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The heptacoordinate cadmium(II) complex [tris(2-benzimidazolylmethyl)amine]dinitratocadmium(II)

Jin-Lei Tian, Ming-Jin Xie, Shi-Ping Yan,* Dai-Zheng Liao, Zhong-Hui Jiang and Peng Cheng

Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: yansp@nankai.edu.cn

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The crystal structure of the title compound, $[Cd(NTB)(NO_3)_2]$ [NTB is tris(2-benzimidazolylmethyl)amine, $C_{24}H_{21}N_7$], contains a neutral monomeric cadmium(II) unit. The cadmium(II) ion is coordinated by four N atoms from the NTB ligand and three O atoms from the two nitrate anions. The coordination polyhedron for each Cd atom can be regarded as distorted pentagonal bipyramidal.

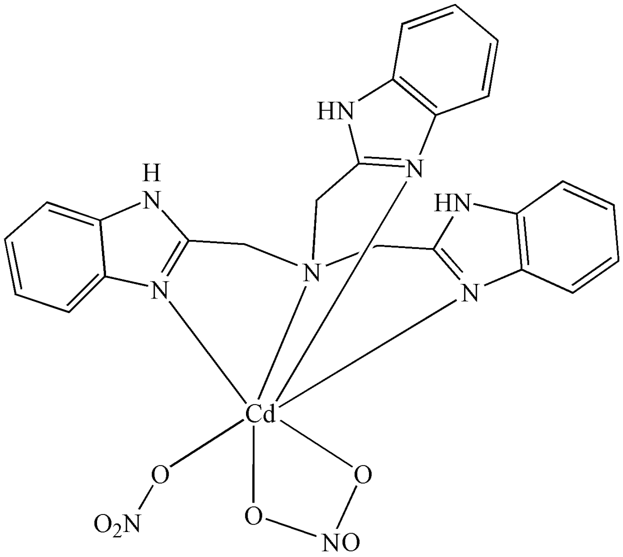
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.039
wR factor = 0.077
Data-to-parameter ratio = 13.3

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

Comment

The coordination chemistry of cadmium in both biological and non-biological areas has attracted the interest of many researchers (Gillard *et al.*, 1987). Cadmium(II) has a d^{10} electron configuration that adapts to a wide variety of stereochemical environments. A review of 200 crystal structures of cadmium(II) complexes showed that cadmium(II) has coordination numbers of 4, 5 and 6 in about 19, 8 and 56%, respectively (Martin & Sigel, 1994). Seven-coordinated cadmium(II) has been obtained in a few cases (Bruckmann *et al.*, 1999; Chen *et al.*, 2002; Chantrapromma *et al.*, 2000; Brusau *et al.*, 2000; Fujita *et al.*, 1994). In this paper, we report the preparation and structure determination of a heptacoordinate cadmium(II) monomer complex.



(I)

The crystal structure of the title complex, (I), is composed of neutral monomeric cadmium(II) complex molecules, $[Cd(NTB)(NO_3)_2]$, as illustrated in Fig. 1. Selected bond

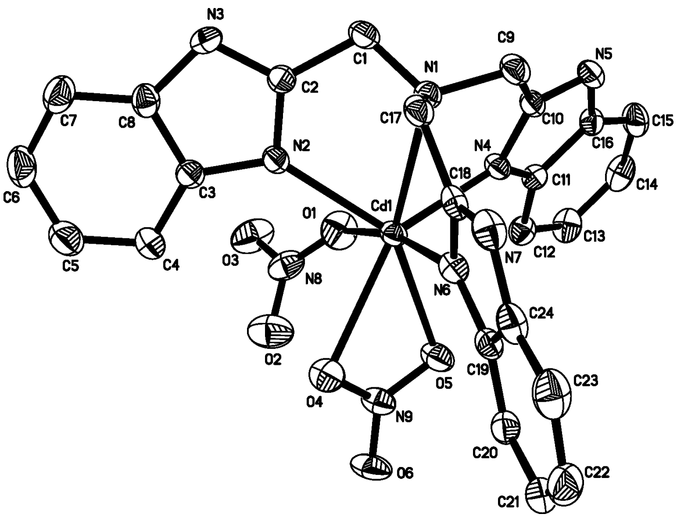


Figure 1

Structure of [Cd(NTB)$(NO_3)_2$]. *ORTEP*III (Burnett & Johnson, 1996) drawing showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

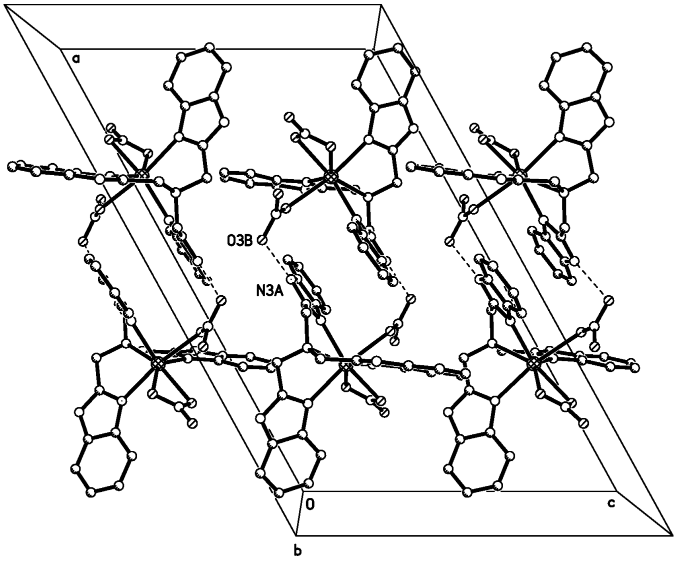


Figure 2

Packing diagram of the title compound. Dashed lines indicate hydrogen bonds.

