

# Bis(acetylacetonato- $\kappa^2O,O'$ )( $N,N,N',N'$ -tetramethylethylenediamine- $\kappa^2N,N'$ )magnesium(II)

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Received 2 September 2022

Accepted 26 October 2022

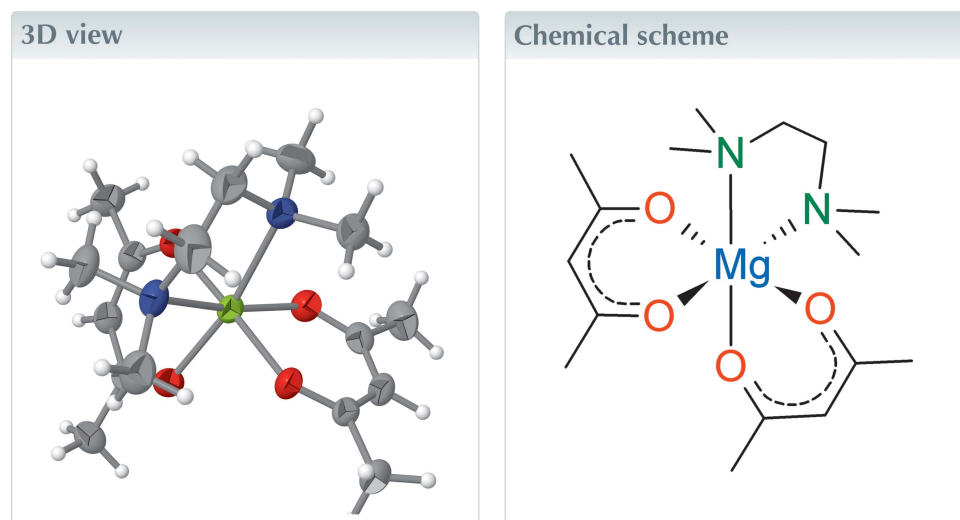
Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; magnesium; acetylacetonate; tetramethylethylenediamine; isotypism.

CCDC reference: 2215481

Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

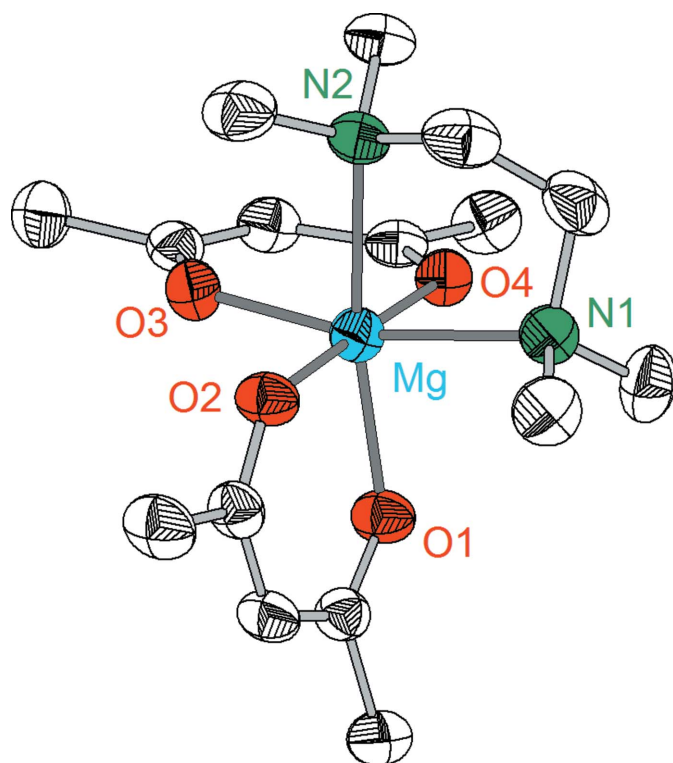
The title complex,  $[\text{Mg}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_6\text{H}_{16}\text{N}_2)]$ , has been synthesized from magnesium acetylacetonate  $[\text{Mg}(\text{acac})_2]$  and tetramethylethylenediamine (TMEDA) in *n*-hexane. The monomeric complex consists of a central magnesium(II) atom, which is surrounded nearly octahedrally by two chelating acetylacetonato ligands and one chelating TMEDA ligand.  $[\text{Mg}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_6\text{H}_{16}\text{N}_2)]$  is isotypic with its Zn analogue.



