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Diaquabis(pyridine-2-carboxylato)-magnesium(II) 0.15-hydrate

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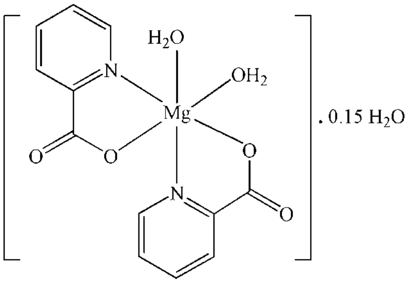
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; disorder in solvent or counterion; R factor = 0.032; wR factor = 0.090; data-to-parameter ratio = 18.0.

The reaction of magnesium(II) chloride tetrahydrate with the proton-transfer compound piperazinediium pyridine-2-carboxylate, $(\mathrm{pipzH_2})(\mathrm{pyc})_2$ (pipz is pirerazine and pycH is pyridine-2-carboxylic acid) in aqueous solution leads to the formation of the title compound, $[\mathrm{Mg(C_6H_4NO_2)_2(H_2O)_2}]\cdot 0.15\mathrm{H_2O}$. The Mg atom is six-coordinated in a distorted octahedral environment by two bidentate pyridine-2-carboxylate groups and two O atoms of coordinated water molecules, which are located in *cis* positions. In the crystal structure, intermolecular O—H⋯O and C—H⋯O hydrogen bonds, and π–π [π–π distance = 3.5616 (8) Å for pyridine rings; symmetry code: $2-x, 1-y, 1-z$] and C—H⋯π stacking, connect the various components into a supramolecular structure.

Related literature

In order to develop new types of proton-transfer compounds and hydrogen-bonding systems, our research group has already selected pyridine-2,6-dicarboxylic acid ($\mathrm{pydcH_2}$) and 1,10-phenanthroline-2,9-dicarboxylic acid ($\mathrm{phendcH_2}$) as proton donors and pyridine-2,6-diamine (pyda), creatinine (creat) and propane-1,3-diamine (pda) as proton acceptors. These resulted in the formation of the new proton-transfer compounds (pydcH)(pydaH) (Aghabozorg *et al.*, 2005), (creatH)(phendcH)·$\mathrm{H_2O}$ (Soleimannejad *et al.*, 2005) and (pda)(pydc)($\mathrm{pydcH_2}$) (Aghabozorg, Ghadermazi & Ramezanipour, 2006). For further details, see: Aghabozorg, Zabihi *et al.* (2006); Aghabozorg, Ghasemikhah *et al.* (2006); Aghabozorg, Ghadermazi & Attar Gharamaleki (2006).



Experimental

Crystal data

$[\mathrm{Mg(C_6H_4NO_2)_2(H2O)_2}]\cdot 0.15\mathrm{H_2O}$
M_r = 307.25
Monoclinic, $P2_1/n$
a = 11.6385 (6) Å
b = 8.7955 (5) Å
c = 14.9357 (8) Å
β = 107.221 (1)°
V = 1460.37 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 100 (2) K
0.23 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min}$ = 0.954, $T_{\max}$ = 0.966
20864 measured reflections
3487 independent reflections
2879 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.090
S = 1.04
3487 reflections
194 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.82 e Å^{-3}
$\Delta\rho_{\min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mg1—O7	2.0313 (9)	Mg1—O2	2.0512 (9)
Mg1—O6	2.0408 (10)	Mg1—N1	2.2049 (11)
Mg1—O3	2.0449 (9)	Mg1—N2	2.2222 (12)
O7—Mg1—O6	86.90 (4)	O3—Mg1—N1	163.68 (4)
O7—Mg1—O2	169.21 (4)	O6—Mg1—N2	168.95 (4)
O2—Mg1—O3—C12	93.50 (9)	O2—Mg1—N2—C7	91.43 (13)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O6—H6A⋯O4$^{\mathrm{i}}$	0.82	1.89	2.697 (1)	170
O6—H6B⋯O1$^{\mathrm{ii}}$	0.82	1.88	2.697 (1)	176
O7—H7A⋯O3$^{\mathrm{i}}$	0.82	1.87	2.669 (1)	167
O7—H7B⋯O1$^{\mathrm{iii}}$	0.82	1.93	2.726 (1)	165
C9—H9A⋯O2$^{\mathrm{iv}}$	0.95	2.57	3.328 (2)	137
C7—H7C⋯Cg	0.95	3.22	4.112 (1)	156
C8—H8A⋯Cg	0.95	3.42	4.162 (1)	137

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+2, -y, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x+1, -y, -z+1$.

