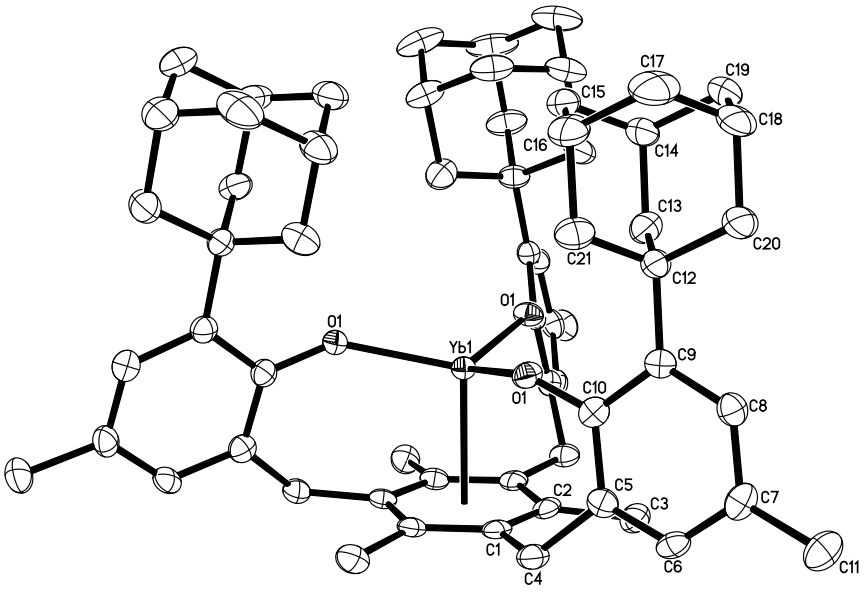

Figure S4. Molecular structure of [((^{Ad,Me}ArO)$_3$mes)Yb], **1-Yb**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

Table S2. Crystal data and structure refinement for [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Ln] (Ln = La, Ce, Pr, Sm, Yb), **2-Ln**.

	2-La	**2-Ce**	**2-Pr**	**2-Sm**	**2-Yb**
Empirical formula	$C_{81}H_{111}LaKN_2O_9$	$C_{81}H_{111}CeKN_2O_9$	$C_{81}H_{111}KN_2O_9$Pr	$C_{81}H_{111}KN_2O_9Sm•C_4H_{10}O$	$C_{81}H_{111}KN_2O_9Yb•C_4H_{10}O$
Formula weight	1434.72	1435.93	1436.72	1520.28	1542.97
Temperature (K)	133(2)	88(2)	133(2)	88(2)	133(2)
Space group	$P2_13$	$P2_13$	$P2_13$	$P2_13$	$P2_13$
a (Å)	19.755(3)	19.7828(19)	19.7501(17)	19.79747(10)	19.755(3)
b (Å)	19.755(3)	19.7828(19)	19.7501(17)	19.79747(10)	19.755(3)
c (Å)	19.755(3)	19.7828(19)	19.7501(17)	19.79747(10)	19.755(3)
α (°)	90	90	90	90	90
β (°)	90	90	90	90	90
γ (°)	90	90	90	90	90
Volume (Å^3)	7710(3)	7742(2)	7704(2)	7756.2(12)	7710(4)
Z	4	4	4	4	4
ρ_{calcd} (g/cm^3)	1.236	1.232	1.239	1.302	1.329
μ (mm^{-1})	0.663	0.697	0.742	0.870	1.326
$R1^a$	0.0577	0.0378	0.0367	0.0374	0.0253
$wR2^b$	0.1686	0.0852	0.897	0.0965	0.0591

Definitions: ^{a}R1 = $\sum||Fo| - |Fc||/\sum|Fo|$; ^{b}wR2 = $[\sum[w(Fo^2 - Fc^2)^2]/\sum[w(Fo^2)^2]\ ]^{1/2}$.

X-ray Data Collection, Structure Solution and Refinement for [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)La], **2-La**.

