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The crystal structure of diaqua-bis(6-aminopicolinato- $\kappa^2 N,O$)magnesium(II), $C_{12}H_{14}O_6N_4Mg$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.12 × 0.11 × 0.1 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.17 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	2898, 1217, 0.030
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1047
$N(\text{param})_{\text{refined}}$:	117
Programs:	Bruker programs [1], OLEX2 [2], SHELX [3], DIAMOND [4]

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Abstract

$C_{12}H_{14}O_6N_4Mg$, monoclinic, $P2_1/c$ (no. 14), $a = 8.2501(10)$ Å, $b = 12.7943(12)$ Å, $c = 7.1562(7)$ Å, $\beta = 113.912(13)^\circ$, $V = 690.53(14)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0386$, $wR_{\text{ref}}(F^2) = 0.0921$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

An amount of 0.138 g 2-amino-6-pyridinecarboxylic acid (1.0 mmol) and 0.180 g 4-formylphenoxyacetic acid (1.0 mmol) were dissolved into 10 mL ethanol at room temperature. After 1 h, 5 mL sodium hydroxide (0.040 g, 1.0 mmol) solution and 0.102 g magnesium chloride hexahy-

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mg1	0.500000	0.500000	1.000000	0.0105(3)
O1	0.62981(18)	0.65029(11)	0.5761(2)	0.0136(4)
O2	0.63974(18)	0.54980(11)	0.83612(19)	0.0130(4)
O3	0.4348(2)	0.36247(11)	0.8319(2)	0.0152(4)
H3A	0.426463	0.353392	0.710659	0.023*
H3B	0.420085	0.301875	0.871224	0.023*
N1	0.0610(3)	0.57137(15)	0.8476(3)	0.0161(4)
N2	0.2959(2)	0.58226(12)	0.7488(2)	0.0103(4)
C1	0.3580(3)	0.61420(15)	0.6080(3)	0.0111(5)
C2	0.2517(3)	0.65487(15)	0.4205(3)	0.0126(5)
H2	0.299247	0.676323	0.329116	0.015*
C3	0.0696(3)	0.66307(16)	0.3710(3)	0.0145(5)
H3	−0.006826	0.687302	0.243006	0.017*
C4	0.0051(3)	0.63517(16)	0.5125(3)	0.0141(5)
H4	−0.115068	0.642175	0.482756	0.017*
H1A	0.130(3)	0.541(2)	0.955(4)	0.025(7)*
H1B	−0.051(4)	0.577(2)	0.820(4)	0.038(8)*
C5	0.1220(3)	0.59575(15)	0.7035(3)	0.0111(5)
C6	0.5572(3)	0.60314(15)	0.6761(3)	0.0111(5)

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drate (0.5 mmol) was added. The mixture was stirred for 5 h at 80 °C. The colorless crystals of the title compound were obtained by slowly volatilizing the filtrate in 16 days.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å, O–H = 0.85 Å and N–H = 0.84–0.87 Å).

Comment

Over the past decades, many heterocycle derivatives and their metal complexes have received attention, because they display widespread applications [5–8]. We have already reported the synthesis and properties of heterocycle and their alkaline-earth metal complex [9, 10]. In our previous work, a new Mg(II), bis(ethanol-*k*O)-bis(6-aminopicolinato-*k*²N,*O*)magnesium(II), has been reported which is closely related with the title complex [11]. It should be mentioned that the picolinato complex also works fine with other metals [12]. In this paper, we reported the structure of a new Mg(II) complex, bis(2-amino-6-pyridinecarboxylate-aqua)magnesium(II).

The title complex is made up of one Mg(II) ion, two 2-amino-6-pyridinecarboxylate ligands and two coordinated water molecules located at an inversion center. The central Mg(II) ion is six-coordinated with four O atoms from two 2-amino-6-pyridinecarboxylate ligands (O2 and O2A) and two coordinated water molecules (O3 and O3A), two N atoms from two 2-amino-6-pyridinecarboxylate ligands (N2 and N2A), and forms a distorted octahedral coordination. The Mg–O bond lengths are 2.0510(14) and 2.0757(14) Å respectively; and the Mg–N bond length is 2.1729(16) Å. The coordination mode of Mg(II) and the bond lengths and bond angles are consistent with that reported in the literature [11]. The Mg(II) complex molecules form 1D chains by OH···O and NH···O hydrogen bonds.

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