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Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2012).

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supplementary materials

Acta Cryst. (2007). E**63**, m2235-m2236   [**doi:10.1107/S1600536807036604**]

Diaquabis(pyridine-2-carboxylato)magnesium(II) 0.15-hydrate

M. A. Sharif, H. Aghabozorg, E. Motyeian, M. Ghadermazi and **J. Attar Gharamaleki**

Comment

Intermolecular interactions, such as hydrogen bonding, π–π stacking, ion pairing and donor acceptor interactions, are famous for making aggregates of molecules. One or more of these interactions may result in the formation of specific and spontaneous self-associations or self-assemblies of compounds. Research has shown that hydrogen bonding plays the key role in the preparation of self-assembled or self-associated compounds. There is a very close relationship between hydrogen bonding and formation of proton-transfer compounds (Aghabozorg *et al.*, 2006). In order to develop new types of proton transfer compounds and hydrogen bonding systems, our research group has already selected pyridine-2,6-dicarboxylic acid (pydcH$_2$) and 1,10-phenanthroline-2,9-dicarboxylic acid (phendcH$_2$) as proton donors and pyridine-2,6-diamine (pyda), creatinine (creat) and propane-1,3-diamine (pda) as proton acceptors. These resulted in the formation of new proton transfer compounds (pydcH)(pydaH) (Aghabozorg *et al.*, 2005), (creatH)(phendcH)·H$_2$O (Soleimannejad *et al.*, 2005) and (pda)(pydc)(pydcH$_2$) (Aghabozorg, Ghadermazi & Ramezanipour, 2006). Here, we report the synthesis and X-ray crystal structure of the title compound, (I). The asymmetric unit of compound (I) contains a neutral complex and one water molecule (Fig. 1). The Mg^{II} atom is six-coordinated by two pyridine-2-carboxylate, (pyc)$^-$, groups and two coordinated water molecules. The O6—Mg1—O7 angel is 86.90 (4)°, showing that the two coordinated water molecules are located at *cis* to each other. Also, torsion angels show that the two (pyc)$^-$ fragments are almost perpendicular to each other. Therefore, the coordination around Mg^{II} is distorted octahedral. A considerable feature of the compound (I) is the presence of π–π and C—H···π stacking interactions. The average distance between the planes are 3.5616 (8) Å ($2 - x$, $1 - y$, $1 - z$). The C—H···π distances (measured to the centre of phenyl ring) are 3.225 (1) Å and 3.417 (1) Å and the C–H···π angles are 156.3 (1)° and 136.9 (1)°, respectively (Figs 2 and 3). Intermolecular O—H···O and C—H···O hydrogen bonds ranging from 2.669 (1) to 3.328 (2) Å (Table 2) seem to be effective in the stabilization of the crystal structure, resulting in the formation of an interesting supramolecular structure (Fig. 4).

Experimental

A solution of MgCl$_2$·4H$_2$O (143 mg, 0.5 mmol) in water (20 ml) was added to an aqueous solution of (pipzH$_2$)(pyc)$_2$ (253 mg, 1.0 mmol) in water (20 ml) in a 1:2 molar ratio. Colorless crystals of (I) were obtained after allowing the mixture to stand for two weeks at room temperature.

Refinement

The hydrogen atoms of water molecules were found in difference Fourier synthesis. The H(C) atom positions were calculated. All hydrogen atoms were refined in isotropic approximation in riding model with with the U_{iso}(H) parameters equal to 1.2 U_{eq}(Ci) and 1.2 U_{eq}(Oi) where U(Ci) and U(Oi) are respectively the equivalent thermal parameters of the carbon and oxygen atoms to which corresponding H atoms are bonded.