A red crystal of approximate dimensions 0.093 x 0.112 x 0.202 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (90 sec/frame scan time for a hemisphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The systematic absences were consistent with the cubic space group $P2_13$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The molecule and counter-ion were located on three-fold rotation axes.

Least-squares analysis yielded wR2 = 0.1686 and Goof = 1.063 for 285 variables refined against 4391 data (0.85), R1 = 0.0577 for those 3523 data with I > 2.0σ(I). The absolute structure was assigned by refinement of the Flack parameter.[8]

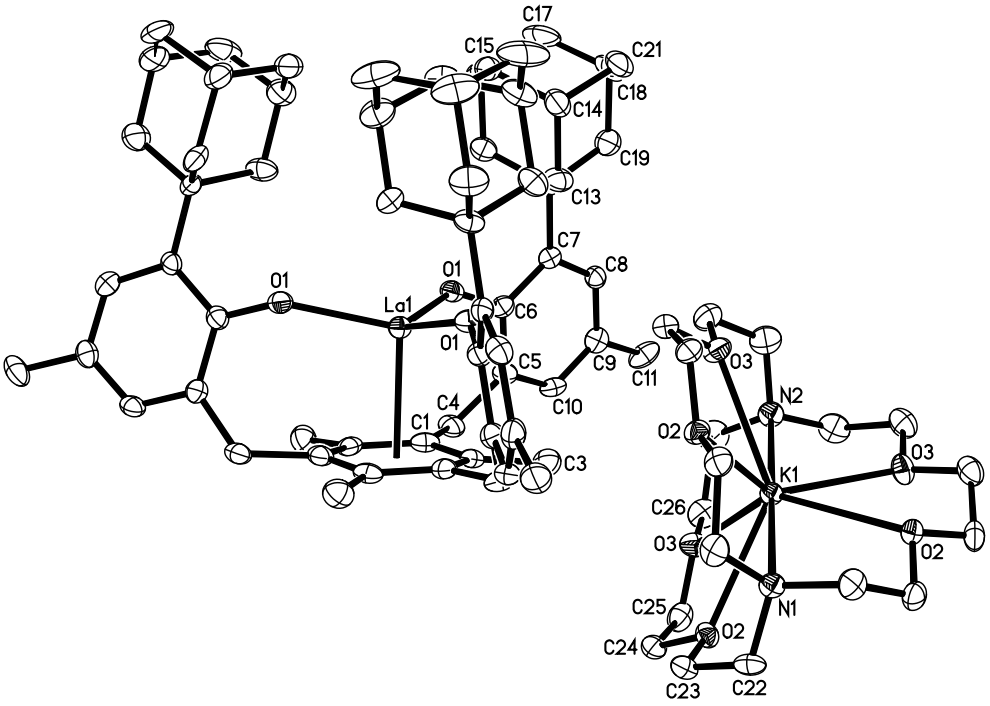

Figure S5. Molecular structure of [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)La], **2-La**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Ce], **2-Ce**.

A red crystal of approximate dimensions 0.158 x 0.272 x 0.330 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (60 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The systematic absences were consistent with the cubic space group $P2_13$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The molecule and counter-ion were located on three-fold rotation axes. The cerium atom was disordered approximately 0.95:0.05 and included with two components to account for the disorder. Ce(2) was assigned an isotropic thermal parameter.

At convergence, wR2 = 0.0852 and Goof = 1.155 for 287 variables refined against 4923 data (0.82), R1 = 0.0378 for those 4709 data with $I > 2.0\sigma(I)$. The absolute structure was assigned by refinement of the Flack parameter.[8]

There were several high residuals present in the final difference-Fourier map. It was not possible to determine the nature of the residuals although it was probable that diethylether or tertahydrofuran was present. The SQUEEZE[6] routine in the PLATON[7] program package was used to account for the electrons in the solvent accessible voids.

