

Bis[*E*]-2-(3-hydroxy-4-methoxyphenyl)-ethenyl]-1-methylquinolinium tetraiodozincate(II) methanol solvate¹

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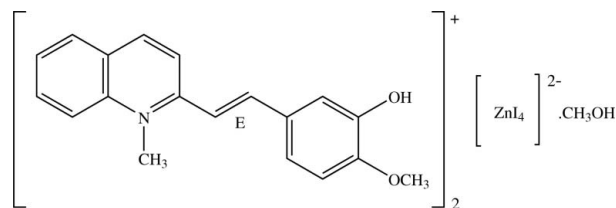
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 40.8.

In the title compound, $(\text{C}_{19}\text{H}_{18}\text{NO}_2)_2[\text{ZnI}_4]\cdot\text{CH}_3\text{OH}$, each cation is nearly planar and exists in an *E* configuration, the dihedral angles between the quinolinium systems and the benzene rings being 1.78 (10) and 5.44 (10)° for the two cations. The $[\text{ZnI}_4]^{2-}$ anion displays a very slightly distorted tetrahedral geometry. There are intramolecular O—H...O hydrogen bonds between the hydroxy and methoxy groups in each cation which generate *S*(5) ring motifs. In the crystal structure, cations are linked together by O—H...O hydrogen bonds and weak C—H...O interactions, whereas the anions are linked to the cations through weak C—H...I interactions. The asymmetric unit also contains a methanol solvent molecule which is linked to one of the cations by an O—H...O hydrogen bond and the anion through an O—H...I hydrogen bond. The crystal is further stabilized by C—H... π and π — π interactions [centroid-centroid distances 3.6054 (15) and 3.6057 (15) Å].

Related literature

For bond-length data, see: Allen *et al.* (1987). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see for example: Chantrapromma *et al.* (2006*a,b*; 2007*a,b,c*); Fun *et al.* (2006); Glavcheva *et al.* (2004); Jindawong *et al.* (2005). For background to non-linear optics, see for example: Oudar & Chemla (1977); Williams (1984).



Experimental

Crystal data

$(\text{C}_{19}\text{H}_{18}\text{NO}_2)_2[\text{ZnI}_4]\cdot\text{CH}_3\text{O}$ $V = 4004.08$ (10) Å³
 $M_r = 1189.72$ $Z = 4$
 Monoclinic, $P2_1/c$ $\text{Mo } K\alpha$ radiation
 $a = 8.6449$ (1) Å $\mu = 3.74$ mm⁻¹
 $b = 23.4312$ (4) Å $T = 100.0$ (1) K
 $c = 19.7763$ (3) Å $0.43 \times 0.28 \times 0.13$ mm
 $\beta = 91.724$ (1)°

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer 100181 measured reflections
 18959 independent reflections
 Absorption correction: multi-scan (SADABS; Bruker, 2005) 15305 reflections with $I > 2\sigma(I)$
 $T_{\min} = 0.295$, $T_{\max} = 0.646$ $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$ 465 parameters
 $wR(F^2) = 0.091$ H-atom parameters constrained
 $S = 1.10$ $\Delta\rho_{\text{max}} = 4.98$ e Å⁻³
 18959 reflections $\Delta\rho_{\text{min}} = -1.46$ e Å⁻³

Table 1

Hydrogen-bond 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> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| O1—H1O1...O2 | 0.82 | 2.15 | 2.611 (3) | 116 |
| O3—H1O3...O4 | 0.82 | 2.23 | 2.673 (3) | 114 |
| O3—H1O3...O5 ⁱ | 0.82 | 1.92 | 2.693 (3) | 156 |
| O5—H1O5...I1 ⁱⁱ | 0.82 | 2.82 | 3.6161 (17) | 163 |
| C2—H2A...O3 ⁱⁱⁱ | 0.93 | 2.56 | 3.476 (3) | 167 |
| C18—H18B...O3 ⁱⁱⁱ | 0.96 | 2.60 | 3.355 (3) | 136 |
| C27—H27A...I4 ^{iv} | 0.93 | 3.02 | 3.899 (3) | 158 |
| C19—H19B...Cg4 | 0.96 | 2.99 | 3.944 (3) | 172 |
| C38—H38B...Cg2 | 0.96 | 2.94 | 3.871 (3) | 165 |

Symmetry codes: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x - 1, y, z - 1$. Cg2 and Cg4 are the centroids of the C12—C17 and C31—C36 benzene rings, respectively.