## Structure description

Complexes of the type  $[\text{M}(\text{acac})_2(\text{TMEDA})]$  (acac is acetylacetonate, TMEDA is tetramethylethylenediamine) are valuable starting materials for the preparation of coordination compounds (Kaschube *et al.*, 1988; Nelkenbaum *et al.*, 2005; Albrecht *et al.*, 2019; Halz *et al.*, 2021). Recently, we reported on the crystal structures of three complexes  $[\text{M}(\text{acac})_2(\text{TMEDA})]$  with  $M = \text{Mn}, \text{Fe}, \text{Zn}$  (Halz *et al.*, 2020), and in the course of these studies we were interested in a structure determination of the magnesium analogue from X-ray data. The crystal structure of  $[\text{Mg}(\text{acac})_2(\text{TMEDA})]$  is isotypic to that of the recently reported zinc(II) representative  $[\text{Zn}(\text{acac})_2(\text{TMEDA})]$  (Halz *et al.*, 2020). This fits well with the observation that the related complex pairs  $[\text{Mg}(\text{acac})_2(2,2'\text{-bipyridine})]/[\text{Zn}(\text{acac})_2(2,2'\text{-bipyridine})]$  and  $[\text{Mg}(\text{acac})_2(1,10\text{-phenanthroline})]/[\text{Zn}(\text{acac})_2(1,10\text{-phenanthroline})]$  are isostructural as well (Brahma *et al.*, 2008, 2013).

The molecular structure of the title compound consists of a magnesium(II) atom, which is nearly octahedrally coordinated by two acetylacetonato ligands and a TMEDA ligand (Fig. 1). The Mg–O distances range from 2.0314 (10)–2.0368 (10) Å, and comparable separations have been observed in  $[\text{Mg}(\text{acac})_2(\text{H}_2\text{O})_2]$  [2.0299 (7)–2.0419 (7) Å; Janczak, 2018]. Currently, the CSD database (Groom *et al.*, 2016) comprises two entries for mixed  $[\text{Mg}(\text{acac})_2L]$  complexes with bidentate N-donor ligands *L*. In the case of *L* = 1,10-phenanthroline, the Mg–O distances are 2.019 (2)–2.049 (2) Å and similar values



**Figure 1**  
The molecular structure of  $[\text{Mg}(\text{acac})_2]\text{TMEDA}$  in the crystal. Displacement ellipsoids are drawn at the 50% probability level; H atoms are omitted for clarity.

[2.020 (3) – 2.044 (4) Å] have been reported for the 2,2'-bipyridine complex (Brahma *et al.*, 2013). Both reference complexes exhibit a slight elongation of the Mg–O bonds *trans* to the acac units [2.038 (4) Å–2.049 (2) Å] compared to the remaining Mg–O bonds *trans* to the nitrogen atoms [2.019 (2)–2.024 (4) Å]. There is no comparable effect in the case of the title compound, and from this aspect  $[\text{Mg}(\text{acac})_2(\text{TMEDA})]$  resembles the isotopic  $[\text{Zn}(\text{acac})_2(\text{TMEDA})]$ . The Mg–N distances in  $[\text{Mg}(\text{acac})_2(\text{TMEDA})]$  [2.3048 (11)–2.3132 (12) Å] are roughly comparable to those in  $[\text{Mg}(\text{thd})_2(\text{TMEDA})]$  [thd = 2,2,6,6-tetramethyl-3,5-heptanedionate, 2.261 (2)–2.292 (3) Å; Hatanpää *et al.*, 2001] and expectedly larger than in the 1,10-phenanthroline [2.238 (2) Å] and 2,2'-bipyridine derivatives [2.232 (4)–2.249 (4) Å].  $[\text{Mg}(\text{hfa})_2(\text{TMEDA})]$  (hfa = 1,1,1,5,5,5-hexafluoropentane-2,4-dionate) and  $[\text{Mg}(\text{tfa})_2(\text{TMEDA})]$  (tfa = 1,1,1-trifluoropentane-2,4-dionate) exhibit shorter Mg–N distances [2.227 (2) Å and 2.262 (2)–2.287 (2) Å, respectively], obviously due to the electron-withdrawing effect of the hfa and tfa ligands (Wang *et al.*, 2005; Vikulova *et al.*, 2017). Regarding the *trans* O–Mg–O and O–Mg–N angles, the deviations from linearity are minor [O2–Mg–O4 = 177.16 (4)°] to medium [O3–Mg–N1 = 166.40 (4)°]. The acac bite angles [86.67 (4) and 86.98 (4)°] are comparable to those found in  $[\text{Mg}(\text{acac})_2(2,2'\text{-bipyridine})]$  and  $[\text{Mg}(\text{acac})_2(1,10\text{-phenanthroline})]$  [87.06 (7)–87.7 (2)°]. The TMEDA bite angle [78.77 (4)°] is slightly smaller. Both the acac–Mg six-membered chelate rings are nearly planar with a maximum

