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Di-μ-acetato-κ^4O:O'-μ-oxido-κ^2O:O-bis[(acetic acid-κO)bis(1H-imidazole-κN^3)magnesium(**II**)]

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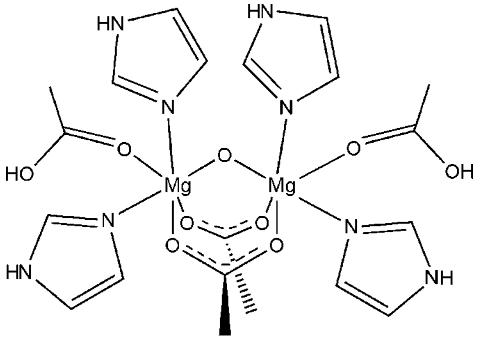
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.071; wR factor = 0.147; data-to-parameter ratio = 7.2.

Magnesium acetate crystallizes upon reaction with imidazole in dimethylformamide at elevated temperatures to form the title magnesium acetate imidazole cluster species, $[Mg_2(C_2H_3O_2)_2O(C_3H_4N_2)_4(C_2H_4O_2)_2]$, with two Mg atoms in octahedral coordination. The complex has crystallographic twofold rotation symmetry. Each Mg atom is coordinated by two imidazole ligands, two linking acetate bridging ligands, a terminal acetic acid ligand, and a bridging O atom lying on the symmetry axis.

Related literature

For related literature, see: Brese & O'Keeffe (1991); Chen *et al.* (2005); Dincã & Long (2005); Huang *et al.* (2004, 2005); Irish *et al.* (1991); Park *et al.* (2006); Rood *et al.* (2006); Rowsell & Yaghi (2006); Roswell *et al.* (2005); Schlapbach & Züttel (2001); Sturm *et al.* (1975); Tian *et al.* (2002, 2003); Tian, Chen *et al.* (2004); Tian, Xu *et al.* (2004).



Experimental

Crystal data

$[Mg_2(C_2H_3O_2)_2O(C_3H_4N_2)_4(C_2H_4O_2)_2]$
M_r = 575.14
Orthorhombic, $Aba2$
a = 8.6927 (14) Å
b = 19.106 (3) Å
c = 16.834 (3) Å
V = 2795.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 298 (2) K
0.12 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004) T_{min} = 0.986, T_{max} = 0.994
10414 measured reflections
1287 independent reflections
1034 reflections with $I > 2\sigma(I)$
R_{int} = 0.112

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.147
S = 1.17
1287 reflections
179 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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, 2001); 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: LH2433).

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supplementary materials

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Di-μ-acetato-κ^4O:O'-μ-oxido-κ^2O:O-bis[(acetic acid-κO)bis(1H-imidazole-κN^3)magnesium(II)\]

N. P. Stadie, **R. Sanchez-Smith** and **T. L. Groy**

Comment

Crystal frameworks incorporating imidazole are of special interest in materials chemistry, especially in the design of metal-organic frameworks (MOFs) that imitate important zeolite topologies. It was found that imidazole may be placed as an organic linker between two coordination centers to bridge metals at the identical angle to the essential bond in most zeolites: the Si—O—Si bond exhibiting a bond angle of 145° (Park *et al.*, 2006). Therefore, this five membered ring makes an ideal organic linker for zeolite analogue frameworks.

Many examples of imidazole zeolite analog structures have been reported, spanning nearly every zeolite topology, a number of different transition metal centers, and various organic linkers incorporating the imidazole ring. The earliest such example is in crystal frameworks of cobalt and imidazole that date back to the 1970 s (Sturm *et al.*, 1975). Numerous other examples of cobalt imidazoles have bee reported to show such zeolite topologies as CAG, among others (Tian *et al.*, 2002, 2003; Tian, Xu *et al.*, 2004; Tian, Chen *et al.*, 2004). Similar copper imidazoles revealing analagous structures to zeolites have also been reported (Huang *et al.*, 2004, 2005). It is important to note that to date, all zeolite analog structures incorporating imidazole have been made with transition metals, mostly from the first row of the d-block.

Our interests in these MOFs have been directed toward synthesizing imidazole structures that incorporate smaller alkali and alkaline earth metals, specifically magnesium. This is appealing because such materials have the potential to be lightweight in comparison to transition metal equivalents and may serve as better candidates for hydrogen or methane gas storage (Rowsell *et al.*, 2005; Rowsell & Yaghi, 2006; Schlapbach & Züttel, 2001; Dincã & Long, 2005; Chen *et al.*, 2005). Other research has begun to be conducted with magnesium and formate as a linking agent; a structural and gas sorption study was recently reported of a porous magnesium formate framework with similar intentions (Rood *et al.*, 2006).

