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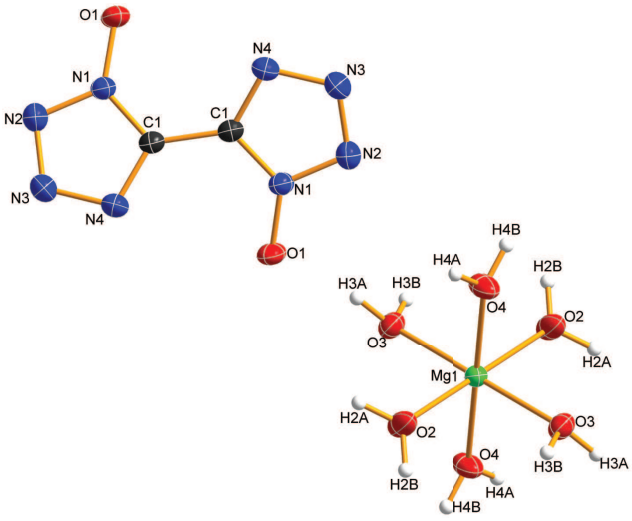
Crystal structure of hexaaquamagnesium(II) 5,5′-bitetrazole-1,1′-diolate, $C_2H_{12}N_8O_8Mg$



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Abstract

$C_2H_{12}N_8O_8Mg$, orthorhombic, *Pbcn*, $a = 9.858(8)$ Å, $b = 6.852(5)$ Å, $c = 18.276(3)$ Å, $V = 1185.6(16)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0245$, $wR_{ref}(F^2) = 0.0693$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Dihydroxylammonium 5,5′-bitetrazole-1,1′-diolate (1.18 g, 5 mmol) was a dissolved in distilled water (30 mL). A solution of magnesium acetate (1.3 g, 6 mmol) in water (20 mL) was added, the suspension was stirred for 30 min at 65 °C, then cooled down and filtered. The obtained solid was washed with water then dried in air to a colorless solid (1.29 g, 86%). TG–DTA (5 °C/min): 320.2 °C (dec.). IR (KBr, cm^{-1}): ν = 3424 (m), 2336 (w), 1676 (m), 1434 (w), 1274 (vs), 1183 (m), 1007 (s), 995 (m), 728 (m), 659 (w); EA (found, calc. for $C_2H_{12}N_8O_8Mg$, MW = 300.15): C (10.61, 10.53), H (1.87, 1.75), N (48.08, 49.12)%.

Table 1: Data collection and handling.

Crystal:	Yellow, block, size 0.20×0.21×0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.07 cm^{-1}
Diffractometer, scan mode:	Bruker-AXS SMART APEX2 CCD, φ and ω scans
$2\theta_{max}$:	50.6°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6720, 1069
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1006
$N(param)_{refined}$:	104
Programs:	SHELX [1], Diamond [2]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2B)	8*d*	0.375(2)	0.228(3)	−0.0866(7)	0.065(6)
H(2A)	8*d*	0.294(2)	0.240(3)	−0.019(1)	0.072(7)
H(3B)	8*d*	0.638(2)	0.235(2)	−0.075(1)	0.056(6)
H(3A)	8*d*	0.718(2)	0.420(3)	−0.0812(9)	0.054(6)
H(4A)	8*d*	0.4847	0.2164	0.1055	0.049
H(4B)	8*d*	0.5749	0.3453	0.1302	0.049

Discussion

Tetrazoles belong to the class of energetic materials [3]. The crystallographic studies reveal that the asymmetric unit consists of one half of a $[Mg(H_2O)_6]^{2+}$ complex and one half of a 5,5′-bitetrazole-1,1′-diolate dianion (see the figure). The magnesium complex is located on an inversion center, whereas the dianion is positioned around a twofold axis. The Mg–O bond lengths are: Mg(1)–O(2) 2.0523(15) Å, Mg(1)–O(3) 2.0802(3) Å and Mg(1)–O(4) 2.0675(14) Å. Hydrogen bonds connect all moyieties.

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mg(1)	4*a*	0.5	0.5	0	0.0187(3)	0.0255(3)	0.0166(3)	−0.0022(2)	0.0003(2)	−0.0007(2)
O(1)	8*d*	0.13342(9)	0.4890(2)	0.12961(5)	0.0300(5)	0.0341(5)	0.0169(5)	0.0022(4)	0.0024(4)	0.0038(4)
N(1)	8*d*	0.1596(1)	0.4469(2)	0.19903(6)	0.0227(5)	0.0244(6)	0.0180(5)	0.0013(5)	0.0009(4)	0.0003(4)
C(1)	8*d*	0.0728(1)	0.4107(2)	0.25399(6)	0.0237(7)	0.0227(7)	0.0174(6)	0.0002(5)	0.0012(5)	−0.0004(5)
O(2)	8*d*	0.3698(1)	0.2868(2)	−0.04222(5)	0.0335(6)	0.0493(7)	0.0247(5)	−0.0188(5)	0.0053(4)	−0.0110(5)
N(2)	8*d*	0.2862(1)	0.4359(2)	0.22467(7)	0.0223(6)	0.0342(7)	0.0286(6)	0.0010(5)	−0.0002(5)	0.0004(5)
O(3)	8*d*	0.66033(9)	0.3524(2)	−0.05152(5)	0.0253(5)	0.0300(5)	0.0246(5)	−0.0014(4)	0.0055(4)	−0.0012(4)
N(3)	8*d*	0.2747(1)	0.3933(2)	0.29442(6)	0.0253(6)	0.0379(7)	0.0269(6)	0.0014(5)	−0.0036(5)	0.0009(5)
O(4)	8*d*	0.5323(1)	0.3181(2)	0.09056(5)	0.0350(5)	0.0402(6)	0.0227(5)	−0.0108(5)	−0.0072(4)	0.0098(4)
N(4)	8*d*	0.1441(1)	0.3774(2)	0.31440(6)	0.0266(6)	0.0340(7)	0.0201(6)	0.0003(5)	−0.0023(4)	0.0021(5)

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