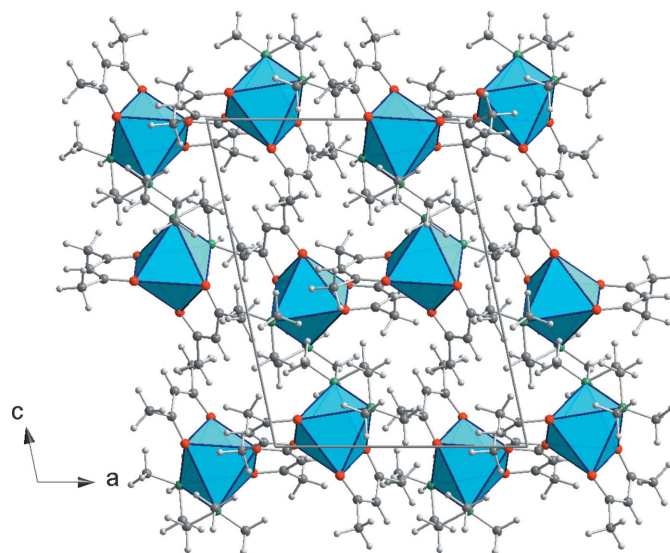
deviation of 0.054 (1) Å from the mean  $\text{C}_3\text{O}_2\text{Mg}$  plane for O2. The five-membered  $\text{C}_2\text{N}_2\text{Mg}$  ring adopts a nearly  $\text{C}_2$ -symmetric twist conformation with the non-crystallographic  $\text{C}_2$  axis running through the center of the C11–C12 bond and the magnesium atom. Fig. 1 displays the  $\text{C}_2\text{N}_2\text{Mg}$  chelate ring in  $\lambda$  conformation. As a result of the centrosymmetric crystal structure, the enantiomeric  $\lambda$  and  $\delta$  conformers are present in an equal ratio.

The crystal packing of  $[\text{Mg}(\text{acac})_2]\text{TMEDA}$  (Fig. 2) is governed by van der Waals interactions and displays no particular supramolecular features.

### Synthesis and crystallization

A mixture of  $[\text{Mg}(\text{acac})_2]$  (2.08 g, 9.35 mmol), TMEDA (2.4 ml, 19 mmol) and 5 ml of *n*-hexane was gently heated to give a clear solution. After cooling down to room temperature, the solution was stored at 248 K to precipitate clear colorless crystals of  $[\text{Mg}(\text{acac})_2(\text{TMEDA})]$ . The crystals were separated by filtration, washed with a few ml of cold *n*-hexane and carefully dried in vacuum. Yield: 2.5 g (83%). On exposure to air the crystals slowly turn turbid due to the loss of TMEDA.

$[\text{Mg}(\text{acac})_2]\text{TMEDA}$  (338.73)  $\text{C}_{16}\text{H}_{30}\text{N}_2\text{O}_4\text{Mg}$ , Mg (complexometric) 7.17%, calc. 7.18%; TGA: 34.33% mass loss between 333 K and 398 K, calc. 34.31% for  $[\text{Mg}(\text{acac})_2(\text{TMEDA})] - \text{TMEDA}$ ,  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 399.962 MHz)  $\delta$  = 5.27 [s, 2H, C(O)CHC(O)], 2.16 (s, 4H,  $\text{Me}_2\text{N}-\text{CH}_2$ ), 2.03 (s, 12H,  $(\text{CH}_3)_2\text{N}$ ), 1.76 [s, 12H,  $\text{CH}_3\text{C}(\text{O})$ ];  $^{13}\text{C}$  NMR ( $\text{C}_6\text{D}_6$ , 100.581 MHz)  $\delta$  = 190.3 [C(O)], 99.2 [C(O)CHC(O)], 56.1 (NCH<sub>2</sub>), 45.9 [(CH<sub>3</sub>)<sub>2</sub>N], 27.7 [C(O)CH<sub>3</sub>] p.p.m.; IR (ATR):  $\nu$  = 2972 w, 2765 w, 1670 w, 1602 m, 1517 s, 1468 s, 1397 vs, 1354 m, 1288 m, 1259 m, 1188 w, 1127 w, 1099 w, 1062 w, 1015 s, 953 w, 919 w, 798 w, 766 w, 660 w, 583 w, 435 w, 405 m, 311 m, 247 m, 220 w  $\text{cm}^{-1}$ .



