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# Bis[(1*Z*,3*Z*)-1,3-bis(4-fluorophenyl)-*N*,*N*′-diphenylpropanediiminato]magnesium(II)

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.041
*wR* factor = 0.113
Data-to-parameter ratio = 15.0

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

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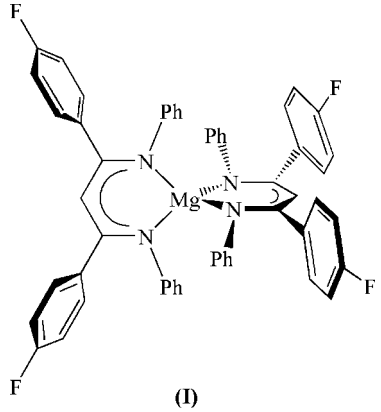
In the title complex, $[Mg(C_{27}H_{19}F_2N_2)_2]$, the $Mg^{II}$ atom, lying on a crystallographic twofold rotation axis, is tetrahedrally coordinated by four N atoms from two diiminate ligands.

## Comment

Over the past two decades, significant advances have been made in the development of biocompatible and biodegradable materials for biomedical applications. Among biodegradable polymers, the aliphatic polyesters, such as poly(ε-caprolactone) (PCL; Endo *et al.*, 1987), poly(lactide) (PLA; Chamberlain *et al.*, 1999) and their copolymers, are especially interesting for their applications in the medical field as biodegradable surgical sutures or as a delivery medium for controlled release of drugs (Ni & Yu, 1998). Therefore, there has been increasing interest in the development of efficient catalytic systems for the preparation of PLA and PCL. The major polymerization method used to synthesize these polymers has been the ring-opening polymerization (ROP) of lactones/lactides and functionally related compounds. Aluminium alkoxides (Duda *et al.*, 1990), stannous (Sawhney *et al.*, 1993), yttrium (Stevels *et al.*, 1996) and trivalent lanthanide derivatives (Simic *et al.*, 1997) have been reported to be effective initiators for ROP of lactones/lactides, giving polymers with both high molecular weights and high yields. However, the cytotoxicity and difficulties in removal of the catalyst from the resulting polymer have limited their utilization when a medical-grade polymer is required. An important task for developing new catalytic systems is to make the catalyst more compatible with the purpose of biomedical application. Lithium- (Ko & Lin, 2001), magnesium- (Shueh *et al.*, 2004; Chamberlain *et al.*, 2001), calcium- (Chisholm *et al.*, 2003) and zinc-based (Chamberlain *et al.*, 2001; Rieth *et al.*, 2002) initiator systems seem to be active and to be suited for this purpose owing to their low toxicity and high activity.




(I)

In the title mononuclear magnesium(II) compound, (I), the $Mg^{II}$ atom is coordinated by four N atoms from two diiminato ligands, forming a distorted tetrahedral geometry (Fig. 1). The $Mg^{II}$ atom lies on a twofold rotation axis. The Mg—N bond distances (Table 1) are somewhat shorter than those [2.123 (3) and 2.124 (3) Å] of the similar complex $[Mg(BDI\text{-}\mathbf{1})(O\mathit{i}Pr)]_2$ {BDI-**1** = 2-[(2,6-diisopropylphenyl)amido]-4-[(2,6-diisopropylphenyl)imino]-2-pentene; O*i*Pr = isopropoxide; Chamberlain *et al.*, 2001}.

## Experimental

The title compound was prepared by the reaction of (1*Z*,3*Z*)-1,3-bis(4-fluorophenyl)-*N*,*N*′-diphenylpropanediimine (0.82 g, 2.0 mmol) with dibutylmagnesium (1.1 ml of 1.0 *M* heptane solution, 1.1 mmol) in hexane (20 ml) at 298 K. The mixture was stirred for 4 h and was evaporated to dryness under vacuum. The residue was extracted with hexane (30 ml), and the extract was then concentrated to *ca* 15 ml. Yellow crystals were obtained after 16 h (yield 0.55 g, 85%).

