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(6,6′-Dimethyl-2,2′-bipyridine-κ^2N,N')-diiodidozinc(II)

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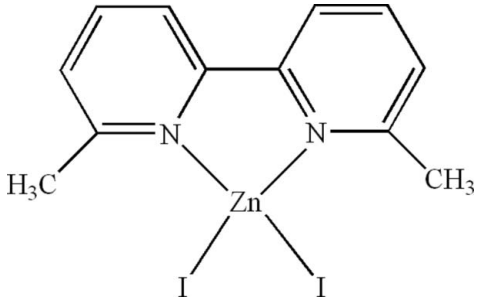
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.043; wR factor = 0.127; data-to-parameter ratio = 25.3.

The complete molecule of the title compound, $[ZnI_2(C_{12}H_{12}N_2)]$, is generated by crystallograpic twofold symmetry, with the Zn^{II} atom lying on the rotation axis. The Zn^{II} atom is coordinated by the *N*,*N*-bidentate 6,6′-dimethyl-2,2′-bipyridine ligand and two iodide ions, resulting in a distorted ZnN_2I_2 tetrahedral geometry for the metal. In the crystal, there are weak π–π contacts between the pyridine rings [centroid–centroid distance = 3.978 (3) Å].

Related literature

For related structures, see: Ahmadi *et al.* (2008, 2009); Alizadeh, Heidari *et al.* (2009); Alizadeh, Kalateh *et al.* (2009); Alizadeh, Khoshtarkib *et al.* (2009); Blake *et al.* (2007); Khalighi *et al.* (2008); Khan & Tuck (1984); Khavasi *et al.* (2008); Khoshtarkib *et al.* (2009); Kwak *et al.* (2008); Lee *et al.* (2007); Marjani *et al.* (2009); Reimann *et al.* (1966); Seebacher *et al.* (2004); Wriedt *et al.* (2008).



Experimental

Crystal data

$[ZnI_2(C_{12}H_{12}N_2)]$
M_r = 503.43
Monoclinic, $C2/c$
a = 13.421 (2) Å
b = 8.441 (2) Å
c = 13.752 (3) Å
β = 105.140 (14)°
V = 1503.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.72 mm^{-1}
T = 298 K
0.48 × 0.12 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.425, T_{max} = 0.539
5694 measured reflections
1997 independent reflections
1748 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.12
1997 reflections
79 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.058 (3)	Zn1—I1	2.5501 (6)
N1—Zn1—N1^{i}	81.9 (2)		

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5152).

References

Ahmadi, R., Kalateh, K., Alizadeh, R., Khoshtarkib, Z. & Amani, V. (2009). *Acta Cryst.* E**65**, m848–m849.
Ahmadi, R., Kalateh, K., Ebadi, A., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m1266.
Alizadeh, R., Heidari, A., Ahmadi, R. & Amani, V. (2009). *Acta Cryst.* E**65**, m483–m484.
Alizadeh, R., Kalateh, K., Ebadi, A., Ahmadi, R. & Amani, V. (2009). *Acta Cryst.* E**65**, m1250.
Alizadeh, R., Khoshtarkib, Z., Chegeni, K., Ebadi, A. & Amani, V. (2009). *Acta Cryst.* E**65**, m1311.
Blake, A. J., Giunta, D., Shannon, J., Solinas, M., Walzer, F. & Woodward, S. (2007). *Collect. Czech. Chem. Commun.* **72**, 1107–1121.
Bruker (1998). *SMART*, *SAINT* and *SADABS*. Bruker AXS, Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Khalighi, A., Ahmadi, R., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m1211–m1212.
Khan, M. A. & Tuck, D. G. (1984). *Acta Cryst.* C**40**, 60–62.
Khavasi, H. R., Abedi, A., Amani, V., Notash, B. & Safari, N. (2008). *Polyhedron*, **27**, 1848–1854.
Khoshtarkib, Z., Ebadi, A., Alizadeh, R., Ahmadi, R. & Amani, V. (2009). *Acta Cryst.* E**65**, m739–m740.
Kwak, H., Lee, S. H., Kim, S. H., Lee, Y. M., Lee, E. Y., Park, B. K., Kim, E. Y., Kim, C., Kim, S. J. & Kim, Y. (2008). *Eur. J. Inorg. Chem.* pp. 408–415.

