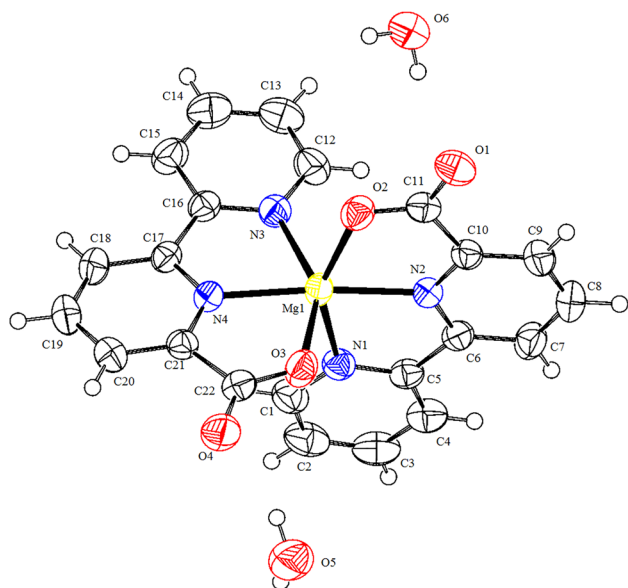


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The crystal structure of [bis(2,2'-bipyridine-6-carboxylato- $\kappa^3 N,N,O$)magnesium(II)]dihydrate, $C_{22}H_{18}N_4O_6Mg$

**Table 1:** Data collection and handling.

Crystal:	Colorless block
Size:	0.14 × 0.12 × 0.09 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	1.17 mm ⁻¹
Diffractometer, scan mode:	XtALAB synergy, ω -scans
$\theta_{\max}$, completeness:	77.5°, >99 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	16,694, 4272, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3742
$N(\text{param})_{\text{refined}}$:	311
Programs:	Bruker programs [1], OLEX2 [2], SHELX [3], DIAMOND [4]

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Abstract

$C_{22}H_{18}N_4O_6Mg$, orthorhombic, *Pbca* (no. 61), $a = 15.3055(2)$ Å, $b = 15.1214(2)$ Å, $c = 18.1048(2)$ Å, $V = 4190.19(9)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0376$, $wR_{\text{ref}}(F^2) = 0.1069$, $T = 296$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

0.100 g 2,2'-Bipyridine-6-carboxylic acid (0.5 mmol), 0.1017 g $MgCl_2 \cdot 6H_2O$ (0.50 mmol), and 0.040 g NaOH (0.50 mmol) were

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dissolved into 25 mL of ethanol(95 %)-water (v:v = 3:2) with stirring. The reactant was heated to 75 °C and continued to react for 4 h. The reaction mixture was then cooled to room temperature and filtered. The filtrate was transferred to a small reagent vial and slowly volatilized at room temperature. The block colorless crystals of the title complex were obtained in 15 days.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å, and O–H = 0.84–0.87 Å). Their U_{iso} values were set to $1.2U_{\text{eq}}$ and $1.5U_{\text{eq}}$ of the parent atoms.

3 Comment

The synthesis, structural characterization, and study of magnesium(II) complexes has been growth in the past two decades. Because magnesium(II) complexes show promising applications in many aspects such as antioxidant activity [5], initiators for forming polylactide [6], fluorescence property [7], and catalyzing the hydrogen-boron reactions [8]. Our research group has also synthesized and structurally characterized some magnesium(II) complexes and studied their properties [9–13]. To further explore the structure and properties of the magnesium(II) complexes, we have synthesized and structurally characterized a new