*Crystal data*

$[Mg(C_{27}H_{19}F_2N_2)_2]$
$M_r$ = 843.19
Monoclinic, $C2/c$
$a$ = 22.0564 (15) Å
$b$ = 10.5743 (7) Å
$c$ = 19.4356 (13) Å
$\beta$ = 106.201 (1)°
$V$ = 4353.0 (5) Å$^3$
$Z$ = 4
$D_x$ = 1.287 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 298 (2) K
Parallelepiped, yellow
0.37 × 0.34 × 0.26 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
12188 measured reflections
4270 independent reflections
2339 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046
$\theta_{max}$ = 26.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
$S$ = 0.91
4270 reflections
285 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Mg—N1 | 2.0266 (17) | N1—C1 | 1.341 (2) |
| Mg—N2 | 2.0439 (15) | N2—C3 | 1.333 (2) |
| F1—C13 | 1.359 (2) | C1—C2 | 1.402 (3) |
| F2—C19 | 1.358 (2) | C2—C3 | 1.404 (3) |
| | | | |
| N1—Mg—N1$^{i}$ | 118.76 (10) | N1—Mg—N2$^{i}$ | 114.47 (6) |
| N1—Mg—N2 | 92.91 (6) | N2—Mg—N2$^{i}$ | 125.67 (10) |

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and constrained to ride on their parent atoms with $U_{iso}$(H) = 1.2$U_{eq}$(C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

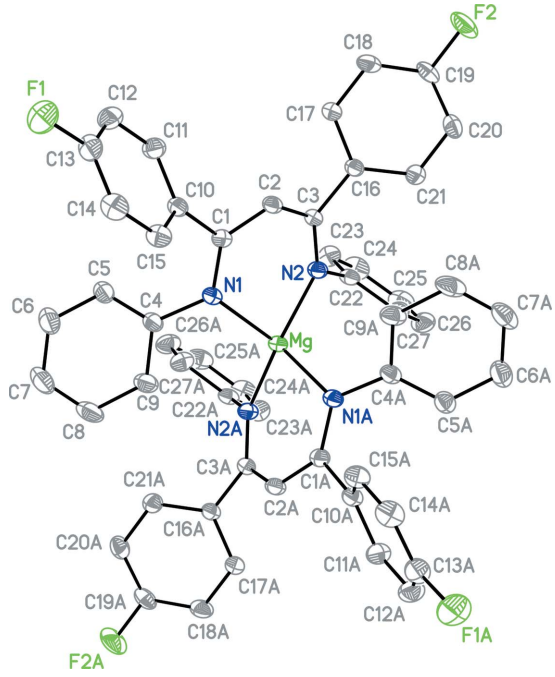



**Figure 1**
A view of the molecular structure of (I) with displacement ellipsoids shown at the 20% probability level. All the H atoms have been omitted for clarity. The suffix A corresponds to symmetry code (i) in Table 1.

Financial support from the National Science Council of the Republic of China is gratefully acknowledged. Helpful comments from the reviewers are also greatly appreciated.

## References

Bruker (1999). *SMART* (Version 5.0), *SAINT* (Version 5.0) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Chamberlain, B. M., Cheng, M., Moore, D. R., Ovitt, T. M., Lobkovsky, E. B. & Coates, G. W. (2001). *J. Am. Chem. Soc.* **123**, 3229–3238.
Chamberlain, B. M., Sun, Y., Hagadorn, J. R., Hemmesch, E. W., Young, V. G. Jr, Pink, M., Hillmyer, M. A. & Tolman, W. B. (1999). *Macromolecules*, **32**, 2400–2402.
Chisholm, M. H., Gallucci, J. & Phomphrai, K. (2003). *Chem. Commun.* pp. 48–49.
Duda, A., Florjanczyk, Z., Hofman, A., Slomkowski, S. & Penczek, S. (1990). *Macromolecules*, **23**, 1640–1646.
Endo, M., Aida, T. & Inoue, S. (1987). *Macromolecules*, **20**, 2982–2988.
Ko, B.-T. & Lin, C.-C. (2001). *J. Am. Chem. Soc.* **123**, 7973–7977.
Ni, Q. & Yu, L. (1998). *J. Am. Chem. Soc.* **120**, 1645–1646.
Rieth, L. R., Moore, D. R., Lobkovsky, E. B. & Coates, G. W. (2002). *J. Am. Chem. Soc.* **124**, 15239–15248.
Sawhney, A., Pathak, C. P. & Hubbell, J. A. (1993). *Macromolecules*, **26**, 581–587.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shueh, M.-L., Wang, Y.-S., Huang, B.-H., Kuo, C.-Y. & Lin, C.-C. (2004). *Macromolecules*, **37**, 5155–5162.
Simic, V., Spassky, N. & Hubert-Pfalzgraf, I. G. (1997). *Macromolecules*, **30**, 7338–7340.
Stevels, W. M., Ankone, M. T., Dijkstra, P. J. & Feijen, J. (1996). *Macromolecules*, **29**, 3332–3333.

