Electronic Supplementary Information for Dalton Transactions

Electronic Supporting information

for

Coordination Complexes Bearing Potentially Tetradentate Phenoxy-Amine Ligands

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Table S1. Crystal Data, Data Collection and Refinement Parameters for compounds **4c** and **5a**.

data	4c	5a
formula	$C_{42}H_{72}MgN_2O_6$	$C_{54}H_{100}CaN_6O_2$
solvent	—	C_7H_8
formula weight	725.33	997.61
colour, habit	colourless blocky needles	colourless tabular needles
crystal size / mm	$0.15 \times 0.13 \times 0.07$	$0.12 \times 0.11 \times 0.04$
temperature / K	173	173
crystal system	monoclinic	triclinic
space group	$P2_1/n$ (no. 14)	$P\bar{1}$ (no. 2)
***a* / Å**	15.7123(6)	10.8234(10)
***b* / Å**	30.5819(12)	12.9659(12)
***c* / Å**	18.7720(7)	13.1370(11)
α / deg	—	110.331(8)
β / deg	90.923(3)	107.408(8)
γ / deg	—	100.882(8)
***V* / Å^3**	9019.0(6)	1558.8(2)
Z	8 [a]	1 [b]
***D*$_c$ / g cm^{-3}**	1.068	1.063
radiation used	Mo-Kα	Mo-Kα
μ / mm^{-1}	0.082	0.144
θ max / deg	66	65
no. of unique reflns		
measured	30993	10277
obs, $\|F_o\| > 4\sigma(\|F_o\|)$	24491	8941
no. of variables	949	372
***R*$_1$, *wR*$_2$** [c]	0.298, 0.447	0.175, 0.356
CCDC	293483	293484

[a] There are two crystallographically independent molecules in the asymmetric unit. [b] The molecule has crystallographic C_i symmetry. [c] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$.

Data were collected using an Oxford Diffraction Xcalibur 3 diffractometer, and the structures were refined based on F^2 using the SHELXTL and SHELX-97 program systems.[1]

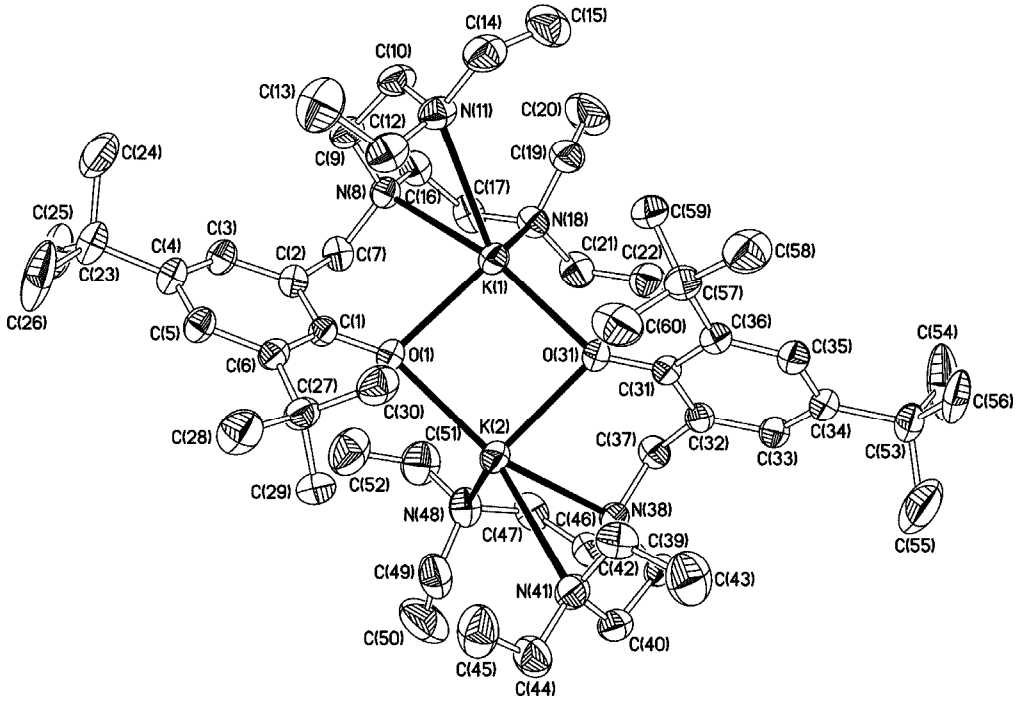

Fig. S1 The molecular structure of **2a** (50% probability ellipsoids).