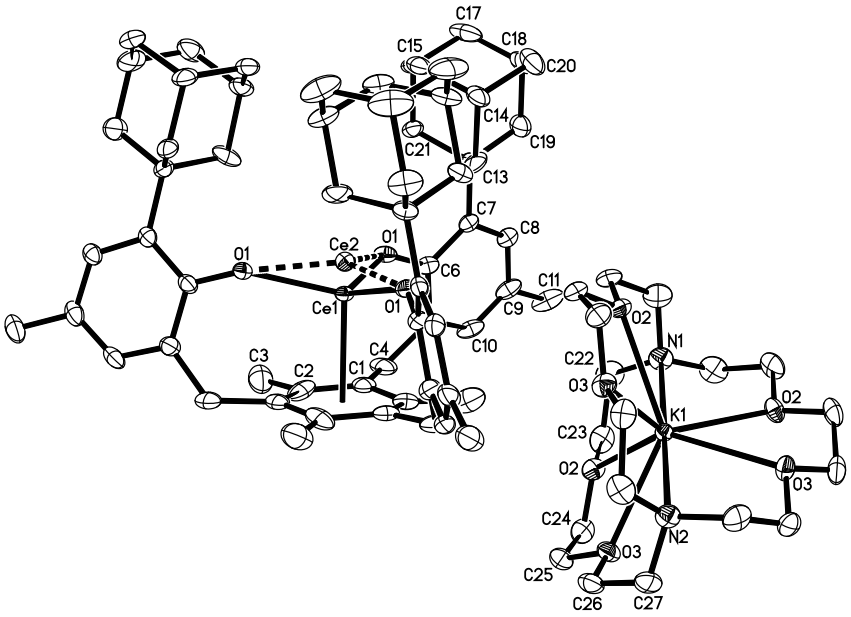

Figure S6. Molecular structure of [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Ce], **2-Ce**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Pr], **2-Pr**.

A red crystal of approximate dimensions 0.185 x 0.244 x 0.352 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (60 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The systematic absences were consistent with the cubic space group $P2_13$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The molecule and counter-ion were located on three-fold rotation axes. The praseodymium atom was disordered approximately 0.96:0.04 and included with two components to account for the disorder. Pr(2) was assigned an isotropic thermal parameter.

At convergence, wR2 = 0.0897 and Goof = 1.175 for 287 variables refined against 4872 data (0.82), R1 = 0.0367 for those 4729 data with $I > 2.0\sigma(I)$. The absolute structure was assigned by refinement of the Flack parameter.[8]

There were several high residuals present in the final difference-Fourier map. It was not possible to determine the nature of the residuals although it was probable that diethylether or tertahydrofuran was present. The SQUEEZE[6] routine in the PLATON[7] program package was used to account for the electrons in the solvent accessible voids.