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2450).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version V7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
- Chantrapromma, S., Jindawong, B. & Fun, H.-K. (2006a). *Acta Cryst.* **E62**, o4004–o4006.
- Chantrapromma, S., Jindawong, B. & Fun, H.-K. (2007a). *Acta Cryst.* **E63**, o2020–o2022.
- Chantrapromma, S., Jindawong, B., Fun, H.-K. & Patil, P. S. (2007c). *Anal. Sci.* **23**, x81–x82.
- Chantrapromma, S., Jindawong, B., Fun, H.-K., Patil, P. S. & Karalai, C. (2006a). *Acta Cryst.* **E62**, o1802–o1804.
- Chantrapromma, S., Jindawong, B., Fun, H.-K., Patil, P. S. & Karalai, C. (2007b). *Anal. Sci.* **23**, x27–x28.
- Fun, H.-K., Rodwatcharapiban, P., Jindawong, B. & Chantrapromma, S. (2006). *Acta Cryst.* **E62**, o2725–o2727.
- Glavcheva, Z., Umezawa, H., Okada, S. & Nakanishi, H. (2004). *Mat. Lett.*, **58**, 2466–2471.
- Jindawong, B., Chantrapromma, S., Fun, H.-K. & Karalai, C. (2005). *Acta Cryst.* **E61**, o3237–o3239.
- Oudar, J.-L. & Chemla, D. S. (1977). *J. Chem. Phys.* **66**, 2664–2668.
- Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Williams, D. J. (1984). *Ang. Chem. Int. Ed. Engl.* **23**, 690–703.

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Bis[(*E*)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]-1-methylquinolinium tetraiodidozincate(II) methanol solvate

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Comment

There is considerable interest in the synthesis of new materials with large second-order nonlinear properties because of their potential usage in a variety of applications such as in optical data storage, optical information processing and telecommunication. We have previously reported the structures of several quinolinium salts (Chantrapromma *et al.*, 2006*a,b*, 2007*a,b,c*; Fun *et al.*, 2006; Jindawong *et al.*, 2005), which were synthesized to study their nonlinear optical (NLO) properties. At the molecular level, a generally popular approach towards NLO materials is to design and synthesize compounds with extended conjugated π systems with donor and acceptor groups because such compounds are likely to exhibit large values of molecular hyperpolarizability (β) and to possess polarizable electrons (as in a conjugated π system) spread over a large distance (Oudar & Chemla, 1977). Quinolinium derivatives are considered to be good conjugated π systems. Organic–inorganic hybrid complexes also present a promising new type of materials for various applications. Thus, we extended our synthesis to this class of materials. This single-crystal X-ray structural study of the title compound was carried out in order to obtain detailed information about its crystal structure. However, the title compound crystallized in the centrosymmetric monoclinic space group $P2_1/c$ and therefore does not exhibit nonlinear optical properties (Williams, 1984).

The asymmetric unit of the title compound consists of two $C_{19}H_{18}NO_2^+$ cations, a ZnI_4^{2-} anion and a methanol solvate molecule (Fig. 1). Each cation is nearly planar as indicated by the dihedral angle between the quinolinium planes and the benzene rings in each cation being 1.78 (10) and 5.44 (10)°, respectively. The H atoms attached to the alkene C atoms C10 and C11 and C29 and C30 are mutually *trans*; torsion angles C9—C10—C11—C12 = 179.1 (2)° and C28—C29—C30—C31 = -179.3 (2)°. Both the hydroxy and methoxy groups are reasonably coplanar with the benzene rings to which they are attached with torsion angles C19—O2—C15—C16 = -0.4 (4)° and C38—O4—C34—C35 = 1.2 (4)°. Both cations form intramolecular O—H \cdots O hydrogen bonds between the hydroxy and methoxy groups which generate S(5) ring motifs (Bernstein *et al.*, 1995). The two cations are approximately parallel to one another with dihedral angles 7.55 (7)° between the two quinolinium planes (C1—C9/N1 and C20—C28/N2) and 12.82 (12)° between the two benzene rings (C12—C17 and C31—C36). The ZnI_4^{2-} anion shows only small distortions from a regular tetrahedron as was found previously (Glavcheva *et al.*, 2004). Zn—I bond distances are in the range 2.6035 (3)–2.6409 (3) Å, and I—Zn—I bond angles lie in the range 106.583 (11)–114.187 (11)°. Bond distances and angles of the cations show normal values (Allen *et al.*, 1987) and are comparable with closely related structures (Chantrapromma *et al.*, 2006*a,b*, 2007*a,b,c*; Fun *et al.*, 2006; Jindawong *et al.*, 2005).