Figures

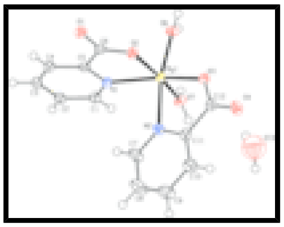

Fig. 1. The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

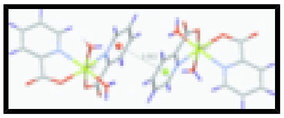

Fig. 2. π–π Stacking interactions between two aromatic rings of (I), The average distance between the planes are 3.5616 (8) Å.

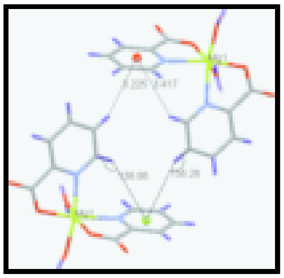

Fig. 3. The C—H···π distances (measured to the centre of phenyl ring) are 3.225 and 3.417 Å and the C–H···π angles are 156.26° and 136.86°, respectively.

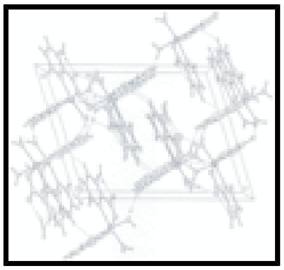

Fig. 4. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Diaquabis(pyridine-2-carboxylato)magnesium(II) 0.15-hydrate

Crystal data

$[Mg(C_6H_4NO_2)_2(H_2O)_2]\cdot 0.15H_2O$	$F_{000} = 638$
$M_r = 307.25$	$D_x = 1.397$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 290 reflections
$a = 11.6385$ (6) Å	$\theta = 3$–28º
$b = 8.7955$ (5) Å	$\mu = 0.15$ mm^{-1}
$c = 14.9357$ (8) Å	$T = 100$ (2) K
$\beta = 107.221$ (1)º	Prism, colourless
$V = 1460.37$ (14) Å^3	0.23 × 0.20 × 0.19 mm
$Z = 4$	

Data collection

Bruker APEXII CCD area-detector	3487 independent reflections

diffractometer	
Radiation source: fine-focus sealed tube	2879 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.029$
$T = 100(2)$ K	$\theta_{\text{max}} = 28.0^\circ$
ω scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -15\rightarrow15$
$T_{\text{min}} = 0.954$, $T_{\text{max}} = 0.966$	$k = -11\rightarrow11$
20864 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.090$	$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3487 reflections	$\Delta\rho_{\text{max}} = 0.82$ e Å^{-3}
194 parameters	$\Delta\rho_{\text{min}} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mg1	0.75274 (4)	0.14609 (4)	0.36741 (3)	0.01536 (11)	
O1	0.95964 (8)	0.13410 (10)	0.64227 (6)	0.0212 (2)	
O2	0.84302 (8)	0.07036 (10)	0.49940 (6)	0.01827 (19)	
O3	0.68286 (8)	−0.06450 (10)	0.32554 (6)	0.01797 (19)	
O4	0.53051 (9)	−0.22785 (11)	0.30834 (7)	0.0281 (2)	
N1	0.80774 (9)	0.35929 (11)	0.44608 (7)	0.0164 (2)	
N2	0.57295 (10)	0.15093 (12)	0.39090 (8)	0.0195 (2)	
C1	0.78783 (11)	0.50379 (14)	0.41751 (9)	0.0189 (3)	

