metal-organic papers

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Key indicators

Single-crystal X-ray study T = 293 K Mean σ (C–C) = 0.005 Å Disorder in main residue R factor = 0.041 wR factor = 0.120 Data-to-parameter ratio = 11.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Di- μ -aqua-bis{aqua[N,N'-bis(furan-2-ylmethylene)hydrazine- $\kappa^2 N,O$](perchlorato- κO)sodium}

The Na atom of the title complex, $[Na_2(ClO_4)_2(C_{10}H_8-N_2O_2)_2(H_2O)_4]$, is six-coordinate in a distorted octahedron. The *N*,*N'*-bis(furan-2-ylmethylene)hydrazine ligand is approximately planar, with a *transoid* configuration. Two coordinated water molecules bridge two Na atoms, with an Na…Na separation of 3.542 (2) Å. The molecule lies on an inversion centre. Intermolecular π - π stacking interactions and O-H···O, O-H···N and C-H···O hydrogen bonds link the molecules together to form a three-dimensional structure.

Comment

Schiff base ligands are excellent ligands and are commonly used in metal-organic chemistry, owing to their ease of synthesis and high yield in a single-step reaction from commercially inexpensive reagents. Among them, diazine Schiff base ligands, with two coordination portions linked by a single N-N bridge, display several possible mono- and multinucleating coordination modes, due to the flexibility of the ligand around the N-N single bond (Xu et al., 2000). Their coordination to d group metals leads to a variety of different structural motifs, such as chains, metallomacrocycles and metallocrowns (Abedin et al. 2003; Onions et al. 2003; Zhao et al., 2004). Such complexes formed by self-assembly exhibit many special functional properties, such as chirality, magnetism, optical activity and redox activity (Bai, Dang et al., 2005; Gao et al., 2003; Grove et al., 2004; Sun et al., 2006). As part of our continuing investigation of this type of diazine ligands and their transition metal compounds (Bai, Duan et al., 2005; Bai et al., 2006), we have used the ligand N,N'-bis-(furan-2-vlmethylene)-hydrazine (L) to construct the title threedimensional sodium coordination polymer, (I).



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In complex (I), the ligand L is approximately planar, with the furan rings adopting a *transoid* configuration. It acts as a bidentate donor and coordinates to Na through one furanyl O Received 25 August 2006 Accepted 25 August 2006



Figure 1

The molecular structure of the title complex, with displacement ellipsoids drawn at the 50% probability level. Half of the disordered O atoms have been omitted. [Symmetry code: (i) 1 - x, 1 - y, -z].



Figure 2

A perspective view of the two-dimensional sheets, showing the intermolecular π - π stacking (open dashed lines) and O-H···O and O-H···N hydrogen-bond (solid dashed lines) interactions. H atoms other than those involved in hydrogen bonding have been omitted.



Figure 3

A perspective view of the three-dimensional structure formed through the $C-H\cdots O$ hydrogen bonds (solid dashed lines) between the sheets. H atoms other than those involved in $C-H\cdots O$ hydrogen bonds have been omitted for clarity.

and one imine N atom. Two coordinated water molecules bridge two Na centres, with an $Na \cdots Na$ separation of

3.541 (2) Å. The dinculear complex is disposed about an inversion centre located mid-way along the Na1···Na1ⁱ vector [Fig. 1; symmetry code: (i) 1 - x, 1 - y, -z]. The asymmetric unit consists of one ligand, one Na⁺ cation, one coordinated perchlorate anion and two coordinated water molecules. Each Na centre is bound to one imine N atom, one furan O atom, three O atoms from three water molecules and one O atom from a disordered perchlorate anion to attain a distorted octahedral coordination geometry.

Intermolecular O–H···O and O–H···N hydrogen bonds (Table 2) and π - π stacking interactions between adjacent molecules link the molecules together to form a sheet parallel to the *ab* plane (Fig. 2). These sheets are further connected through C–H···O hydrogen bonds (Table 2) to form a threedimensional structure (Fig. 3). For the π - π stacking, the fivemembered furan ring is approximately parallel to the two neighbouring furan rings [centroid-to-centroid distances are 3.748 (1) Å between rings C1–C4/O1 and C7ⁱⁱ–C10ⁱⁱ/O2ⁱⁱ, and 3.677 (2) Å between rings C1–C4/O1 and C7ⁱⁱⁱ–C10ⁱⁱⁱ/O2ⁱⁱⁱ [symmetry codes: (ii) 1 – x, -y, -z; (iii) 2 – x, -y, -z].

