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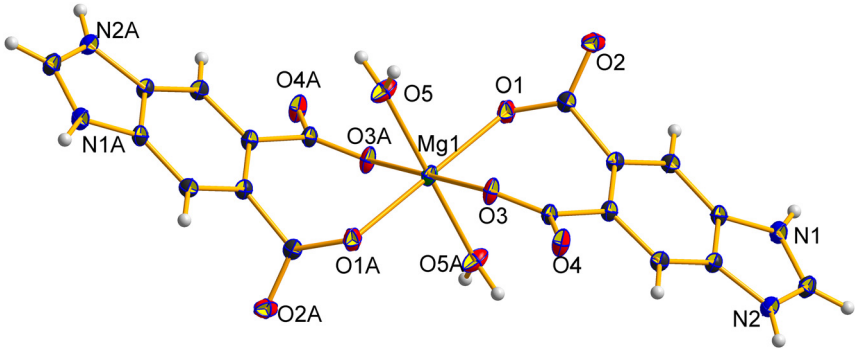
Crystal structure of [diaqua-{1*H*-benzo[*d*]imidazol-3-ium-5,6-dicarboxylato-κ^2*O*,*O*′}magnesium(II)] $C_{18}H_{14}MgN_4O_{10}$



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Abstract

$C_{18}H_{14}MgN_4O_{10}$, orthorhombic, *Pbca* (no. 61), a = 6.9266(14) Å, b = 15.444(3) Å, c = 17.371(4) Å, V = 1858.3(6) Å^3, Z = 4, $R_{gt}(F)$ = 0.0442, $wR_{ref}(F^2)$ = 0.0980, T = 293 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

A mixture of 10 mL H_2O, 0.3 mmol (252 mg) magnesium carbonate and 0.2 mmol (412 mg) 1*H*-benzo[d]imidazole-5,6-dicarboxylic acid (H_2BIDA) was sealed in a 23 mL Teflon lined stainless steel container, and then it was heated at 403 K for 72 h. Finally, colorless block crystals were obtained with a yield of about 70 % (calculated based on BIDA ligand) through filtering.

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Table 1: Data collection and handling.

Crystal:	Clear colourless block
Size:	0.34 × 0.30 × 0.28 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.17 mm^{-1}
Diffractometer, scan mode:	Excalibur, ω scans
θ_{max}, completeness:	27.5°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	17560, 2120, 0.074
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1796
$N(param)_{refined}$:	160
Programs:	Oxford,[1] Olex2,[2] SHELX[3]

2 Experimental details

The data were collected and processed using CrysAlis^{PRO}.[1] The structure was solved by Direct Methods using Olex2 software[2] and refined with the SHELXL.[3] The hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on the parent atoms. The U_{iso} of the H-atoms were set to 1.5 times U_{eq} of the parent atoms with C–H = 0.93 Å (aromatic).

3 Comment

The design and preparation of magnesium-based complexes has attracted attention due to their potential applications in fields such as luminescence, gas storage and catalysis due to the metal's low density and strong Lewis acidity.[4–9] The title

Mg(II) complex crystallizes in the orthorhombic system, and the asymmetric unit contains one Mg(II) ion, one HBIDA mono anion, one coordinated water molecule. The magnesium(II) ion is located at the centre of a slightly distorted octahedral geometry, with the equator of the octahedron consisting of four carboxylic acid oxygen atoms(O1, O3, O1A, O3A, A = −x, 1−y, 1−z) derived from two BIDA ligands, and the axial direction of the equatorial octahedron made up of two coordinated water molecules. The Mg(II)–O bond distances are 2.0577(13), 2.0769(14) and 2.0922(15) Å, which are within the normal range.[5,7] The asymmetric unit undergoes a centrosymmetric inversion to form a complete complex Mg(II) $(H_2BIDA)_2(H_2O)_2$. Notably, both nitrogen atoms on the benzimidazole are protonated, resulting in an ylidic ligand. The title complex further forms a three-dimensional supramolecular structure *via* the O–H···O hydrogen bonds between carboxyl oxygen and coordinated water and N–H···O hydrogen bonds between carboxyl oxygen and nitrogen atoms on the benzimidazole.

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