# supporting information

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## S1. Comment

Over the past two decades, significant advances have been made in the development of biocompatible and biodegradable materials for biomedical applications. Among biodegradable polymers, the aliphatic polyesters, such as poly(ε-caprolactone) (PCL; Endo *et al.*, 1987), poly(lactide) (PLA; Chamberlain *et al.*, 1999) and their copolymers, are especially interested for their applications in the medical field as biodegradable surgical sutures or as a delivery medium for controlled release of drugs (Ni & Yu, 1998). Therefore, there has been increasing interest in the development of efficient catalytic systems for the preparation of PLA and PCL. The major polymerization method used to synthesize these polymers has been the ring-opening polymerization (ROP) of lactones/lactides and functionally related compounds. Aluminium alkoxides (Duda *et al.*, 1990), stannous (Sawhney *et al.*, 1993), yttrium (Stevels *et al.*, 1996) and trivalent lanthanide derivatives (Simic *et al.*, 1997) have been reported to be effective initiators that initiate ROP of lactones/lactides giving polymers with both high molecular weights and high yields. However, the cytotoxicity and difficulties in removal of the catalyst from the resulting polymer have limited their utilization when a medical-grade polymer is required. An important task for developing new catalytic systems is to make the catalyst more compatible with the purpose of biomedical application. Lithium- (Ko & Lin, 2001), magnesium- (Shueh *et al.*, 2004; Chamberlain *et al.*, 2001), calcium- (Chisholm *et al.*, 2003) and zinc-based (Chamberlain *et al.*, 2001; Rieth *et al.*, 2002) initiator systems seem to be active and suited for this purpose owing to their low toxicity and high activity.