Experimental

All chemicals were of reagent grade quality obtained from commercial sources. *N*,*N'*-Bis-(furan-2-ylmethylene)hydrazine was readily prepared by the reaction of hydrazine hydrate with furfural in a 1:2 ratio in methanol solution (50 ml). The ligand (0.50 mmol, 0.095 g) and NaClO₄·6H₂O (0.40 mmol, 0.115 g) were mixed in ethanol (20 ml). The solution was left for a few weeks at room temperature to afford yellow crystals of (I) (yield 76%). Analysis, calculated for $C_{20}H_{24}Cl_2N_4Na_2O_{16}$: C 34.7, H 3.5, N 8.1%; found: C 34.2, H 3.7, N 7.9%.

Crystal data

$Na_2(ClO_4)_2(C_{10}H_8N_2O_2)_2(H_2O)_4]$	V = 746.73 (2) Å ³
$M_r = 693.31$	Z = 1
Friclinic, P1	$D_x = 1.542 \text{ Mg m}^{-3}$
a = 6.5565 (1) Å	Mo $K\alpha$ radiation
b = 9.9647 (2) Å	$\mu = 0.33 \text{ mm}^{-1}$
z = 12.4108 (2) Å	T = 293 (2) K
$\alpha = 73.882 \ (1)^{\circ}$	Block, yellow
$\beta = 81.473 \ (1)^{\circ}$	$0.20 \times 0.15 \times 0.15 \text{ mm}$
$\nu = 74.058 \ (1)^{\circ}$	

Data collection

Bruker SMART CCD area-detector diffractometer φ/ω scans Absorption correction: none 8844 measured reflections

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.041$ $wR(F^2) = 0.120$ S = 1.012621 reflections 237 parameters H-atom parameters constrained 2621 independent reflections 2407 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.020$ $\theta_{\text{max}} = 25.0^{\circ}$

$$\begin{split} &w = 1/[\sigma^2(F_o^2) + (0.072P)^2 \\ &+ 0.3846P] \\ &where \ P = (F_o^2 + 2F_c^2)/3 \\ (\Delta/\sigma)_{max} < 0.001 \\ \Delta\rho_{max} = 0.56 \ e^{\Lambda^{-3}} \\ \Delta\rho_{min} = -0.36 \ e^{\Lambda^{-3}} \\ Extinction \ correction: \ SHELXTL \\ (Bruker, 2000) \\ Extinction \ coefficient: \ 0.095 \ (10) \end{split}$$

Table 1

			0	
Selected	geometric	parameters	(Å	°)
Serected	Scometrie	purumeters	(1 1,	<i>.</i>

Na1-O3	2.292 (5)	Na1-O3'	2.496 (12)
Na1-O7	2.381 (2)	Na1-O1	2.499 (2)
Na1-O7 ⁱ	2.421 (2)	Na1-N1	2.522 (2)
Na1-O8	2.424 (2)		
O3-Na1-O7	84.99 (18)	O7-Na1-O1	98.60 (8)
O3-Na1-O7 ⁱ	88.71 (17)	O7 ⁱ -Na1-O1	90.52 (8)
O7-Na1-O7 ⁱ	84.99 (7)	O8-Na1-O1	84.87 (7)
O3-Na1-O8	96.22 (17)	O3'-Na1-O1	165.0 (3)
O7-Na1-O8	90.51 (7)	O3-Na1-N1	109.44 (18)
O7 ⁱ -Na1-O8	173.02 (9)	O7-Na1-N1	164.34 (9)
O7-Na1-O3'	92.2 (3)	O7 ⁱ -Na1-N1	89.16 (7)
O7 ⁱ -Na1-O3'	80.0 (3)	O8-Na1-N1	93.83 (7)
O8-Na1-O3'	105.5 (3)	O3'-Na1-N1	101.1 (3)
O3-Na1-O1	176.25 (19)	O1-Na1-N1	66.88 (7)

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

Table 2Hydrogen-bond geometry (Å, °).

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdots A$
$O7-H7A\cdots O4^{ii}$	0.85	2.49	3.155 (8)	136
$O7 - H7B \cdot \cdot \cdot O8^{ii}$	0.85	1.98	2.822 (3)	172
$O8-H8B\cdots O4^{ii}$	0.85	2.14	2.941 (6)	157
O8−H8A···N2 ⁱⁱⁱ	0.85	2.04	2.893 (3)	178
$C2-H2\cdots O5^{iv}$	0.93	2.57	3.415 (6)	151

Symmetry codes: (ii) -x + 2, -y + 1, -z; (iii) -x + 2, -y, -z; (iv) x, y, z - 1.

The O atoms of the CIO_4^- anion were refined as disordered over two positions, O3, O4, O5 and O6, and O3', O4', O5' and O6'; these two positions were refined to occpancies of 0.70 (1) and 0.30 (1), respectively. Displacement parameters of adjacent atoms in the disordered units were restrained to be similar (48 restraints). H atoms bonded to C and O atoms were constrained to ride on their parent atoms, at distances of 0.93 and 0.85 Å, respectively. All $U_{iso}(H)$ values were constrained to be 1.2 times U_{eq} of the carrier atom.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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