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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.054
 wR factor = 0.125
Data-to-parameter ratio = 15.7

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

Diazidobis(1,10-phenanthroline- κ^2N,N')cadmium(II)

The hydrothermal reaction of NaN_3 , 1,10-phenanthroline and Cd^{II} in basic aqueous solution gave rise to the title complex, $[\text{Cd}(\text{N}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$. The Cd^{II} atom (site symmetry 2) is six-coordinated with distorted octahedral geometry and the two azido ions in *cis* positions.

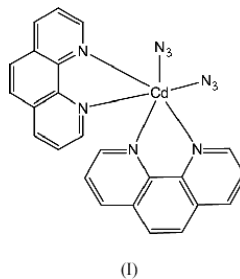
Received 5 July 2004

Accepted 7 July 2004

Online 17 July 2004

Comment

We are currently interested in pursuing synthetic strategies using the N_3^- azide ligand. This is a versatile species that can act as a monodentate as well as a bridging ligand, adopting the end-on or end-to-end modes to generate interesting complexes with different structures varying from mononuclear to three-dimensional (Cheng *et al.*, 2002; Li *et al.*, 2002; Viau *et al.*, 1997; Wang *et al.*, 2004; Shen *et al.*, 1999). We report here the preparation and crystal structure of the title complex, (I) (Fig. 1).



The asymmetric unit of (I) consists of one-half of the title complex, with the other half generated by twofold symmetry, the Cd atom lying on a twofold axis. The Cd atom is coordinated octahedrally (Table 1) by four N atoms from two 1,10-phenanthroline (phen) ligands and two N atoms from two azide (az) groups, with the two azide ligands in *cis* positions. The $\text{Cd1}-\text{N}_{\text{phen}}$ bond lengths are in the range 2.355 (4)–2.415 (5) Å, and are longer than the $\text{Cd1}-\text{N}_{\text{az}}$ bond of 2.280 (5) Å. The *cis* $\text{N}-\text{Cd}-\text{N}$ angles range from 70.48 (5) to 103.03 (7)°, while the azide ligands are essentially linear, with $\text{N5}-\text{N4}-\text{N3} = 178.5$ (6)°. One azide N atom acts as an acceptor for a weak $\text{C8}-\text{H8}\cdots\text{N3}^{\text{i}}$ intermolecular interaction (see Table 2 for symmetry code).

Experimental

$\text{CdSO}_4\cdot 8\text{H}_2\text{O}$ (0.04 g, 0.05 mmol), NaN_3 (0.02 g, 0.3 mmol) and phen (0.016 g, 0.1 mmol) were mixed in 20 ml H_2O and heated at 433 K for 3 d in a sealed 30 ml Teflon-lined stainless steel vessel under autogenous pressure. After the reaction mixture had been cooled slowly to room temperature, colorless prism-shaped crystals of the title complex appeared.

Crystal data

[Cd(N₃)₂(C₁₂H₈N₂)₂]
M_r = 556.87
 Orthorhombic, *Pbcn*
a = 14.071 (7) Å
b = 8.985 (6) Å
c = 17.23 (3) Å
V = 2178 (4) Å³
Z = 4
D_x = 1.698 Mg m⁻³

Data collection

Bruker SMART CCD
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (SADABS; Siemens, 1996)
T_{min} = 0.551, *T_{max}* = 0.901
 15133 measured reflections

Mo *K* α radiation
 Cell parameters from 112
 reflections
 θ = 1.9–27.5°
 μ = 1.04 mm⁻¹
T = 293 (2) K
 Prism, colorless
 0.60 × 0.40 × 0.10 mm

2502 independent reflections
 1908 reflections with *I* > 2 σ (*I*)
R_{int} = 0.062
 θ_{\max} = 27.5°
h = -18 → 12
k = -11 → 10
l = -22 → 22

Refinement

Refinement on *F*²
R[*F*² > 2 σ (*F*²)] = 0.054
wR(*F*²) = 0.125
S = 1.08
 2502 reflections
 159 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 17.7008P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.47 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.44 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1—N3	2.280 (5)	N3—N4	1.185 (6)
Cd1—N2	2.355 (4)	N4—N5	1.155 (6)
Cd1—N1	2.415 (5)		
N3—Cd1—N3 ⁱ	98.2 (3)	N2—Cd1—N1	70.47 (15)
N3—Cd1—N2	96.47 (16)	N2 ⁱ —Cd1—N1	87.81 (15)
N3 ⁱ —Cd1—N2	103.02 (17)	N1—Cd1—N1 ⁱ	87.5 (2)
N2—Cd1—N2 ⁱ	150.1 (2)	N4—N3—Cd1	134.7 (4)
N3—Cd1—N1	166.47 (15)	N5—N4—N3	178.5 (6)

Symmetry code: (i) $-x, y, \frac{3}{2} - z$.

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H8A...N3 ⁱⁱ	0.93	2.37	3.242 (7)	157

Symmetry code: (ii) $x - \frac{1}{2}, y - \frac{1}{2}, \frac{3}{2} - z$.

H atoms were geometrically placed in idealized positions (C—H = 0.93 Å) and allowed to ride on their respective parent C atoms, with *U_{iso}*(H) = 1.2*U_{eq}*(C). The highest peak and deepest hole in the

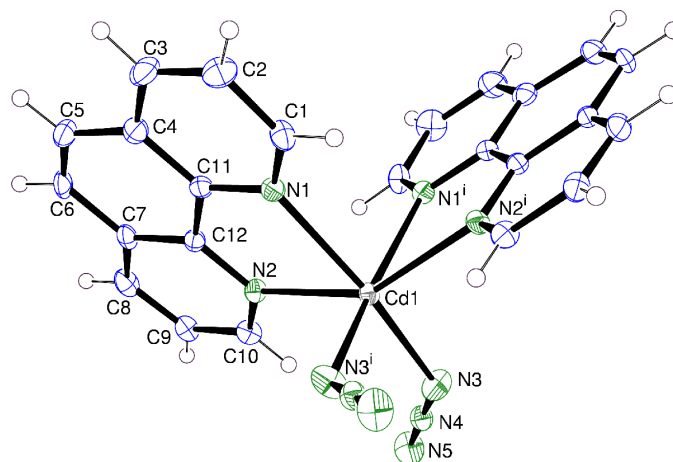


Figure 1

View of (I), shown with 40% probability displacement ellipsoids. The symmetry code is as in Table 1.

difference map were located 0.90 and 1.22 Å from atoms Cd1 and N3, respectively.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by the 973 Program of MOST (001CB108906), the National Natural Science Foundation of China (90206040, 20073048, 20333070 and 20303021), the NSF of Fujian Province (2002 F015 and 2002 J006) and the Chinese Academy of Sciences.

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