Although this is not a three-dimensional zeolite analog framework, it proves that such a framework may be possible with magnesium. Imidazole does not here serve in its intended role as a zeolitic linker. However, a new and interesting cluster species has been discovered.

The local coordination environment around each magnesium atom may be described as distorted octahedral. The magnesium atoms are related by symmetry and both are coordinated by two terminal imidazole ligands, two bridging acetate ligands, a terminal acetate ligand, and a bridging oxygen. The bond angles reported here match very closely to those reported for magnesium diacetate tetrahydrate (Irish *et al.*, 1991). Bond valences for each coordinative bond may be derived from the bond lengths by specific parameters for a given bond (Brese & O'Keeffe, 1991).

The stucture of the title compound is shown in Figure 1.

Experimental

A solid mixture of magnesium acetate tetrahydrate Mg(CH$_3$COO)$_2$ 4H$_2$O (0.670 g, 3.12 × 10 $^{−3}$mol) and imidazole (1.546 g, 2.27 × 10 $^{−2}$mol) was dissolved in 20 mL of dimethylformamide in a 50 mL centrifuge tube. The tube was stirred for 30 minutes until all reagents were well dissolved, capped, and heated at a rate of 5 K per minute to 358 K in a progammable oven; this temperature was held constant for 48 h. The oven was then cooled at 0.4 K per minute to room temperature. The mother liquor was decanted off following centrifuge and the sample washed with DMF (10 mL × 3). The colorless plate-like crystals harvested from solution were analyzed by single-crystal *x*-ray diffraction.

Refinement

Although the space group is noncentrosymmetric, an absolute configuration could not be obtained, as shown by an indeterminate Flack parameter value of 0.0 (8). This is attributable to the structure containing only light atoms. Therefore, the Friedel opposites were merged before the final refinement. The R_{int} value of 0.1184 shows the poor agreement between equivalent reflections, and the overall weakness of scattering by the preferentially chosen crystal is indicated by the average σ(I)/I$_{\text{net}}$ value of 0.0564. These lead to low bond precision in the C—C bonds (0.012 Å). The methyl H atoms were refined as idealized rotating groups with isotropic thermal parameters set to 1.5 times the isotropic thermal parameter of the corresponding methyl carbon. The H atoms on the imidazoles were refined as idealized aromatic H atoms riding on their bonding partners with isotropic thermal parameters set to 1.2 times that of their corresponding bonding partner. The hydrogen on the carboxylate oxygen was refined as an idealized hydroxyl hydrogen with an isotropic thermal parameter set to 1.5 times the isotropic thermal parameter of the hydroxyl oxygen. It should be noted that the chosen crystal was the best of many that were examined.

Figures

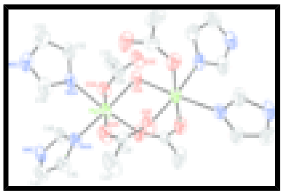


Fig. 1. The title structure showing the octahedral coordination of each magnesium atom. Thermal ellipsoids are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity. Unlabeled atoms are related by the symmetry operator (1 − *x*, −*y*, *z*).

Di-μ-acetato-κ^4*O*:*O*'-μ-oxido-κ^2*O*:*O*-bis[(acetic acid-κ*O*)bis(1*H*-imidazole-κ*N*^{3})magnesium(II)]

Crystal data

[Mg$_2$(C$_2$H$_3$O$_2$)$_2$O(C$_3$H$_4$N$_2$)$_4$(C$_2$H$_4$O$_2$)$_2$]	F_{000} = 1208
M_r = 575.14	D_x = 1.366 Mg m$^{−3}$
Orthorhombic, *Aba*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: A 2 -2ac	Cell parameters from 1685 reflections
a = 8.6927 (14) Å	θ = 2.4–22.2°
b = 19.106 (3) Å	μ = 0.15 mm$^{−1}$

$c = 16.834$ (3) Å	$T = 298$ (2) K
$V = 2795.8$ (8) Å^3	Block, colourless
$Z = 4$	0.12 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer	1287 independent reflections
Radiation source: fine-focus sealed tube	1034 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.112$
$T = 298(2)$ K	$\theta_{\text{max}} = 25.0°$
ω scans	$\theta_{\text{min}} = 2.1°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.986$, $T_{\text{max}} = 0.994$	$k = -22 \rightarrow 22$
10414 measured reflections	$l = -20 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.071$	H-atom parameters constrained
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 3.9683P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1287 reflections	$\Delta\rho_{\text{max}} = 0.24$ e Å^{-3}
179 parameters	$\Delta\rho_{\text{min}} = -0.25$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}*/U_{\text{eq}}$
Mg1	0.3999 (3)	0.08395 (10)	0.18240 (17)	0.0326 (6)