In the crystal packing, the cations are linked together through O—H \cdots O hydrogen bonds and weak C—H \cdots O interactions (Table 1). The cations are also linked to the ZnI_4^{2-} anions through weak C27—H27A \cdots I4 interactions (symmetry code: $-1 + x, y, -1 + z$). The methanol molecule links with the cation by an O3—H1O3 \cdots O5 hydrogen bond (symmetry code: $1 - x, -1/2 + y, 1/2 - z$) and with the ZnI_4^{2-} anion by an O5—H1O5 \cdots I1 hydrogen bond (symmetry code: $1 - x, 1 - y, 1 - z$). The cations are arranged in an antiparallel manner and stacked along the *a* axis in such a way that the centroid–centroid distance between the C1–C6 (Cg_1) and C12–C17 (Cg_2) rings is 3.6054 (15) Å (symmetry code: $1 - x, 1 - y, 1 - z$) and

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that between the C20–C25 (Cg_3) and C31–C36 (Cg_4) rings is 3.6057 (15) Å (symmetry code: $1 - x, 1 - y, -z$), indicating π – π interactions. The crystal is further stabilized by C—H \cdots π interactions (Table 1); Cg_2 and Cg_4 are the centroids of the C12–C17 and C31–C36 benzene rings, respectively.

Experimental

The title compound was synthesized by mixing a solution of 2-[(*E*)-2-(3-Hydroxy-4-methoxyphenyl)ethynyl]-1-methylquinolinium iodide (Chantrapromma *et al.*, 2006a) (0.20 g, 0.48 mmol) in hot methanol (50 ml) and a solution of ZnI₂ (0.19 g, 0.48 mmol) in hot methanol (30 ml). The mixture was stirred for half an hour and then left at room-temperature. The title compound formed as a red solid after 2 days. Red plates suitable for X-ray diffraction analysis were obtained by recrystallization from a methanol/ethanol (1:2 v/v) by slow evaporation of the solvents at ambient temperature after several days, *M.p.* 493–494 K.

Refinement

All H atoms were placed in calculated positions with an O—H distance of 0.82 Å and C—H distances in the range 0.93–0.97 Å. The $U_{iso}(H)$ values were constrained to be $1.5U_{eq}$ of the carrier atom for hydroxyl and methyl H atoms, and $1.2U_{eq}(C)$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.76 Å from I4 and the deepest hole is located at 0.50 Å from I4.

Figures

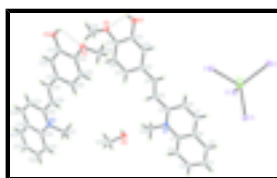


Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed lines indicate O—H \cdots O hydrogen bonds.

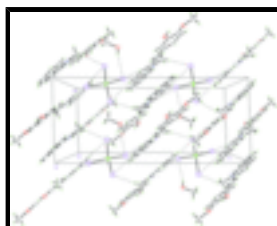


Fig. 2. The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

(C₁₉H₁₈NO₂)₂[ZnI₄]·CH₄O

$M_r = 1189.72$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.6449$ (1) Å

$F_{000} = 2280$

$D_x = 1.974$ Mg m⁻³

Melting point: 493–494 K

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 18959 reflections

| | |
|----------------------------------|---|
| $b = 23.4312 (4) \text{ \AA}$ | $\theta = 1.4\text{--}36.0^\circ$ |
| $c = 19.7763 (3) \text{ \AA}$ | $\mu = 3.74 \text{ mm}^{-1}$ |
| $\beta = 91.724 (1)^\circ$ | $T = 100.0 (1) \text{ K}$ |
| $V = 4004.08 (10) \text{ \AA}^3$ | Plate, orange |
| $Z = 4$ | $0.43 \times 0.28 \times 0.13 \text{ mm}$ |

