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Bis[2-(dimethylamino-κN)-α,α-diphenylbenzenemethanolato-κO](tetrahydrofuran-κO)magnesium(II)

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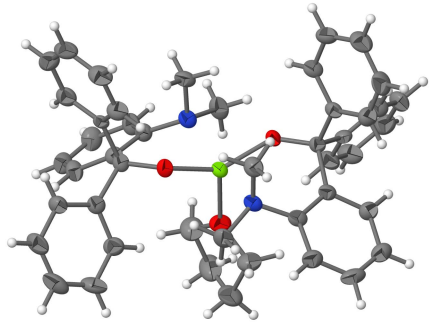
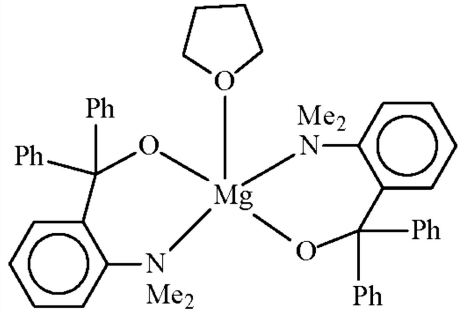
Structural data: full structural data are available from iucrdata.iucr.org

The title magnesium complex, $[Mg(C_{21}H_{20}NO_2)_2(C_4H_8O)]_n$, exhibits two *N*,*O*-bidentate 2-(dimethylamino)-α,α-diphenylbenzenemethanolate ligands, forming two six-membered chelate rings. The distorted square-pyramidal coordination sphere of the Mg^{II} atom is completed by the O atom of a tetrahydrofuran ligand, with its O atom in the apical position. The O and N atoms are in a mutual *trans* arrangement. Except for two C—H$\cdots\pi$ interactions, no significant intermolecular interactions are observed in the crystal.

3D view



Chemical scheme



Structure description

Compounds with *O*,*N*- or *N*,*N*-bidentate functionalities can be reacted with many main-group and transition-metal compounds, in which they act as hemilabile ligands, forming six- or seven-membered chelate rings (Al-Masri *et al.*, 2004*a*). As a continuation of our work on the syntheses and crystal structures of such complexes (Al-Masri *et al.*, 2004*b*), herein the synthesis and molecular and crystal structures of a magnesium(II) complex with two *N*,*O*-chelating ligands, (**I**), are reported.

The crystal structure of complex (**I**) (Fig. 1) exhibits a monomeric molecule with two *N*,*O*-bidentate 2-(dimethylamino)-α,α-diphenylbenzenemethanolate ligands, forming two six-membered chelate rings. The Mg^{II} atom is pentacoordinated by the pair of *N*,*O*-bidentate ligands in a mutual *trans* orientation, and by the O atom of the tetrahydrofuran (THF) molecule. The six-membered chelate rings adopt screw-boat conformations, with puckering parameters (Cremer & Pople, 1975) of Q = 0.694 (5) Å, θ = 109.6 (5)° and φ = 154.4 (5)° for the Mg1/O1/C19/C1/C2/N1 ring, and Q = 0.687 (5) Å, θ = 70.6 (5)° and φ = 28.9 (5)° for the Mg1/N2/C23/C22/C40/O2 ring. The coordination geometry around the Mg atom tends towards square pyramidal, as evidenced by the τ_5 parameter (Addison *et al.*, 1984) of 0.38 (ideal values: τ_5 = 1 for a trigonal bipyramid and 0 for a square pyramid).

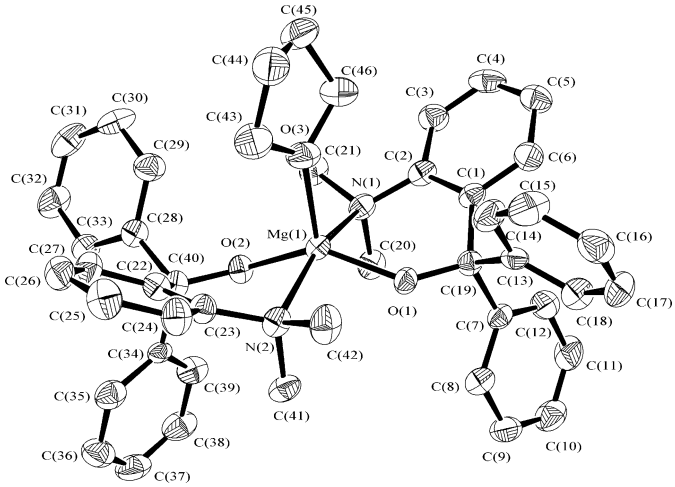


Figure 1
The molecular structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level.

To the best of my knowledge, there is only one other structurally characterized monomeric complex with five-coordinated magnesium(II) and bidentate *N*,*O*-chelating ligands, namely [(^{CMe_2Ph}BTP)$_2$Mg(THF)], (**II**) (Li *et al.*, 2012).