H1A	0.7432	0.5232	0.3542	0.023*	
C2	0.82985 (11)	0.62649 (14)	0.47670 (9)	0.0201 (3)	
H2A	0.8148	0.7277	0.4541	0.024*	
C3	0.89413 (12)	0.59849 (15)	0.56922 (9)	0.0217 (3)	
H3A	0.9235	0.6803	0.6114	0.026*	
C4	0.91508 (11)	0.44843 (15)	0.59947 (9)	0.0211 (3)	
H4A	0.9586	0.4261	0.6626	0.025*	
C5	0.87139 (10)	0.33242 (14)	0.53592 (9)	0.0161 (2)	
C6	0.89342 (10)	0.16539 (14)	0.56167 (9)	0.0164 (2)	
C7	0.51747 (14)	0.26405 (16)	0.42112 (11)	0.0292 (3)	
H7C	0.5588	0.3578	0.4379	0.035*	
C8	0.40216 (15)	0.25093 (18)	0.42914 (13)	0.0382 (4)	
H8A	0.3654	0.3343	0.4504	0.046*	
C9	0.34146 (15)	0.11477 (18)	0.40569 (13)	0.0358 (4)	
H9A	0.2627	0.1025	0.4111	0.043*	
C10	0.39795 (13)	−0.00355 (16)	0.37412 (10)	0.0278 (3)	
H10A	0.3584	−0.0984	0.3571	0.033*	
C11	0.51309 (11)	0.01883 (14)	0.36780 (9)	0.0194 (3)	
C12	0.57951 (11)	−0.10300 (15)	0.33120 (8)	0.0183 (3)	
O6	0.90157 (8)	0.11746 (10)	0.32355 (6)	0.0194 (2)	
H6A	0.9151	0.1602	0.2789	0.023*	
H6B	0.9465	0.0436	0.3360	0.023*	
O7	0.67881 (8)	0.25894 (10)	0.24522 (6)	0.01865 (19)	
H7A	0.7209	0.3019	0.2177	0.022*	
H7B	0.6088	0.2754	0.2149	0.022*	
O1S	0.3507 (12)	−0.3966 (16)	0.3526 (9)	0.089 (4)*	0.15
H1SA	0.4061	−0.3424	0.3481	0.106*	0.15
H1SB	0.2825	−0.3612	0.3359	0.106*	0.15

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0147 (2)	0.0129 (2)	0.0172 (2)	−0.00015 (15)	0.00268 (16)	−0.00011 (15)
O1	0.0191 (4)	0.0191 (5)	0.0207 (4)	0.0034 (4)	−0.0013 (4)	0.0011 (3)
O2	0.0178 (4)	0.0149 (4)	0.0195 (4)	−0.0010 (3)	0.0016 (3)	0.0001 (3)
O3	0.0158 (4)	0.0158 (4)	0.0223 (4)	−0.0012 (3)	0.0057 (3)	−0.0022 (3)
O4	0.0286 (5)	0.0225 (5)	0.0384 (6)	−0.0104 (4)	0.0178 (4)	−0.0118 (4)
N1	0.0143 (5)	0.0155 (5)	0.0186 (5)	0.0002 (4)	0.0037 (4)	0.0001 (4)
N2	0.0209 (5)	0.0165 (5)	0.0222 (5)	0.0010 (4)	0.0081 (4)	0.0001 (4)
C1	0.0189 (6)	0.0179 (6)	0.0198 (6)	0.0005 (5)	0.0058 (5)	0.0015 (5)
C2	0.0197 (6)	0.0152 (6)	0.0275 (7)	0.0005 (5)	0.0101 (5)	0.0002 (5)
C3	0.0191 (6)	0.0177 (6)	0.0271 (7)	−0.0019 (5)	0.0049 (5)	−0.0064 (5)
C4	0.0187 (6)	0.0208 (6)	0.0204 (6)	0.0020 (5)	0.0009 (5)	−0.0021 (5)
C5	0.0116 (5)	0.0172 (6)	0.0191 (6)	0.0009 (4)	0.0038 (4)	0.0001 (5)
C6	0.0119 (5)	0.0168 (6)	0.0200 (6)	0.0013 (5)	0.0039 (4)	0.0006 (5)
C7	0.0312 (8)	0.0181 (6)	0.0443 (8)	−0.0009 (6)	0.0205 (7)	−0.0032 (6)
C8	0.0385 (9)	0.0256 (8)	0.0621 (11)	0.0027 (7)	0.0328 (8)	−0.0044 (7)
C9	0.0287 (8)	0.0309 (8)	0.0567 (10)	−0.0015 (6)	0.0263 (7)	−0.0011 (7)

C10	0.0258 (7)	0.0238 (7)	0.0379 (8)	−0.0043 (6)	0.0159 (6)	−0.0021 (6)
C11	0.0200 (6)	0.0191 (6)	0.0202 (6)	−0.0008 (5)	0.0075 (5)	0.0005 (5)
C12	0.0195 (6)	0.0185 (6)	0.0169 (6)	−0.0014 (5)	0.0054 (5)	−0.0009 (5)
O6	0.0175 (4)	0.0164 (4)	0.0244 (5)	0.0028 (3)	0.0066 (4)	0.0045 (3)
O7	0.0139 (4)	0.0201 (4)	0.0199 (4)	−0.0002 (3)	0.0019 (3)	0.0044 (3)