Data collection

| | |
|--|---|
| Bruker SMART APEX2 CCD area-detector diffractometer | 18959 independent reflections |
| Radiation source: fine-focus sealed tube | 15305 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.033$ |
| Detector resolution: $8.33 \text{ pixels mm}^{-1}$ | $\theta_{\text{max}} = 36.0^\circ$ |
| $T = 100.0(1) \text{ K}$ | $\theta_{\text{min}} = 1.4^\circ$ |
| ω scans | $h = -14 \rightarrow 14$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | $k = -38 \rightarrow 38$ |
| $T_{\text{min}} = 0.295, T_{\text{max}} = 0.646$ | $l = -32 \rightarrow 32$ |
| 100181 measured reflections | |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | H-atom parameters constrained |
| $wR(F^2) = 0.091$ | $w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 5.8575P]$ |
| $S = 1.10$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 18959 reflections | $(\Delta/\sigma)_{\text{max}} = 0.003$ |
| 465 parameters | $\Delta\rho_{\text{max}} = 4.98 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -1.46 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

Special details

Experimental. The low-temperature data was collected with the Oxford Cryosystem Cobra low-temperature attachment.

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 $F^2 > 2\sigma(F^2)$ 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.

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|---------------|----------------------------------|
| Zn1 | 1.00933 (3) | 0.428527 (12) | 0.759635 (14) | 0.01632 (5) |
| I1 | 0.961758 (19) | 0.360714 (7) | 0.654410 (8) | 0.01980 (4) |
| I2 | 0.763779 (18) | 0.492846 (7) | 0.768472 (8) | 0.02042 (4) |
| I3 | 1.242365 (18) | 0.496650 (7) | 0.741500 (8) | 0.01896 (3) |
| I4 | 1.06173 (2) | 0.361619 (7) | 0.865320 (8) | 0.02277 (4) |
| O1 | 0.4535 (3) | 0.23008 (8) | 0.41531 (10) | 0.0276 (4) |
| H1O1 | 0.3889 | 0.2141 | 0.3908 | 0.041* |
| O2 | 0.2948 (2) | 0.26419 (8) | 0.30840 (10) | 0.0228 (4) |
| N1 | 0.7449 (2) | 0.57253 (9) | 0.48296 (10) | 0.0157 (3) |
| C1 | 0.8311 (3) | 0.61157 (10) | 0.52232 (11) | 0.0157 (4) |
| C2 | 0.8240 (3) | 0.67052 (11) | 0.50971 (12) | 0.0195 (4) |
| H2A | 0.7600 | 0.6848 | 0.4751 | 0.023* |
| C3 | 0.9135 (3) | 0.70685 (12) | 0.54942 (13) | 0.0217 (5) |
| H3A | 0.9080 | 0.7459 | 0.5414 | 0.026* |
| C4 | 1.0122 (3) | 0.68662 (12) | 0.60141 (13) | 0.0226 (5) |
| H4A | 1.0736 | 0.7119 | 0.6266 | 0.027* |
| C5 | 1.0179 (3) | 0.62947 (12) | 0.61501 (13) | 0.0218 (5) |
| H5A | 1.0824 | 0.6160 | 0.6499 | 0.026* |
| C6 | 0.9259 (3) | 0.59056 (11) | 0.57618 (12) | 0.0179 (4) |
| C7 | 0.9253 (3) | 0.53154 (11) | 0.59081 (12) | 0.0202 (4) |
| H7A | 0.9854 | 0.5174 | 0.6268 | 0.024* |
| C8 | 0.8368 (3) | 0.49546 (11) | 0.55219 (13) | 0.0204 (4) |
| H8A | 0.8354 | 0.4568 | 0.5626 | 0.024* |
| C9 | 0.7464 (3) | 0.51611 (10) | 0.49612 (12) | 0.0166 (4) |
| C10 | 0.6567 (3) | 0.47728 (11) | 0.45303 (13) | 0.0209 (4) |
| H10A | 0.5975 | 0.4932 | 0.4178 | 0.025* |
| C11 | 0.6525 (3) | 0.42026 (11) | 0.46004 (12) | 0.0182 (4) |
| H11A | 0.7128 | 0.4042 | 0.4948 | 0.022* |
| C12 | 0.5606 (3) | 0.38162 (10) | 0.41721 (12) | 0.0166 (4) |
| C13 | 0.5545 (3) | 0.32353 (10) | 0.43517 (12) | 0.0184 (4) |
| H13A | 0.6117 | 0.3103 | 0.4725 | 0.022* |
| C14 | 0.4634 (3) | 0.28614 (10) | 0.39728 (12) | 0.0180 (4) |
| C15 | 0.3786 (3) | 0.30571 (10) | 0.34013 (11) | 0.0165 (4) |
| C16 | 0.3839 (3) | 0.36292 (10) | 0.32192 (12) | 0.0175 (4) |
| H16A | 0.3272 | 0.3760 | 0.2843 | 0.021* |
| C17 | 0.4750 (3) | 0.40049 (11) | 0.36050 (12) | 0.0186 (4) |
| H17A | 0.4789 | 0.4388 | 0.3483 | 0.022* |
| C18 | 0.6509 (3) | 0.59471 (11) | 0.42510 (13) | 0.0217 (5) |
| H18A | 0.6655 | 0.5710 | 0.3863 | 0.033* |
| H18B | 0.6825 | 0.6330 | 0.4152 | 0.033* |
| H18C | 0.5436 | 0.5946 | 0.4363 | 0.033* |
| C19 | 0.2009 (3) | 0.27958 (12) | 0.25072 (13) | 0.0235 (5) |
| H19A | 0.1487 | 0.2463 | 0.2332 | 0.035* |
| H19B | 0.2649 | 0.2954 | 0.2166 | 0.035* |
| H19C | 0.1258 | 0.3074 | 0.2636 | 0.035* |