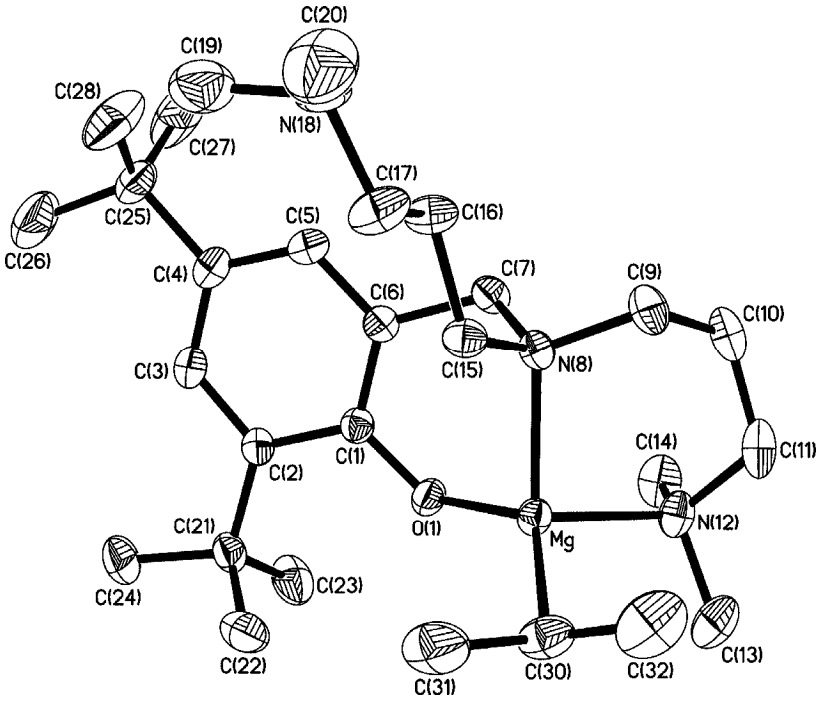

Fig. S2 The molecular structure of **3b** (50% probability ellipsoids).

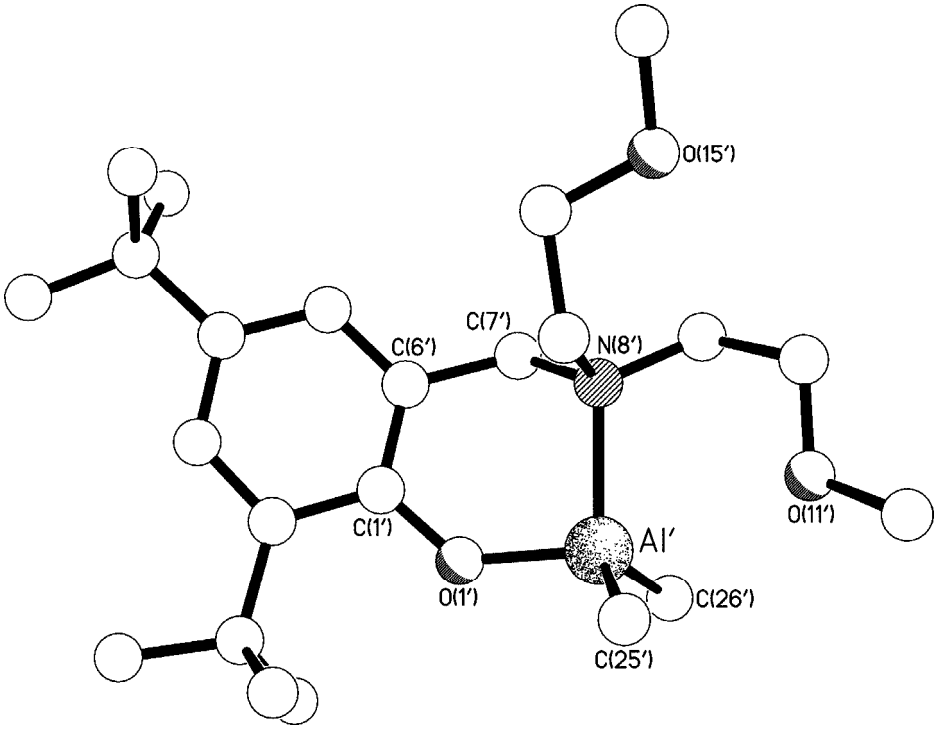

Fig. S3 The molecular structure of one (**II**) of the two independent complexes present in the crystals of **6c**.

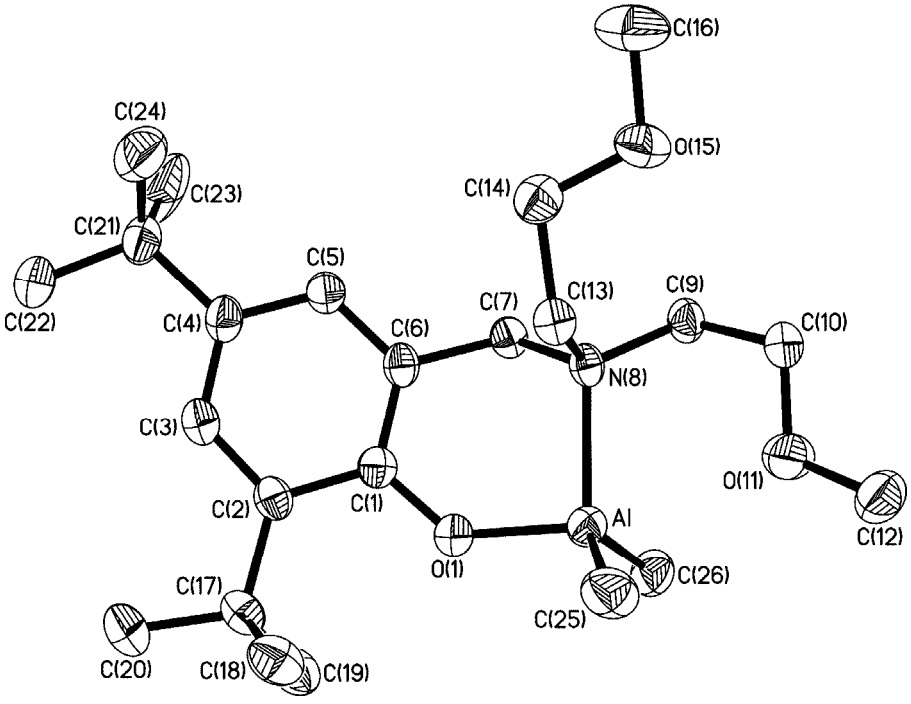

Fig. S4 The molecular structure of one (**I**) of the two independent complexes present in the crystals of **6c** (50% probability ellipsoids).