Geometric parameters (Å, °)

Mg1—O7	2.0313 (9)	C3—H3A	0.9500
Mg1—O6	2.0408 (10)	C4—C5	1.3837 (18)
Mg1—O3	2.0449 (9)	C4—H4A	0.9500
Mg1—O2	2.0512 (9)	C5—C6	1.5210 (17)
Mg1—N1	2.2049 (11)	C7—C8	1.387 (2)
Mg1—N2	2.2222 (12)	C7—H7C	0.9500
O1—C6	1.2529 (15)	C8—C9	1.382 (2)
O2—C6	1.2588 (15)	C8—H8A	0.9500
O3—C12	1.2763 (15)	C9—C10	1.386 (2)
O4—C12	1.2379 (16)	C9—H9A	0.9500
N1—C1	1.3389 (16)	C10—C11	1.3851 (19)
N1—C5	1.3478 (16)	C10—H10A	0.9500
N2—C7	1.3354 (17)	C11—C12	1.5149 (18)
N2—C11	1.3461 (16)	O6—H6A	0.8199
C1—C2	1.3890 (18)	O6—H6B	0.8200
C1—H1A	0.9500	O7—H7A	0.8196
C2—C3	1.3848 (19)	O7—H7B	0.8197
C2—H2A	0.9500	O1S—H1SA	0.8200
C3—C4	1.3930 (18)	O1S—H1SB	0.8200

O7—Mg1—O6	86.90 (4)	C5—C4—H4A	120.6
O7—Mg1—O3	98.25 (4)	C3—C4—H4A	120.6
O6—Mg1—O3	95.08 (4)	N1—C5—C4	122.39 (11)
O7—Mg1—O2	169.21 (4)	N1—C5—C6	115.01 (10)
O6—Mg1—O2	91.52 (4)	C4—C5—C6	122.59 (11)
O3—Mg1—O2	92.52 (4)	O1—C6—O2	125.70 (11)
O7—Mg1—N1	92.42 (4)	O1—C6—C5	117.70 (11)
O6—Mg1—N1	97.81 (4)	O2—C6—C5	116.60 (11)
O3—Mg1—N1	163.68 (4)	N2—C7—C8	122.97 (13)
O2—Mg1—N1	77.21 (4)	N2—C7—H7C	118.5
O7—Mg1—N2	87.95 (4)	C8—C7—H7C	118.5
O6—Mg1—N2	168.95 (4)	C9—C8—C7	119.04 (14)
O3—Mg1—N2	75.99 (4)	C9—C8—H8A	120.5
O2—Mg1—N2	95.33 (4)	C7—C8—H8A	120.5
N1—Mg1—N2	92.17 (4)	C8—C9—C10	118.59 (14)
C6—O2—Mg1	119.25 (8)	C8—C9—H9A	120.7
C12—O3—Mg1	121.15 (8)	C10—C9—H9A	120.7
C1—N1—C5	118.42 (11)	C11—C10—C9	118.84 (13)
C1—N1—Mg1	129.94 (9)	C11—C10—H10A	120.6
C5—N1—Mg1	111.64 (8)	C9—C10—H10A	120.6
C7—N2—C11	117.67 (11)	N2—C11—C10	122.89 (12)
C7—N2—Mg1	129.78 (9)	N2—C11—C12	114.98 (11)

C11—N2—Mg1	112.52 (8)	C10—C11—C12	122.10 (12)
N1—C1—C2	122.66 (12)	O4—C12—O3	125.68 (12)
N1—C1—H1A	118.7	O4—C12—C11	118.98 (11)
C2—C1—H1A	118.7	O3—C12—C11	115.33 (11)
C3—C2—C1	118.77 (12)	Mg1—O6—H6A	126.1
C3—C2—H2A	120.6	Mg1—O6—H6B	124.7
C1—C2—H2A	120.6	H6A—O6—H6B	106.6
C2—C3—C4	118.89 (12)	Mg1—O7—H7A	121.3
C2—C3—H3A	120.6	Mg1—O7—H7B	132.1
C4—C3—H3A	120.6	H7A—O7—H7B	106.6
C5—C4—C3	118.86 (12)	H1SA—O1S—H1SB	117.9