Lee, Y. M., Hong, S. J., Kim, H. J., Lee, S. H., Kwak, H., Kim, C., Kim, S. J. & Kim, Y. (2007). *Inorg. Chem. Commun.* **10**, 287–291.
Marjani, K., Asgarian, J., Mousavi, M. & Amani, V. (2009). *Z. Anorg. Allg. Chem.* **635**, 1633–1637.
Reimann, C. W., Block, S. & Perloff, A. (1966). *Inorg. Chem.* **5**, 1185–1189.
Seebacher, J., Ji, M. & Vahrenkamp, H. (2004). *Eur. J. Inorg. Chem.* pp. 409–417.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wriedt, M., Jess, I. & Näther, C. (2008). *Acta Cryst.* E**64**, m315.

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Acta Cryst. (2009). E**65**, m1439–m1440 [https://doi.org/10.1107/S1600536809043049]

(6,6′-Dimethyl-2,2′-bipyridine-κ^2N,N')diiodidozinc(II)

Robabeh Alizadeh, Khadijeh Kalateh, Zeinab Khoshtarkib, Roya Ahmadi and Vahid Amani

S1. Comment

Recently, we reported the synthes and crystal structure of [$ZnCl_2$(phend)], (II), (Khoshtarkib *et al.*, 2009), [$HgBr_2$(2,9-dmphen)], (III), (Alizadeh, Heidari *et al.*, 2009) and [$Pb_4(NO_3)_8$(6-mbpy)$_4$], (IV), (Ahmadi, Kalateh, Alizadeh *et al.*, 2009) [where phend is phenanthridine, 2,9-dmphen is 2,9-dimethyl-1,10-phenanthroline and 6-mbpy is 6-methyl-2,2′-bipyridine].

There are several Zn^{II} complexes, with formula, [ZnX_2(N—N)], (X = Cl, Br and I), such as [$ZnCl_2$(bipy)], (V), (Khan & Tuck, 1984), [$ZnCl_2$(phen)], (VI), (Reimann *et al.*, 1966), [$ZnCl_2$(dm4bt)], (VII), (Khavasi *et al.*, 2008), [$ZnCl_2$(5,5′-dmbpy)], (VIII), (khalighi *et al.*, 2008), [$ZnCl_2$(6-mbpy)], (IX), (Ahmadi, Kalateh, Ebadi *et al.*, 2008), [$ZnCl_2$(6,6′-dmbpy)], (*X*), (Alizadeh, Kalateh *et al.*, 2009), [$ZnCl_2$(PBD)]}, (XI), (Marjani *et al.*, 2009), [$ZnBr_2$(4,4′-(dtbpy)].(Et_2O), (XII), (Blake *et al.*, 2007), {$ZnBr_2$[$NH(py)_2$]},(XIII), (Lee *et al.*, 2007), {$ZnBr_2$[$S(py)_2$]}, (XIV) (Wriedt *et al.*, 2008), [$ZnBr_2$(6,6′-dmbpy)], (XV), (Alizadeh, Khoshtarkib *et al.*, 2009), [ZnI_2(2,9-dmphen)], (XVI), (Seebacher *et al.*, 2004) and {ZnI_2[$NH(py)_2$]}, (XVII) (Kwak *et al.*, 2008) [where bipy is 2,2′-bipyridine, phen is 1,10-phenanthroline, dm4bt is 2,2′-dimethyl-4,4′-bithiazole, 5,5′-dmbpy is 5,5′-dimethyl-2,2′-bipyridine, 6,6′-dmbpy is 6,6′-dimethyl-2,2′-bipyridine, PBD is *N*-(pyridin-2-ylmethylene)benzene-1,4-diamine, dtbpy is 4,4′-di-*tert*-butyl-2,2′-bipyridine, $NH(py)_2$ is bis(2-pyridyl)amine, $S(py)_2$ is bis(2-pyridyl)sulfide and $NH(py)_2$ is bis(2-pyridyl)amine] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound (I).