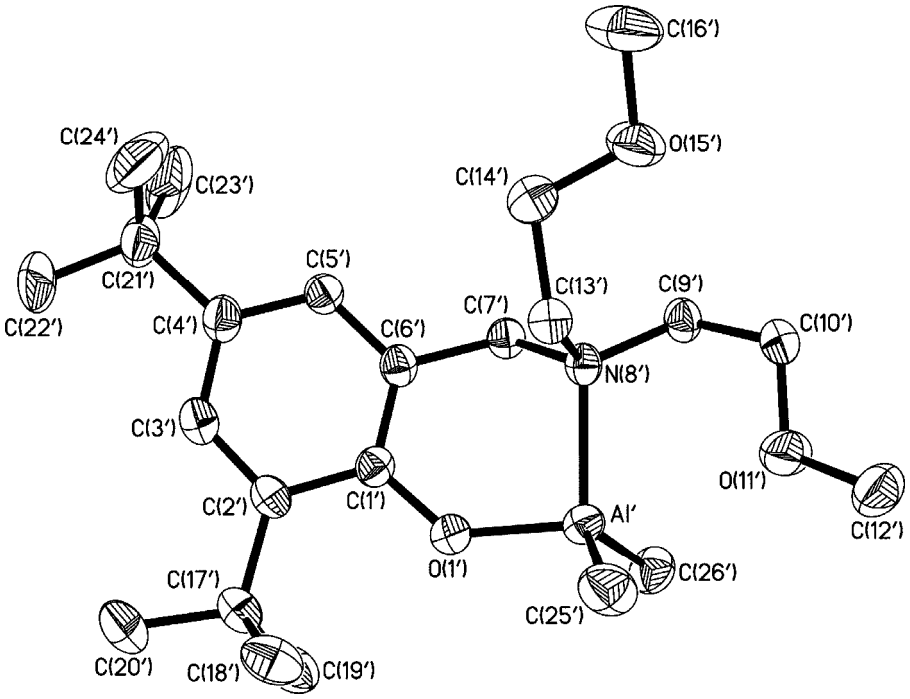

Fig. S5 The molecular structure of one (**II**) of the two independent complexes present in the crystals of **6c** (50% probability ellipsoids).

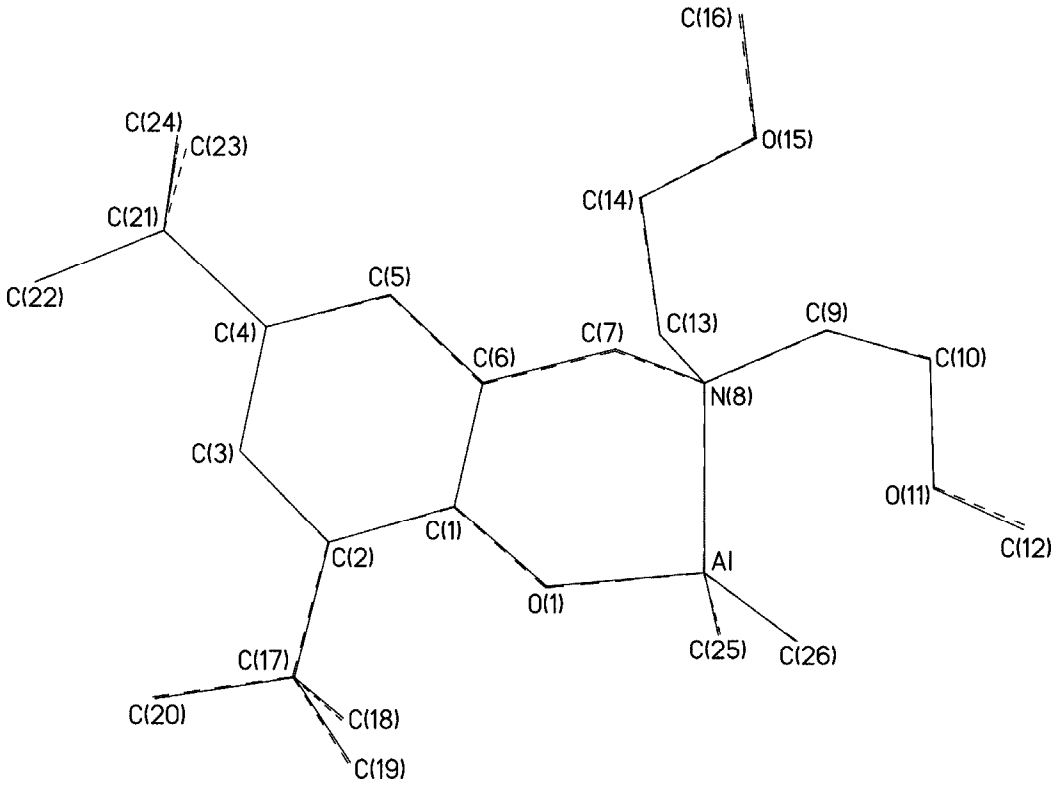

Fig. S6 Overlay of the two independent complexes (**I** and **II**) present in the crystals of **6c**. The r.m.s. fit of all the non-hydrogen atoms of the two complexes is *ca.* 0.057 Å.

