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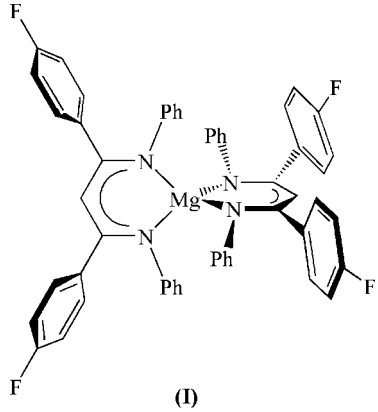
In the title complex, $[Mg(C_{27}H_{19}F_2N_2)_2]$, the Mg^{II} atom, lying on a crystallographic twofold rotation axis, is tetrahedrally coordinated by four N atoms from two diiminate ligands.

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
β = 106.201 (1)°
V = 4353.0 (5) Å^3
Z = 4
D_x = 1.287 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Parallelepiped, yellow
0.37 × 0.34 × 0.26 mm

Data collection

Bruker SMART 1000 CCD diffractometer
φ and ω scans
Absorption correction: none
12188 measured reflections
4270 independent reflections
2339 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{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) = 1.2U_{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*.

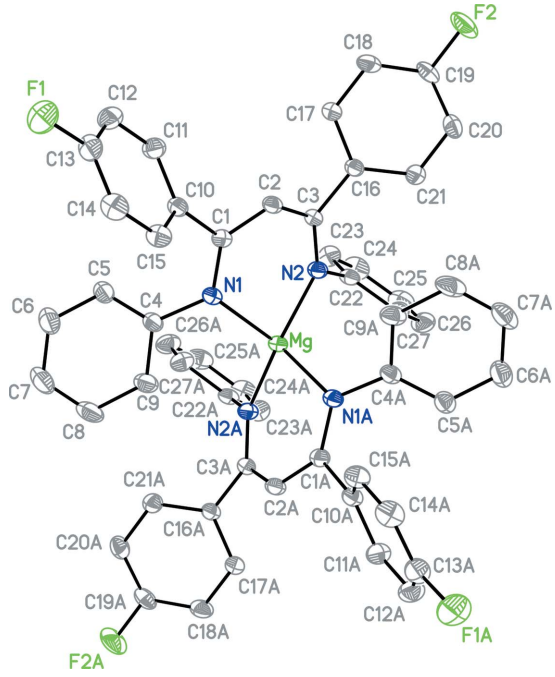


Figure 1
A view of the molecular structure of (I) with displacement ellipsoids shown at the 20% probability level. All the H atoms have been omitted for clarity. The suffix A corresponds to symmetry code (i) in Table 1.

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