| | | | | |
|------|------------|--------------|---------------|------------|
| O3 | 0.4542 (2) | 0.23128 (8) | 0.09856 (10) | 0.0247 (4) |
| H1O3 | 0.5009 | 0.2121 | 0.1272 | 0.037* |
| O4 | 0.6512 (2) | 0.26270 (8) | 0.19848 (10) | 0.0218 (4) |
| N2 | 0.2764 (2) | 0.58183 (9) | 0.01849 (10) | 0.0164 (3) |
| C20 | 0.1990 (3) | 0.62274 (10) | -0.02175 (11) | 0.0162 (4) |
| C21 | 0.2255 (3) | 0.68161 (10) | -0.01304 (12) | 0.0183 (4) |
| H21A | 0.2984 | 0.6945 | 0.0189 | 0.022* |
| C22 | 0.1422 (3) | 0.71975 (11) | -0.05247 (13) | 0.0211 (4) |
| H22A | 0.1611 | 0.7586 | -0.0473 | 0.025* |
| C23 | 0.0292 (3) | 0.70159 (12) | -0.10046 (14) | 0.0228 (5) |
| H23A | -0.0293 | 0.7282 | -0.1251 | 0.027* |
| C24 | 0.0065 (3) | 0.64442 (11) | -0.11052 (13) | 0.0209 (4) |
| H24A | -0.0664 | 0.6322 | -0.1429 | 0.025* |
| C25 | 0.0921 (3) | 0.60365 (11) | -0.07241 (12) | 0.0175 (4) |
| C26 | 0.0762 (3) | 0.54494 (11) | -0.08489 (12) | 0.0201 (4) |
| H26A | 0.0072 | 0.5320 | -0.1185 | 0.024* |
| C27 | 0.1627 (3) | 0.50671 (11) | -0.04747 (13) | 0.0201 (4) |
| H27A | 0.1556 | 0.4680 | -0.0574 | 0.024* |
| C28 | 0.2627 (3) | 0.52520 (10) | 0.00606 (11) | 0.0159 (4) |
| C29 | 0.3499 (3) | 0.48449 (10) | 0.04726 (12) | 0.0180 (4) |
| H29A | 0.4236 | 0.4988 | 0.0780 | 0.022* |
| C30 | 0.3313 (3) | 0.42729 (10) | 0.04406 (12) | 0.0166 (4) |
| H30A | 0.2583 | 0.4130 | 0.0129 | 0.020* |
| C31 | 0.4171 (3) | 0.38655 (10) | 0.08570 (11) | 0.0158 (4) |
| C32 | 0.3966 (3) | 0.32777 (10) | 0.07350 (12) | 0.0165 (4) |
| H32A | 0.3285 | 0.3159 | 0.0390 | 0.020* |
| C33 | 0.4759 (3) | 0.28738 (10) | 0.11199 (12) | 0.0168 (4) |
| C34 | 0.5794 (3) | 0.30554 (10) | 0.16424 (11) | 0.0156 (4) |
| C35 | 0.5998 (3) | 0.36337 (10) | 0.17718 (12) | 0.0167 (4) |
| H35A | 0.6670 | 0.3752 | 0.2120 | 0.020* |
| C36 | 0.5195 (3) | 0.40361 (10) | 0.13794 (12) | 0.0172 (4) |
| H36A | 0.5342 | 0.4423 | 0.1466 | 0.021* |
| C37 | 0.3706 (3) | 0.60281 (11) | 0.07710 (12) | 0.0208 (4) |
| H37A | 0.3660 | 0.5758 | 0.1135 | 0.031* |
| H37B | 0.3308 | 0.6389 | 0.0916 | 0.031* |
| H37C | 0.4760 | 0.6074 | 0.0642 | 0.031* |
| C38 | 0.7552 (3) | 0.27751 (12) | 0.25358 (13) | 0.0231 (5) |
| H38A | 0.7961 | 0.2433 | 0.2741 | 0.035* |
| H38B | 0.7005 | 0.2990 | 0.2866 | 0.035* |
| H38C | 0.8385 | 0.3001 | 0.2370 | 0.035* |
| O5 | 0.4508 (2) | 0.64459 (8) | 0.32101 (11) | 0.0268 (4) |
| H1O5 | 0.3567 | 0.6404 | 0.3178 | 0.040* |
| C39 | 0.5133 (4) | 0.64612 (14) | 0.25496 (16) | 0.0316 (6) |
| H39A | 0.4609 | 0.6749 | 0.2283 | 0.047* |
| H39B | 0.4993 | 0.6096 | 0.2336 | 0.047* |
| H39C | 0.6217 | 0.6549 | 0.2585 | 0.047* |