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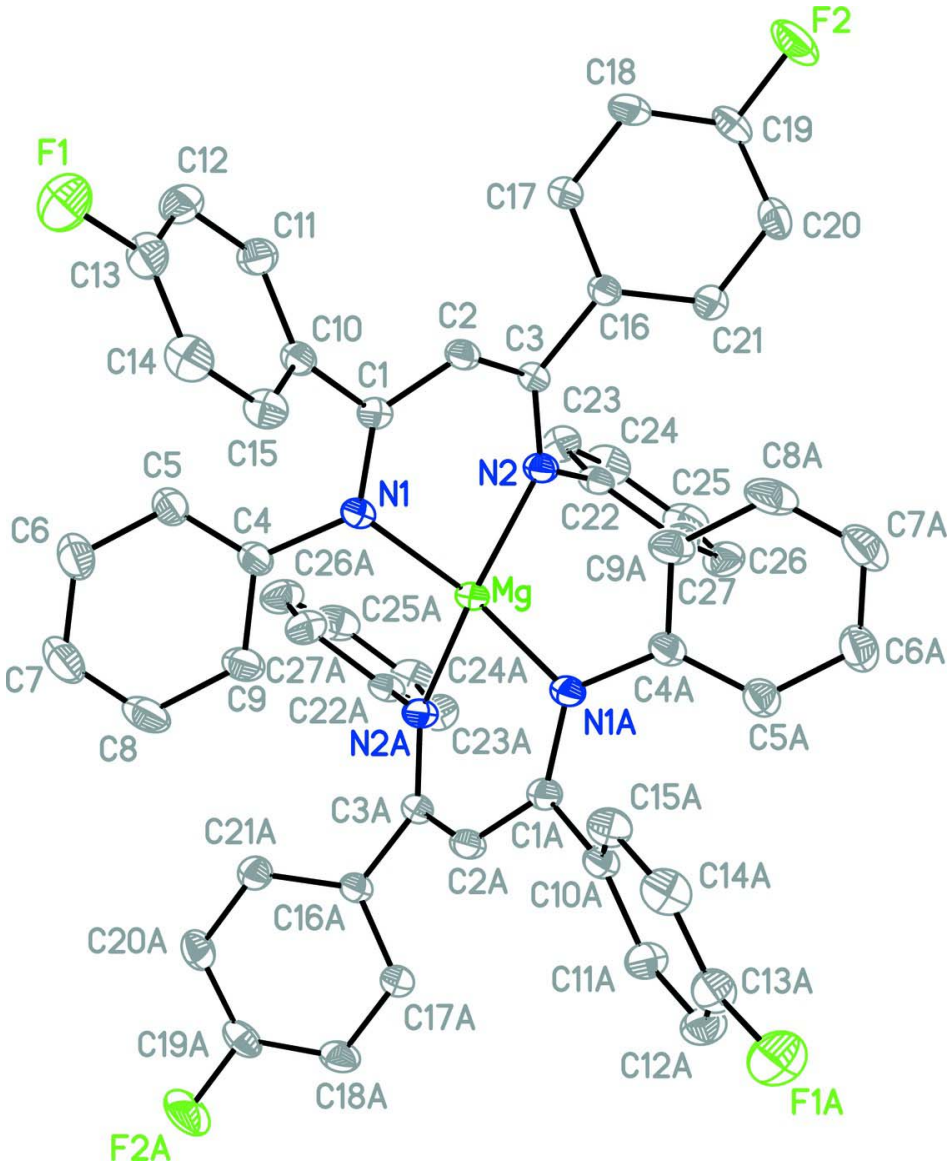


**Figure 1**

A view of the molecular structure of (I) with displacement ellipsoids shown at the 20% probability level. All the H atoms have been omitted for clarity. The suffix A corresponds to symmetry code (i) in Table 1.

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$M_r = 843.19$
Monoclinic, *C*2/*c*
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$a = 22.0564\ (15)$ Å
$b = 10.5743\ (7)$ Å
$c = 19.4356\ (13)$ Å
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$\theta = 2.3–22.9°$
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Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
12188 measured reflections
4270 independent reflections
2339 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
$h = -27 \rightarrow 27$
$k = -13 \rightarrow 10$
$l = -23 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.113$
$S = 0.91$
4270 reflections
285 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
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mg | 0.5000 | 0.15309 (9) | 0.2500 | 0.0432 (3) |
| F1 | 0.33159 (8) | 0.65235 (14) | −0.07840 (8) | 0.1010 (5) |
| F2 | 0.72941 (7) | 0.01347 (15) | −0.02150 (9) | 0.1013 (6) |
| N1 | 0.44314 (7) | 0.25070 (15) | 0.16709 (8) | 0.0464 (4) |
| N2 | 0.54626 (8) | 0.06484 (15) | 0.18583 (8) | 0.0451 (4) |
| C1 | 0.46219 (9) | 0.28050 (18) | 0.10935 (10) | 0.0445 (5) |
| C2 | 0.51500 (9) | 0.22538 (19) | 0.09460 (10) | 0.0466 (5) |
| H2A | 0.5284 | 0.2648 | 0.0586 | 0.056* |
| C3 | 0.55084 (9) | 0.11980 (18) | 0.12578 (10) | 0.0422 (5) |
| C4 | 0.38015 (10) | 0.27652 (19) | 0.16888 (11) | 0.0473 (5) |
| C5 | 0.32870 (10) | 0.24184 (19) | 0.11343 (12) | 0.0552 (6) |
| H5A | 0.3349 | 0.2125 | 0.0708 | 0.066* |
| C6 | 0.26824 (11) | 0.2500 (2) | 0.12012 (15) | 0.0744 (7) |
| H6A | 0.2341 | 0.2264 | 0.0821 | 0.089* |
| C7 | 0.25832 (14) | 0.2927 (3) | 0.18265 (18) | 0.0858 (9) |
| H7A | 0.2176 | 0.2971 | 0.1873 | 0.103* |
| C8 | 0.30860 (15) | 0.3290 (2) | 0.23819 (15) | 0.0794 (8) |

