

A donor–acceptor compound composed of a dinuclear zinc(II) complex of a Robson macrocycle with 8-methylquinoline

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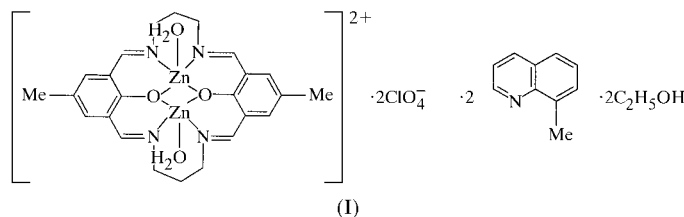
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A donor–acceptor compound, diaqua-1κO,2κO-[μ-11,23-dimethyl-3,7,15,19-tetraazatricyclo[19.3.1.1^{9,13}]hexacos-1(25),-2,7,9,11,13(26),14,19,21,23-decaene-25,26-diolato-1κ⁴N³,N⁷,-O²⁵,O²⁶;2κ⁴N¹⁵,N¹⁹,O²⁵,O²⁶]dizinc(II) diperchlorate bis(8-methylquinoline) ethanol disolvate, [Zn₂(C₂₄H₂₆N₄O₂)(H₂O)₂](ClO₄)₂·2C₁₀H₉N·2C₂H₆O, obtained by the reaction of a dinuclear zinc(II) complex of a Robson macrocycle (acceptor) and 8-methylquinoline (donor), lies about an inversion centre and the coordination about the unique Zn atom is a distorted square pyramid. The fifth coordination site is occupied by the water molecule, Zn–O = 2.016 (2) Å, and the average macrocyclic Zn–O and Zn–N distances are 2.059 (6) and 2.059 (3) Å, respectively.

Comment

Since the synthesis of crown ethers and the discovery of their complexing properties towards alkali metal cations in 1967 (Pedersen, 1967), host–guest chemistry has developed rapidly and now includes ancillary fields of study such as supermolecular chemistry, biomimetic chemistry and materials science (Lehn, 1995). The self-assembly process driven by non-covalent interactions, such as hydrogen bonding, π–π stacking, electrostatic and van der Waals forces, and hydrophobic and hydrophilic interactions, is now universally recognized to be crucial in the proliferation of all biological organisms (Stang & Olenyuk, 1997). A variety of receptor molecules have been devised, and various anion-binding strategies have been exploited which yield a plethora of novel structures of possible biological and chemical significance (Hawthorne & Zheng, 1997; Fyfe & Stoddart, 1997). Here, we

chose a dinuclear zinc(II) complex of a Robson macrocycle as a host and 8-methylquinoline as a guest to form a donor–acceptor compound, (I), in order to study the interactions between the two kinds of molecules.



The asymmetric unit contains half a molecule, with the Zn atom lying near the inversion centre. The coordination geometry around each metal atom may be considered to be a distorted square pyramid whose base plane is composed of O1, O1ⁱ, N1 and N2 [symmetry code: (i) 1 – x, –y, 1 – z]. These crystal data are similar to those of a reported dinuclear zinc(II) complex of a Robson macrocycle diperchlorate (Adams *et al.*, 1995). The water molecule (O1W) occupies the fifth coordinating site of Zn [Zn1–O1W = 2.016 (2) Å]. The crystal structure of the title complex contains two parallel planes, *i.e.* the macrocyclic plane and 8-methylquinoline plane. In the macrocyclic plane, there are two five-coordinate Zn^{II} atoms derived from four donors (two phenolic O and two imine N atoms) on the macrocyclic framework with the water molecule out of the plane.

The six-membered ring (Zn1, N1, O1, C4, C5 and C10), adopts an envelope conformation. The 8-methylquinoline ring is planar and is essentially coplanar with the macrocyclic plane, making a dihedral angle of 2.19 (5)°. The two Zn atoms are 3.228 (1) Å apart. The water molecule is involved in intermolecular O–H···N and O–H···O hydrogen bonds with the methylquinoline ring and solvent ethanol (Table 2). The highly disordered perchlorate ion, connects the methylquinoline ring to the anion to form a two-dimensional network. An intra- and intermolecular C–H···π interaction is observed between the methylquinoline ring and the centroid of the planar four-membered ring (Zn1, O1, Zn1ⁱ and O1ⁱ).

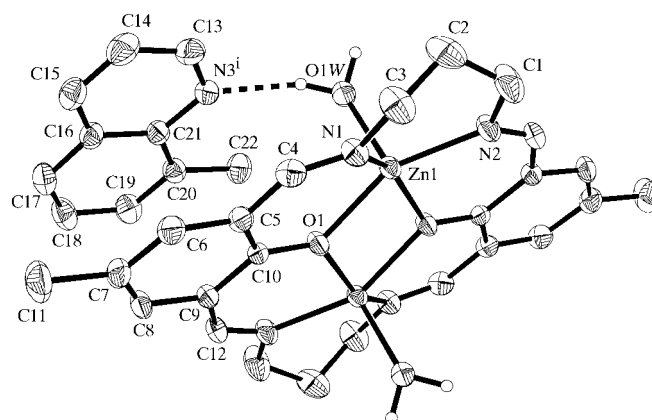


Figure 1

The structure of the cation of (I) with the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level.