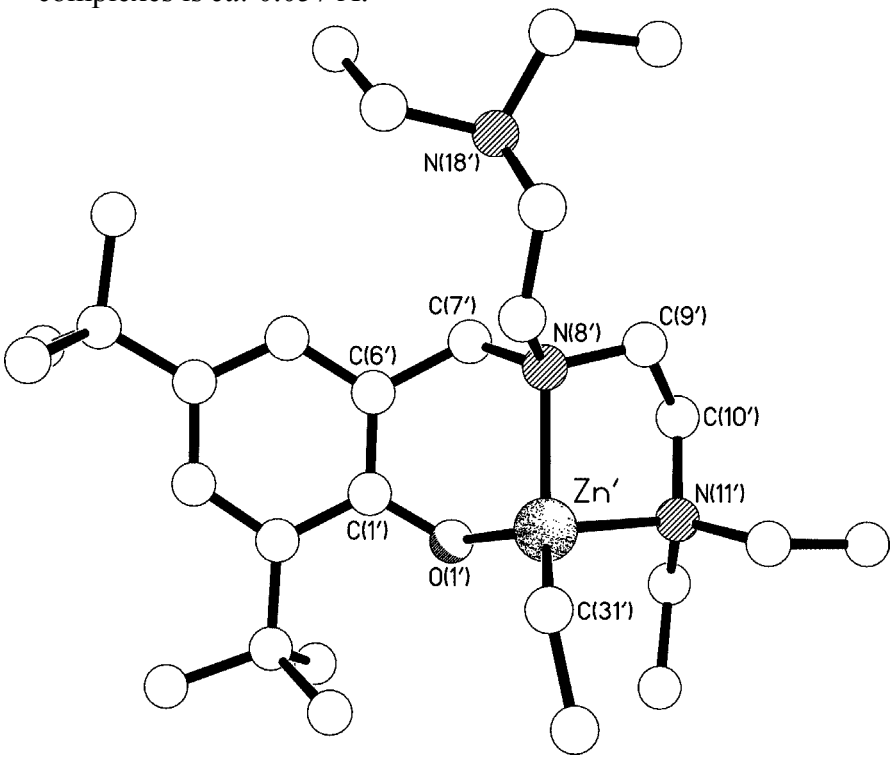

Fig. S7 The molecular structure of one (**II**) of the two independent complexes present in the crystals of **7a**.

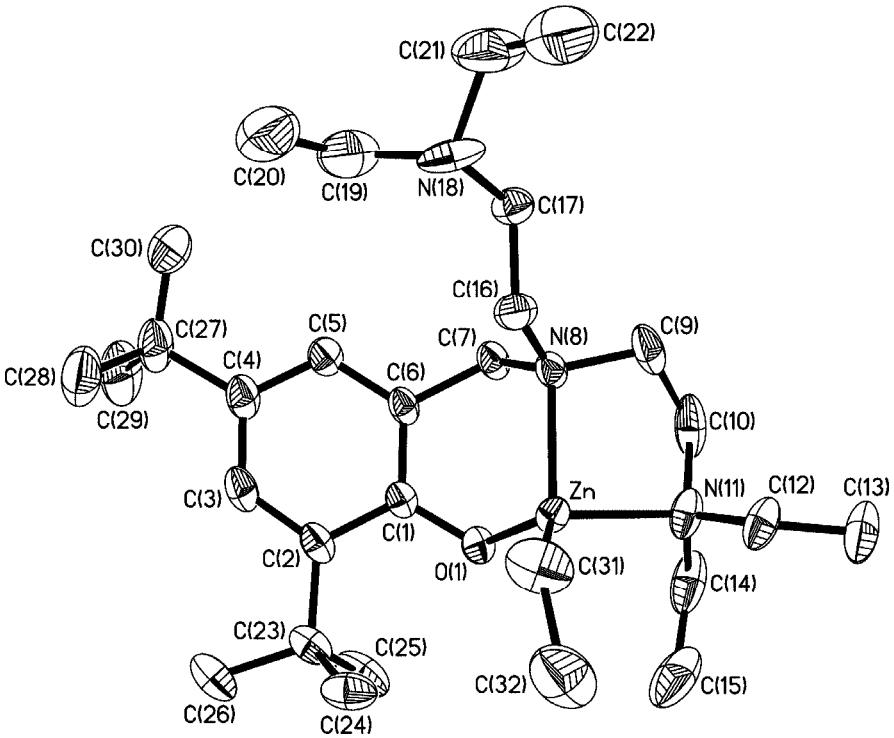

Fig. S8 The molecular structure of one (**I**) of the two independent complexes present in the crystals of **7a** (30% probability ellipsoids).