The basal plane in (**I**) is occupied by pairs of N and O atoms from the two *N*,*O*-bidentate ligands (O1, N1, O2 and N2). The Mg^{II} atom is displaced by 0.4931 (19) Å from the basal plane in the direction of the apical O3 atom. The distances between the Mg^{II} atom and basal atoms O1, O2, N1 and N2 are 1.887 (4), 1.891 (4), 2.306 (6) and 2.277 (5) Å, respectively, for (**I**). The corresponding angles of O1—Mg1—N1 = 83.25 (19)°, O1—Mg1—N2 = 89.85 (19)°, O2—Mg1–N1= 90.97 (19)° and O2—Mg1—N2 = 84.29 (19)° and their sum (348.36°; ideal = 360°) confirm the distortion towards trigonal bipyramidal. The angles N2—Mg1—N1 [162.9 (2)°] and O2—Mg1—O1 [140.1 (2)°] are narrower than N1—Mg—N4 [178.22 (8)°] and O1—Mg—O2 [147.42 (8)°] in (**II**).

The Mg—O bonds in (**I**) are slightly shorter than the distances [1.9113 (17) and 1.9099 (16) Å] in (**II**). The apical position being occupied by the O atom of the THF molecule, with an Mg—O3 bond length of 2.095 (4) Å, is somewhat longer than the corresponding Mg—O(THF) bond of 2.0501 (17) Å in (**II**). The Mg—N bond lengths for (**I**) are similar, but are longer than for (**II**) [2.144 (2) and 2.159 (2) Å] (Li *et al.*, 2012) or in other complexes with N-containing ligands, including [$MgBr_2(NHMe_2)_3$] [2.159 (5), 2.177 (3) and 2.177 (3) Å; Vitze *et al.*, 2009], the dimeric complex Mg^{II} [(SalenMe)Mg(OBn)]$_2$ [2.161 (2) and 2.260 (2) Å; Wua *et al.*, 2005], [(*N*,*N*,*O*-tridentate ketiminate ligand)Mg(μ-OBn)]$_2$ [2.123 (3) and 2.262 (3) Å; Tang *et al.*, 2007] and di-μ-chlorido-bis{[*N*,*N*′-dicyclohexyl-*N*″,*N*″-bis(trimethylsilyl)guanidinato-

