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Supplementary Material

Extremely bulky β-diketiminate complexes of calcium(II) and ytterbium(II)

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Table S1. Crystal data for compounds **1**-**4**.

	1·(hexane)	**2**·(benzene)$_6$	**3**·(toluene)	**4**·(hexane)
empirical formula	$C_{77}H_{75}CaIN_2$	$C_{107}H_{97}IN_2Yb$	$C_{156}H_{136}Ca_2N_4$	$C_{83}H_{91}BN_2Yb$
formula weight	1195.37	1710.80	2146.84	1300.42
crystal system	triclinic	triclinic	monoclinic	monoclinic
space group	*P*-1	*P*-1	*C*2/*c*	$P2_1/n$
a (Å)	12.7462(3)	12.9219(3)	17.862(4)	11.6382(3)
b (Å)	14.3054(3)	13.4569(3)	25.995(5)	31.1049(10)
c (Å)	17.3946(4)	25.4495(7)	25.089(5)	18.5341(7)
α (º)	99.900(2)	79.664(2)	90	90
β (º)	94.512(2)	83.898(2)	93.01(3)	100.871(3)
γ (º)	99.256(2)	75.878(2)	90	90
V (Å^3)	3065.32(12)	4214.92(18)	11633(4)	6589.0(4)
Z	2	2	4	4
T (K)	123(2)	123(2)	100(2)	123(2)
ρ_{calcd} (g·cm^3)	1.295	0.1.349	1.226	1.311
μ (mm^{-1})	0.652	1.527	0.156	1.467
F(000)	1248	1752	4560	2712
reflns collected	28547	37518	47897	42923
unique reflns	14772	16534	12635	12829
R_{int}	0.0270	0.0319	0.0614	0.0519
R1 [I > 2σ(I)]	0.0430	0.0307	0.0563	0.0507
wR2 (all data)	0.1198	0.0646	0.1595	0.1391
largest peak and hole (e·Å^{-3})	0.92, -0.83	1.23, -0.80	0.55, -0.39	0.95, -1.28
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