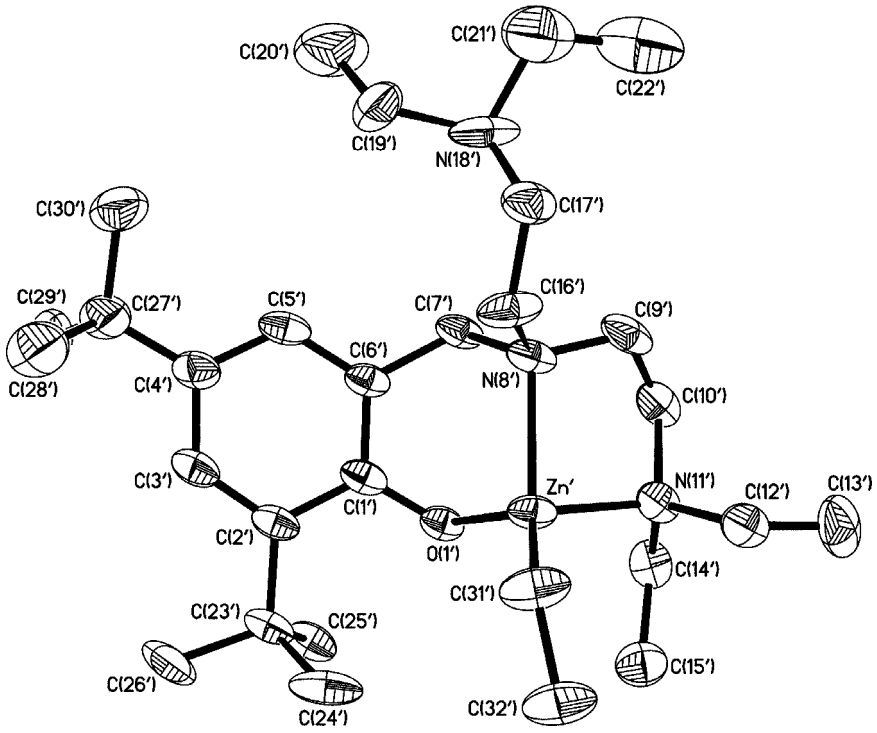

Fig. S9 The molecular structure of one (**II**) of the two independent complexes present in the crystals of **7a** (30% probability ellipsoids).

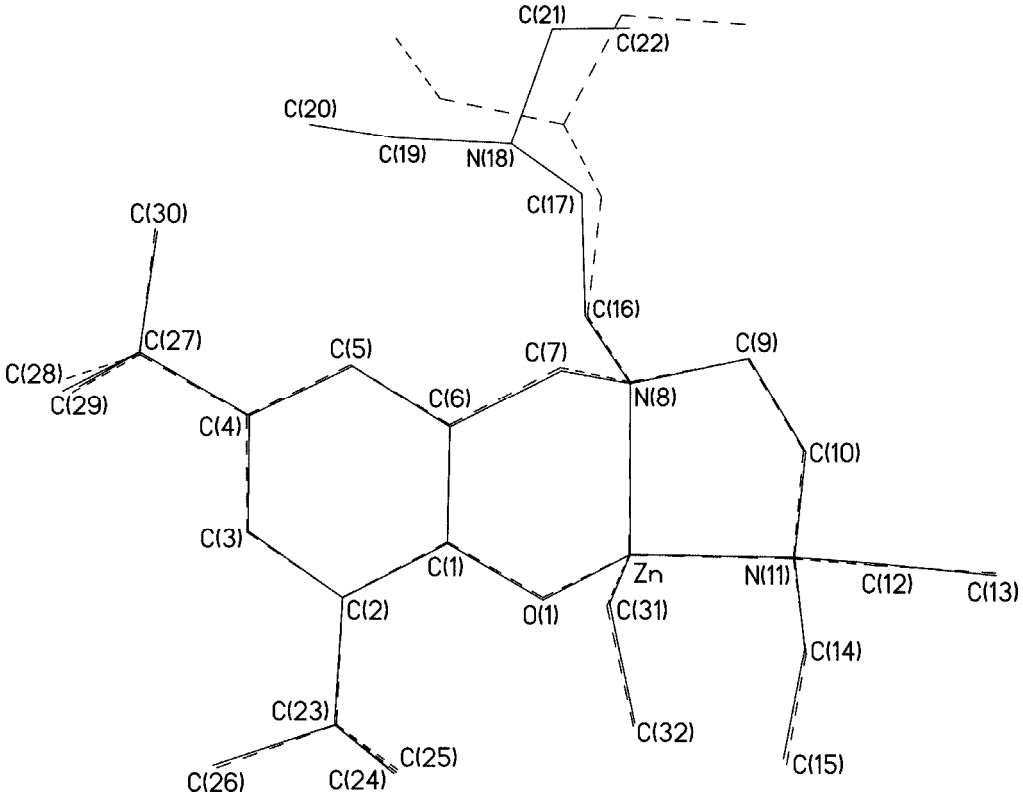

Fig. S10 Overlay of the two independent complexes (**I** and **II**) present in the crystals of **7a**. With the exception of the disordered C(16) to C(22) sidearm, the non-hydrogen atoms of the two complexes have an r.m.s. fit of *ca.* 0.069 Å.

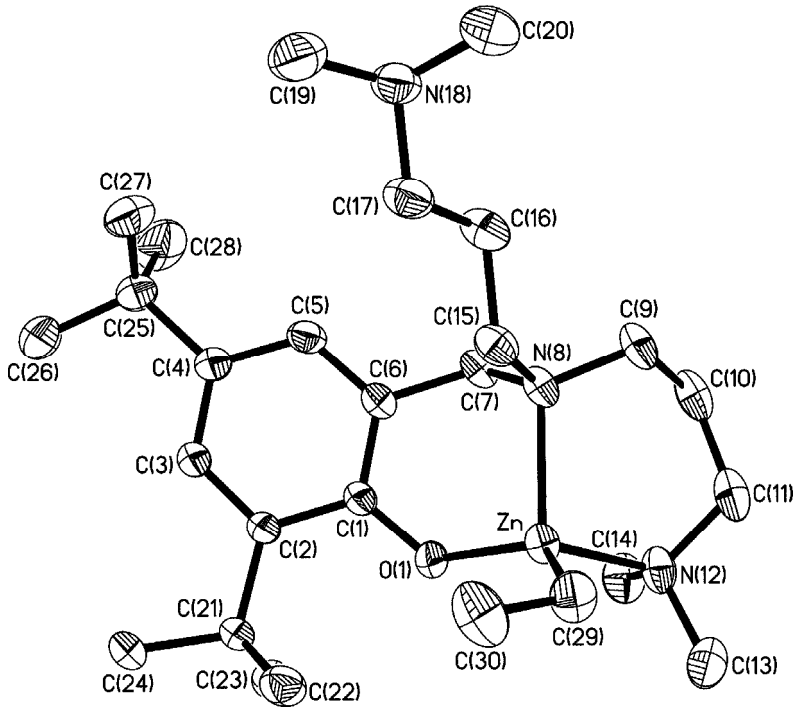

Fig. S11 The molecular structure of **7b** (50% probability ellipsoids).