supplementary materials

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Zn1 | 0.01907 (12) | 0.01326 (12) | 0.01669 (11) | -0.00056 (9) | 0.00160 (9) | -0.00004 (9) |
| I1 | 0.02518 (7) | 0.01483 (7) | 0.01937 (7) | -0.00102 (5) | 0.00049 (6) | -0.00314 (5) |
| I2 | 0.01964 (7) | 0.02145 (8) | 0.02027 (7) | 0.00436 (5) | 0.00210 (5) | 0.00072 (5) |
| I3 | 0.01906 (6) | 0.01890 (7) | 0.01889 (6) | -0.00450 (5) | -0.00014 (5) | -0.00183 (5) |
| I4 | 0.03423 (9) | 0.01546 (7) | 0.01869 (7) | 0.00205 (6) | 0.00207 (6) | 0.00244 (5) |
| O1 | 0.0404 (11) | 0.0138 (8) | 0.0280 (10) | -0.0005 (7) | -0.0109 (9) | 0.0017 (7) |
| O2 | 0.0283 (9) | 0.0184 (8) | 0.0214 (8) | -0.0023 (7) | -0.0062 (7) | -0.0020 (7) |
| N1 | 0.0155 (8) | 0.0180 (9) | 0.0135 (8) | 0.0002 (6) | -0.0010 (6) | 0.0006 (6) |
| C1 | 0.0145 (8) | 0.0188 (10) | 0.0139 (8) | -0.0014 (7) | 0.0013 (7) | -0.0015 (7) |
| C2 | 0.0218 (10) | 0.0202 (11) | 0.0167 (9) | -0.0032 (8) | 0.0000 (8) | -0.0009 (8) |
| C3 | 0.0237 (11) | 0.0216 (12) | 0.0199 (10) | -0.0044 (9) | 0.0016 (9) | -0.0011 (9) |
| C4 | 0.0203 (10) | 0.0275 (13) | 0.0200 (10) | -0.0048 (9) | -0.0009 (9) | -0.0049 (9) |
| C5 | 0.0196 (10) | 0.0271 (13) | 0.0185 (10) | -0.0020 (9) | -0.0020 (8) | -0.0044 (9) |
| C6 | 0.0155 (9) | 0.0232 (11) | 0.0150 (9) | -0.0008 (8) | 0.0000 (7) | -0.0003 (8) |
| C7 | 0.0200 (10) | 0.0236 (12) | 0.0168 (10) | 0.0017 (8) | -0.0017 (8) | 0.0001 (8) |
| C8 | 0.0233 (10) | 0.0197 (11) | 0.0179 (10) | 0.0000 (8) | -0.0020 (8) | 0.0028 (8) |
| C9 | 0.0171 (9) | 0.0171 (10) | 0.0157 (9) | -0.0008 (7) | 0.0000 (7) | 0.0002 (7) |
| C10 | 0.0267 (11) | 0.0168 (11) | 0.0188 (10) | -0.0022 (8) | -0.0056 (9) | 0.0016 (8) |
| C11 | 0.0174 (9) | 0.0193 (11) | 0.0179 (9) | 0.0008 (8) | -0.0017 (8) | 0.0005 (8) |
| C12 | 0.0165 (9) | 0.0172 (10) | 0.0160 (9) | 0.0003 (7) | 0.0000 (8) | 0.0002 (7) |
| C13 | 0.0203 (10) | 0.0180 (10) | 0.0168 (9) | 0.0011 (8) | -0.0023 (8) | 0.0018 (8) |
| C14 | 0.0224 (10) | 0.0135 (10) | 0.0179 (9) | 0.0017 (8) | -0.0018 (8) | 0.0011 (7) |