| | | | | |
|---|---|---|---|---|
| H8A | 0.3018 | 0.3592 | 0.2804 | 0.095* |
| C9 | 0.36968 (12) | 0.3210 (2) | 0.23186 (12) | 0.0628 (6) |
| H9A | 0.4036 | 0.3454 | 0.2699 | 0.075* |
| C10 | 0.42826 (9) | 0.37966 (19) | 0.05840 (10) | 0.0451 (5) |
| C11 | 0.40926 (10) | 0.3594 (2) | −0.01487 (11) | 0.0582 (6) |
| H11A | 0.4186 | 0.2829 | −0.0332 | 0.070* |
| C12 | 0.37675 (11) | 0.4508 (2) | −0.06106 (13) | 0.0677 (7) |
| H12A | 0.3632 | 0.4363 | −0.1102 | 0.081* |
| C13 | 0.36485 (11) | 0.5632 (2) | −0.03289 (14) | 0.0662 (7) |
| C14 | 0.38430 (12) | 0.5893 (2) | 0.03818 (14) | 0.0674 (7) |
| H14A | 0.3765 | 0.6678 | 0.0556 | 0.081* |
| C15 | 0.41584 (10) | 0.4965 (2) | 0.08377 (13) | 0.0577 (6) |
| H15A | 0.4291 | 0.5125 | 0.1327 | 0.069* |
| C16 | 0.59807 (9) | 0.07764 (17) | 0.08816 (10) | 0.0424 (5) |
| C17 | 0.58006 (10) | 0.06118 (19) | 0.01429 (10) | 0.0513 (5) |
| H17A | 0.5375 | 0.0663 | −0.0108 | 0.062* |
| C18 | 0.62418 (12) | 0.0373 (2) | −0.02267 (12) | 0.0614 (6) |
| H18A | 0.6118 | 0.0246 | −0.0720 | 0.074* |
| C19 | 0.68597 (12) | 0.0331 (2) | 0.01501 (14) | 0.0624 (6) |
| C20 | 0.70626 (11) | 0.0478 (2) | 0.08743 (13) | 0.0616 (6) |
| H20A | 0.7490 | 0.0436 | 0.1115 | 0.074* |
| C21 | 0.66193 (10) | 0.06915 (19) | 0.12451 (11) | 0.0520 (5) |
| H21A | 0.6750 | 0.0779 | 0.1741 | 0.062* |
| C22 | 0.57449 (10) | −0.05449 (19) | 0.20918 (11) | 0.0472 (5) |
| C23 | 0.54983 (11) | −0.1652 (2) | 0.17496 (12) | 0.0631 (6) |
| H23A | 0.5171 | −0.1615 | 0.1328 | 0.076* |
| C24 | 0.57331 (14) | −0.2816 (2) | 0.20272 (15) | 0.0774 (8) |
| H24A | 0.5565 | −0.3554 | 0.1789 | 0.093* |
| C25 | 0.62108 (14) | −0.2885 (3) | 0.26491 (15) | 0.0773 (8) |
| H25A | 0.6364 | −0.3669 | 0.2837 | 0.093* |
| C26 | 0.64644 (13) | −0.1795 (3) | 0.29959 (13) | 0.0720 (7) |
| H26A | 0.6795 | −0.1841 | 0.3415 | 0.086* |
| C27 | 0.62290 (11) | −0.0626 (2) | 0.27230 (12) | 0.0610 (6) |
| H27A | 0.6397 | 0.0108 | 0.2965 | 0.073* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mg | 0.0445 (6) | 0.0547 (6) | 0.0338 (5) | 0.000 | 0.0164 (4) | 0.000 |