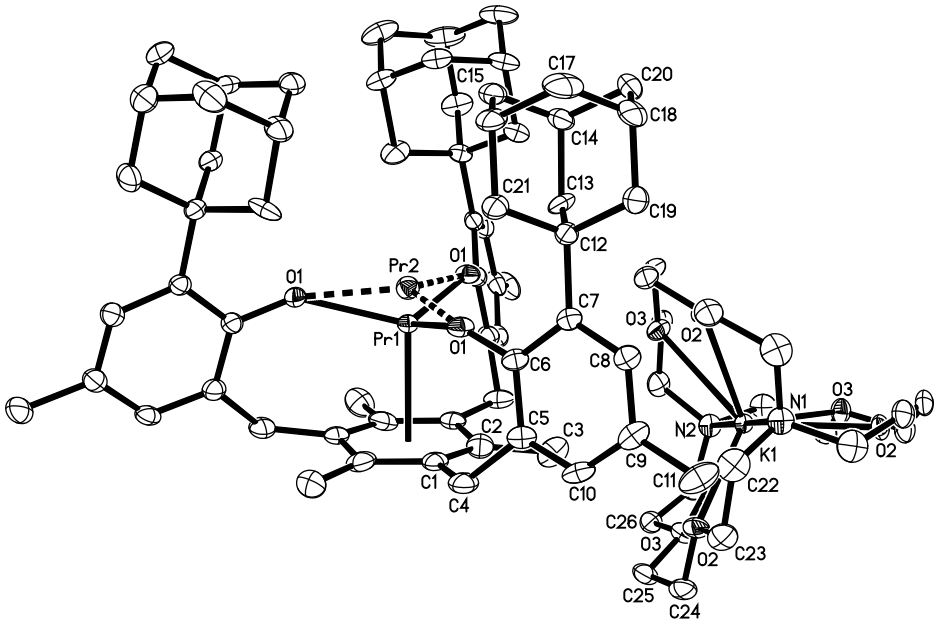

Figure S7. Molecular structure of [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Pr], **2-Pr**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Sm], **2-Sm**.

A red crystal of approximate dimensions 0.280 x 0.305 x 0.318 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The systematic absences were consistent with the cubic space group $P2_13$ that was later determined to be correct.

The structure was solved by dual space methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The molecule and counter-ion were located on three-fold rotation axes. An ether solvent molecule was disordered about a three-fold rotation axis and included with partial site-occupancy-factors.

At convergence, wR2 = 0.0965 and Goof = 1.136 for 297 variables refined against 6196 data (0.76), R1 = 0.0374 for those 6012 data with I > 2.0σ(I). The absolute structure was assigned by refinement of the Flack parameter.[8]

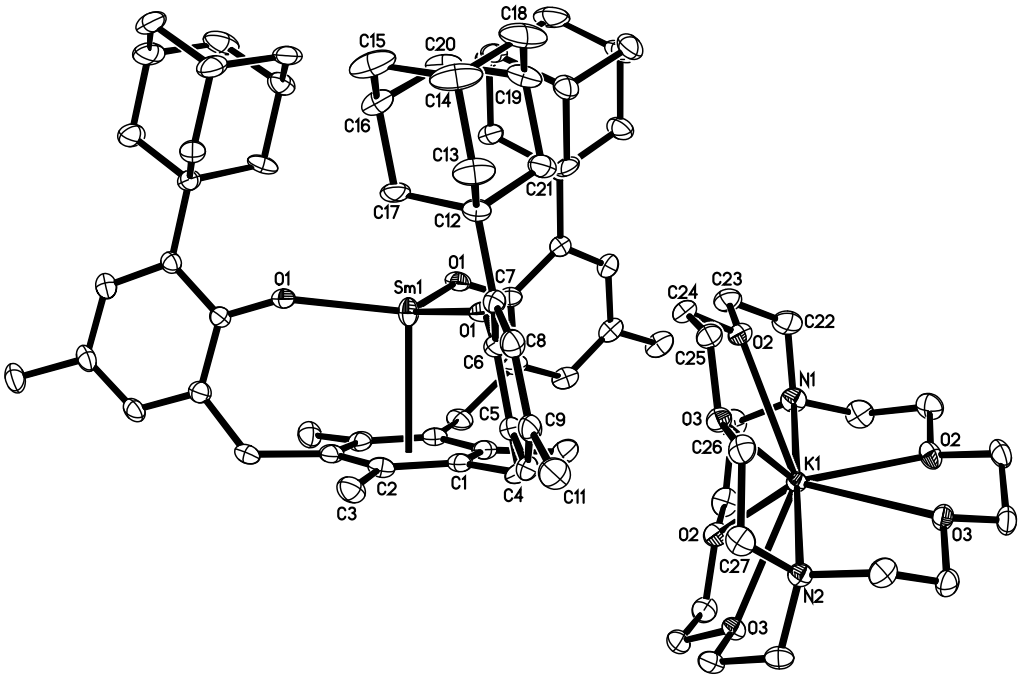

Figure S8. Molecular structure of [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Sm], **2-Sm**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

X-ray Data Collection, Structure Solution and Refinement for [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Yb], **2-Yb**.

A green crystal of approximate dimensions 0.093 x 0.138 x 0.152 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (90 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The systematic absences were consistent with the cubic space group $P2_13$ that was later determined to be correct.