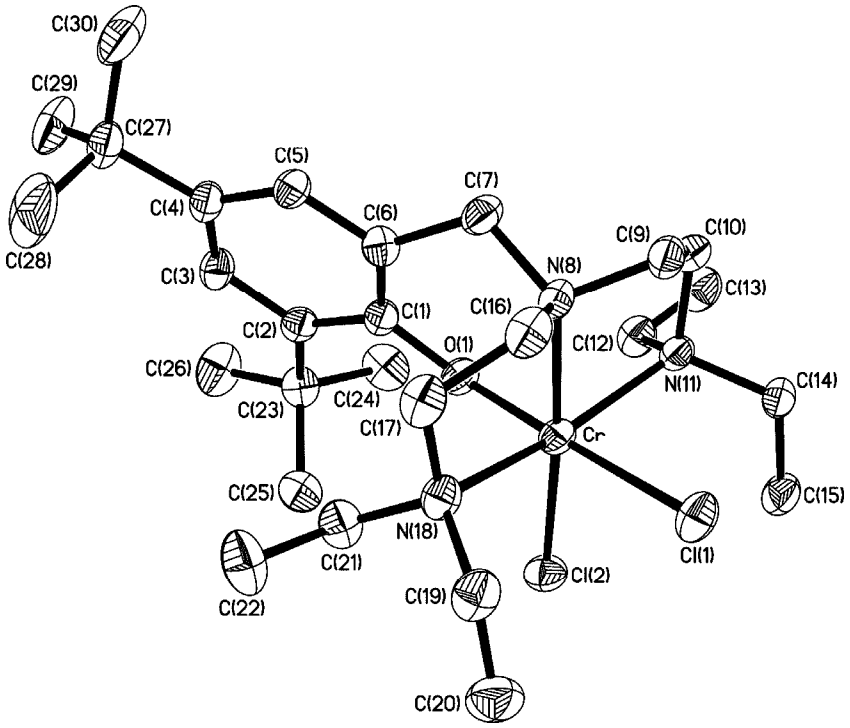

Fig. S12 The molecular structure of **8a** (50% probability ellipsoids).

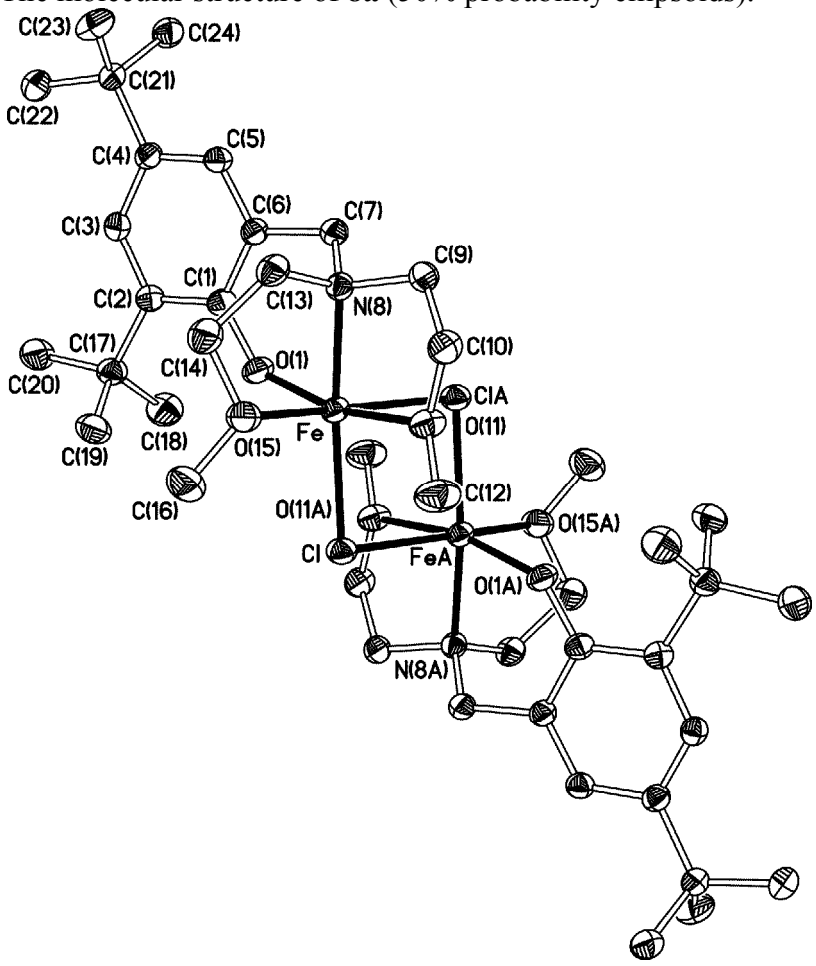

Fig. S13 The molecular structure of **9c** (50% probability ellipsoids).