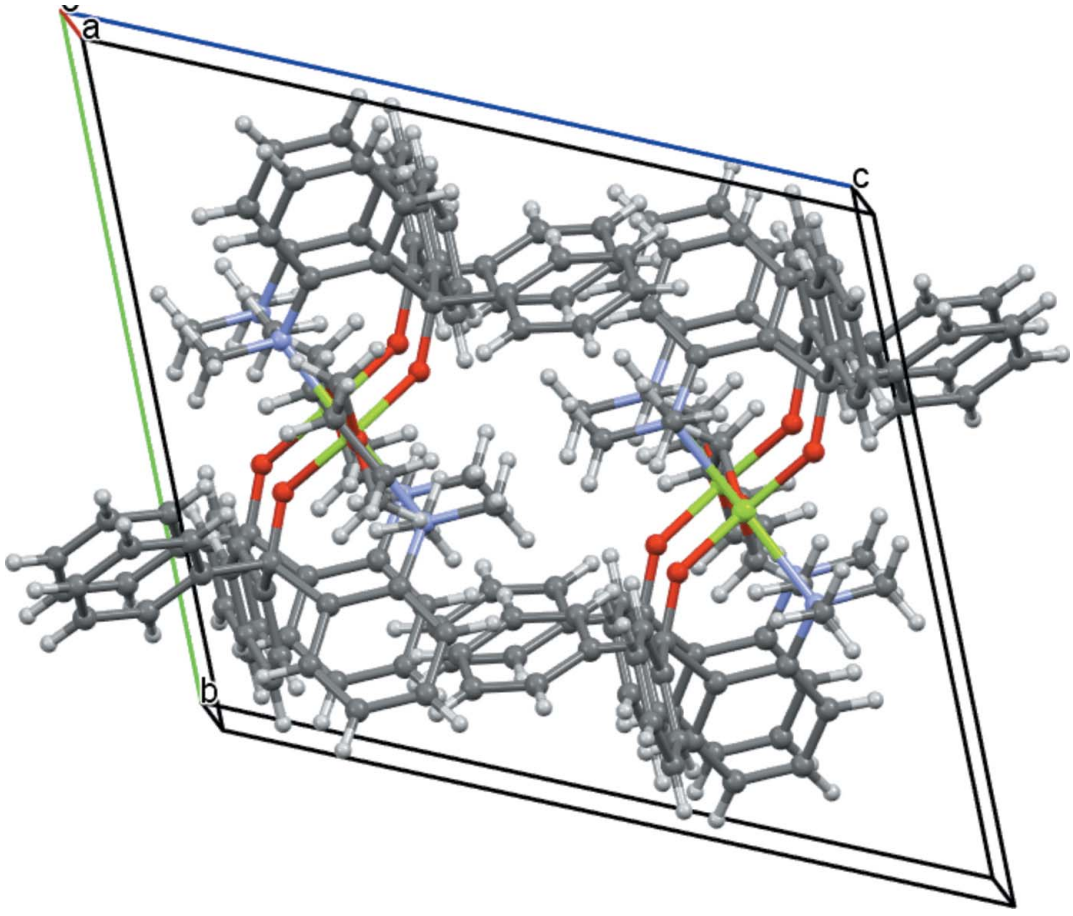


Figure 2
Packing view of the title complex along the *a* axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Mg(C_{21}H_{20}NO_2)_2(C_4H_8O)]$
M_r	701.17
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	208
a, b, c (Å)	9.5014 (15), 13.801 (2), 15.834 (3)
α, β, γ (°)	66.375 (4), 89.911 (4), 81.735 (4)
V (Å^3)	1878.9 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.15 × 0.10 × 0.08
Data collection	
Diffractometer	Bruker SMART APEX area detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.989, 0.993
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6887, 5408, 2783
R_{int}	0.061
θ_{max} (°)	23.3
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.555
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.087, 0.250, 1.09
No. of reflections	5408
No. of parameters	469
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.60, −0.33

Computer programs: *SMART* (Bruker, 2007), *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *ORTEP-3* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

κ^2N,N'](tetrahydrofuran-κO)magnesium(II)} [2.0734 (18) and 2.1247 (17) Å; Cheng, 2011].

Except for two C—H$\cdots Cg$ interactions, namely C20—H20$C\cdots Cg6(-x, -y + 1, -z)$ = 3.871 (8) Å and C41—H41$C\cdots Cg6(-x, -y + 1, -z + 1)$ = 3.790 (8) Å ($Cg6$ and $Cg4$ are the centroids of the C28–C33 and C13–C18 rings, respectively), no other significant intermolecular interactions exist. The packing of the molecules is shown in Fig. 2.

Synthesis and crystallization

A 100 ml Schlenk flask was charged with 1-HOCPh$_2$-2-NMe$_2$C$_6$H$_4$ (0.48 g, 1.6 mmol) and THF (50 ml). (n-Bu)$_2$Mg (0.8 ml, 0.8 mmol) was then added dropwise at 273 K. The solution was warmed to room temperature and left to stir for about 1 h. The solvent was removed and the remaining solid washed with n-hexane. Colourless crystals were obtained from a THF solution at 269 K in 80% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.41 [br, 12H, N(CH$_3$)$_2$], 3.26 (THF), 6.22–7.31 (m, vbr, 28H, C$_6$H$_4$ and C$_6$H$_5$). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 44.4, 45.7 [N(CH$_3$)$_2$], 56.9 (THF), 66.8, 112.5, 113.9, 118.1, 124.9, 127.7, 128.4, 137.1, 145.5, 152.6, 161.7.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x191412 [https://doi.org/10.1107/S2414314619014123]

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Crystal data

$[Mg(C_{21}H_{20}NO_2)_2(C_4H_8O)]$
M_r = 701.17
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.5014 (15) Å
b = 13.801 (2) Å
c = 15.834 (3) Å
α = 66.375 (4)°
β = 89.911 (4)°
γ = 81.735 (4)°
V = 1878.9 (5) Å^3
Z = 2
$F(000)$ = 748
char
D_x = 1.239 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6887 reflections
θ = 1.4–23.3°
μ = 0.09 mm^{-1}
T = 208 K
Plate, colorless
0.15 × 0.10 × 0.08 mm

Data collection

Bruker SMART APEX area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.989, T_{max} = 0.993
6887 measured reflections
5408 independent reflections
2783 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 23.3°, θ_{min} = 1.4°
h = −7→10
k = −15→13
l = −17→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.087
$wR(F^2)$ = 0.250
S = 1.09
5408 reflections
469 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1205P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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.

