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Crystal structure of di- μ_2 -aqua-tetraaqua-bis(4-(1*H*-1,2,4-triazol-1-yl)benzoato- κN)disodium(I) $C_{18}H_{24}N_6Na_2O_{10}$

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Abstract

$C_{18}H_{24}N_6Na_2O_{10}$, triclinic, $P\bar{1}$, $a = 6.223(2)$ Å, $b = 7.385(2)$ Å, $c = 14.295(4)$ Å, $\alpha = 75.491(6)^\circ$, $\beta = 77.953(6)^\circ$, $\gamma = 70.523(6)^\circ$, $V = 593.9(3)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0517$, $wR_{ref}(F^2) = 0.1533$, $T = 296(2)$ K.

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A part of the crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The ligand, 4-(1*H*-1,2,4-triazol-1-yl)benzoic acid, was purchased from alfa aesar company. Sodium hydrate (0.004 g, 0.1 mmol), Hbpt24 (0.0189 g, 0.1 mmol) and distilled water (20 mL) were placed in a 20.0 mL Teflon-lined stainless steel autoclave. It was heated at 383 K for 2 days. After cooling

Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.2 × 0.2 × 0.2 mm
Wavelength:	Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å)
μ :	0.151 mm ^{−1}
Diffractometer, scan mode:	Bruker APEX-II CCD, ϕ and ω -scans
θ_{max} , completeness:	28.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	4678, 3075, 0.0253
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1837
$N(param)_{refined}$:	173
Programs:	Bruker programs [1], SHELX [2–4]

to room temperature, colourless block crystals of the title complex were obtained.

Experimental details

The carbon H-atoms were placed in calculated positions ($C-H_{phenyl \text{ or triazolyl}} = 0.93$ Å) using a riding model (AFIX 43 or AFIX 137 option of the SHELX program [11–13], and were included with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H-atoms were placed in calculated positions ($O \cdots H = 0.85$ Å), and were included with $U_{iso}(H) = 1.2U_{eq}(O)$.

Comment

The exploration of alkali-metal complexes has attracted significant interest, due to its potential application in catalysts [5–8]. The exo-multidentate compounds are often employed as ligands to produce polymeric networks due to their rich coordination sites and various coordination modes [9–12]. Recently, our group studied the reactions of 4-(1*H*-1,2,4-triazol-1-yl)benzoic acid (HL) with silver, obtaining a series of coordination compounds [13, 14]. As a follow up study, we report the title complex.

The title complex consists of two Na(I) ion, two L ligands and six coordinated water molecules. Each Na(I) is five-coordinated by one N atom from L and four O atoms from four water molecules. The Na–N distance is 2.437(2) Å and Na–O bond lengths are in the range of 2.3158(17) – 2.530(2) Å. The

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
Na1	0.32484(14)	0.71525(15)	0.94416(6)	0.0573(3)
O1	0.7263(9)	0.822(4)	0.1605(3)	0.070(3)
O1A	0.736(3)	0.733(8)	0.1628(14)	0.045(6)
N1	0.3680(3)	0.7611(2)	0.61720(11)	0.0380(4)
C1	0.8401(4)	0.7252(4)	0.23146(15)	0.0465(5)
O2	1.0516(3)	0.6408(2)	0.22396(11)	0.0521(4)
C2	0.7111(3)	0.7384(3)	0.33250(13)	0.0377(5)
N2	0.1350(3)	0.8255(3)	0.63609(13)	0.0523(5)
O3	−0.0731(2)	0.8101(2)	0.97557(10)	0.0432(4)
H3A	−0.140118	0.795045	1.034305	0.052
H3B	−0.166769	0.919138	0.954986	0.052
C3	0.4739(4)	0.7912(4)	0.35125(16)	0.0608(7)
H3	0.389219	0.821522	0.299984	0.073
N3	0.2907(4)	0.7324(3)	0.77516(13)	0.0581(6)
O5	0.7205(2)	0.5765(2)	0.92465(11)	0.0509(4)
H5A	0.817056	0.518382	0.882099	0.061
H5B	0.799986	0.637838	0.936953	0.061
C5	0.4833(3)	0.7568(3)	0.52000(13)	0.0340(4)
O4	0.3425(3)	0.8182(2)	1.09180(11)	0.0488(4)
H4A	0.445678	0.811179	1.122965	0.059
H4B	0.262266	0.759502	1.135456	0.059
C4	0.3594(4)	0.7997(4)	0.44502(16)	0.0552(6)
H4	0.199576	0.834476	0.456618	0.066
C7	0.8308(4)	0.7001(4)	0.40855(15)	0.0495(6)
H7	0.990610	0.665192	0.397209	0.059
C6	0.7191(4)	0.7120(4)	0.50228(16)	0.0542(6)
H6	0.802947	0.689908	0.552922	0.065
C8	0.4557(4)	0.7055(4)	0.70096(15)	0.0543(6)
H8	0.611895	0.654778	0.706254	0.065
C9	0.1001(4)	0.8050(4)	0.73174(16)	0.0538(6)
H9	−0.046506	0.838691	0.766712	0.065

coordination environment is a distorted trigonal bipyramid, since the N—Na—O and N—Na—O bond angles in the trigonal plane are in the range of 78.13 – 160.18°. The water O5 atom acts as a μ_2 -bridge linking the Na(I) centers into a the dinuclear complex. Intermolecular hydrogen bonds link dinuclear complexes into a three-dimensional supramolecular framework.

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