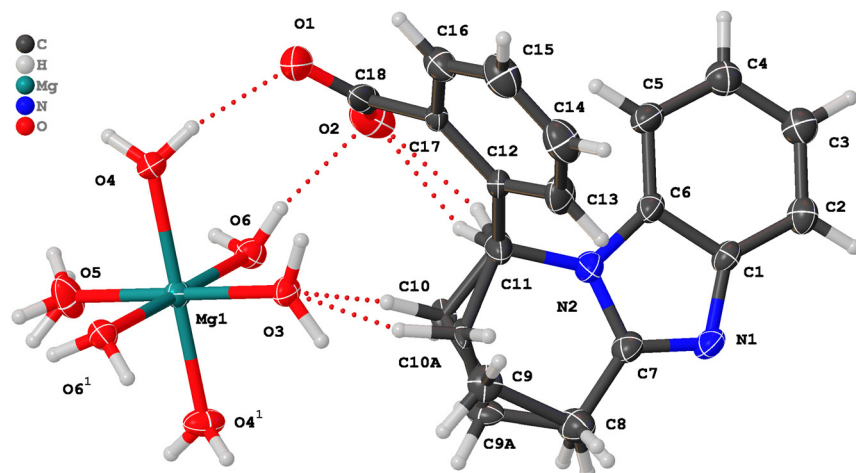


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The crystal structure of hexaaquamagnesium(II) bis-3-(1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2- α]pyridin-1-yl)benzoate, $C_{36}H_{42}N_4O_{10}Mg$



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Abstract

$C_{36}H_{42}N_4O_{10}Mg$, monoclinic, $C2/c$ (no. 15), $a = 16.4977(12)$ Å, $b = 16.3866(10)$ Å, $c = 12.5814(10)$ Å, $\beta = 101.922(8)^\circ$, $V = 3327.9(4)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0794$, $wR_{\text{ref}}(F^2) = 0.2021$, $T = 260$ 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

An amount of 0.0585 g 2-(1H-benzo[d]imidazol-2-yl)ethanamine dihydrochloride (0.25 mmol), 0.0375 g 2-carboxybenzaldehyde

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.16 \times 0.13 \times 0.11$ mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.12 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.0° , >99 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7457, 2931, 0.027
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2335
$N(\text{param})_{\text{refined}}$:	258
Programs:	Bruker, ¹ Olex2, ² SHELX, ³ Diamond ⁴

(0.25 mmol), 0.030 g NaOH (0.75 mmol), and 0.0508 g magnesium chloride hexahydrate (0.25 mmol) were dissolved to the 20 ml ethanol-water (v:v = 3:1) solution under stirring. The above solution was heated and stirred for 4 h at 85 °C. The solution was then stirred for an additional 3 h at room temperature. The colorless block crystals were received from the filtrate after 10 days.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93–0.97 Å, O–H = 0.85–0.93 Å). Their U_{iso} values were set to $1.2U_{\text{eq}}$ or $1.5U_{\text{eq}}$ of the parent atoms.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2728 (2)	0.9015 (2)	0.5441 (3)	0.0350 (7)
C2	0.2566 (3)	0.9455 (3)	0.6322 (3)	0.0449 (9)
H2	0.210328	0.979081	0.624943	0.054*
C3	0.3113 (3)	0.9376 (3)	0.7306 (4)	0.0502 (10)
H3	0.301527	0.966463	0.790323	0.060*
C4	0.3809 (3)	0.8875 (3)	0.7430 (4)	0.0494 (10)
H4	0.416557	0.883711	0.810531	0.059*
C5	0.3979 (3)	0.8432 (3)	0.6563 (3)	0.0457 (9)
H5	0.444160	0.809510	0.663986	0.055*
C6	0.3427 (2)	0.8515 (2)	0.5577 (3)	0.0369 (8)
C7	0.2722 (2)	0.8472 (2)	0.3877 (3)	0.0410 (8)
C8	0.2515 (3)	0.8198 (3)	0.2726 (4)	0.0540 (11)
H8AA ^a	0.238107	0.865882	0.223618	0.065*
H8AB ^a	0.205269	0.782083	0.260385	0.065*
H8BC ^b	0.193428	0.80483	0.254665	0.065*
H8BD ^b	0.259265	0.865428	0.226465	0.065*
C9A ^b	0.2988 (6)	0.7534 (6)	0.2482 (7)	0.0389 (19)
H9AA ^b	0.289902	0.747255	0.169939	0.047*
H9AB ^b	0.279626	0.703848	0.277396	0.047*
C9 ^a	0.3386 (7)	0.7738 (6)	0.2558 (8)	0.043 (2)
H9A ^a	0.326533	0.744979	0.186955	0.051*
H9B ^a	0.378909	0.815782	0.250031	0.051*
C10A ^b	0.3870 (5)	0.7631 (5)	0.2921 (8)	0.034 (2)
H10A ^b	0.406290	0.813538	0.265576	0.040*
H10B ^b	0.417164	0.718264	0.267984	0.040*
C10 ^a	0.3758 (4)	0.7184 (4)	0.3363 (6)	0.0281 (16)
H10C ^a	0.335602	0.678997	0.350858	0.034*
H10D ^a	0.420735	0.689456	0.313894	0.034*
C11	0.4047 (2)	0.7646 (3)	0.4254 (4)	0.0519 (10)
H11 ^a	0.412884	0.723786	0.483538	0.062*
H11A ^b	0.406608	0.710125	0.457936	0.062*
C12	0.4885 (2)	0.8068 (2)	0.4454 (3)	0.0331 (7)
C13	0.4925 (3)	0.8892 (2)	0.4187 (4)	0.0520 (10)
H13	0.443578	0.917179	0.391495	0.062*
C14	0.5668 (3)	0.9302 (3)	0.4315 (4)	0.0626 (11)
H14	0.567712	0.985141	0.413202	0.075*
C15	0.6389 (3)	0.8900 (3)	0.4712 (4)	0.0605 (11)
H15	0.689197	0.917529	0.480850	0.073*
C16	0.6371 (3)	0.8087 (3)	0.4968 (3)	0.0461 (9)
H16	0.686749	0.781600	0.523054	0.055*
C17	0.5627 (2)	0.7654 (2)	0.4845 (3)	0.0296 (7)
C18	0.5704 (3)	0.6764 (2)	0.5129 (3)	0.0514 (9)
Mg1	0.500000	0.52137 (10)	0.250000	0.0309 (4)
N1	0.22938 (19)	0.8973 (2)	0.4367 (3)	0.0416 (7)
N2	0.3412 (2)	0.8185 (2)	0.4560 (3)	0.0466 (8)
O1	0.6369 (2)	0.6420 (2)	0.5048 (3)	0.0849 (12)
O2	0.5121 (3)	0.6408 (2)	0.5415 (3)	0.0719 (10)
O3	0.500000	0.6451 (2)	0.250000	0.0355 (8)
H3A ^c	0.544952	0.673469	0.289958	0.053*
H3B ^c	0.455048	0.673469	0.210042	0.053*
O4	0.61544 (17)	0.52157 (17)	0.3526 (2)	0.0472 (7)
H4A	0.630963	0.557062	0.401866	0.071*
H4B	0.643356	0.479211	0.375514	0.071*
O5	0.500000	0.3966 (2)	0.250000	0.0578 (12)
H5A ^c	0.513301	0.368000	0.307278	0.087*