**Figure 2**  
Packing diagram for  $[\text{Mg}(\text{acac})_2]\text{TMEDA}$  in a view along [010] with a polyhedral representation around the magnesium(II) atom.

Table 1

Experimental details.

Crystal data	
Chemical formula	[Mg(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> )]
<i>M<sub>r</sub></i>	338.73
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	170
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.3036 (3), 14.1907 (5), 13.6808 (7)
$\beta$ (°)	101.967 (2)
<i>V</i> (Å <sup>3</sup> )	1956.87 (14)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.11
Crystal size (mm)	0.50 × 0.30 × 0.30
Data collection	
Diffractometer	Stoe IPDS2
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	10632, 4259, 3462
<i>R</i> <sub>int</sub>	0.027
(sin $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.639
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.036, 0.105, 1.03
No. of reflections	4259
No. of parameters	216
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.21, -0.16

Computer programs: *X-AREA* (Stoe & Cie, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *DIAMOND* (Brandenburg, 2019) and *OLEX2* (Dolomanov *et al.*, 2009).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

## Acknowledgements

We thank Dr Roberto Köferstein for the TGA analysis and Andreas Kiowski for technical support.

## Funding information

We acknowledge the financial support within the funding programme Open Access Publishing by the German Research Foundation (DFG).

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## full crystallographic data

*IUCrData* (2022). 7, x221035 [https://doi.org/10.1107/S2414314622010355]

## Bis(acetylacetonato- $\kappa^2O,O'$ )( $N,N,N',N'$ -tetramethylethylenediamine- $\kappa^2N,N'$ )magnesium(II)

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Bis(acetylacetonato- $\kappa^2O,O'$ )( $N,N,N',N'$ -tetramethylethylenediamine- $\kappa^2N,N'$ )magnesium(II)

### Crystal data

[Mg(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>16</sub>N<sub>2</sub>)]

$M_r = 338.73$

Monoclinic,  $P2_1/n$

$a = 10.3036$  (3) Å

$b = 14.1907$  (5) Å

$c = 13.6808$  (7) Å

$\beta = 101.967$  (2)°

$V = 1956.87$  (14) Å<sup>3</sup>

$Z = 4$

$F(000) = 736$

$D_x = 1.150$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 10102 reflections

$\theta = 1.4$ – $29.6$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 170$  K

Block, colorless

$0.50 \times 0.30 \times 0.30$  mm

### Data collection

Stoe IPDS2

diffractometer

rotation scans

10632 measured reflections

4259 independent reflections

3462 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\text{max}} = 27.0$ °,  $\theta_{\text{min}} = 2.1$ °

$h = -12 \rightarrow 13$

$k = -18 \rightarrow 16$

$l = -17 \rightarrow 17$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.105$

$S = 1.03$

4259 reflections

216 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.3308P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.16$  e Å<sup>-3</sup>

### Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mg	0.73539 (4)	0.26603 (3)	0.54050 (3)	0.03160 (12)
O3	0.57619 (9)	0.17878 (7)	0.50564 (7)	0.0406 (2)
O4	0.61060 (8)	0.36201 (6)	0.58213 (7)	0.0352 (2)
O1	0.73219 (9)	0.33737 (7)	0.41083 (7)	0.0407 (2)
O2	0.85612 (9)	0.17168 (7)	0.49172 (7)	0.0397 (2)
N2	0.78681 (11)	0.19671 (8)	0.69609 (8)	0.0380 (3)
N1	0.91223 (11)	0.35780 (9)	0.61862 (9)	0.0413 (3)
C6	0.36376 (16)	0.11102 (13)	0.48657 (12)	0.0555 (4)
H6A	0.372979	0.084281	0.422318	0.083*
H6B	0.272363	0.132687	0.481885	0.083*
H6C	0.384978	0.062753	0.538676	0.083*
C7	0.45770 (13)	0.19322 (10)	0.51253 (9)	0.0385 (3)
C8	0.40896 (12)	0.27786 (11)	0.54250 (10)	0.0396 (3)
H8	0.316681	0.281565	0.541694	0.048*
C9	0.48651 (12)	0.35783 (9)	0.57373 (9)	0.0342 (3)
C10	0.41890 (14)	0.44581 (11)	0.59948 (12)	0.0466 (3)
H10A	0.477538	0.478764	0.654427	0.070*
H10B	0.336241	0.428760	0.619890	0.070*
H10C	0.398936	0.487131	0.540888	0.070*
C1	0.76348 (16)	0.38372 (11)	0.25150 (11)	0.0487 (3)
H1A	0.670005	0.402333	0.233031	0.073*
H1B	0.790149	0.353958	0.194086	0.073*
H1C	0.818365	0.439616	0.271684	0.073*
C2	0.78188 (12)	0.31474 (10)	0.33739 (9)	0.0369 (3)
C3	0.85356 (14)	0.23238 (10)	0.33053 (10)	0.0415 (3)
H3	0.881122	0.220325	0.269621	0.050*
C4	0.88733 (13)	0.16657 (10)	0.40757 (10)	0.0380 (3)
C5	0.97013 (17)	0.08251 (12)	0.39097 (12)	0.0537 (4)
H5A	1.049281	0.079154	0.444786	0.081*
H5B	0.996978	0.089060	0.326650	0.081*
H5C	0.917846	0.024787	0.390710	0.081*
C12	0.91892 (14)	0.23291 (13)	0.74428 (11)	0.0529 (4)
H12A	0.987902	0.198867	0.717547	0.063*
H12B	0.934479	0.220931	0.817066	0.063*
C11	0.93036 (16)	0.33683 (14)	0.72627 (11)	0.0554 (4)
H11A	0.862464	0.371005	0.754102	0.066*
H11B	1.018785	0.359273	0.761306	0.066*
C15	0.68884 (14)	0.22022 (12)	0.75699 (10)	0.0460 (3)
H15A	0.684183	0.288791	0.764016	0.069*
H15B	0.715659	0.191433	0.823219	0.069*
H15C	0.601543	0.196056	0.724211	0.069*
C16	0.79117 (18)	0.09384 (11)	0.68770 (12)	0.0549 (4)
H16A	0.703083	0.070324	0.655925	0.082*
H16B	0.818003	0.066168	0.754468	0.082*
H16C	0.855325	0.076251	0.647080	0.082*

C13	0.88414 (16)	0.45858 (11)	0.60113 (14)	0.0547 (4)
H13A	0.869596	0.471786	0.529373	0.082*
H13B	0.959599	0.495693	0.636548	0.082*
H13C	0.804472	0.475507	0.625816	0.082*
C14	1.03394 (14)	0.33530 (13)	0.58274 (13)	0.0529 (4)
H14A	1.019513	0.347677	0.510815	0.079*
H14B	1.056192	0.268678	0.595527	0.079*
H14C	1.107062	0.374585	0.617995	0.079*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mg	0.0288 (2)	0.0357 (2)	0.0315 (2)	0.00339 (16)	0.00908 (16)	-0.00113 (16)
O3	0.0387 (5)	0.0404 (5)	0.0423 (5)	-0.0016 (4)	0.0074 (4)	-0.0055 (4)
O4	0.0277 (4)	0.0387 (5)	0.0411 (5)	0.0020 (3)	0.0109 (3)	-0.0018 (4)
O1	0.0453 (5)	0.0420 (5)	0.0373 (5)	0.0097 (4)	0.0144 (4)	0.0037 (4)
O2	0.0423 (5)	0.0423 (5)	0.0376 (5)	0.0097 (4)	0.0152 (4)	0.0014 (4)
N2	0.0360 (5)	0.0453 (6)	0.0335 (5)	0.0063 (5)	0.0090 (4)	0.0023 (5)
N1	0.0303 (5)	0.0505 (7)	0.0442 (6)	-0.0040 (5)	0.0104 (4)	-0.0044 (5)
C6	0.0529 (9)	0.0614 (10)	0.0510 (9)	-0.0206 (8)	0.0077 (7)	-0.0071 (7)
C7	0.0370 (6)	0.0486 (8)	0.0282 (6)	-0.0076 (6)	0.0027 (5)	0.0019 (5)
C8	0.0275 (6)	0.0542 (8)	0.0374 (7)	-0.0013 (6)	0.0070 (5)	0.0019 (6)
C9	0.0310 (6)	0.0435 (7)	0.0296 (6)	0.0057 (5)	0.0097 (4)	0.0053 (5)
C10	0.0383 (7)	0.0497 (8)	0.0563 (9)	0.0104 (6)	0.0202 (6)	0.0028 (7)
C1	0.0573 (9)	0.0501 (9)	0.0401 (7)	-0.0013 (7)	0.0134 (6)	0.0064 (6)
C2	0.0343 (6)	0.0427 (7)	0.0337 (6)	-0.0037 (5)	0.0073 (5)	0.0000 (5)
C3	0.0462 (7)	0.0479 (8)	0.0339 (6)	0.0030 (6)	0.0161 (5)	-0.0031 (6)
C4	0.0362 (6)	0.0405 (7)	0.0391 (7)	0.0021 (5)	0.0119 (5)	-0.0061 (5)
C5	0.0618 (9)	0.0520 (9)	0.0521 (9)	0.0171 (7)	0.0231 (7)	-0.0050 (7)
C12	0.0368 (7)	0.0808 (12)	0.0385 (7)	0.0037 (7)	0.0017 (6)	0.0081 (7)
C11	0.0439 (8)	0.0797 (12)	0.0406 (8)	-0.0160 (8)	0.0043 (6)	-0.0119 (7)
C15	0.0441 (7)	0.0621 (9)	0.0345 (7)	0.0057 (7)	0.0142 (6)	0.0042 (6)
C16	0.0710 (10)	0.0460 (9)	0.0503 (9)	0.0150 (8)	0.0183 (7)	0.0125 (7)
C13	0.0450 (8)	0.0457 (9)	0.0748 (11)	-0.0115 (7)	0.0155 (7)	-0.0107 (7)
C14	0.0304 (6)	0.0688 (10)	0.0617 (9)	-0.0053 (7)	0.0145 (6)	-0.0049 (8)