In the molecule of the title compound, (I), (Fig. 1), the Zn^{II} atom is four-coordinated in distorted tetrahedral configurations by two N atoms from one 6,6′-dimethyl-2,2′-bipyridine and two terminal I atoms. The Zn—I and Zn—I bond lengths and angles (Table 1) are within normal range (XVI).

The π-π contacts between the pyridine rings, $Cg2\cdots Cg2^{i}$ [symmetry cods: (i) –X,1-Y,1-Z, where, $Cg2$ is centroids of the ring (N1/C2—C6)] further stabilize the structure, with centroid-centroid distance of 3.978 (3) Å. It seems this π-π stacking is effective in the stabilization of the crystal structure (Fig. 2).

S2. Experimental

A solution of 6,6′-dimethyl-2,2′-bipyridine (0.20 g, 1.10 mmol) in methanol (10 ml) was added to a solution of ZnI_2 (0.35 g, 1.10 mmol) in acetonitrile (10 ml) and the resulting colourless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, colourless needles of (I) were isolated (yield 0.41 g, 74.1%).

S3. Refinement

All H atoms were positioned geometrically, with C—H = 0.93–0.96Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

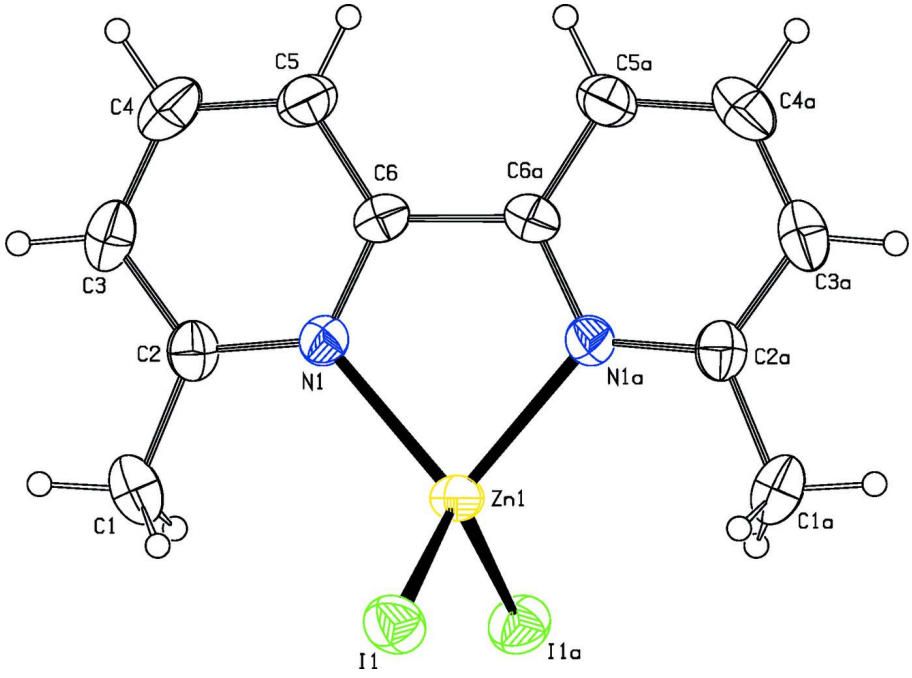

Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

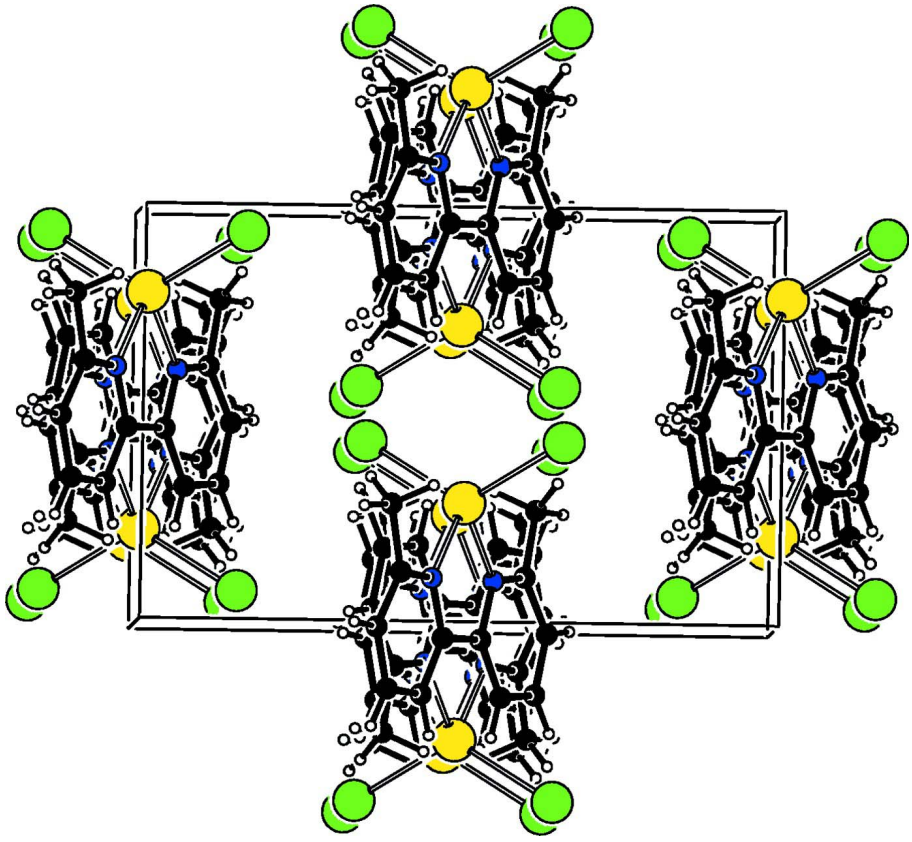

Figure 2

Unit-cell packing diagram for (I).

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Crystal data

$[ZnI_2(C_{12}H_{12}N_2)]$
$M_r = 503.43$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 13.421\ (2)$ Å
$b = 8.441\ (2)$ Å
$c = 13.752\ (3)$ Å
$\beta = 105.140\ (14)°$
$V = 1503.8\ (5)$ Å^3
$Z = 4$
$F(000) = 936$
$D_x = 2.224$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 896 reflections
$\theta = 2.9–29.2°$
$\mu = 5.72$ mm^{-1}
$T = 298$ K
Needle, colourless
0.48 × 0.12 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.425$, $T_{max} = 0.539$