| F1 | 0.1136 (13) | 0.0817 (11) | 0.1039 (12) | 0.0315 (9) | 0.0241 (10) | 0.0455 (9) |
| F2 | 0.0802 (11) | 0.1323 (13) | 0.1172 (13) | 0.0020 (9) | 0.0703 (11) | −0.0205 (10) |
| N1 | 0.0458 (10) | 0.0580 (11) | 0.0397 (9) | 0.0055 (8) | 0.0189 (8) | 0.0016 (8) |
| N2 | 0.0510 (11) | 0.0492 (10) | 0.0390 (9) | 0.0062 (8) | 0.0188 (8) | 0.0052 (8) |
| C1 | 0.0472 (13) | 0.0486 (12) | 0.0395 (11) | 0.0008 (9) | 0.0152 (10) | −0.0003 (9) |
| C2 | 0.0484 (13) | 0.0557 (13) | 0.0410 (11) | 0.0078 (10) | 0.0212 (10) | 0.0091 (10) |
| C3 | 0.0397 (12) | 0.0512 (12) | 0.0389 (11) | 0.0013 (9) | 0.0161 (9) | −0.0010 (9) |
| C4 | 0.0495 (13) | 0.0491 (12) | 0.0493 (12) | 0.0100 (10) | 0.0233 (11) | 0.0083 (10) |
| C5 | 0.0504 (14) | 0.0579 (14) | 0.0608 (14) | 0.0053 (11) | 0.0214 (12) | 0.0028 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0540 (16) | 0.0829 (19) | 0.0902 (19) | 0.0092 (13) | 0.0263 (15) | 0.0137 (15) |
| C7 | 0.071 (2) | 0.097 (2) | 0.107 (2) | 0.0275 (16) | 0.055 (2) | 0.0299 (18) |
| C8 | 0.099 (2) | 0.0854 (19) | 0.0729 (18) | 0.0385 (16) | 0.0557 (18) | 0.0165 (15) |
| C9 | 0.0744 (17) | 0.0699 (16) | 0.0524 (14) | 0.0201 (12) | 0.0314 (13) | 0.0060 (11) |
| C10 | 0.0462 (13) | 0.0466 (12) | 0.0469 (12) | 0.0053 (9) | 0.0202 (10) | 0.0050 (10) |
| C11 | 0.0666 (16) | 0.0605 (15) | 0.0488 (13) | 0.0130 (11) | 0.0183 (12) | 0.0042 (11) |
| C12 | 0.0760 (18) | 0.0735 (18) | 0.0534 (14) | 0.0112 (13) | 0.0178 (13) | 0.0155 (13) |
| C13 | 0.0641 (16) | 0.0589 (16) | 0.0776 (18) | 0.0140 (12) | 0.0231 (14) | 0.0288 (14) |
| C14 | 0.0826 (19) | 0.0440 (14) | 0.0821 (19) | 0.0086 (12) | 0.0338 (15) | 0.0080 (13) |
| C15 | 0.0689 (16) | 0.0491 (14) | 0.0594 (14) | 0.0011 (11) | 0.0252 (13) | 0.0023 (11) |
| C16 | 0.0441 (13) | 0.0448 (12) | 0.0419 (11) | 0.0042 (9) | 0.0182 (10) | 0.0043 (9) |
| C17 | 0.0479 (13) | 0.0646 (14) | 0.0443 (12) | −0.0005 (10) | 0.0179 (10) | −0.0020 (10) |