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.
All H atoms were positioned geometrically (C—H = 0.93–0.97?Å) and refined as riding, with Uiso(H) = 1.2Ueq(C) or 1.5Ueq(methyl C).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mg1	0.1554 (2)	0.50201 (16)	0.24814 (14)	0.0261 (5)
O1	0.1102 (4)	0.3872 (3)	0.3537 (3)	0.0292 (10)
O2	0.0645 (4)	0.6179 (3)	0.1421 (3)	0.0282 (10)
O3	0.3757 (4)	0.5028 (4)	0.2476 (3)	0.0413 (12)
N1	0.1431 (5)	0.3850 (4)	0.1785 (3)	0.0315 (13)
N2	0.0968 (5)	0.6150 (4)	0.3196 (3)	0.0302 (13)
C1	0.2249 (6)	0.2298 (5)	0.3302 (4)	0.0279 (15)
C2	0.2241 (6)	0.2794 (5)	0.2314 (4)	0.0297 (15)
C3	0.3067 (7)	0.2242 (5)	0.1876 (5)	0.0390 (17)
H3	0.3031	0.2540	0.1227	0.047*
C4	0.3934 (7)	0.1279 (6)	0.2344 (5)	0.0437 (19)
H4	0.4499	0.0949	0.2016	0.052*
C5	0.3973 (7)	0.0804 (5)	0.3285 (5)	0.0398 (18)
H5	0.4559	0.0145	0.3613	0.048*
C6	0.3127 (7)	0.1314 (5)	0.3748 (5)	0.0368 (17)
H6	0.3147	0.0979	0.4396	0.044*
C7	−0.0133 (6)	0.2342 (5)	0.4035 (4)	0.0283 (15)
C8	−0.1289 (6)	0.2962 (5)	0.4213 (4)	0.0312 (16)
H8	−0.1177	0.3624	0.4221	0.037*
C9	−0.2602 (7)	0.2618 (6)	0.4378 (5)	0.0417 (18)
H9	−0.3364	0.3052	0.4496	0.050*
C10	−0.2816 (8)	0.1655 (6)	0.4373 (5)	0.048 (2)
H10	−0.3703	0.1419	0.4499	0.058*
C11	−0.1671 (8)	0.1044 (6)	0.4175 (5)	0.048 (2)
H11	−0.1794	0.0391	0.4152	0.057*
C12	−0.0359 (7)	0.1381 (5)	0.4013 (5)	0.0417 (18)
H12	0.0397	0.0950	0.3886	0.050*
C13	0.2103 (6)	0.2382 (5)	0.4881 (4)	0.0279 (15)
C14	0.3345 (7)	0.2805 (5)	0.4934 (5)	0.0404 (18)
H14	0.3685	0.3284	0.4392	0.048*
C15	0.4076 (8)	0.2524 (6)	0.5781 (5)	0.049 (2)
H15	0.4900	0.2816	0.5808	0.058*
C16	0.3590 (8)	0.1814 (6)	0.6583 (5)	0.0460 (19)
H16	0.4086	0.1622	0.7154	0.055*

C17	0.2375 (8)	0.1387 (5)	0.6542 (5)	0.0409 (18)
H17	0.2046	0.0901	0.7084	0.049*
C18	0.1641 (7)	0.1681 (5)	0.5695 (5)	0.0366 (17)
H18	0.0808	0.1394	0.5676	0.044*
C19	0.1316 (6)	0.2769 (5)	0.3901 (4)	0.0265 (15)
C20	−0.0118 (7)	0.3809 (5)	0.1751 (5)	0.0378 (17)
H20A	−0.0631	0.4521	0.1393	0.057*
H20B	−0.0440	0.3547	0.2374	0.057*
H20C	−0.0298	0.3331	0.1465	0.057*
C21	0.1823 (8)	0.4356 (5)	0.0812 (4)	0.0419 (18)
H21A	0.1241	0.5053	0.0505	0.063*
H21B	0.1664	0.3906	0.0494	0.063*
H21C	0.2821	0.4439	0.0802	0.063*
C22	0.1243 (6)	0.7708 (5)	0.1704 (4)	0.0289 (15)
C23	0.1367 (6)	0.7208 (5)	0.2690 (4)	0.0302 (16)
C24	0.1913 (7)	0.7727 (5)	0.3169 (5)	0.0380 (17)
H24	0.1947	0.7413	0.3818	0.046*
C25	0.2409 (7)	0.8686 (5)	0.2738 (5)	0.0435 (19)
H25	0.2771	0.9014	0.3090	0.052*
C26	0.2372 (7)	0.9166 (5)	0.1781 (5)	0.0394 (18)
H26	0.2735	0.9809	0.1477	0.047*
C27	0.1783 (7)	0.8672 (5)	0.1284 (5)	0.0356 (17)
H27	0.1747	0.9001	0.0635	0.043*
C28	0.1133 (7)	0.7659 (5)	0.0112 (4)	0.0310 (16)
C29	0.2492 (7)	0.7159 (5)	0.0031 (5)	0.0405 (18)
H29	0.2995	0.6622	0.0562	0.049*
C30	0.3110 (8)	0.7438 (6)	−0.0809 (5)	0.049 (2)
H30	0.4021	0.7094	−0.0847	0.059*
C31	0.2372 (8)	0.8228 (6)	−0.1596 (5)	0.053 (2)
H31	0.2790	0.8419	−0.2168	0.063*
C32	0.1054 (8)	0.8729 (6)	−0.1549 (5)	0.048 (2)
H32	0.0555	0.9259	−0.2084	0.057*
C33	0.0444 (7)	0.8446 (5)	−0.0691 (4)	0.0363 (17)
H33	−0.0462	0.8803	−0.0661	0.044*
C34	−0.1109 (6)	0.7775 (5)	0.0944 (4)	0.0249 (15)
C35	−0.1616 (7)	0.8754 (5)	0.0983 (5)	0.0394 (18)
H35	−0.0970	0.9143	0.1107	0.047*
C36	−0.3063 (8)	0.9166 (6)	0.0843 (5)	0.047 (2)
H36	−0.3382	0.9823	0.0881	0.056*
C37	−0.4032 (8)	0.8619 (6)	0.0648 (5)	0.050 (2)
H37	−0.5009	0.8897	0.0551	0.060*
C38	−0.3532 (7)	0.7650 (6)	0.0599 (5)	0.047 (2)
H38	−0.4176	0.7266	0.0465	0.057*
C39	−0.2086 (7)	0.7241 (6)	0.0746 (4)	0.0390 (18)
H39	−0.1769	0.6583	0.0709	0.047*
C40	0.0491 (6)	0.7286 (5)	0.1068 (4)	0.0284 (15)
C41	−0.0609 (6)	0.6210 (5)	0.3222 (5)	0.0355 (17)
H41A	−0.0841	0.5497	0.3554	0.053*