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

	X	Y	Z	U_{iso}^*/U_{eq}
Mg1	0.28416 (3)	0.38106 (3)	0.49473 (2)	0.03698 (14)
O1	0.40402 (8)	0.39674 (8)	0.29158 (6)	0.0551 (3)
O2	0.35416 (7)	0.42922 (7)	0.40456 (6)	0.0455 (3)
O3	0.38804 (8)	0.32982 (7)	0.55480 (6)	0.0489 (3)
O4	0.46983 (9)	0.34259 (8)	0.65648 (7)	0.0591 (3)
N1	0.18447 (8)	0.28324 (8)	0.53939 (6)	0.0400 (3)
N2	0.26228 (8)	0.28611 (7)	0.41205 (6)	0.0352 (3)
N3	0.17669 (8)	0.48237 (8)	0.48411 (7)	0.0405 (3)
N4	0.29476 (8)	0.46623 (7)	0.58643 (6)	0.0352 (3)
C1	0.14272 (11)	0.28851 (11)	0.60397 (9)	0.0495 (4)
H1	0.156303	0.334871	0.635706	0.059*
C2	0.08007 (12)	0.22784 (13)	0.62567 (10)	0.0580 (4)
H2	0.052588	0.233132	0.671272	0.070*
C3	0.05917 (11)	0.15976 (12)	0.57879 (10)	0.0568 (4)
H3	0.017147	0.118360	0.592230	0.068*
C4	0.10088 (11)	0.15330 (11)	0.51183 (9)	0.0489 (4)
H4	0.087410	0.107761	0.479230	0.059*
C5	0.16359 (9)	0.21609 (9)	0.49374 (8)	0.0379 (3)
C6	0.21102 (9)	0.21520 (9)	0.42234 (8)	0.0374 (3)
C7	0.20500 (11)	0.15004 (10)	0.36874 (9)	0.0488 (4)
H7	0.168970	0.101191	0.375529	0.059*
C8	0.25361 (13)	0.15932 (11)	0.30518 (9)	0.0556 (4)
H8	0.250163	0.116416	0.268487	0.067*
C9	0.30754 (12)	0.23189 (11)	0.29538 (8)	0.0486 (4)
H9	0.341619	0.237896	0.253148	0.058*
C10	0.30900 (9)	0.29506 (9)	0.35047 (7)	0.0373 (3)
C11	0.36065 (10)	0.38110 (9)	0.34784 (8)	0.0399 (3)
C12	0.11918 (12)	0.48881 (12)	0.42868 (9)	0.0516 (4)
H12	0.119303	0.445174	0.392482	0.062*
C13	0.05964 (12)	0.55711 (13)	0.42261 (11)	0.0602 (5)
H13	0.020828	0.559667	0.383148	0.072*
C14	0.05933 (13)	0.62121 (13)	0.47649 (11)	0.0621 (5)
H14	0.020506	0.668380	0.473463	0.075*
C15	0.11653 (12)	0.61540 (11)	0.53483 (10)	0.0515 (4)
H15	0.116394	0.657893	0.571961	0.062*
C16	0.17437 (9)	0.54499 (9)	0.53721 (8)	0.0374 (3)
C17	0.23909 (9)	0.53349 (8)	0.59724 (8)	0.0358 (3)
C18	0.24488 (11)	0.58444 (10)	0.66084 (8)	0.0448 (3)
H18	0.205092	0.629759	0.669487	0.054*
C19	0.31035 (12)	0.56695 (11)	0.71095 (9)	0.0499 (4)
H19	0.315892	0.601637	0.753109	0.060*
C20	0.36797 (11)	0.49784 (10)	0.69871 (8)	0.0454 (3)
H20	0.412541	0.485483	0.732059	0.054*
C21	0.35724 (9)	0.44767 (9)	0.63531 (7)	0.0370 (3)
C22	0.41073 (10)	0.36663 (9)	0.61438 (8)	0.0411 (3)
O5	0.53560 (12)	0.16856 (10)	0.68357 (9)	0.0762 (4)
H5A	0.5167 (19)	0.2190 (14)	0.6672 (15)	0.114*
H5B	0.4938 (16)	0.1523 (19)	0.7104 (15)	0.114*
O6	0.42572 (10)	0.56899 (9)	0.23104 (7)	0.0635 (3)
H6A	0.4129 (18)	0.5211 (13)	0.2535 (14)	0.095*
H6B	0.4519 (17)	0.5990 (15)	0.2641 (12)	0.095*

magnesium(II) complex with 2,2'-bipyridine-6-carboxylic acid ligand.

The molecular structure of the title magnesium(II) complex is shown in the Figure. The title magnesium(II) complex consists of one Mg(II) ion, two *N, N, O*-bonded 2,2'-bipyridine-6-carboxylato ligands and two lattice water molecules. The Mg(II) is six-coordinated with two oxygen atoms (O1, O3) from two 2,2'-bipyridine-6-carboxylato ligands, four nitrogen atoms (N1, N2, N3, N4) from two 2,2'-bipyridine-6-carboxylato ligands to form a distorted $[MgN_4O_2]$ octahedral polyhedron. The 2,2'-bipyridine-6-carboxylato acts as a *N, N, O*-chelating tridentate ligand coordinating to the Mg(II) ion via its two pyridyl N atoms and one of the carboxylate oxygen atoms to form two stable five membered rings. The Mg–O and Mg–N distances are in the range of 2.0763(12)–2.0841(11) Å and 2.1010(12)–2.2737(13) Å, respectively. The N2–Mg1–N4 bond angle is 172.38(5)°, indicating that the N2 and N4 atoms occupy the equatorial positions, and the N1, N3, O1 and O3 atoms are at the axial positions with the summation of bond angles, N1–Mg1–N3, O2–Mg1–N3, O2–Mg1–O3, and O3–Mg1–N1 equals to 376.39°. The carboxyl oxygen atoms of 2,2'-bipyridine-6-carboxylato ligands and oxygen atoms of lattice water molecules are involved in intermolecular O–H...O hydrogen bonds.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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