| C18 | 0.0717 (18) | 0.0718 (16) | 0.0505 (13) | −0.0015 (12) | 0.0333 (13) | −0.0079 (11) |
| C19 | 0.0574 (16) | 0.0686 (16) | 0.0766 (17) | 0.0044 (12) | 0.0443 (14) | −0.0072 (13) |
| C20 | 0.0426 (14) | 0.0687 (16) | 0.0772 (17) | 0.0086 (11) | 0.0229 (13) | 0.0037 (13) |
| C21 | 0.0499 (14) | 0.0579 (14) | 0.0483 (12) | 0.0049 (10) | 0.0137 (11) | 0.0024 (10) |
| C22 | 0.0556 (14) | 0.0509 (13) | 0.0428 (12) | 0.0054 (11) | 0.0265 (11) | 0.0034 (10) |
| C23 | 0.0693 (16) | 0.0610 (16) | 0.0578 (14) | 0.0009 (12) | 0.0159 (12) | −0.0009 (12) |
| C24 | 0.099 (2) | 0.0525 (16) | 0.090 (2) | −0.0013 (14) | 0.0403 (18) | −0.0033 (14) |
| C25 | 0.100 (2) | 0.0663 (18) | 0.0774 (19) | 0.0235 (16) | 0.0448 (18) | 0.0224 (15) |
| C26 | 0.0833 (19) | 0.0796 (19) | 0.0526 (14) | 0.0231 (15) | 0.0185 (13) | 0.0147 (14) |
| C27 | 0.0739 (17) | 0.0601 (15) | 0.0481 (13) | 0.0113 (12) | 0.0155 (12) | 0.0034 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mg—N1$^{i}$ | 2.0266 (17) | C11—H11A | 0.9300 |
| Mg—N1 | 2.0266 (17) | C12—C13 | 1.364 (3) |
| Mg—N2 | 2.0439 (15) | C12—H12A | 0.9300 |
| Mg—N2$^{i}$ | 2.0439 (15) | C13—C14 | 1.356 (3) |
| F1—C13 | 1.359 (2) | C14—C15 | 1.374 (3) |
| F2—C19 | 1.358 (2) | C14—H14A | 0.9300 |
| N1—C1 | 1.341 (2) | C15—H15A | 0.9300 |
| N1—C4 | 1.426 (2) | C16—C17 | 1.390 (3) |
| N2—C3 | 1.333 (2) | C16—C21 | 1.391 (3) |
| N2—C22 | 1.424 (2) | C17—C18 | 1.385 (3) |
| C1—C2 | 1.402 (3) | C17—H17A | 0.9300 |
| C1—C10 | 1.492 (3) | C18—C19 | 1.356 (3) |
| C2—C3 | 1.404 (3) | C18—H18A | 0.9300 |
| C2—H2A | 0.9300 | C19—C20 | 1.362 (3) |
| C3—C16 | 1.498 (2) | C20—C21 | 1.385 (3) |
| C4—C5 | 1.379 (3) | C20—H20A | 0.9300 |
| C4—C9 | 1.389 (3) | C21—H21A | 0.9300 |
| C5—C6 | 1.378 (3) | C22—C23 | 1.381 (3) |
| C5—H5A | 0.9300 | C22—C27 | 1.386 (3) |
| C6—C7 | 1.370 (3) | C23—C24 | 1.386 (3) |
| C6—H6A | 0.9300 | C23—H23A | 0.9300 |
| C7—C8 | 1.369 (4) | C24—C25 | 1.366 (4) |
| C7—H7A | 0.9300 | C24—H24A | 0.9300 |