H41B	−0.1034	0.6506	0.2596	0.053*
H41C	−0.0977	0.6664	0.3532	0.053*
C42	0.1561 (8)	0.5613 (5)	0.4173 (4)	0.0433 (18)
H42A	0.1259	0.4917	0.4463	0.065*
H42B	0.1215	0.6048	0.4505	0.065*
H42C	0.2593	0.5523	0.4187	0.065*
C43	0.4484 (7)	0.5857 (6)	0.2551 (6)	0.054 (2)
H43A	0.4169	0.6013	0.3079	0.065*
H43B	0.4292	0.6517	0.1988	0.065*
C44	0.6045 (8)	0.5402 (7)	0.2684 (6)	0.065 (3)
H44A	0.6627	0.5971	0.2414	0.078*
H44B	0.6337	0.5003	0.3341	0.078*
C45	0.6175 (8)	0.4679 (7)	0.2189 (6)	0.063 (2)
H45A	0.7014	0.4123	0.2430	0.076*
H45B	0.6240	0.5080	0.1525	0.076*
C46	0.4823 (7)	0.4202 (6)	0.2386 (5)	0.048 (2)
H46A	0.4534	0.4023	0.1879	0.057*
H46B	0.4951	0.3551	0.2958	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0268 (12)	0.0277 (11)	0.0243 (12)	−0.0074 (9)	0.0041 (9)	−0.0102 (9)
O1	0.037 (3)	0.025 (2)	0.023 (2)	−0.0056 (19)	0.0079 (19)	−0.0076 (19)
O2	0.036 (3)	0.028 (2)	0.020 (2)	−0.0043 (19)	−0.0021 (19)	−0.0098 (19)
O3	0.027 (3)	0.048 (3)	0.049 (3)	−0.007 (2)	0.006 (2)	−0.020 (2)
N1	0.036 (3)	0.037 (3)	0.022 (3)	−0.008 (3)	0.006 (2)	−0.012 (3)
N2	0.036 (3)	0.034 (3)	0.024 (3)	−0.009 (2)	0.002 (2)	−0.013 (3)
C1	0.030 (4)	0.030 (4)	0.030 (4)	−0.011 (3)	0.008 (3)	−0.016 (3)
C2	0.034 (4)	0.036 (4)	0.028 (4)	−0.011 (3)	0.006 (3)	−0.020 (3)
C3	0.040 (4)	0.042 (4)	0.040 (4)	−0.005 (3)	0.007 (3)	−0.021 (4)
C4	0.032 (4)	0.054 (5)	0.062 (6)	−0.007 (4)	0.013 (4)	−0.041 (4)
C5	0.038 (4)	0.039 (4)	0.048 (5)	−0.002 (3)	0.003 (4)	−0.024 (4)
C6	0.042 (4)	0.034 (4)	0.038 (4)	−0.005 (3)	0.007 (3)	−0.018 (3)
C7	0.030 (4)	0.033 (4)	0.021 (4)	−0.007 (3)	0.004 (3)	−0.009 (3)
C8	0.034 (4)	0.039 (4)	0.028 (4)	−0.013 (3)	0.004 (3)	−0.019 (3)
C9	0.035 (4)	0.051 (5)	0.039 (5)	−0.004 (3)	0.010 (3)	−0.018 (4)
C10	0.036 (4)	0.057 (5)	0.048 (5)	−0.017 (4)	0.006 (4)	−0.013 (4)
C11	0.048 (5)	0.035 (4)	0.060 (6)	−0.022 (4)	0.005 (4)	−0.015 (4)
C12	0.045 (5)	0.035 (4)	0.047 (5)	−0.007 (3)	0.010 (4)	−0.018 (4)
C13	0.024 (4)	0.031 (4)	0.029 (4)	0.000 (3)	0.006 (3)	−0.014 (3)
C14	0.042 (4)	0.047 (4)	0.027 (4)	−0.009 (3)	0.007 (3)	−0.009 (3)
C15	0.037 (4)	0.071 (5)	0.037 (5)	−0.010 (4)	0.002 (4)	−0.021 (4)
C16	0.047 (5)	0.050 (5)	0.036 (5)	0.009 (4)	−0.002 (4)	−0.017 (4)
C17	0.051 (5)	0.045 (4)	0.022 (4)	−0.008 (4)	0.005 (3)	−0.008 (3)
C18	0.040 (4)	0.040 (4)	0.033 (4)	−0.009 (3)	0.003 (3)	−0.018 (3)
C19	0.030 (4)	0.028 (4)	0.022 (4)	−0.005 (3)	0.003 (3)	−0.011 (3)
C20	0.039 (4)	0.041 (4)	0.033 (4)	−0.009 (3)	0.000 (3)	−0.013 (3)