The structure was solved by dual space methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The molecule and counter-ion were located on three-fold rotation axes. An ether solvent molecule was disordered about a three-fold rotation axis and included with partial site-occupancy-factors.

At convergence, wR2 = 0.0591and Goof = 1.100 for 297 variables refined against 5908 data (0.77), R1 = 0.0253 for those 5565 data with I > 2.0σ(I). The absolute structure was assigned by refinement of the Flack parameter.[8]

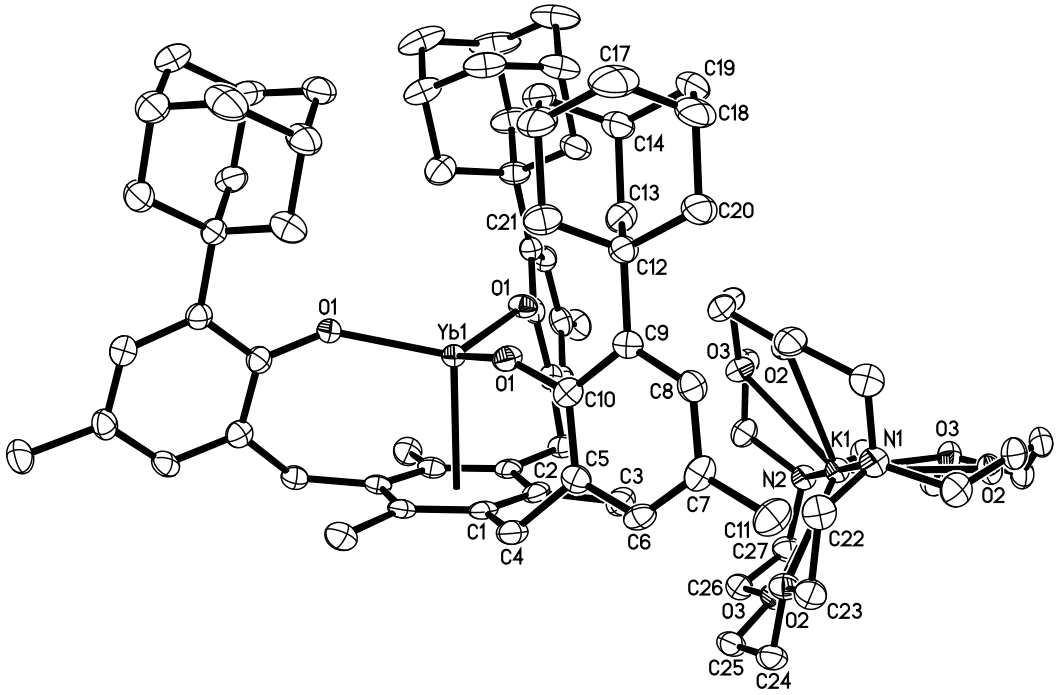

Figure S9. Molecular structure of [K(2.2.2-cryptand)][((^{Ad,Me}ArO)$_3$mes)Yb], **2-Yb**, with thermal ellipsoids drawn at the 50% probability level and hydrogen atoms omitted for clarity.