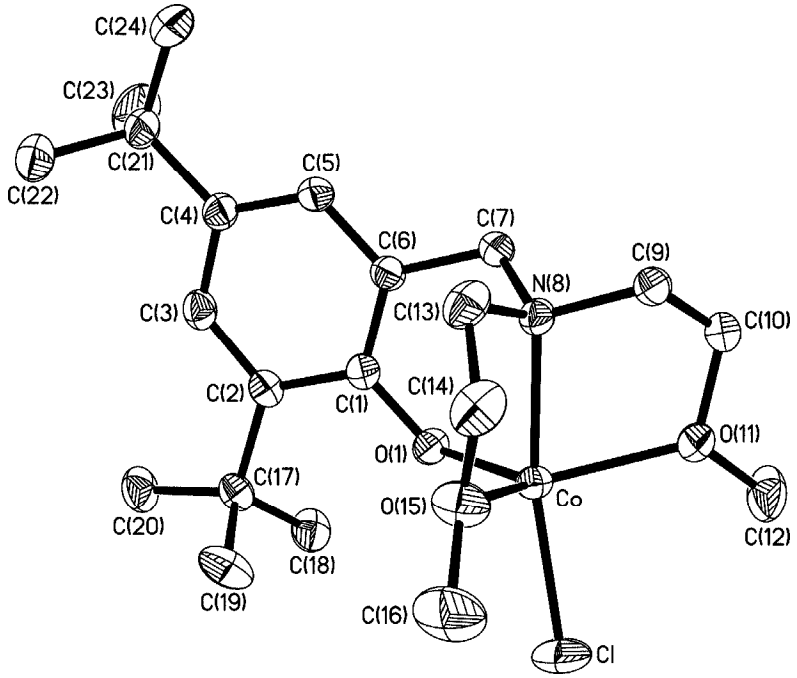

Fig. S14 The molecular structure of **10c** (50% probability ellipsoids).

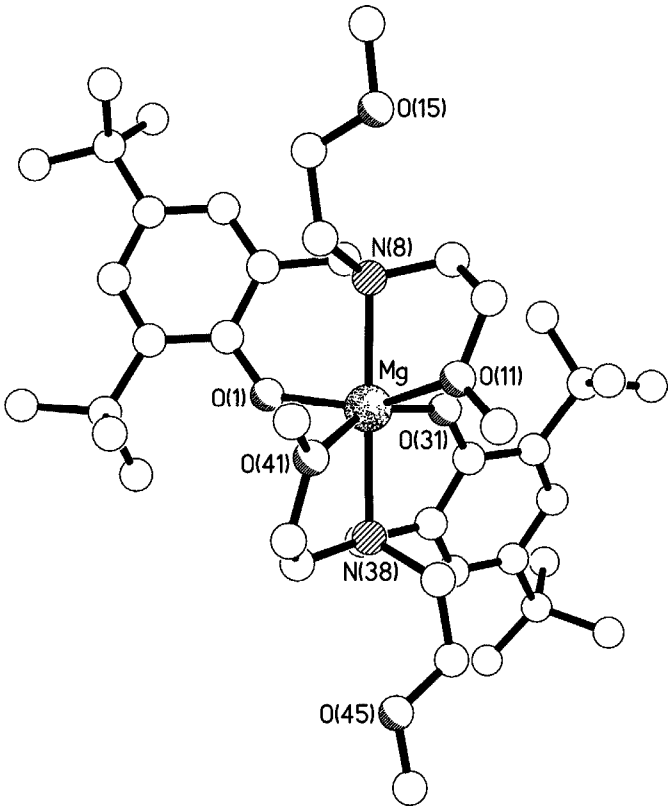

Fig. S15 The molecular structure of one (**I**) of the two independent complexes present in the crystals of **4c**.

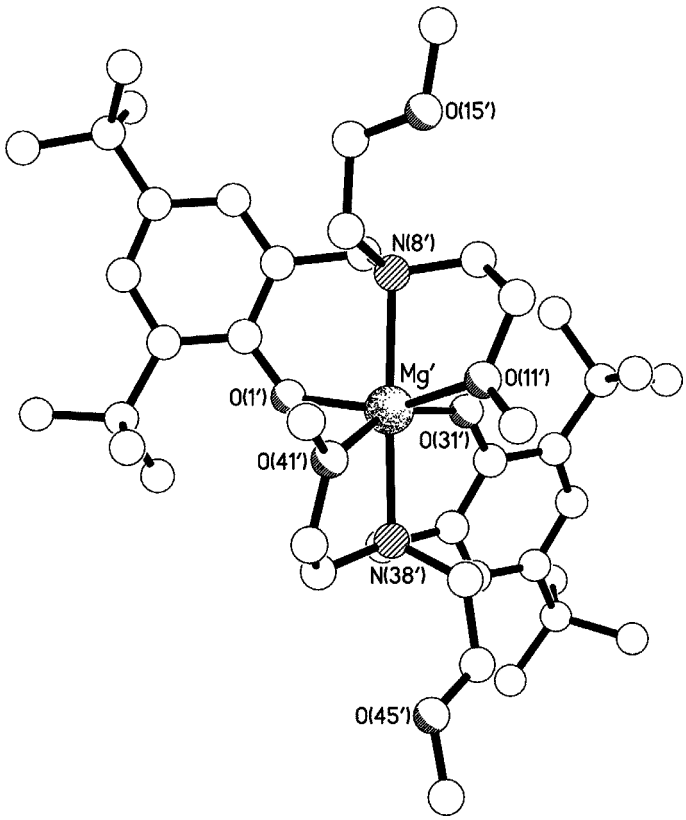

Fig. S16 The molecular structure of one (**II**) of the two independent complexes present in the crystals of **4c**.