C21	0.059 (5)	0.043 (4)	0.025 (4)	−0.006 (3)	0.011 (3)	−0.016 (3)
C22	0.029 (4)	0.031 (4)	0.027 (4)	−0.001 (3)	−0.003 (3)	−0.013 (3)
C23	0.034 (4)	0.029 (4)	0.030 (4)	−0.007 (3)	0.002 (3)	−0.013 (3)
C24	0.047 (4)	0.035 (4)	0.029 (4)	−0.007 (3)	−0.004 (3)	−0.010 (3)
C25	0.048 (5)	0.042 (4)	0.046 (5)	−0.012 (4)	−0.007 (4)	−0.022 (4)
C26	0.029 (4)	0.032 (4)	0.056 (5)	−0.011 (3)	−0.002 (3)	−0.016 (4)
C27	0.036 (4)	0.032 (4)	0.036 (4)	−0.011 (3)	−0.002 (3)	−0.009 (3)
C28	0.035 (4)	0.034 (4)	0.027 (4)	−0.007 (3)	0.001 (3)	−0.014 (3)
C29	0.035 (4)	0.047 (4)	0.035 (4)	−0.001 (3)	0.002 (3)	−0.014 (4)
C30	0.033 (4)	0.073 (6)	0.047 (5)	−0.017 (4)	0.017 (4)	−0.027 (4)
C31	0.061 (6)	0.072 (6)	0.033 (5)	−0.032 (5)	0.018 (4)	−0.023 (4)
C32	0.051 (5)	0.059 (5)	0.023 (4)	−0.011 (4)	0.003 (3)	−0.005 (4)
C33	0.042 (4)	0.038 (4)	0.027 (4)	−0.005 (3)	0.007 (3)	−0.012 (3)
C34	0.024 (3)	0.030 (4)	0.016 (3)	−0.002 (3)	0.005 (3)	−0.006 (3)
C35	0.040 (5)	0.046 (4)	0.029 (4)	−0.007 (4)	0.004 (3)	−0.012 (3)
C36	0.046 (5)	0.048 (5)	0.036 (5)	0.008 (4)	0.003 (4)	−0.012 (4)
C37	0.029 (4)	0.067 (6)	0.039 (5)	0.003 (4)	0.005 (3)	−0.009 (4)
C38	0.030 (4)	0.067 (5)	0.040 (5)	−0.009 (4)	−0.001 (3)	−0.016 (4)
C39	0.034 (4)	0.049 (4)	0.033 (4)	−0.006 (3)	0.000 (3)	−0.016 (4)
C40	0.032 (4)	0.029 (4)	0.025 (4)	−0.007 (3)	−0.001 (3)	−0.010 (3)
C41	0.037 (4)	0.044 (4)	0.034 (4)	−0.014 (3)	0.013 (3)	−0.021 (3)
C42	0.065 (5)	0.042 (4)	0.022 (4)	−0.010 (4)	0.001 (3)	−0.012 (3)
C43	0.037 (5)	0.056 (5)	0.067 (6)	−0.011 (4)	−0.002 (4)	−0.021 (4)
C44	0.036 (5)	0.058 (5)	0.079 (7)	−0.009 (4)	−0.006 (4)	−0.004 (5)
C45	0.036 (5)	0.069 (6)	0.066 (6)	−0.011 (4)	0.014 (4)	−0.008 (5)
C46	0.032 (4)	0.058 (5)	0.055 (5)	−0.005 (4)	0.004 (4)	−0.026 (4)

Geometric parameters (Å, º)

Mg1—O1	1.887 (4)	C21—H21B	0.9700
Mg1—O2	1.891 (4)	C21—H21C	0.9700
Mg1—O3	2.095 (4)	C22—C27	1.401 (8)
Mg1—N2	2.277 (5)	C22—C23	1.429 (8)
Mg1—N1	2.306 (6)	C22—C40	1.566 (9)
O1—C19	1.378 (7)	C23—C24	1.378 (9)
O2—C40	1.386 (7)	C24—C25	1.376 (9)
O3—C43	1.461 (8)	C24—H24	0.9400
O3—C46	1.464 (8)	C25—C26	1.387 (10)
N1—C2	1.456 (8)	C25—H25	0.9400
N1—C20	1.484 (8)	C26—C27	1.393 (9)
N1—C21	1.486 (8)	C26—H26	0.9400
N2—C23	1.462 (7)	C27—H27	0.9400
N2—C41	1.490 (7)	C28—C33	1.384 (9)
N2—C42	1.492 (8)	C28—C29	1.405 (9)
C1—C6	1.396 (9)	C28—C40	1.547 (9)
C1—C2	1.433 (9)	C29—C30	1.383 (10)
C1—C19	1.560 (8)	C29—H29	0.9400
C2—C3	1.389 (9)	C30—C31	1.389 (10)