| | | | |
|---|---|---|---|
| C8—C9 | 1.389 (3) | C25—C26 | 1.373 (3) |
| C8—H8A | 0.9300 | C25—H25A | 0.9300 |
| C9—H9A | 0.9300 | C26—C27 | 1.388 (3) |
| C10—C11 | 1.384 (3) | C26—H26A | 0.9300 |
| C10—C15 | 1.386 (3) | C27—H27A | 0.9300 |
| C11—C12 | 1.376 (3) | | |

| | | | |
|---|---|---|---|
| N1—Mg—N1$^{i}$ | 118.76 (10) | C11—C12—H12A | 120.9 |
| N1$^{i}$—Mg—N2 | 114.47 (6) | C14—C13—F1 | 118.8 (2) |
| N1—Mg—N2 | 92.91 (6) | C14—C13—C12 | 123.0 (2) |
| N1$^{i}$—Mg—N2$^{i}$ | 92.91 (6) | F1—C13—C12 | 118.2 (2) |
| N1—Mg—N2$^{i}$ | 114.47 (6) | C13—C14—C15 | 118.1 (2) |
| N2—Mg—N2$^{i}$ | 125.67 (10) | C13—C14—H14A | 121.0 |
| C1—N1—C4 | 120.68 (16) | C15—C14—H14A | 121.0 |
| C1—N1—Mg | 121.08 (13) | C14—C15—C10 | 121.5 (2) |
| C4—N1—Mg | 117.98 (11) | C14—C15—H15A | 119.3 |
| C3—N2—C22 | 122.16 (15) | C10—C15—H15A | 119.3 |
| C3—N2—Mg | 120.53 (13) | C17—C16—C21 | 118.28 (17) |
| C22—N2—Mg | 117.28 (11) | C17—C16—C3 | 120.28 (18) |
| N1—C1—C2 | 123.07 (18) | C21—C16—C3 | 120.98 (17) |
| N1—C1—C10 | 120.29 (17) | C18—C17—C16 | 121.3 (2) |
| C2—C1—C10 | 116.61 (16) | C18—C17—H17A | 119.4 |
| C1—C2—C3 | 129.96 (17) | C16—C17—H17A | 119.4 |
| C1—C2—H2A | 115.0 | C19—C18—C17 | 118.1 (2) |
| C3—C2—H2A | 115.0 | C19—C18—H18A | 120.9 |
| N2—C3—C2 | 123.61 (16) | C17—C18—H18A | 120.9 |
| N2—C3—C16 | 122.05 (17) | F2—C19—C18 | 118.2 (2) |
| C2—C3—C16 | 114.24 (16) | F2—C19—C20 | 118.8 (2) |
| C5—C4—C9 | 118.4 (2) | C18—C19—C20 | 123.1 (2) |
| C5—C4—N1 | 121.67 (18) | C19—C20—C21 | 118.7 (2) |
| C9—C4—N1 | 119.3 (2) | C19—C20—H20A | 120.7 |
| C6—C5—C4 | 121.1 (2) | C21—C20—H20A | 120.7 |
| C6—C5—H5A | 119.4 | C20—C21—C16 | 120.5 (2) |
| C4—C5—H5A | 119.4 | C20—C21—H21A | 119.7 |
| C7—C6—C5 | 120.2 (3) | C16—C21—H21A | 119.7 |
| C7—C6—H6A | 119.9 | C23—C22—C27 | 118.5 (2) |
| C5—C6—H6A | 119.9 | C23—C22—N2 | 121.3 (2) |
| C6—C7—C8 | 119.8 (2) | C27—C22—N2 | 119.81 (19) |
| C6—C7—H7A | 120.1 | C22—C23—C24 | 120.8 (2) |
| C8—C7—H7A | 120.1 | C22—C23—H23A | 119.6 |
| C7—C8—C9 | 120.3 (2) | C24—C23—H23A | 119.6 |
| C7—C8—H8A | 119.8 | C25—C24—C23 | 120.3 (2) |
| C9—C8—H8A | 119.8 | C25—C24—H24A | 119.9 |
| C8—C9—C4 | 120.2 (2) | C23—C24—H24A | 119.9 |
| C8—C9—H9A | 119.9 | C24—C25—C26 | 119.8 (2) |
| C4—C9—H9A | 119.9 | C24—C25—H25A | 120.1 |
| C11—C10—C15 | 118.08 (19) | C26—C25—H25A | 120.1 |
| C11—C10—C1 | 121.73 (18) | C25—C26—C27 | 120.2 (2) |

| | | | |
|---|---|---|---|
| C15—C10—C1 | 120.18 (18) | C25—C26—H26A | 119.9 |
| C12—C11—C10 | 121.0 (2) | C27—C26—H26A | 119.9 |
| C12—C11—H11A | 119.5 | C26—C27—C22 | 120.5 (2) |
| C10—C11—H11A | 119.5 | C26—C27—H27A | 119.8 |
| C13—C12—C11 | 118.2 (2) | C22—C27—H27A | 119.8 |
| C13—C12—H12A | 120.9 | | |

Symmetry code: (i) $-x+1, y, -z+1/2$.