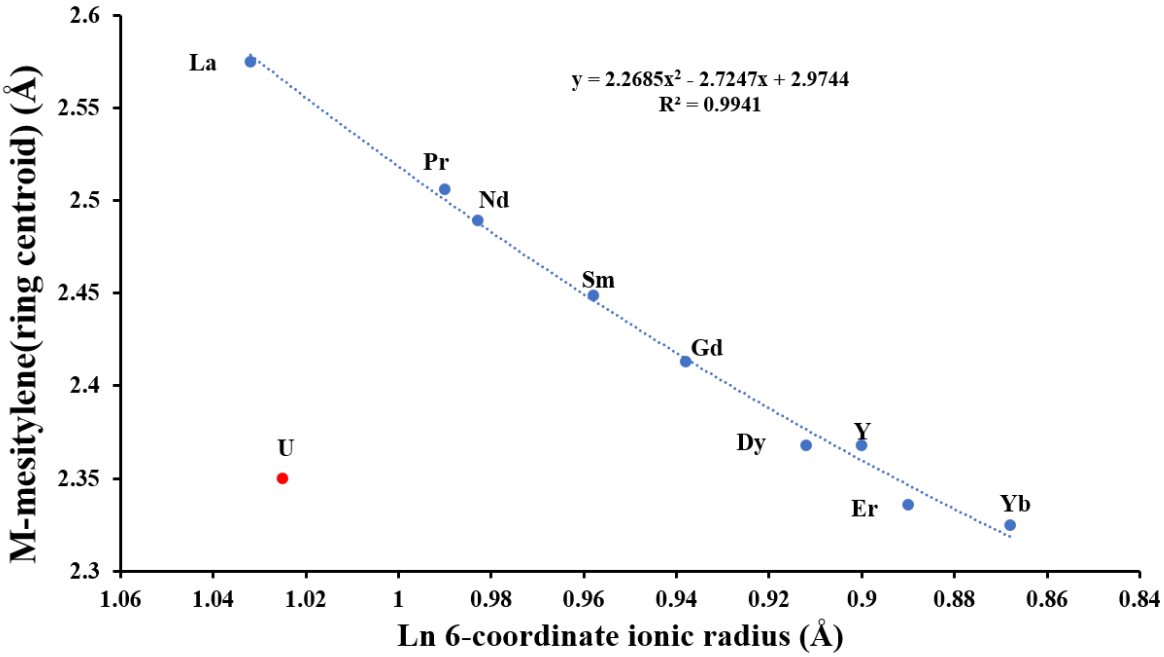

Figure S10. Plot of M–C_6(ring centroid) bond distances versus 6-coordinate ionic radius.[9]