C3—C4	1.375 (9)	C30—H30	0.9400
C3—H3	0.9400	C31—C32	1.358 (10)
C4—C5	1.365 (10)	C31—H31	0.9400
C4—H4	0.9400	C32—C33	1.403 (9)
C5—C6	1.388 (9)	C32—H32	0.9400
C5—H5	0.9400	C33—H33	0.9400
C6—H6	0.9400	C34—C39	1.373 (9)
C7—C12	1.387 (9)	C34—C35	1.393 (9)
C7—C8	1.393 (8)	C34—C40	1.550 (8)
C7—C19	1.556 (8)	C35—C36	1.392 (9)
C8—C9	1.386 (9)	C35—H35	0.9400
C8—H8	0.9400	C36—C37	1.377 (10)
C9—C10	1.375 (9)	C36—H36	0.9400
C9—H9	0.9400	C37—C38	1.387 (10)
C10—C11	1.393 (10)	C37—H37	0.9400
C10—H10	0.9400	C38—C39	1.391 (9)
C11—C12	1.381 (9)	C38—H38	0.9400
C11—H11	0.9400	C39—H39	0.9400
C12—H12	0.9400	C41—H41A	0.9700
C13—C18	1.382 (9)	C41—H41B	0.9700
C13—C14	1.407 (9)	C41—H41C	0.9700
C13—C19	1.575 (9)	C42—H42A	0.9700
C14—C15	1.393 (9)	C42—H42B	0.9700
C14—H14	0.9400	C42—H42C	0.9700
C15—C16	1.384 (9)	C43—C44	1.505 (10)
C15—H15	0.9400	C43—H43A	0.9800
C16—C17	1.382 (9)	C43—H43B	0.9800
C16—H16	0.9400	C44—C45	1.489 (12)
C17—C18	1.390 (9)	C44—H44A	0.9800
C17—H17	0.9400	C44—H44B	0.9800
C18—H18	0.9400	C45—C46	1.503 (9)
C20—H20A	0.9700	C45—H45A	0.9800
C20—H20B	0.9700	C45—H45B	0.9800
C20—H20C	0.9700	C46—H46A	0.9800
C21—H21A	0.9700	C46—H46B	0.9800

O1—Mg1—O2	140.1 (2)	H21B—C21—H21C	109.5
O1—Mg1—O3	110.6 (2)	C27—C22—C23	116.9 (6)
O2—Mg1—O3	109.3 (2)	C27—C22—C40	118.1 (5)
O1—Mg1—N2	89.85 (19)	C23—C22—C40	125.0 (5)
O2—Mg1—N2	84.29 (19)	C24—C23—C22	118.9 (6)
O3—Mg1—N2	98.27 (19)	C24—C23—N2	119.6 (6)
O1—Mg1—N1	83.25 (19)	C22—C23—N2	121.4 (5)
O2—Mg1—N1	90.97 (19)	C25—C24—C23	122.8 (7)
O3—Mg1—N1	98.81 (19)	C25—C24—H24	118.6
N2—Mg1—N1	162.9 (2)	C23—C24—H24	118.6
C19—O1—Mg1	138.6 (4)	C24—C25—C26	119.8 (6)
C40—O2—Mg1	136.4 (4)	C24—C25—H25	120.1