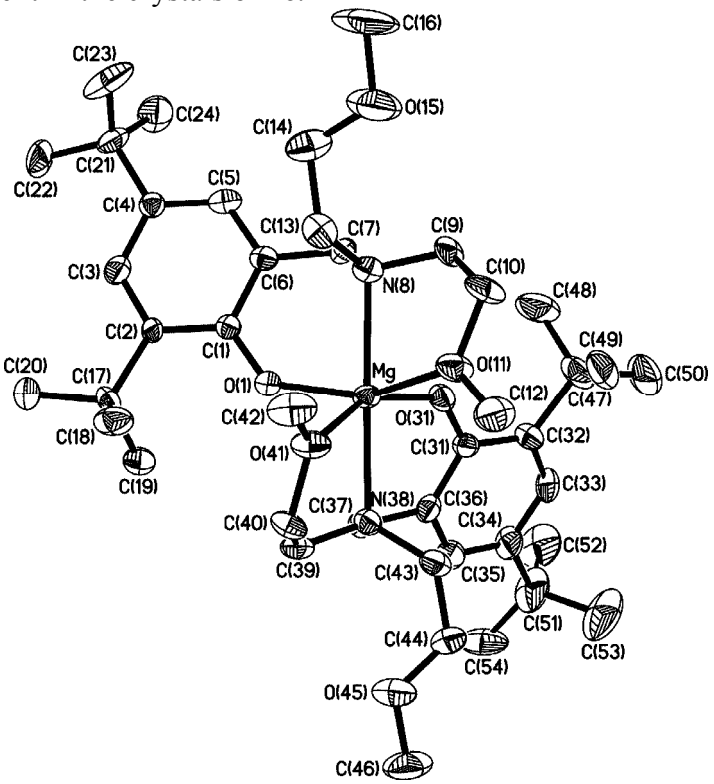

Fig. S17 The molecular structure of one (**I**) of the two independent complexes present in the crystals of **4c** (50% probability ellipsoids).

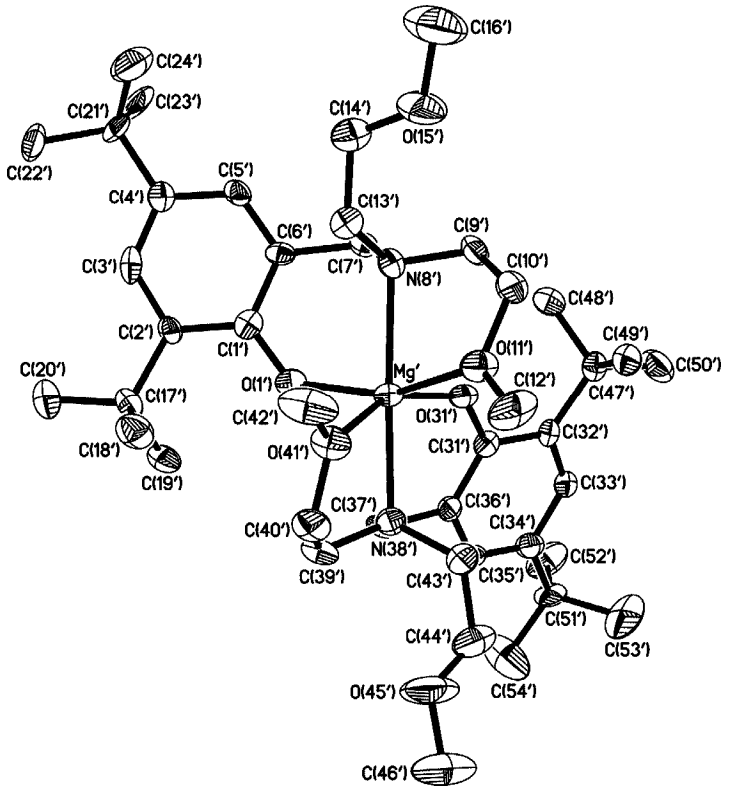

Fig. S18 The molecular structure of one (**II**) of the two independent complexes present in the crystals of **4c** (50% probability ellipsoids).

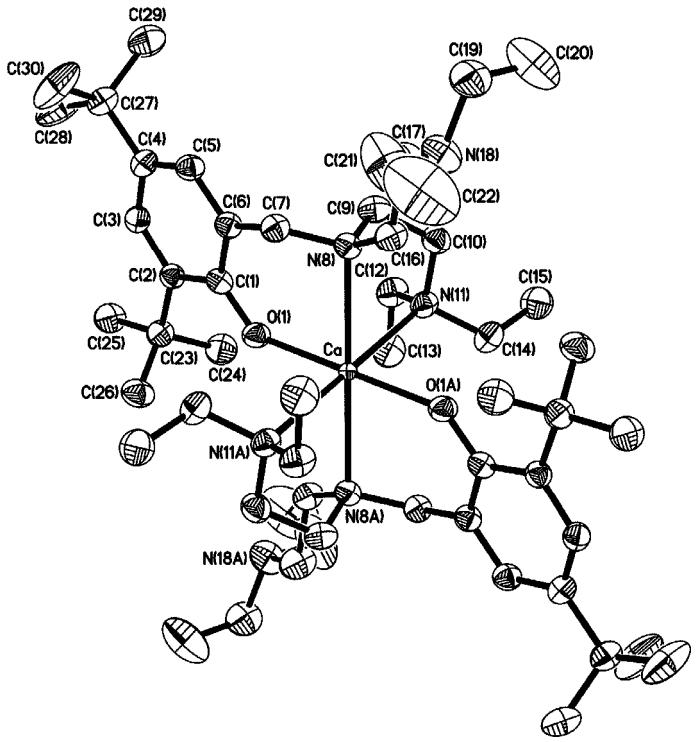

Fig. S19 The molecular structure of the C_i-symmetric complex **5a** (50% probability ellipsoids).

Reference

[1] SHELXTL PC version 5.1, Bruker AXS, Madison, WI, 1997; SHELX-97, G. Sheldrick, Institut Anorg. Chemie, Tammannstr. 4, D37077 Göttingen, Germany, 199