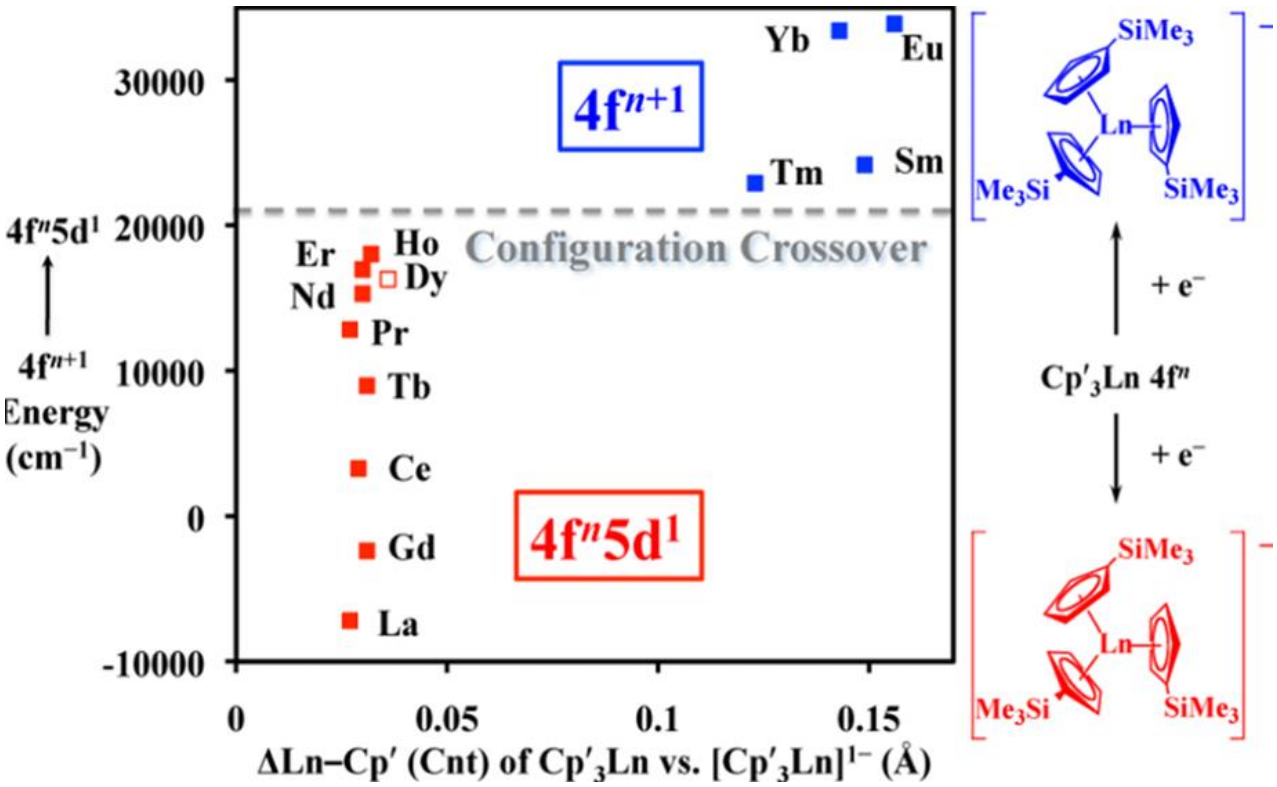

Figure S11. Plot of the $4f^{n+1}$ to $4f^n5d^1$ promotion energies[10] (only an estimated energy is available for Dy) vs the differences in Ln−(Cp′ centroid) distances of $(Cp'_3Ln)^{1-}$ and Cp'_3Ln.[11,12] The gray dashed line indicates the barrier in promotion energies to reduce the $4f^n$ Cp'_3Ln to a $4f^{n+1}$ (blue squares on right) or $4f^n5d^1$ (red squares on left) configuration of $(Cp'_3Ln)^{1-}$.