C43—O3—C46	108.7 (5)	C26—C25—H25	120.1
C43—O3—Mg1	126.0 (4)	C25—C26—C27	118.3 (6)
C46—O3—Mg1	125.3 (4)	C25—C26—H26	120.8
C2—N1—C20	111.2 (5)	C27—C26—H26	120.8
C2—N1—C21	114.3 (5)	C26—C27—C22	123.1 (6)
C20—N1—C21	106.7 (5)	C26—C27—H27	118.4
C2—N1—Mg1	112.5 (4)	C22—C27—H27	118.4
C20—N1—Mg1	102.3 (4)	C33—C28—C29	116.7 (6)
C21—N1—Mg1	109.0 (4)	C33—C28—C40	124.4 (6)
C23—N2—C41	111.3 (5)	C29—C28—C40	118.9 (5)
C23—N2—C42	114.0 (5)	C30—C29—C28	121.7 (6)
C41—N2—C42	106.7 (5)	C30—C29—H29	119.2
C23—N2—Mg1	112.8 (4)	C28—C29—H29	119.2
C41—N2—Mg1	102.3 (3)	C29—C30—C31	119.5 (7)
C42—N2—Mg1	108.8 (4)	C29—C30—H30	120.2
C6—C1—C2	117.2 (6)	C31—C30—H30	120.2
C6—C1—C19	118.3 (5)	C32—C31—C30	120.7 (7)
C2—C1—C19	124.5 (5)	C32—C31—H31	119.7
C3—C2—C1	117.6 (6)	C30—C31—H31	119.7
C3—C2—N1	120.7 (6)	C31—C32—C33	119.3 (7)
C1—C2—N1	121.7 (5)	C31—C32—H32	120.4
C4—C3—C2	123.2 (7)	C33—C32—H32	120.4
C4—C3—H3	118.4	C28—C33—C32	122.2 (7)
C2—C3—H3	118.4	C28—C33—H33	118.9
C5—C4—C3	119.9 (6)	C32—C33—H33	118.9
C5—C4—H4	120.1	C39—C34—C35	117.5 (6)
C3—C4—H4	120.1	C39—C34—C40	118.7 (6)
C4—C5—C6	118.6 (7)	C35—C34—C40	123.8 (6)
C4—C5—H5	120.7	C36—C35—C34	121.2 (7)
C6—C5—H5	120.7	C36—C35—H35	119.4
C5—C6—C1	123.4 (7)	C34—C35—H35	119.4
C5—C6—H6	118.3	C37—C36—C35	120.7 (7)
C1—C6—H6	118.3	C37—C36—H36	119.7
C12—C7—C8	117.4 (6)	C35—C36—H36	119.7
C12—C7—C19	125.3 (6)	C36—C37—C38	118.5 (7)
C8—C7—C19	117.4 (5)	C36—C37—H37	120.8
C9—C8—C7	121.0 (6)	C38—C37—H37	120.8
C9—C8—H8	119.5	C37—C38—C39	120.5 (7)
C7—C8—H8	119.5	C37—C38—H38	119.8
C10—C9—C8	121.6 (6)	C39—C38—H38	119.8
C10—C9—H9	119.2	C34—C39—C38	121.7 (7)
C8—C9—H9	119.2	C34—C39—H39	119.2
C9—C10—C11	117.6 (6)	C38—C39—H39	119.2
C9—C10—H10	121.2	O2—C40—C28	106.9 (5)
C11—C10—H10	121.2	O2—C40—C34	110.3 (5)
C12—C11—C10	121.1 (7)	C28—C40—C34	109.0 (5)
C12—C11—H11	119.5	O2—C40—C22	113.1 (5)
C10—C11—H11	119.5	C28—C40—C22	110.0 (5)

C11—C12—C7	121.4 (6)	C34—C40—C22	107.4 (5)
C11—C12—H12	119.3	N2—C41—H41A	109.5
C7—C12—H12	119.3	N2—C41—H41B	109.5
C18—C13—C14	117.7 (6)	H41A—C41—H41B	109.5
C18—C13—C19	124.8 (6)	N2—C41—H41C	109.5
C14—C13—C19	117.5 (5)	H41A—C41—H41C	109.5
C15—C14—C13	120.7 (6)	H41B—C41—H41C	109.5
C15—C14—H14	119.6	N2—C42—H42A	109.5
C13—C14—H14	119.6	N2—C42—H42B	109.5
C16—C15—C14	120.1 (7)	H42A—C42—H42B	109.5
C16—C15—H15	119.9	N2—C42—H42C	109.5
C14—C15—H15	119.9	H42A—C42—H42C	109.5
C17—C16—C15	119.8 (7)	H42B—C42—H42C	109.5
C17—C16—H16	120.1	O3—C43—C44	105.3 (6)
C15—C16—H16	120.1	O3—C43—H43A	110.7
C16—C17—C18	119.8 (7)	C44—C43—H43A	110.7
C16—C17—H17	120.1	O3—C43—H43B	110.7
C18—C17—H17	120.1	C44—C43—H43B	110.7
C13—C18—C17	121.8 (6)	H43A—C43—H43B	108.8
C13—C18—H18	119.1	C45—C44—C43	103.7 (7)
C17—C18—H18	119.1	C45—C44—H44A	111.0
O1—C19—C7	110.7 (5)	C43—C44—H44A	111.0
O1—C19—C1	113.0 (5)	C45—C44—H44B	111.0
C7—C19—C1	109.6 (5)	C43—C44—H44B	111.0
O1—C19—C13	106.3 (5)	H44A—C44—H44B	109.0
C7—C19—C13	108.0 (5)	C44—C45—C46	103.2 (6)
C1—C19—C13	109.0 (5)	C44—C45—H45A	111.1
N1—C20—H20A	109.5	C46—C45—H45A	111.1
N1—C20—H20B	109.5	C44—C45—H45B	111.1
H20A—C20—H20B	109.5	C46—C45—H45B	111.1
N1—C20—H20C	109.5	H45A—C45—H45B	109.1
H20A—C20—H20C	109.5	O3—C46—C45	105.4 (6)
H20B—C20—H20C	109.5	O3—C46—H46A	110.7
N1—C21—H21A	109.5	C45—C46—H46A	110.7
N1—C21—H21B	109.5	O3—C46—H46B	110.7
H21A—C21—H21B	109.5	C45—C46—H46B	110.7
N1—C21—H21C	109.5	H46A—C46—H46B	108.8
H21A—C21—H21C	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20*C*···O1	0.97	2.57	3.095 (8)	114
C21—H21*A*···O2	0.97	2.53	3.105 (8)	118
C41—H41*C*···O2	0.97	2.58	3.103 (8)	114
C42—H42*A*···O1	0.97	2.46	3.037 (8)	118