Experimental

The dinuclear zinc(II)–diperchlorate complex of a Robson macrocycle (0.732 g, 1 mmol) was prepared *via* a sodium template method as reported previously (Gou & Fenton, 1994), dissolved in ethanol (50 ml) and 8-methylquinoline (0.286 g, 2 mmol) was added. The mixture was refluxed for 1 h, then cooled to room temperature. The yellow precipitate was collected, washed with a small amount of ethanol and dried *in vacuo*. Yellow single crystals suitable for X-ray structure analysis were grown from an ethanol solution.

Crystal data

$[\text{Zn}_2(\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_2)(\text{H}_2\text{O})_2](\text{ClO}_4)_2 \cdot 2\text{C}_{10}\text{H}_9\text{N} \cdot 2\text{C}_2\text{H}_6\text{O}$	$D_x = 1.459 \text{ Mg m}^{-3}$
$M_r = 1146.70$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8192 reflections
$a = 12.8258 (2) \text{ \AA}$	$\theta = 2.70\text{--}28.36^\circ$
$b = 15.1039 (1) \text{ \AA}$	$\mu = 1.091 \text{ mm}^{-1}$
$c = 14.7734 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 114.228 (1)^\circ$	Slab, light yellow
$V = 2609.82 (6) \text{ \AA}^3$	$0.44 \times 0.34 \times 0.28 \text{ mm}$
$Z = 2$	

Data collection

Siemens SMART CCD area-detector diffractometer	6445 independent reflections
ω scans	4334 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.066$
$T_{\text{min}} = 0.645$, $T_{\text{max}} = 0.750$	$\theta_{\text{max}} = 28.31^\circ$
18483 measured reflections	$h = -10 \rightarrow 17$
	$k = -20 \rightarrow 20$
	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	H atoms: see text
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2]$
$wR(F^2) = 0.115$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{\text{max}} < 0.001$
6445 reflections	$\Delta\rho_{\text{max}} = 0.57 \text{ e \AA}^{-3}$
412 parameters	$\Delta\rho_{\text{min}} = -0.52 \text{ e \AA}^{-3}$

H atoms were introduced at calculated positions and refined using a riding model, except for the H atoms of the water molecule, which were included in the refinement. The perchlorate ion and the ethanol solvent are disordered, with major and minor components in ratios of 54:46 and 52:48, respectively.

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996); program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 1990).

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Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1—O1	2.0615 (15)	N1—C4	1.278 (3)
Zn1—O1 ⁱ	2.0562 (16)	N2—C1	1.479 (4)
Zn1—O1W	2.016 (2)	N2—C12 ⁱ	1.277 (3)
Zn1—N1	2.064 (2)	C12—N2 ⁱ	1.277 (3)
Zn1—N2	2.052 (2)	N3—C13	1.325 (4)
O1—C10	1.325 (3)	N3—C21	1.367 (3)
N1—C3	1.475 (4)		
O1W—Zn1—O1 ⁱ	101.37 (8)	O1W—Zn1—O1	99.03 (8)
O1W—Zn1—N1	103.66 (9)	O1 ⁱ —Zn1—O1	76.77 (6)
O1W—Zn1—N2	102.96 (9)	O1—Zn1—N1	88.55 (7)
N1—Zn1—N2	95.80 (9)	O1 ⁱ —Zn1—N1	152.66 (8)
N2—Zn1—O1	155.84 (8)	C10—O1—Zn1 ⁱ	128.62 (14)
N2—Zn1—O1 ⁱ	89.12 (8)		

Symmetry code: (i) $1 - x, -y, 1 - z$.

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O1W—H1W \cdots N3 ⁱ	0.84 (3)	1.90 (3)	2.731 (3)	172 (4)
O1W—H2W \cdots O7A ⁱⁱ	0.88 (3)	1.78 (4)	2.648 (17)	171 (4)
C3—H3A \cdots O3A ⁱⁱⁱ	0.97	2.54	3.508 (12)	177
C3—H3B \cdots O1A ^{iv}	0.97	2.48	3.348 (11)	149
C15—H15 \cdots O3A ⁱⁱⁱ	0.93	2.52	3.377 (10)	154

Symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $1 - x, -y, 1 - z$; (iii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (iv) $1 + x, \frac{1}{2} - y, \frac{1}{2} + z$.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GG1016). Services for accessing these data are described at the back of the journal.

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