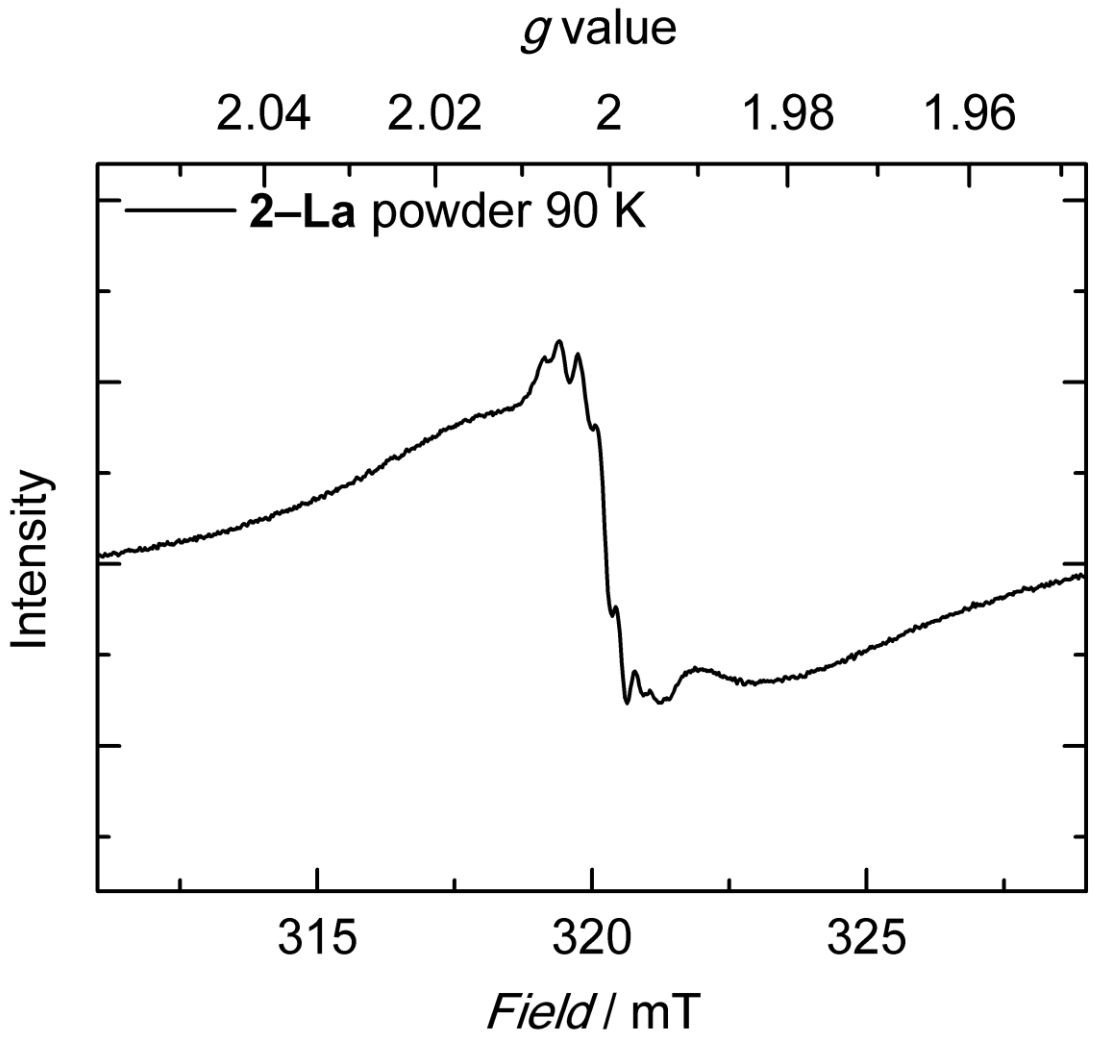

Figure S12. Experimental X-band EPR spectrum of a powdered sample of **2-La** at 90 K (Mode: perpendicular; g = 2.001; A = 3.0 G; ν = 8.967 GHz; P = 1.00 mW; modulation amplitude = 0.20 G).

DFT-based structural parameters and populations analysis of 2-Ln complexes:

Table S3. Computed bond lengths (Å) and angles (°) of **2-Ln** (Ln = La, Ce, Pr, Sm, Yb) obtained from DFT calculations in solution phase

	2-La	**2-Ce**	**2-Pr**	**2-Sm**	**2-Yb**
M–O	2.32	2.26	2.30	2.27	2.17
M–Cnt	2.41	2.31	2.38	2.42	2.27
M–C_{arene}	2.80	2.72	2.78	2.81	2.68
M out of O_3 plane[a]	0.49	0.55	0.49	0.42	0.56
O–M–O Angle	115.7	114.3	115.5	116.7	113.6
Largest C_6 Torsion Angle[b]	15.0	7.7	7.5	3.4	3.4

[a] Distance of M from the plane defined by the three O atoms of the $((^{Ad,Me}ArO)_3mes)^{3-}$ ligand. [b] The largest dihedral angle between adjacent three carbon plane in the mesitylene ring.

Table S4. Difference between the experimental and computed bond lengths (Å) and angles (°) of **2-Ln** (Ln = La, Ce, Pr, Sm, Yb) obtained from DFT calculations in solution phase

	2-La	**2-Ce**	**2-Pr**	**2-Sm**	**2-Yb**
M–O	−0.05	0.00	−0.06	0.00	0.04
M–Cnt	0.05	0.10	0.02	0.15	0.14
M–C_{arene}	0.05	0.08	0.02	0.12	0.12
M out of O_3 plane[a]	−0.06	−0.04	−0.02	−0.15	−0.12
O–M–O Angle	0.8	0.8	−0.4	1.8	2.5
Largest C_6 Torsion Angle[b]	−5.2	3.8	3.4	1.4	1.4

[a] Distance of M from the plane defined by the three O atoms of the $(({}^{Ad,Me}ArO)_3mes)^{3-}$ ligand.

[b] The largest dihedral angle between adjacent three carbon plane in the mesitylene ring.

Table S5. Mulliken spin-density population analysis for **2-Ln** (Ln = La, Ce, Pr, Sm) obtained from DFT calculations in solution phase.

	2-La	**2-Ce**	**2-Pr**	**2-Sm**
C_{arene}	0.87	0.80	0.49	0.23
M	0.08	1.21	2.54	5.79

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