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cis-Bis(2,2′-bipyridine)diiodocadmium(II)

Hong-Xu Guo,* Hai-Bin Lin and Qing-Hua Wang

Zhangzhou Teacher's College, Department of Chemistry and Environmental Science, Zhangzhou, Fujian 363000, People's Republic of China

Correspondence e-mail:
guohongxu919@yahoo.com.cn

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Key indicators

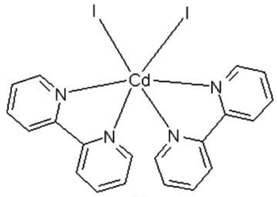
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.036
wR factor = 0.111
Data-to-parameter ratio = 19.5

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

The title compound, [$CdI_2(C_{10}H_8N_2)_2$], synthesized by hydrothermal methods from CdI_2 and 2,2′-bipyridine, has the Cd atom coordinated by two I and four N atoms from two 2,2′-bipyridine ligands in a distorted octahedral geometry.

Comment

The chemistry of novel metal–organic hybrid coordination complexes has been the subject of intensive research in recent years owing to their interesting topologies and unexpected properties for potential applications (Li *et al.*, 2003; Hammond *et al.*, 1999). Recently, there has been increasing interest in cadmium–halogen compounds because of their applications in molecular materials (Strasdeit *et al.*, 1988; Liu *et al.*, 2002; Zhou *et al.*, 2003). In this communication, we have introduced 2,2′-bipyridine (bpy) as a terminal ligand which favors crystal growth of the product. Through a mild-temperature hydrothermal process, we have successfully synthesized the title crystalline iodo-coordinated Cd complex, [$CdI_2(bpy)_2$], (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The compound is a mononuclear complex in which the Cd atom is coordinated by two iodide anions and four N atoms from two bpy ligands in a distorted octahedral geometry. As shown in Table 1, The Cd—I and Cd—N bond lengths are in the expected ranges.

Experimental

The hydrothermal reaction of cadmium diiodide (0.095 g, 0.26 mmol), 2,2′-bipyridine (0.086 g, 0.55 mmol) and water (15.0 ml) was carried out at 433 K for 4 d. After cooling to room temperature at a rate of 5 K h^{-1}, block-shaped brown crystals of (I) suitable for X-ray analysis were obtained.

Crystal data

[$CdI_2(C_{10}H_8N_2)_2$]
M_r = 678.57
Monoclinic, $C2/c$
a = 16.6260 (10) Å
b = 15.7192 (9) Å
c = 17.8778 (13) Å
β = 109.642 (2)°
V = 4400.4 (5) Å^3

Z = 8
D_x = 2.049 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.81 mm^{-1}
T = 293 (2) K
Block, brown
0.40 × 0.20 × 0.12 mm

Data collection

Rigaku Weissenberg IP diffractometer
ω scans
Absorption correction: ψ scan (*TEXRAY*; Molecular Structure Corporation, 1999)
$T_{\min} = 0.713$, $T_{\max} = 0.998$ (expected range = 0.452–0.633)
18349 measured reflections
4660 independent reflections
3343 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.054$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.111$
$S = 1.01$
4660 reflections
239 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 2.0186P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.70$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.377 (4)	Cd1—N3	2.475 (4)
Cd1—N4	2.380 (4)	Cd1—I2	2.8274 (5)
Cd1—N2	2.445 (4)	Cd1—I1	2.8490 (5)
N1—Cd1—N4	146.84 (15)	N2—Cd1—I2	165.87 (10)
N1—Cd1—N2	68.39 (14)	N3—Cd1—I2	92.25 (11)
N4—Cd1—N2	88.50 (15)	N1—Cd1—I1	103.85 (10)
N1—Cd1—N3	84.71 (15)	N4—Cd1—I1	98.67 (10)
N4—Cd1—N3	67.37 (15)	N2—Cd1—I1	88.33 (9)
N2—Cd1—N3	79.56 (15)	N3—Cd1—I1	161.53 (11)
N1—Cd1—I2	99.61 (9)	I2—Cd1—I1	102.208 (17)
N4—Cd1—I2	99.02 (10)		

All H atoms were placed at calculated positions and refined with isotropic displacement parameters using a riding model [C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$]. Atom C13 was refined with isotropic displacement parameters because of problems with anisotropic refinement. The highest density peak is located 1.18 Å from atom I1.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

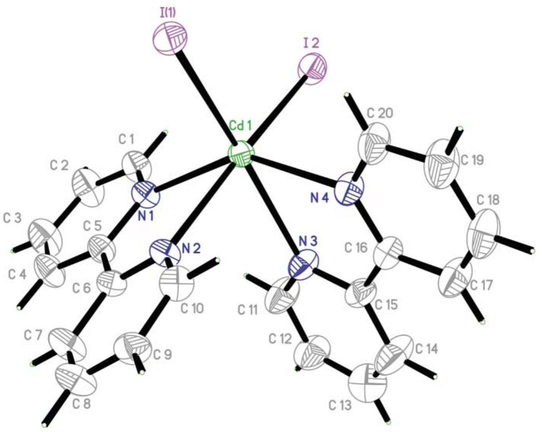


Figure 1
View of the structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.

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