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# Diiodidobis(1,10-phenanthroline-$\kappa^2N,N'$)cadmium(II)

**Ming-Lei Cao,[a,b] Xin Fang,[a,b] Hai-Yang Yu[a,b] and Jun-Dong Wang[a,b]***

[a]Department of Chemistry, University of Fuzhou, Fuzhou 350002, People's Republic of China, and [b]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou 350002, People's Republic of China
Correspondence e-mail: wangjd@fzu.edu.cn

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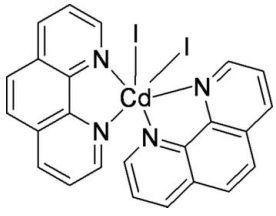
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.014 Å; $R$ factor = 0.045; $wR$ factor = 0.144; data-to-parameter ratio = 17.1.

The title compound, $[CdI_2(C_{12}H_8N_2)_2]$, consists of two 1,10-phenanthroline (phen) ligands, two I atoms and one Cd atom. The coordination geometry around the Cd atom, which lies on a twofold rotation axis, is slightly distorted octahedral. In the crystal structure, the dihedral angle between the two phen ligands is 89.03 (5)°. The crystal packing is stabilized by intermolecular $\pi$–$\pi$ interactions of phen rings, with a parallel distance of 3.362 Å, a centroid–centroid distance of 3.903 Å and a slip distance of 1.983 Å, and C—H···I hydrogen bonding [I···H = 3.091 and 2.990 Å].

## Related literature

For related literature, see: Bowmaker *et al.* (1973); Boys (1988); Boys *et al.* (1981); Healy *et al.* (1985); Pallenberg *et al.* (1995); Wicholas & Wolford (1974); Yang *et al.* (2004).




## Experimental

### Crystal data

$[CdI_2(C_{12}H_8N_2)_2]$
$M_r$ = 726.61
Orthorhombic, *Pbcn*
$a$ = 13.4833 (5) Å
$b$ = 9.5244 (3) Å
$c$ = 17.3385 (5) Å
$V$ = 2226.41 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 3.77 mm$^{-1}$
$T$ = 173 (2) K
0.08 × 0.07 × 0.01 mm

### Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.664, $T_{max}$ = 1.000
20141 measured reflections
2554 independent reflections
1786 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.144
$S$ = 1.15
2554 reflections
149 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 1.84 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.73 e Å$^{-3}$

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2059).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m1951 [ **doi:10.1107/S1600536807029145** ]

# Diiodidobis(1,10-phenanthroline-$\kappa^2N,N'$)cadmium(II)

**M.-L. Cao, X. Fang, H.-Y. Yu and J.-D. Wang**

## Comment

The title compound, (I), is a complex with organic and inorganic ligands, which can be used as a catalyst in chemical and biochemical reactions (Boys *et al.* 1988).

The molecular structure of (I) is shown in Fig. 1. Four N atoms from phen and two I atoms form a distorted octahedron arrangement around the Cd atom. The dihedral angle between the two phen rings of one molecule is 89.03 (5)°. The angles of the axial and equatorial I—Cd—N bonds are different at 161.72 (17) and 90.13 (17), respectively.

In the crystal structure of (I), the crystal packing is stabilized by intermolecular *p*-\p stacking interactions, with the distances between phen rings centroids of 3.362\%A, 3.903\%A, and a slip distance of 1.983\%A. There are also weak I–H secondary interactions with distances of 3.091\%A for I(1)–H(16 A) and 2.990\%A for I(1)–H(9 A).

## Experimental

The title compound was prepared by the slow addition of CdI~2~ (0.0183 g, 0.05 mmol) and phen (0.018 g, 0.1 mmol) to 10 ml DMF, stirred for 30 min. The solution was filtered, after the solvent was slowly evaporated at room temperature, colorless crystals was obtained.

## Figures

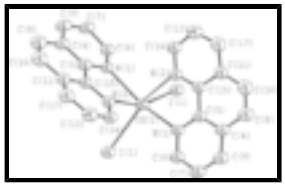


Fig. 1. A view of the molecular structure of (I), with displacement ellipsoids drawn at the 50% probabilty level for non-H atoms.