O7—Mg1—O2—C6	12.0 (3)	N1—C1—C2—C3	−0.53 (19)
O6—Mg1—O2—C6	93.42 (9)	C1—C2—C3—C4	0.44 (19)
O3—Mg1—O2—C6	−171.42 (9)	C2—C3—C4—C5	0.28 (19)
N1—Mg1—O2—C6	−4.24 (9)	C1—N1—C5—C4	0.92 (18)
N2—Mg1—O2—C6	−95.27 (9)	Mg1—N1—C5—C4	−179.50 (10)
O7—Mg1—O3—C12	−87.16 (9)	C1—N1—C5—C6	−178.05 (10)
O6—Mg1—O3—C12	−174.75 (9)	Mg1—N1—C5—C6	1.53 (13)
O2—Mg1—O3—C12	93.50 (9)	C3—C4—C5—N1	−0.99 (19)
N1—Mg1—O3—C12	43.15 (19)	C3—C4—C5—C6	177.90 (11)
N2—Mg1—O3—C12	−1.37 (9)	Mg1—O2—C6—O1	−173.57 (10)
O7—Mg1—N1—C1	3.61 (11)	Mg1—O2—C6—C5	6.37 (14)
O6—Mg1—N1—C1	90.82 (11)	N1—C5—C6—O1	174.80 (11)
O3—Mg1—N1—C1	−127.33 (15)	C4—C5—C6—O1	−4.17 (18)
O2—Mg1—N1—C1	−179.40 (11)	N1—C5—C6—O2	−5.15 (16)
N2—Mg1—N1—C1	−84.43 (11)	C4—C5—C6—O2	175.89 (11)
O7—Mg1—N1—C5	−175.91 (8)	C11—N2—C7—C8	−0.2 (2)
O6—Mg1—N1—C5	−88.71 (8)	Mg1—N2—C7—C8	177.65 (12)
O3—Mg1—N1—C5	53.15 (18)	N2—C7—C8—C9	0.5 (3)
O2—Mg1—N1—C5	1.08 (8)	C7—C8—C9—C10	−0.6 (3)
N2—Mg1—N1—C5	96.05 (8)	C8—C9—C10—C11	0.4 (2)
O7—Mg1—N2—C7	−78.27 (13)	C7—N2—C11—C10	0.0 (2)
O6—Mg1—N2—C7	−140.6 (2)	Mg1—N2—C11—C10	−178.22 (11)
O3—Mg1—N2—C7	−177.30 (13)	C7—N2—C11—C12	178.16 (12)
O2—Mg1—N2—C7	91.43 (13)	Mg1—N2—C11—C12	−0.08 (14)
N1—Mg1—N2—C7	14.08 (13)	C9—C10—C11—N2	−0.1 (2)
O7—Mg1—N2—C11	99.71 (9)	C9—C10—C11—C12	−178.10 (14)
O6—Mg1—N2—C11	37.4 (3)	Mg1—O3—C12—O4	−179.40 (10)
O3—Mg1—N2—C11	0.68 (9)	Mg1—O3—C12—C11	1.73 (14)
O2—Mg1—N2—C11	−90.59 (9)	N2—C11—C12—O4	−179.95 (12)
N1—Mg1—N2—C11	−167.95 (9)	C10—C11—C12—O4	−1.79 (19)
C5—N1—C1—C2	−0.15 (18)	N2—C11—C12—O3	−1.00 (16)
Mg1—N1—C1—C2	−179.64 (9)	C10—C11—C12—O3	177.16 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6A···O4^{i}	0.82	1.89	2.697 (1)	170

O6—H6B···O1$^{\mathrm{ii}}$	0.82	1.88	2.697 (1)	176
O7—H7A···O3$^{\mathrm{i}}$	0.82	1.87	2.669 (1)	167
O7—H7B···O1$^{\mathrm{iii}}$	0.82	1.93	2.726 (1)	165
C9—H9A···O2$^{\mathrm{iv}}$	0.95	2.57	3.328 (2)	137
C7—H7C···Cg	0.95	3.22	4.112 (1)	156
C8—H8A···Cg	0.95	3.42	4.162 (1)	137

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*−1/2, −*y*+1/2, *z*−1/2; (iv) −*x*+1, −*y*, −*z*+1.