distances and angles are shown in Table 1. The cadmium(II) ion is seven-coordinated by four N atoms from the tris(2-benzimidazolylmethyl)amine (NTB) ligand and three O atoms from two nitrate anions. The coordination polyhedron for each cadmium atom can be regarded as a distorted pentagonal bipyramid. The pentagonal plane is composed of atoms O4, O5, N1, N2 and N4. The axial positions are occupied by atoms N6 and O1, with axial distances of 2.366 (4) and 2.515 (4) Å, respectively. The degree of distortortion from ideal pentagonal bipyramidal geometry is reflected in the angles around the Cd atom in the equatorial plane (the ideal value being 72°). The most notable feature of the present structure is the coordination mode of the two nitrate anions; one functions as a monodentate (O1) and the other as a bidentate ligand (O4 and O5). Though two O atoms (O2 and O3) of the monodentate nitrate are free, these atoms do not bind with another cadmium(II) ion to give a polymeric structure, probably as a result of steric hindrance of the cadmium(II) coordination site. The bond distance between atom Cd1 and tertiary atom N1 of NTB is 2.602 (3) Å, which is much longer than the normal bond distance. This phenomenon is attributed to the steric requirements of the tripodal ligand (Gogineni *et al.*, 1997; Cheng *et al.*, 2003). In addition, a weak hydrogen bond is observed between the imine N atom in the benzimidazole ring and the O atom from the monodentate nitrate anion ($N3A\cdots O3B$ = 2.852 Å; Fig. 2).

NTB exhibits two absorptions bands at 1622 and 1588 cm^{-1}, which are assumed to be due to CN stretching in the imidazole ring. The complex exhibits the same two bands; the lower energy band falls in the range 1590–1607 cm^{-1}, while the higher falls in the range 1610–1632 cm^{-1}. In the complex, the characteristic peaks of mondentate and bidentate nitrate are all observed (monodentate: 992, 1310 cm^{-1}; bidentate: 1459, 1310 cm^{-1}).

Experimental

NTB was synthesized by a published procedure (Ramaswamy *et al.*, 1966). A methanol solution (10 ml) of NTB (0.0610 g, 0.15 mmol) was added to a methanol solution (10 ml) of $Cd(NO_3)_2\cdot 4H_2O$ (0.0463 g, 0.15 mmol). The resulting solution was refluxed for about 5 h and then filtered. The filtrate was allowed to stand for several days in a refrigerator and colorless well shaped block crystals were obtained. Analysis found: C 44.86, H 3.18, N 19.42%; calculated for $C_{24}H_{21}CdN_9O_6$: C 44.73, H 3.29, N 19.58%.

Crystal data

$[Cd(NO_3)_2(C_{24}H_{21}N_7)]$
M_r = 643.90
Monoclinic, $C2/c$
a = 26.082 (14) Å
b = 14.385 (7) Å
c = 16.231 (8) Å
β = 118.808 (8)°
V = 5336 (5) Å^3
Z = 8
D_x = 1.603 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 885 reflections
θ = 3.4–25.4°
μ = 0.88 mm^{-1}
T = 293 (2) K
Block, colorless
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.779, T_{max} = 0.880
11 037 measured reflections
4799 independent reflections
3049 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.4°
$h = -31 \rightarrow 24$
$k = -17 \rightarrow 9$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.077
S = 0.96
4799 reflections
361 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0240P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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Table 1

Selected geometric parameters (Å, °).

Cd1—N2	2.263 (4)	Cd1—O1	2.515 (4)
Cd1—N4	2.281 (3)	Cd1—O4	2.539 (3)
Cd1—N6	2.366 (4)	Cd1—N1	2.602 (3)
Cd1—O5	2.369 (3)		
N2—Cd1—N4	116.38 (12)	N4—Cd1—O4	143.77 (12)
N2—Cd1—N6	107.51 (12)	N6—Cd1—O4	82.92 (11)
N4—Cd1—N6	100.99 (12)	O5—Cd1—O4	52.10 (10)
N2—Cd1—O5	140.83 (11)	O1—Cd1—O4	87.32 (12)
N4—Cd1—O5	91.68 (11)	N2—Cd1—N1	69.93 (12)
N6—Cd1—O5	91.94 (12)	N4—Cd1—N1	69.98 (11)
N2—Cd1—O1	79.27 (12)	N6—Cd1—N1	68.48 (12)
N4—Cd1—O1	83.49 (13)	O5—Cd1—N1	148.96 (11)
N6—Cd1—O1	168.61 (12)	O1—Cd1—N1	122.86 (12)
O5—Cd1—O1	77.38 (12)	O4—Cd1—N1	141.24 (10)
N2—Cd1—O4	95.99 (12)		

H atoms bonded to C atoms were included at calculated positions (C—H = 0.93–0.97 Å and N—H = 0.86 Å), with isotropic displacement parameters [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N)], riding on their carrier atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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