5694 measured reflections
1997 independent reflections
1748 reflections with $I > 2\sigma(I)$
$R_{int} = 0.076$
$\theta_{max} = 29.2°$, $\theta_{min} = 2.9°$
$h = -18\rightarrow18$
$k = -9\rightarrow11$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.127$
$S = 1.12$
1997 reflections
79 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 3.240P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.85$ e Å^{-3}

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}
C1	0.1171 (5)	0.2312 (7)	0.4901 (4)	0.0650 (14)

H1A	0.1495	0.1657	0.4501	0.078*
H1B	0.0518	0.1858	0.4914	0.078*
H1C	0.1607	0.2378	0.5575	0.078*
C2	0.1003 (4)	0.3936 (6)	0.4452 (3)	0.0498 (9)
C3	0.1376 (4)	0.5282 (8)	0.5028 (4)	0.0624 (13)
H3	0.1737	0.5192	0.5702	0.075*
C4	0.1190 (5)	0.6766 (8)	0.4564 (5)	0.0677 (14)
H4	0.1435	0.7680	0.4925	0.081*
C5	0.0640 (4)	0.6862 (6)	0.3567 (4)	0.0581 (11)
H5	0.0499	0.7842	0.3251	0.070*
C6	0.0304 (4)	0.5486 (5)	0.3045 (3)	0.0466 (9)
N1	0.0498 (3)	0.4055 (4)	0.3488 (3)	0.0429 (7)
Zn1	0.0000	0.22134 (8)	0.2500	0.0467 (2)
I1	0.15441 (3)	0.07347 (4)	0.21872 (3)	0.06177 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.061 (3)	0.082 (4)	0.049 (3)	0.010 (3)	0.010 (2)	0.017 (2)
C2	0.045 (2)	0.062 (3)	0.043 (2)	0.0025 (19)	0.0125 (17)	−0.0009 (18)
C3	0.051 (2)	0.086 (4)	0.047 (2)	−0.001 (3)	0.0064 (19)	−0.017 (2)
C4	0.062 (3)	0.068 (3)	0.073 (3)	−0.009 (3)	0.017 (3)	−0.030 (3)
C5	0.058 (3)	0.046 (2)	0.068 (3)	−0.003 (2)	0.011 (2)	−0.011 (2)
C6	0.050 (2)	0.0395 (19)	0.052 (2)	−0.0028 (16)	0.0149 (18)	−0.0068 (16)
N1	0.0444 (17)	0.0428 (17)	0.0406 (16)	0.0000 (14)	0.0097 (13)	−0.0026 (13)
Zn1	0.0570 (4)	0.0354 (3)	0.0469 (4)	0.000	0.0121 (3)	0.000
I1	0.0680 (3)	0.0582 (2)	0.0608 (2)	0.01460 (14)	0.01977 (18)	−0.00003 (13)