## Diiodidobis(1,10-phenanthroline-$\kappa^2N,N'$)cadmium(II)

*Crystal data*

| | |
|---|---|
| $[CdI_2(C_{12}H_8N_2)_2]$ | $F_{000}$ = 1368 |
| $M_r$ = 726.61 | $D_x$ = 2.168 Mg m$^{-3}$ |
| Orthorhombic, *Pbcn* | Mo *K*α radiation<br>λ = 0.71069 Å |
| Hall symbol: -P2n2ab | Cell parameters from 12645 reflections |
| *a* = 13.4833 (5) Å | θ = 6.0–55.0º |
| *b* = 9.5244 (3) Å | μ = 3.77 mm$^{-1}$ |
| *c* = 17.3385 (5) Å | *T* = 173 (2) K |

| | |
|---|---|
| $V$ = 2226.41 (13) Å$^3$ | Block, colorless |
| $Z$ = 4 | 0.08 × 0.07 × 0.01 mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS SPIDER diffractometer | 2554 independent reflections |
| Radiation source: fine-focus sealed tube | 1786 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.067 |
| Detector resolution: 10 pixels mm$^{-1}$ | $\theta_{max}$ = 27.5º |
| $T$ = 173(2) K | $\theta_{min}$ = 3.0º |
| ω oscillation scans | $h$ = −17→17 |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | $k$ = −11→12 |
| $T_{min}$ = 0.664, $T_{max}$ = 1.000 | $l$ = −22→22 |
| 20141 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | Only H-atom displacement parameters refined |
| $R[F^2 > 2\sigma(F^2)]$ = 0.046 | $w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 27.7932P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.144 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $S$ = 1.15 | $\Delta\rho_{max}$ = 1.84 e Å$^{-3}$ |
| 2554 reflections | $\Delta\rho_{min}$ = −2.73 e Å$^{-3}$ |
| 149 parameters | Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0013 (2) |
| Secondary atom site location: difference Fourier map | |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| I1 | 0.58713 (4) | 0.08128 (7) | 0.85926 (4) | 0.0384 (2) |
| Cd1 | 0.5000 | 0.27221 (10) | 0.7500 | 0.0314 (3) |
| N1 | 0.6549 (5) | 0.3396 (8) | 0.6981 (4) | 0.0325 (16) |
| N2 | 0.4792 (5) | 0.4653 (8) | 0.6587 (4) | 0.0314 (16) |
| C4 | 0.7434 (7) | 0.4817 (10) | 0.6051 (5) | 0.037 (2) |
| C5 | 0.6541 (6) | 0.4377 (10) | 0.6418 (5) | 0.035 (2) |
| C6 | 0.7409 (7) | 0.2878 (11) | 0.7207 (5) | 0.039 (2) |
| H6A | 0.7406 | 0.2197 | 0.7591 | 0.050* |
| C7 | 0.8321 (7) | 0.3292 (12) | 0.6905 (6) | 0.045 (3) |
| H7A | 0.8913 | 0.2940 | 0.7101 | 0.04 (3)* |
| C8 | 0.7383 (8) | 0.5822 (11) | 0.5438 (6) | 0.047 (3) |
| H8A | 0.7956 | 0.6042 | 0.5165 | 0.06 (4)* |
| C9 | 0.8314 (7) | 0.4227 (11) | 0.6314 (6) | 0.045 (3) |
| H9A | 0.8909 | 0.4477 | 0.6081 | 0.04 (3)* |
| C11 | 0.5627 (7) | 0.6104 (10) | 0.5635 (5) | 0.037 (2) |
| C13 | 0.3902 (8) | 0.6415 (11) | 0.5886 (6) | 0.043 (2) |
| H13A | 0.3304 | 0.6874 | 0.5799 | 0.06 (3)* |
| C14 | 0.3957 (7) | 0.5325 (12) | 0.6420 (6) | 0.041 (2) |
| H14A | 0.3379 | 0.5055 | 0.6672 | 0.05 (3)* |
| C15 | 0.5633 (6) | 0.5036 (11) | 0.6210 (5) | 0.034 (2) |
| C16 | 0.6540 (8) | 0.6442 (11) | 0.5252 (6) | 0.048 (3) |
| H16A | 0.6538 | 0.7115 | 0.4863 | 0.06 (4)* |
| C17 | 0.4733 (8) | 0.6804 (11) | 0.5493 (6) | 0.045 (2) |
| H17A | 0.4705 | 0.7527 | 0.5133 | 0.06 (4)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I1 | 0.0315 (3) | 0.0445 (4) | 0.0391 (4) | −0.0002 (3) | −0.0038 (3) | 0.0038 (3) |
| Cd1 | 0.0224 (4) | 0.0394 (5) | 0.0323 (5) | 0.000 | 0.0013 (4) | 0.000 |
| N1 | 0.025 (4) | 0.044 (4) | 0.028 (4) | 0.001 (3) | 0.003 (3) | 0.002 (3) |
| N2 | 0.030 (4) | 0.034 (4) | 0.030 (4) | 0.007 (3) | −0.002 (3) | 0.001 (3) |
| C4 | 0.028 (4) | 0.041 (5) | 0.041 (5) | −0.012 (4) | 0.012 (4) | −0.012 (4) |
| C5 | 0.027 (4) | 0.043 (5) | 0.033 (5) | −0.006 (4) | 0.001 (4) | −0.008 (4) |
| C6 | 0.030 (4) | 0.049 (6) | 0.037 (5) | 0.003 (4) | 0.002 (4) | −0.004 (4) |
| C7 | 0.023 (4) | 0.065 (7) | 0.047 (6) | 0.008 (4) | −0.001 (4) | −0.021 (5) |
| C8 | 0.043 (6) | 0.051 (6) | 0.046 (6) | −0.013 (5) | 0.018 (5) | −0.003 (5) |
| C9 | 0.028 (5) | 0.060 (7) | 0.049 (6) | −0.017 (5) | 0.008 (4) | −0.019 (5) |
| C11 | 0.041 (5) | 0.041 (5) | 0.028 (5) | −0.004 (4) | 0.003 (4) | 0.002 (4) |
| C13 | 0.045 (6) | 0.040 (5) | 0.044 (6) | 0.009 (4) | −0.004 (5) | 0.015 (5) |
| C14 | 0.028 (4) | 0.061 (6) | 0.036 (5) | −0.008 (4) | 0.001 (4) | 0.000 (5) |
| C15 | 0.028 (4) | 0.046 (5) | 0.029 (5) | −0.017 (4) | 0.002 (3) | −0.007 (4) |
| C16 | 0.058 (7) | 0.045 (6) | 0.041 (6) | −0.005 (5) | 0.011 (5) | 0.001 (5) |
| C17 | 0.051 (6) | 0.044 (6) | 0.041 (6) | −0.007 (5) | −0.005 (5) | 0.007 (5) |