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
H5B ^c	0.514482	0.367960	0.200766	0.087*
O6	0.44228 (16)	0.52030 (16)	0.3832 (2)	0.0383 (6)
H6A	0.447426	0.473110	0.412051	0.058*
H6B	0.468228	0.551762	0.432433	0.058*

^aOccupancy: 0.507(10). ^bOccupancy: 0.493(10). ^cOccupancy: 0.5.

3 Comment

Because the nitrogen and oxygen atoms of some ligands exhibit a variety of coordination modes,^{5,6} and the complexes also show potential applications in many aspects for example antitumor chemodynamic therapy agent,⁷ fluorescent property,⁸ dual functional luminescent sensors,⁹ and ion sensing and dye adsorption.¹⁰ In our previous work, we have synthesized and structurally characterized some metal complexes with nitrogen heterocarboxylic acid ligands.^{11–14} To further enrich the structure of metal complexes with nitrogen heterocarboxylic acid ligands. Thus, we synthesized and structurally characterized a Mg(II) complex using 2-(1H-benzo[d]imidazol-2-yl)ethanamine dihydrochloride, 2-carboxybenzaldehyde, NaOH, and magnesium chloride hexahydrate as materials. The molecular structure of the title complex is shown in the figure. The title complex is made up of one $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$ cation and 3-(1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridin-1-yl)benzoate anion. The asymmetric unit Mg(II) complex contains one half of a Mg^{2+} , one 3-(1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridin-1-yl)benzoate ligand, and six coordinated H_2O molecules. And the Mg^{2+} is six-coordinated with six O atoms (O3, O4, O4¹, O5, O6, O6¹) of six coordinated H_2O molecules, which form a distorted MgO_6 octahedral coordination geometry (figure). And the bond angle of O3–Mg1–O5 is 180.0°, showing that the O3 and O5 atoms are at the axial positions, and the O4, O4¹, O6, O6¹ atoms are at the equatorial plane. The bond lengths of Mg are in the range of 2.027(4)–2.092(2) Å, which are coincident with that reported in reference.¹⁵ The angles around the Mg^{2+} range from 89.27(11) to 90.73(11)° in the basal plane. Unfortunately, the carboxy oxygen atoms of 3-(1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridin-1-yl)benzoate ligand do not take part in coordination with Mg^{2+} . The $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$ cation unit and 3-(1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyridin-1-yl)benzoate anion unit are linked together by O–H...O and C–H...O hydrogen bonds.

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

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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