O1A	0.5000	0.0000	0.2501 (4)	0.0333 (17)
O2A	0.2900 (6)	0.0160 (2)	0.1101 (4)	0.0469 (15)
C2B	0.3038 (8)	−0.0453 (3)	0.0872 (4)	0.0298 (16)
O2C	0.4045 (6)	−0.0881 (2)	0.1118 (4)	0.0438 (14)
C2D	0.1915 (12)	−0.0706 (4)	0.0281 (7)	0.073 (3)
H2D1	0.1459	−0.1134	0.0466	0.109*
H2D2	0.2429	−0.0789	−0.0215	0.109*
H2D3	0.1128	−0.0360	0.0207	0.109*
O3A	0.5018 (6)	0.1576 (2)	0.2544 (3)	0.0436 (14)
C3B	0.6049 (8)	0.1524 (4)	0.3047 (5)	0.0383 (18)
O3C	0.6644 (6)	0.0947 (3)	0.3253 (4)	0.0529 (16)
H3CA	0.6183	0.0625	0.3038	0.079*
C3D	0.6620 (11)	0.2178 (4)	0.3447 (6)	0.059 (2)
H3D1	0.7089	0.2479	0.3060	0.089*
H3D2	0.7364	0.2056	0.3845	0.089*
H3D3	0.5771	0.2417	0.3691	0.089*
N4A	0.2875 (7)	0.1689 (3)	0.1191 (4)	0.0374 (16)
C4E	0.1930 (9)	0.1640 (4)	0.0553 (5)	0.044 (2)
H4E	0.1779	0.1237	0.0254	0.053*
C4D	0.1237 (10)	0.2263 (4)	0.0416 (6)	0.056 (2)
H4D	0.0547	0.2370	0.0012	0.067*
N4C	0.1753 (7)	0.2691 (3)	0.0985 (4)	0.0426 (17)
H4CA	0.1477	0.3119	0.1055	0.051*
C4B	0.2761 (9)	0.2343 (4)	0.1422 (5)	0.045 (2)
H4B	0.3318	0.2537	0.1839	0.054*
N5A	0.2107 (6)	0.0828 (3)	0.2699 (4)	0.0400 (16)
C5B	0.0607 (9)	0.0839 (4)	0.2574 (7)	0.054 (2)
H5B	0.0150	0.0823	0.2075	0.065*
N5C	−0.0174 (7)	0.0874 (4)	0.3264 (5)	0.0530 (19)
H5CA	−0.1158	0.0897	0.3314	0.064*
C5E	0.2252 (9)	0.0836 (4)	0.3508 (5)	0.050 (2)
H5E	0.3181	0.0821	0.3782	0.060*
C5D	0.0842 (10)	0.0868 (5)	0.3855 (6)	0.059 (2)
H5D	0.0630	0.0884	0.4396	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0281 (12)	0.0214 (11)	0.0482 (14)	0.0010 (10)	−0.0043 (11)	−0.0019 (13)
O1A	0.027 (4)	0.024 (3)	0.049 (5)	0.003 (3)	0.000	0.000
O2A	0.049 (3)	0.025 (2)	0.067 (4)	0.006 (2)	−0.015 (3)	−0.008 (3)
C2B	0.030 (4)	0.022 (3)	0.037 (4)	−0.001 (3)	0.002 (3)	−0.002 (3)
O2C	0.040 (3)	0.027 (3)	0.064 (4)	0.002 (2)	−0.010 (3)	−0.001 (3)
C2D	0.074 (7)	0.037 (4)	0.106 (8)	0.012 (5)	−0.040 (7)	−0.013 (5)
O3A	0.043 (3)	0.034 (3)	0.054 (4)	−0.001 (2)	−0.014 (3)	−0.003 (3)
C3B	0.030 (4)	0.046 (5)	0.039 (5)	−0.013 (4)	0.004 (4)	−0.004 (4)
O3C	0.040 (3)	0.041 (3)	0.078 (4)	−0.002 (3)	−0.021 (3)	−0.005 (3)
C3D	0.070 (6)	0.056 (5)	0.053 (6)	−0.003 (5)	−0.031 (5)	−0.011 (5)