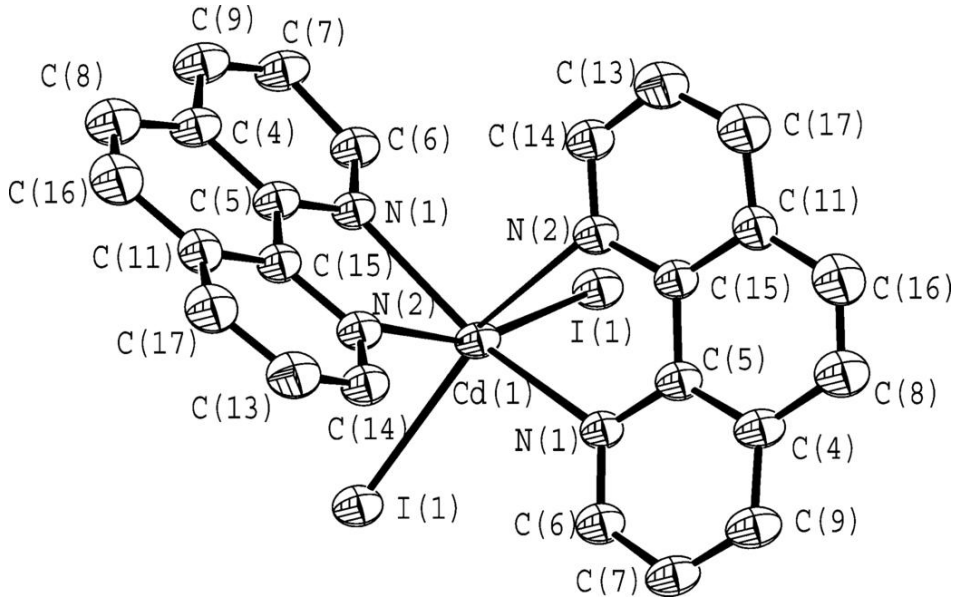
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| I1—Cd1 | 2.8766 (9) | C6—H6A | 0.9300 |
| Cd1—N1 | 2.362 (7) | C7—C9 | 1.357 (15) |

