Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Tris(4,4′,5,5′-tetramethyl-2,2′-biimidazole)-zinc(II) dinitrate

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Received 11 April 2005
Accepted 3 May 2005
Online 14 May 2005

A new six-coordinate monomeric Zn^{II} complex, $[Zn(L)_3](NO_3)_2$, where L is 4,4′,5,5′-tetramethyl-2,2′-biimidazole ($C_{10}H_{14}N_4$), has been synthesized and characterized by X-ray diffraction techniques. The Zn^{II} atom, on a twofold axis, has a ZnN_6 distorted octahedral coordination environment. 4,4′,5,5′-Tetramethyl-2,2′-biimidazole is bonded as a chelating ligand through its unprotonated N atoms. These discrete monomeric units possesses excellent hydrogen-bonding sites which further self-assemble into a three-dimensional supramolecular architecture through intermolecular N—H···O and C—H···O hydrogen bonds.

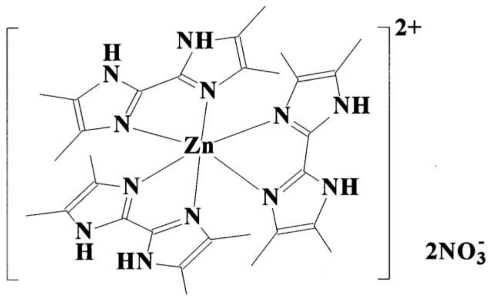
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.043
wR factor = 0.111
Data-to-parameter ratio = 16.1

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

Comment

The unique strength, directionality and complementarity of non-covalent interactions, such as hydrogen bonding and coordination bonding, play an important role in the creation of a variety of molecular architectures (Tadokoro *et al.*, 1999; Lehn, 1995). The building blocks possessing such non-covalent interaction sites can produce one-, two- and three-dimensional molecular arrangements with long-range order (Subramanian & Zaworotko, 1994; Ermer, 1988). We present here a new three-dimensional hydrogen-bonding network with discrete monomeric Zn^{II} building blocks, $[Zn(L)_3](NO_3)_2$, (I), where L is 4,4′,5,5′-tetramethyl-2,2′-biimidazole.



(I)

X-ray structure analysis reveals that (I) is a monomeric Zn^{II} complex (Fig. 1). The coordination geometry around the Zn^{II} atom, which lies on a twofold rotation axis, is octahedral, with Zn—N distances in the range 2.149 (3)–2.208 (2) Å. The 4,4′,5,5′-tetramethyl-2,2′-biimidazole ligand is bonded as a chelating ligand through its unprotonated N atoms. A striking structural feature of (I) is the formation of a three-dimensional supramolecular architecture through intermolecular N—H···O and C—H···O hydrogen-bonding interactions (Table 1).

Experimental

Complex (I) was prepared by reacting an acetonitrile solution (15 ml) of zinc(II) nitrate with 4,4′,5,5′-tetramethyl-2,2′-biimidazole in a 1:3 ratio. Red block-shaped crystals were recovered by filtration and dried in air. The yield was *ca* 78% (based on Zn). IR (KBr, cm^{-1}): 3232 (*m*), 2980 (*m*), 1696 (*s*), 1517 (*s*), 1456 (*m*), 1200 (*m*), 841 (*m*), 751 (*w*), 624 (*w*) cm^{-1}.

Crystal data

$[Zn(C_{10}H_{14}N_4)_3](NO_3)_2$
$M_r = 760.15$
Hexagonal, $P6_4$
$a = 13.900$ (2) Å
$c = 16.809$ (3) Å
$V = 2812.7$ (8) Å^3
$Z = 3$
$D_x = 1.346$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 6512 reflections
$\theta = 2.9$–24.1°
$\mu = 0.72$ mm^{-1}
$T = 293$ (2) K
Block, red
0.20 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.868$, $T_{max} = 0.898$
17035 measured reflections
4093 independent reflections
3093 reflections with $I > 2\sigma(I)$
$R_{int} = 0.116$
$\theta_{max} = 28.3°$
$h = -12 \rightarrow 18$
$k = -18 \rightarrow 15$
$l = -17 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.111$
$S = 0.96$
4093 reflections
254 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Flack (1983), 1683 Friedel pairs
Flack parameter = −0.027 (13)

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{i}	0.86	2.01	2.852 (4)	167
N4—H4A···O3^{i}	0.86	2.01	2.818 (5)	156
N6—H6A···O2^{ii}	0.86	2.03	2.849 (5)	157
N6—H6A···O3^{ii}	0.86	2.60	3.276 (5)	136
C9—H9A···O3^{iii}	0.96	2.47	3.403 (7)	163
C9—H9B···O1^{iv}	0.96	2.51	3.431 (7)	162
C10—H10C···O2^{v}	0.96	2.46	3.235 (6)	138

Symmetry codes: (i) $x-y, x, z-\frac{1}{3}$; (ii) $y, 1-x+y, \frac{1}{3}+z$; (iii) $1-x, 1-y, z$; (iv) $1-x+y, 2-x, z-\frac{1}{3}$; (v) $x-1, y, z$.

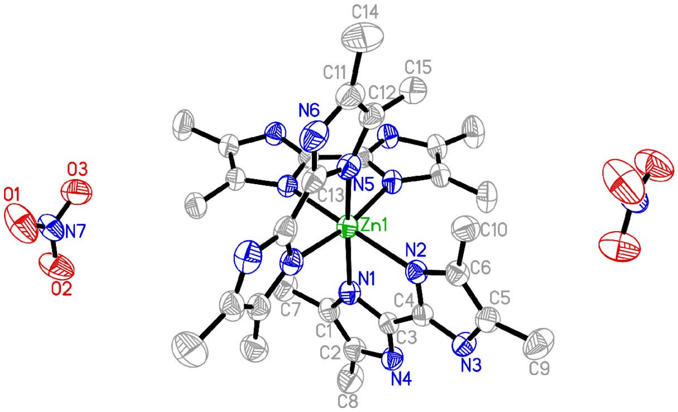


Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted. Unlabeled atoms are related to labeled atoms by $-x, -y, z$.

All H atoms were placed in calculated positions and allowed to ride on their parent atoms [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

The authors thank AIST and Kobe University for financial support.

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