Fig. 1

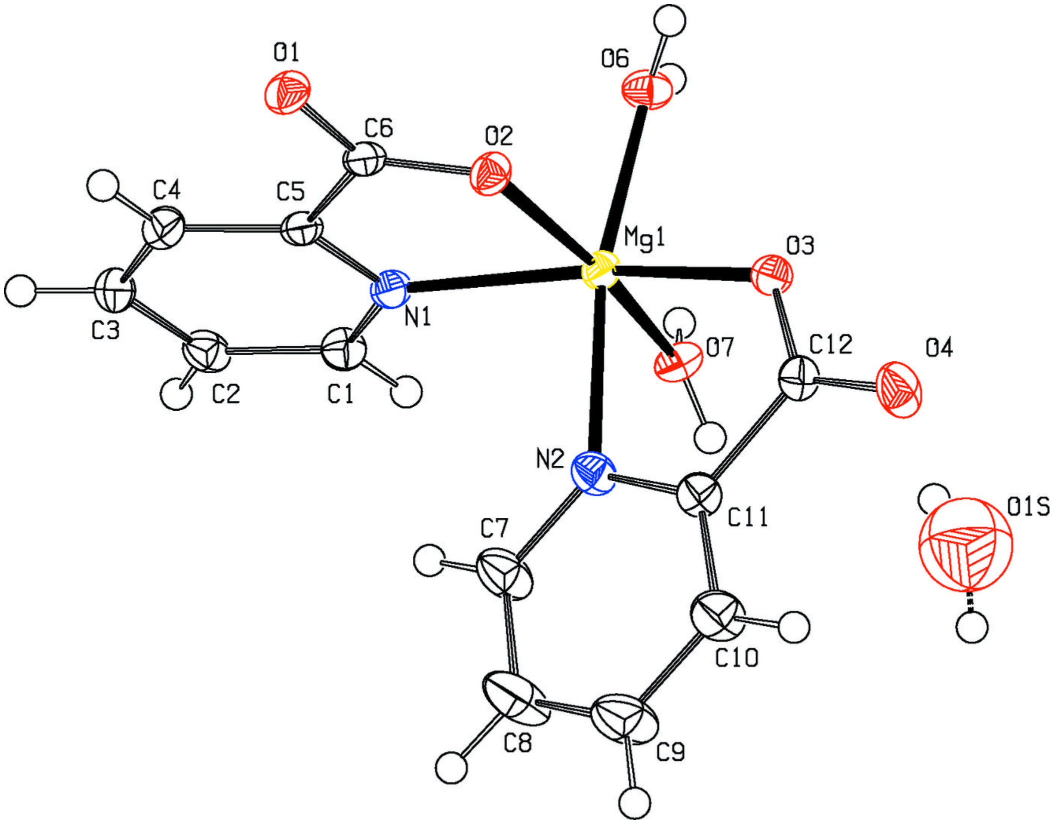

Fig. 2