| | | | |
|---|---|---|---|
| Cd1—N1$^{i}$ | 2.362 (7) | C7—H7A | 0.9300 |
| Cd1—N2$^{i}$ | 2.442 (7) | C8—C16 | 1.321 (15) |
| Cd1—N2 | 2.442 (7) | C8—H8A | 0.9300 |
| Cd1—I1$^{i}$ | 2.8766 (9) | C9—H9A | 0.9300 |
| N1—C6 | 1.319 (12) | C11—C17 | 1.400 (14) |
| N1—C5 | 1.351 (12) | C11—C15 | 1.425 (13) |
| N2—C14 | 1.327 (12) | C11—C16 | 1.435 (14) |
| N2—C15 | 1.358 (11) | C13—C17 | 1.362 (14) |
| C4—C9 | 1.390 (15) | C13—C14 | 1.393 (14) |
| C4—C5 | 1.424 (12) | C13—H13A | 0.9300 |
| C4—C8 | 1.432 (14) | C14—H14A | 0.9300 |
| C5—C15 | 1.423 (13) | C16—H16A | 0.9300 |
| C6—C7 | 1.394 (14) | C17—H17A | 0.9300 |
| N1—Cd1—N1$^{i}$ | 148.5 (4) | C7—C6—H6A | 118.0 |
| N1—Cd1—N2$^{i}$ | 86.6 (3) | C9—C7—C6 | 117.6 (9) |
| N1$^{i}$—Cd1—N2$^{i}$ | 69.5 (3) | C9—C7—H7A | 121.2 |
| N1—Cd1—N2 | 69.5 (2) | C6—C7—H7A | 121.2 |
| N1$^{i}$—Cd1—N2 | 86.6 (3) | C16—C8—C4 | 121.5 (9) |
| N2$^{i}$—Cd1—N2 | 82.3 (3) | C16—C8—H8A | 119.3 |
| N1—Cd1—I1$^{i}$ | 106.37 (18) | C4—C8—H8A | 119.3 |
| N1$^{i}$—Cd1—I1$^{i}$ | 93.52 (18) | C7—C9—C4 | 121.2 (9) |
| N2$^{i}$—Cd1—I1$^{i}$ | 161.72 (17) | C7—C9—H9A | 119.4 |
| N2—Cd1—I1$^{i}$ | 90.13 (17) | C4—C9—H9A | 119.4 |
| N1—Cd1—I1 | 93.52 (18) | C17—C11—C15 | 117.9 (9) |
| N1$^{i}$—Cd1—I1 | 106.37 (18) | C17—C11—C16 | 123.4 (9) |
| N2$^{i}$—Cd1—I1 | 90.13 (17) | C15—C11—C16 | 118.7 (9) |
| N2—Cd1—I1 | 161.72 (17) | C17—C13—C14 | 119.4 (9) |
| I1$^{i}$—Cd1—I1 | 101.59 (4) | C17—C13—H13A | 120.3 |
| C6—N1—C5 | 118.6 (8) | C14—C13—H13A | 120.3 |
| C6—N1—Cd1 | 124.2 (6) | N2—C14—C13 | 123.4 (9) |
| C5—N1—Cd1 | 117.1 (6) | N2—C14—H14A | 118.3 |
| C14—N2—C15 | 118.2 (8) | C13—C14—H14A | 118.3 |
| C14—N2—Cd1 | 127.0 (6) | N2—C15—C5 | 118.5 (8) |
| C15—N2—Cd1 | 114.7 (6) | N2—C15—C11 | 121.6 (9) |
| C9—C4—C5 | 117.1 (9) | C5—C15—C11 | 119.8 (8) |
| C9—C4—C8 | 123.7 (9) | C8—C16—C11 | 121.6 (10) |
| C5—C4—C8 | 119.2 (9) | C8—C16—H16A | 119.2 |
| N1—C5—C15 | 119.6 (8) | C11—C16—H16A | 119.2 |
| N1—C5—C4 | 121.3 (9) | C13—C17—C11 | 119.4 (9) |
| C15—C5—C4 | 119.0 (9) | C13—C17—H17A | 120.3 |
| N1—C6—C7 | 124.0 (10) | C11—C17—H17A | 120.3 |
| N1—C6—H6A | 118.0 | | |

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

**Fig. 1**


C(9)
C(7)
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C(7)