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(*meso*-5,5,7,12,12,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane)zinc(II) diperchlorate

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Key indicators

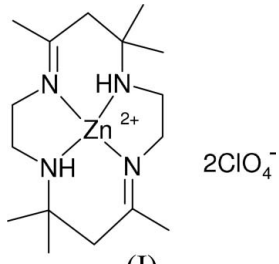
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 17.9

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

In the title mononuclear zinc(II) compound, $[Zn(C_{16}H_{36}N_4)](ClO_4)_2$, the Zn^{2+} atom lies on an inversion center and is coordinated by four N atoms from the macrocyclic ligand. The coordination geometry is slightly distorted square planar.

Comment

In preparing $Zn(ClO_4)_2$ complexes with ethylenediamine in acetone, we isolated some crystals of the title compound, (I), unexpectedly. However, we failed to repeat the experiment. The complex can also be obtained according to a published method (Zhu *et al.*, 1999).



(I)

In the complex cation, the Zn^{II} atom, on an inversion center, is coordinated by four N atoms of the macrocyclic ligand (Fig. 1). The metal atom and the four N atoms are coplanar. The Zn—N bond lengths are close to those in similar zinc(II) complexes (Zhu *et al.*, 2004; You *et al.*, 2004). The perchlorate anions are not coordinated.

Experimental

The ligand *meso*-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane was prepared according to the literature method of Hay *et al.* (1975). Equimolar amounts of the ligand and $Zn(ClO_4)_2\cdot 9H_2O$ were mixed in water in a flask and the solution was kept in air for one week. Large colorless prismatic crystals were precipitated after about 80% of the solvent had evaporated. They were filtered off, washed with water three times and dried in air (yield 24%).

Crystal data

$[Zn(C_{16}H_{32}N_4)](ClO_4)_2$
M_r = 544.74
Monoclinic, $P2_1/c$
a = 10.323 (2) Å
b = 10.630 (2) Å
c = 11.018 (2) Å
β = 111.71 (3)°
V = 1123.3 (4) Å^3
Z = 2
D_x = 1.622 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1989 reflections
θ = 4.8–27.5°
μ = 1.38 mm^{-1}
T = 293 (2) K
Prism, colorless
0.45 × 0.35 × 0.35 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.580, T_{max} = 0.625
9499 measured reflections
2645 independent reflections
2448 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 28.2°
$h = -13 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.14
2645 reflections
148 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 1.108P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.029
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

All the H atoms attached to C atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H distances of 0.96 or 0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The H atom attached to N1 was refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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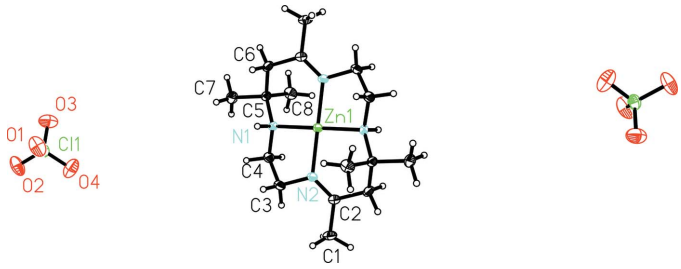

Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabeled atoms are related to labeled atoms by $(2 - x, 2 - y, -z)$.

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