N4A	0.038 (4)	0.032 (3)	0.042 (4)	0.006 (3)	−0.001 (3)	−0.002 (3)
C4E	0.047 (5)	0.035 (4)	0.051 (5)	0.002 (4)	−0.009 (5)	−0.002 (4)
C4D	0.051 (5)	0.060 (5)	0.057 (6)	0.008 (4)	−0.016 (5)	−0.001 (5)
N4C	0.034 (3)	0.023 (3)	0.071 (5)	0.008 (3)	−0.003 (3)	−0.001 (3)
C4B	0.041 (5)	0.034 (4)	0.060 (5)	0.009 (4)	−0.009 (4)	−0.002 (4)
N5A	0.021 (3)	0.042 (3)	0.057 (5)	0.005 (3)	−0.002 (3)	0.006 (3)
C5B	0.034 (4)	0.048 (5)	0.080 (7)	0.003 (4)	−0.003 (5)	−0.001 (5)
N5C	0.027 (3)	0.057 (4)	0.075 (5)	0.005 (3)	0.008 (4)	−0.002 (4)
C5E	0.027 (4)	0.064 (5)	0.058 (6)	−0.001 (4)	−0.006 (4)	−0.003 (5)
C5D	0.048 (5)	0.068 (6)	0.060 (6)	0.001 (4)	0.010 (5)	−0.009 (5)

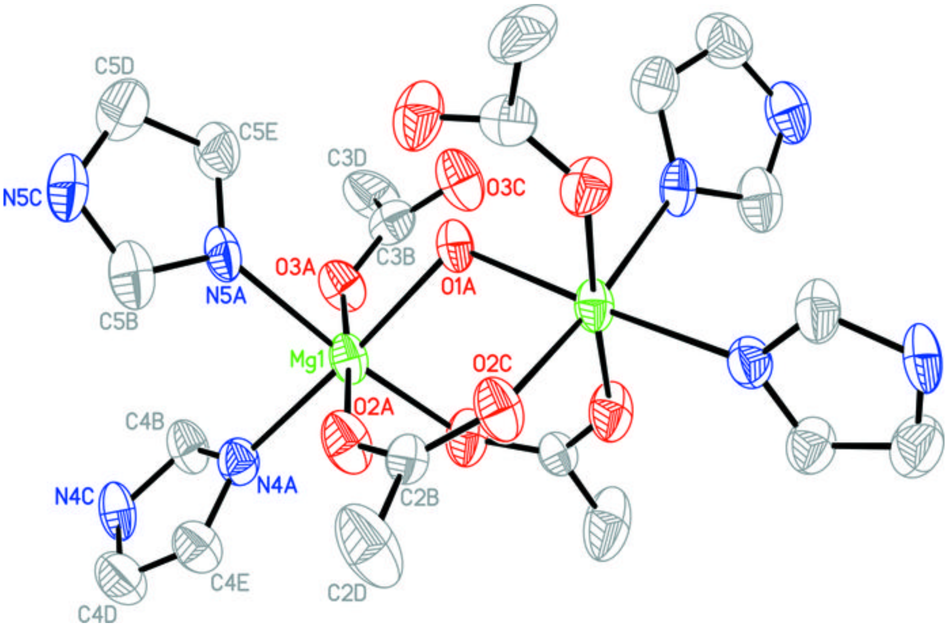
Geometric parameters (Å, °)

