Electronic Supplementary Information

for

Complexes of Group 2 dications with soft thioether- and selenoether-containing macrocycles

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Table S1 X-ray crystallographic data

Compound	$[Sr(MeCN)_8][BAr^F]_2$	$[Ca(18-crown-6)(MeCN)_2][BAr^F]_2$
Formula	$C_{80}H_{48}B_2F_{48}N_8Sr$	$C_{80}H_{54}B_2CaF_{48}N_2O_6$
M/g mol^{-1}	2142.50	2112.95
Crystal system	tetragonal	monoclinic
Space group (No.)	$P\ 4/nnc$ (126)	$C\ 2/c$ (15)
a/Å	15.892(3)	18.707(3)
b/Å	15.892(3)	18.139(3)
c/Å	18.290(4)	25.768(4)
α/°	90	90
β/°	90	97.207(4)
γ/°	90	90
U/Å^3	4619(2)	8675(3)
Z	2	4
μ(Mo-Kα) /mm^{-1}	0.727	0.229
F(000)	2128	4232
Total reflections	31835	29936
Unique reflections	2053	9892
R_{int}	0.120	0.056
Goodness-of-fit on F^2	1.024	1.048
$R_1{}^b$ [$I_o > 2\sigma(I_o)$]	0.077	0.077
R_1 (all data)	0.106	0.130
$wR_2{}^b$ [$I_o > 2\sigma(I_o)$]	0.198	0.201
wR_2 (all data)	0.218	0.236

Common items: T = 100 K, λ_1 = 0.71073 Å (Mo K$_\alpha$), θ_{max} = 27.5°, $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma w(F_o{}^2 - F_c{}^2)^2/\Sigma w F_o{}^2]^{1/2}$.
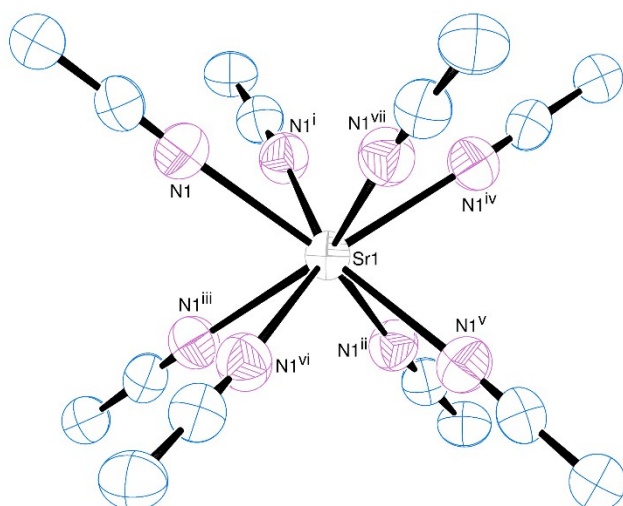
Figure S1. ORTEP representation of the $[Sr(MeCN)_8]^{2+}$ dication. Ellipsoids are shown at the 50% probability level and hydrogen atoms are omitted for clarity. $d(Sr–N) = 2.681(5)$ Å. Symmetry operations: (i) $1.5 – y, 1.5 – x, 0.5 – z$; (ii) $x, 1.5 – y, 0.5 – z$; (iii) $y, 1.5 – x, z$; (iv) $1.5 – x, 1.5 – y, z$; (v) $y, x, 0.5 – z$; (vi) $1.5 – y, x, z$; (vii) $1.5 – x, y, 0.5 – z$.
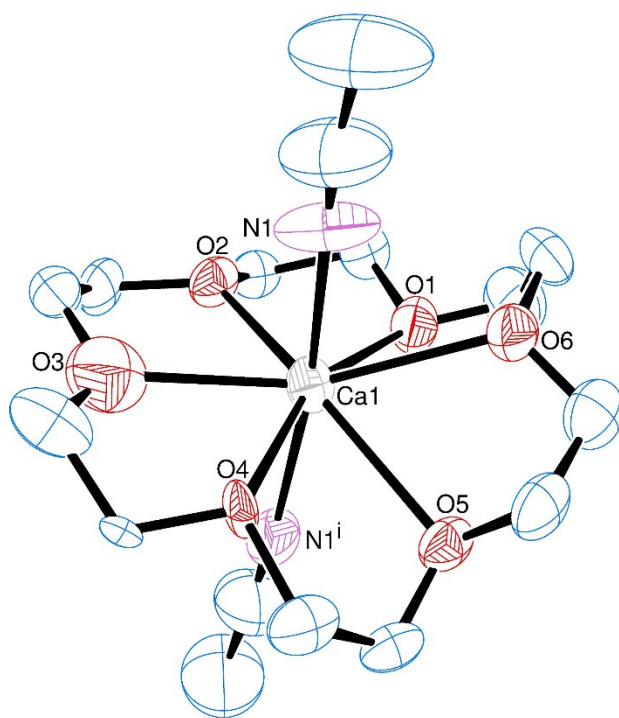

Figure S2. ORTEP representation of the dication in $[Ca(18\text{-crown-}6)(MeCN)_2][BAr^F]_2$. Hydrogen atoms are omitted for clarity and ellipsoids are shown at the 50% probability level. Selected bond lengths (Å) and angles (°): Ca–O1 2.529(6), Ca–O2 2.377(5), Ca–O3 2.50(2), Ca–O4 2.490(8), Ca–O5 2.605(5), Ca–O6 2.550(5), Ca–N1 2.423(4); O1–Ca–O2 65.8(2), O2–Ca–O3 67.1(5), O3–Ca–O4 63.3(3), O4–Ca–O5 63.9(3), O5–Ca–O6 62.0(2), O6–Ca–O1 65.1(2). Symmetry operation: $–x, y, 0.5 – z$.