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Bis(2-anilinobenzoato-κO)diaqua(2,2′-diamino-4,4′-bi-1,3-thiazole-$\kappa^2 N^1,N^{1'}$)magnesium(II)

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In the title complex, $[Mg(C_{13}H_{10}NO_2)_2(C_6H_6N_4S_2)(H_2O)_2]$, the Mg^{II} ion is coordinated by two 2-anilinobenzoate anions, two water molecules and an 2-anilinobenzoate molecule in a distorted octahedral geometry. The two thiazole rings in the diaminobithiazole molecule are nearly coplanar, with a dihedral angle of 3.88 (17)°. The two benzene rings in each 2-anilinobenzoate anion are twisted with respect to each other, the dihedral angles being 56.32 (12) and 45.68 (12)° in the two anions.

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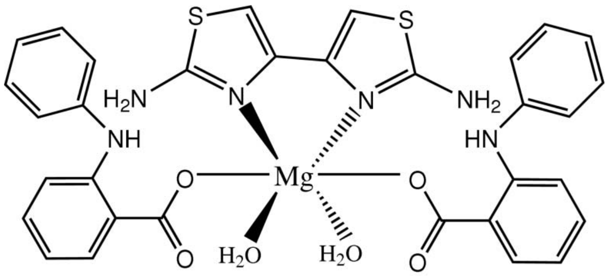
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.137
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

We are interested in metal complexes with diaminobithiazole (DABT) because of their potential magnetic properties (Sun *et al.*, 1997). As part of an ongoing investigation on DABT complexes (Liu *et al.*, 2001), we present here the structure of the title Mg^{II} complex, (I).



(I)

Two 2-anilinobenzoate anions, two water molecules and one DABT molecule coordinate to the Mg^{II} ion in a distorted octahedral geometry (Fig. 1 and Table 1). The DABT molecule is close to planar, with a dihedral angle of 3.88 (17)° between the thiazole rings, comparable to that of 2.35 (12)° found in a Cd^{II} complex of DABT with glycinate (Liu *et al.*, 2005). The two benzene rings in each 2-anilinobenzoate anion are twisted relative to each other, the dihedral angles being 56.32 (12)° and 45.68 (12)°.

An intra- and intermolecular O—H⋯O and N—H⋯O hydrogen-bonding network stabilizes the molecular and crystal structure (Table 2).

Experimental

An aqueous solution (20 ml) containing DABT (1 mmol) and $MgSO_4$ (1 mmol) was mixed with another aqueous solution (10 ml) of *N*-phenylanthranilic acid (2 mmol) and NaOH (2 mmol). The mixture was refluxed for 5 h. The solution was filtered after cooling to room temperature. Single crystals of (I) were obtained from the filtrate after two weeks.

Crystal data

$[Mg(C_{13}H_{10}NO_2)_2(C_6H_6N_4S_2)$-$(H_2O)_2]$
$M_r = 683.05$
Monoclinic, $P2_1/c$
$a = 14.0151$ (3) Å
$b = 19.8832$ (4) Å
$c = 12.0345$ (3) Å
$\beta = 98.3200$ (11)°
$V = 3318.30$ (13) Å^3
$Z = 4$

$D_x = 1.367$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7560 reflections
$\theta = 2.8$–25.0°
$\mu = 0.23$ mm^{-1}
$T = 295$ (2) K
Prism, yellow
0.20 × 0.17 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.945$, $T_{\max} = 0.980$
23565 measured reflections

7620 independent reflections
4001 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.052$
$\theta_{\max} = 27.5°$
$h = -18 \rightarrow 15$
$k = -25 \rightarrow 22$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.137$
$S = 1.02$
7620 reflections
424 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.2965P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Mg—O1	2.0846 (18)	Mg—O31	2.0804 (18)
Mg—O2	2.1087 (18)	Mg—N1	2.184 (2)
Mg—O11	2.0522 (17)	Mg—N2	2.182 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O12$^{\rm i}$	0.89	1.83	2.716 (2)	171
O1—H1*B*···O32	0.84	1.93	2.598 (2)	136
O2—H2*A*···O12	0.90	1.83	2.654 (2)	151
N3—H3*A*···O2	0.82	2.23	3.005 (3)	157
N3—H3*B*···N6$^{\rm ii}$	0.82	2.56	3.203 (3)	137
N4—H4*A*···O1	0.85	2.22	2.983 (3)	150
N4—H4*B*···O32$^{\rm iii}$	0.86	2.07	2.921 (3)	169
N5—H5*B*···O11	0.86	1.91	2.606 (3)	137
N6—H6···O31	0.86	1.97	2.667 (3)	137

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z$.

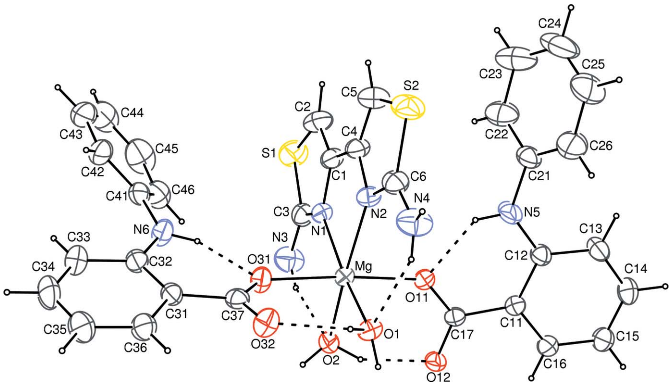


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. Dashed lines indicate the intramolecular hydrogen bonds.

Amino H atoms and water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(carrier). Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(carrier).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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