Mg1—O2A	2.021 (6)	C3D—H3D2	0.9600
Mg1—O3A	2.058 (6)	C3D—H3D3	0.9600
Mg1—O2C^{i}	2.076 (6)	N4A—C4B	1.312 (9)
Mg1—O1A	2.151 (5)	N4A—C4E	1.355 (10)
Mg1—N4A	2.173 (6)	C4E—C4D	1.354 (10)
Mg1—N5A	2.208 (7)	C4E—H4E	0.9300
Mg1—Mg1^{i}	3.649 (4)	C4D—N4C	1.337 (11)
O1A—Mg1^{i}	2.151 (5)	C4D—H4D	0.9300
O2A—C2B	1.239 (8)	N4C—C4B	1.323 (10)
C2B—O2C	1.267 (8)	N4C—H4CA	0.8600
C2B—C2D	1.475 (11)	C4B—H4B	0.9300
O2C—Mg1^{i}	2.076 (6)	N5A—C5B	1.320 (10)
C2D—H2D1	0.9600	N5A—C5E	1.368 (11)
C2D—H2D2	0.9600	C5B—N5C	1.347 (12)
C2D—H2D3	0.9600	C5B—H5B	0.9300
O3A—C3B	1.237 (9)	N5C—C5D	1.330 (11)
C3B—O3C	1.265 (9)	N5C—H5CA	0.8600
C3B—C3D	1.505 (10)	C5E—C5D	1.359 (12)
O3C—H3CA	0.8200	C5E—H5E	0.9300
C3D—H3D1	0.9600	C5D—H5D	0.9300
O2A—Mg1—O3A	176.5 (2)	C3B—O3C—H3CA	109.5
O2A—Mg1—O2C^{i}	93.8 (2)	C3B—C3D—H3D1	109.5
O3A—Mg1—O2C^{i}	87.6 (2)	C3B—C3D—H3D2	109.5
O2A—Mg1—O1A	91.78 (19)	H3D1—C3D—H3D2	109.5
O3A—Mg1—O1A	91.4 (2)	C3B—C3D—H3D3	109.5
O2C^{i}—Mg1—O1A	90.1 (2)	H3D1—C3D—H3D3	109.5
O2A—Mg1—N4A	88.4 (2)	H3D2—C3D—H3D3	109.5
O3A—Mg1—N4A	88.4 (2)	C4B—N4A—C4E	104.7 (7)
O2C^{i}—Mg1—N4A	93.4 (2)	C4B—N4A—Mg1	126.9 (6)
O1A—Mg1—N4A	176.6 (3)	C4E—N4A—Mg1	127.5 (5)
O2A—Mg1—N5A	92.5 (3)	N4A—C4E—C4D	110.1 (7)
O3A—Mg1—N5A	86.3 (2)	N4A—C4E—H4E	125.0
O2C^{i}—Mg1—N5A	173.0 (3)	C4D—C4E—H4E	125.0
O1A—Mg1—N5A	86.6 (2)	N4C—C4D—C4E	105.5 (7)

N4A—Mg1—N5A	90.0 (2)	N4C—C4D—H4D	127.3
O2A—Mg1—Mg1^{i}	70.15 (14)	C4E—C4D—H4D	127.3
O3A—Mg1—Mg1^{i}	113.34 (17)	C4B—N4C—C4D	108.2 (6)
O2C^{i}—Mg1—Mg1^{i}	69.12 (15)	C4B—N4C—H4CA	125.9
O1A—Mg1—Mg1^{i}	31.98 (19)	C4D—N4C—H4CA	125.9
N4A—Mg1—Mg1^{i}	150.55 (18)	N4A—C4B—N4C	111.4 (7)
N5A—Mg1—Mg1^{i}	110.26 (16)	N4A—C4B—H4B	124.3
Mg1—O1A—Mg1^{i}	116.0 (4)	N4C—C4B—H4B	124.3
C2B—O2A—Mg1	138.5 (5)	C5B—N5A—C5E	104.4 (8)
O2A—C2B—O2C	125.2 (7)	C5B—N5A—Mg1	129.0 (7)
O2A—C2B—C2D	117.1 (6)	C5E—N5A—Mg1	126.5 (5)
O2C—C2B—C2D	117.8 (6)	N5A—C5B—N5C	111.2 (9)
C2B—O2C—Mg1^{i}	136.7 (4)	N5A—C5B—H5B	124.4
C2B—C2D—H2D1	109.5	N5C—C5B—H5B	124.4
C2B—C2D—H2D2	109.5	C5D—N5C—C5B	108.0 (7)
H2D1—C2D—H2D2	109.5	C5D—N5C—H5CA	126.0
C2B—C2D—H2D3	109.5	C5B—N5C—H5CA	126.0
H2D1—C2D—H2D3	109.5	C5D—C5E—N5A	110.2 (8)
H2D2—C2D—H2D3	109.5	C5D—C5E—H5E	124.9
C3B—O3A—Mg1	131.2 (5)	N5A—C5E—H5E	124.9
O3A—C3B—O3C	123.7 (7)	N5C—C5D—C5E	106.2 (8)
O3A—C3B—C3D	118.5 (7)	N5C—C5D—H5D	126.9
O3C—C3B—C3D	117.8 (7)	C5E—C5D—H5D	126.9

Symmetry codes: (i) $-x+1, -y, z$.

Fig. 1


C5D
C5E
N5C
C3D
O3C
C3B
O3A
O1A
N5A
C5B
Mg1
O2C
C4B
O2A
N4A
N4C
C2B
C4E
C2D
C4D