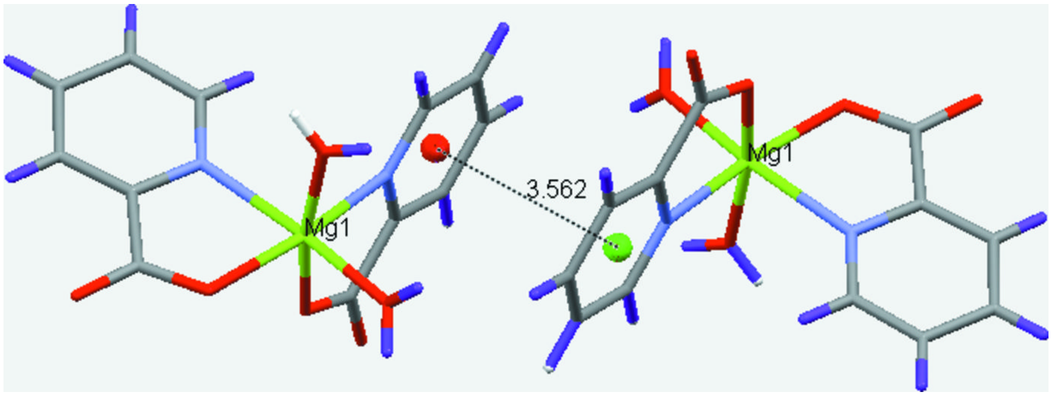

Fig. 3

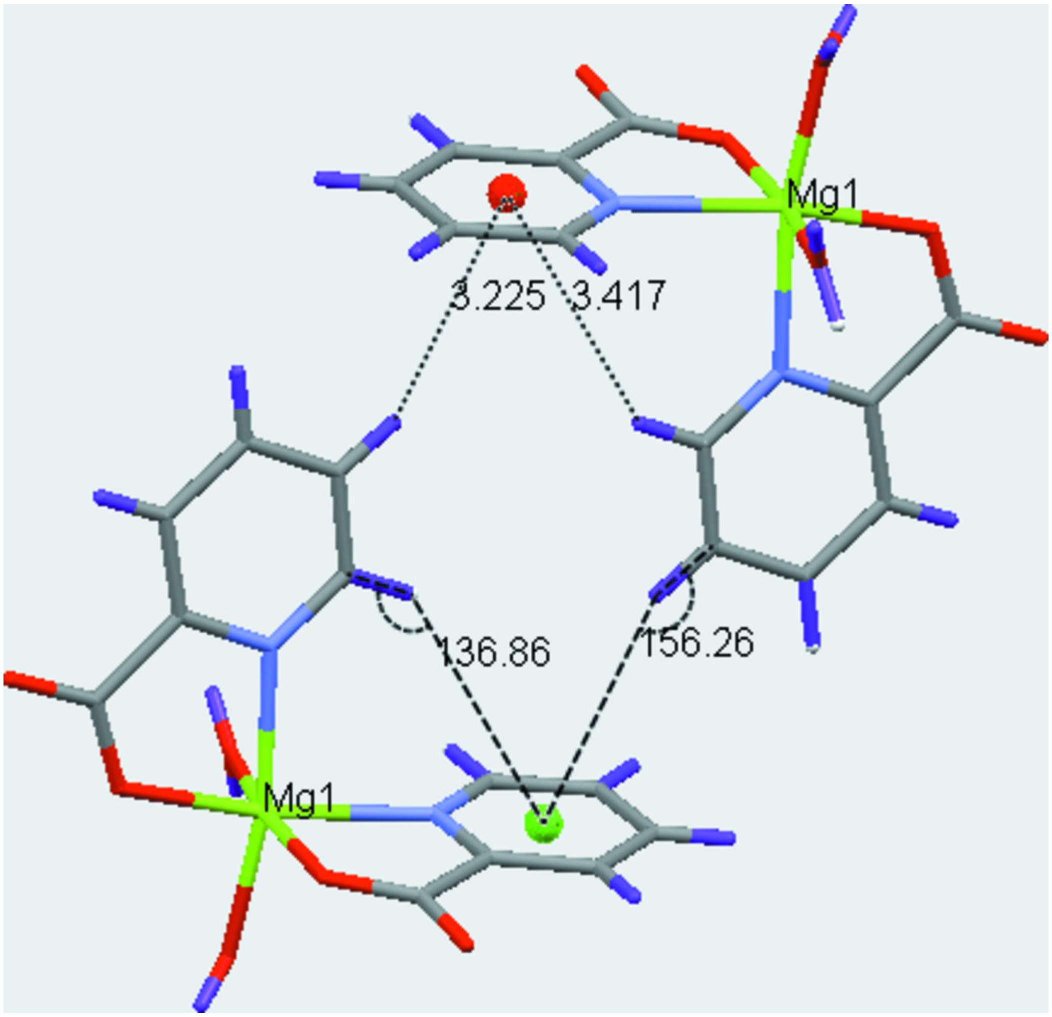

Fig. 4