Geometric parameters (Å, º)

C1—C2	1.496 (8)	C4—H4	0.9300
C1—H1A	0.9600	C5—C6	1.378 (6)
C1—H1B	0.9600	C5—H5	0.9300
C1—H1C	0.9600	C6—N1	1.347 (6)
C2—N1	1.327 (6)	C6—C6^{i}	1.508 (9)
C2—C3	1.400 (8)	Zn1—N1	2.058 (3)
C3—C4	1.398 (9)	Zn1—N1^{i}	2.058 (3)
C3—H3	0.9300	Zn1—I1^{i}	2.5501 (6)
C4—C5	1.379 (8)	Zn1—I1	2.5501 (6)
C2—C1—H1A	109.5	C6—C5—C4	119.0 (5)
C2—C1—H1B	109.5	C6—C5—H5	120.5
H1A—C1—H1B	109.5	C4—C5—H5	120.5
C2—C1—H1C	109.5	N1—C6—C5	121.5 (5)
H1A—C1—H1C	109.5	N1—C6—C6^{i}	116.1 (2)
H1B—C1—H1C	109.5	C5—C6—C6^{i}	122.4 (3)
N1—C2—C3	121.2 (5)	C2—N1—C6	120.5 (4)
N1—C2—C1	117.7 (4)	C2—N1—Zn1	126.6 (3)

C3—C2—C1	121.2 (5)	C6—N1—Zn1	112.8 (3)
C4—C3—C2	118.3 (5)	N1—Zn1—N1^{i}	81.9 (2)
C4—C3—H3	120.8	N1—Zn1—I1^{i}	113.38 (10)
C2—C3—H3	120.8	N1^{i}—Zn1—I1^{i}	110.04 (10)
C5—C4—C3	119.5 (5)	N1—Zn1—I1	110.04 (10)
C5—C4—H4	120.3	N1^{i}—Zn1—I1	113.38 (10)
C3—C4—H4	120.3	I1^{i}—Zn1—I1	121.39 (3)
N1—C2—C3—C4	0.9 (7)	C5—C6—N1—C2	1.6 (7)
C1—C2—C3—C4	−179.8 (5)	C6^{i}—C6—N1—C2	−178.1 (5)
C2—C3—C4—C5	0.8 (8)	C5—C6—N1—Zn1	−175.7 (4)
C3—C4—C5—C6	−1.3 (8)	C6^{i}—C6—N1—Zn1	4.7 (6)
C4—C5—C6—N1	0.1 (8)	C2—N1—Zn1—N1^{i}	−178.8 (5)
C4—C5—C6—C6^{i}	179.8 (6)	C6—N1—Zn1—N1^{i}	−1.7 (2)
C3—C2—N1—C6	−2.1 (7)	C2—N1—Zn1—I1^{i}	72.8 (4)
C1—C2—N1—C6	178.6 (4)	C6—N1—Zn1—I1^{i}	−110.1 (3)
C3—C2—N1—Zn1	174.7 (3)	C2—N1—Zn1—I1	−66.8 (4)
C1—C2—N1—Zn1	−4.6 (6)	C6—N1—Zn1—I1	110.3 (3)

Symmetry code: (i) $-x, y, -z+1/2$.