*Geometric parameters (Å, °)*

Mg—O1	2.0368 (10)	N1—C13	1.469 (2)
Mg—O2	2.0322 (10)	N1—C14	1.4734 (17)
Mg—O3	2.0314 (10)	N1—C11	1.476 (2)
Mg—O4	2.0338 (9)	C6—C7	1.510 (2)
Mg—N1	2.3132 (12)	C7—C8	1.396 (2)
Mg—N2	2.3048 (11)	C8—C9	1.4027 (19)
O3—C7	1.2607 (16)	C9—C10	1.5066 (19)
O4—C9	1.2611 (14)	C1—C2	1.5107 (19)
O1—C2	1.2603 (15)	C2—C3	1.396 (2)
O2—C4	1.2600 (15)	C3—C4	1.397 (2)

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N2—C16	1.466 (2)	C4—C5	1.5109 (19)
N2—C15	1.4741 (16)	C12—C11	1.504 (3)
N2—C12	1.4762 (19)		
O3—Mg—O2	92.34 (4)	C12—N2—Mg	106.14 (9)
O3—Mg—O4	86.98 (4)	C13—N1—C14	108.02 (12)
O2—Mg—O4	177.16 (4)	C13—N1—C11	109.80 (13)
O3—Mg—O1	103.42 (4)	C14—N1—C11	110.39 (12)
O2—Mg—O1	86.67 (4)	C13—N1—Mg	111.29 (9)
O4—Mg—O1	90.80 (4)	C14—N1—Mg	111.55 (9)
O3—Mg—N2	88.65 (4)	C11—N1—Mg	105.79 (9)
O2—Mg—N2	89.02 (4)	O3—C7—C8	125.09 (12)
O4—Mg—N2	93.72 (4)	O3—C7—C6	116.12 (13)
O1—Mg—N2	167.33 (4)	C8—C7—C6	118.79 (13)
O3—Mg—N1	166.40 (4)	C7—C8—C9	124.66 (12)
O2—Mg—N1	92.60 (4)	O4—C9—C8	124.65 (12)
O4—Mg—N1	88.67 (4)	O4—C9—C10	116.68 (12)
O1—Mg—N1	89.51 (4)	C8—C9—C10	118.67 (11)
N2—Mg—N1	78.77 (4)	O1—C2—C3	125.10 (12)
C7—O3—Mg	129.11 (9)	O1—C2—C1	116.66 (12)
C9—O4—Mg	129.11 (9)	C3—C2—C1	118.23 (12)
C2—O1—Mg	129.19 (9)	C2—C3—C4	124.16 (12)
C4—O2—Mg	128.86 (9)	O2—C4—C3	125.45 (12)
C16—N2—C15	107.78 (12)	O2—C4—C5	116.21 (12)
C16—N2—C12	109.95 (12)	C3—C4—C5	118.33 (12)
C15—N2—C12	110.18 (12)	N2—C12—C11	111.38 (12)
C16—N2—Mg	110.95 (9)	N1—C11—C12	111.30 (13)
C15—N2—Mg	111.85 (8)		

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