| C15 | 0.0183 (9) | 0.0167 (10) | 0.0145 (9) | 0.0004 (7) | -0.0002 (7) | 0.0000 (7) |
| C16 | 0.0185 (9) | 0.0176 (10) | 0.0163 (9) | -0.0004 (8) | -0.0016 (8) | 0.0028 (8) |
| C17 | 0.0192 (10) | 0.0165 (10) | 0.0200 (10) | -0.0015 (8) | -0.0004 (8) | 0.0020 (8) |
| C18 | 0.0248 (11) | 0.0194 (11) | 0.0204 (10) | -0.0004 (9) | -0.0067 (9) | -0.0002 (8) |
| C19 | 0.0261 (11) | 0.0274 (13) | 0.0168 (10) | -0.0027 (10) | -0.0036 (9) | -0.0019 (9) |
| O3 | 0.0359 (10) | 0.0135 (8) | 0.0237 (9) | -0.0023 (7) | -0.0147 (8) | 0.0008 (6) |
| O4 | 0.0239 (8) | 0.0195 (8) | 0.0214 (8) | -0.0006 (7) | -0.0082 (7) | 0.0012 (6) |
| N2 | 0.0189 (8) | 0.0157 (9) | 0.0145 (8) | -0.0002 (7) | -0.0006 (7) | -0.0003 (6) |
| C20 | 0.0172 (9) | 0.0179 (10) | 0.0134 (8) | 0.0002 (7) | 0.0020 (7) | 0.0016 (7) |
| C21 | 0.0207 (10) | 0.0152 (10) | 0.0191 (10) | 0.0002 (8) | 0.0029 (8) | 0.0010 (8) |
| C22 | 0.0254 (11) | 0.0169 (11) | 0.0210 (10) | 0.0035 (8) | 0.0033 (9) | 0.0020 (8) |
| C23 | 0.0219 (11) | 0.0233 (12) | 0.0232 (11) | 0.0041 (9) | 0.0004 (9) | 0.0047 (9) |
| C24 | 0.0199 (10) | 0.0239 (12) | 0.0188 (10) | 0.0014 (8) | -0.0002 (8) | 0.0026 (9) |
| C25 | 0.0171 (9) | 0.0200 (11) | 0.0155 (9) | 0.0012 (8) | 0.0011 (8) | 0.0018 (8) |
| C26 | 0.0209 (10) | 0.0219 (11) | 0.0172 (10) | -0.0009 (8) | -0.0027 (8) | -0.0005 (8) |
| C27 | 0.0237 (10) | 0.0174 (11) | 0.0189 (10) | -0.0015 (8) | -0.0021 (8) | -0.0017 (8) |
| C28 | 0.0190 (9) | 0.0142 (10) | 0.0147 (9) | -0.0015 (7) | 0.0012 (8) | -0.0009 (7) |
| C29 | 0.0205 (10) | 0.0172 (10) | 0.0163 (9) | -0.0003 (8) | -0.0016 (8) | 0.0004 (8) |
| C30 | 0.0181 (9) | 0.0149 (10) | 0.0167 (9) | -0.0010 (7) | 0.0005 (8) | 0.0004 (7) |
| C31 | 0.0163 (9) | 0.0160 (10) | 0.0151 (9) | -0.0004 (7) | -0.0015 (7) | -0.0013 (7) |
| C32 | 0.0161 (9) | 0.0170 (10) | 0.0162 (9) | -0.0011 (7) | -0.0030 (7) | -0.0005 (7) |
| C33 | 0.0196 (9) | 0.0143 (9) | 0.0163 (9) | -0.0015 (7) | -0.0031 (8) | -0.0010 (7) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|--------------|
| C34 | 0.0167 (9) | 0.0151 (10) | 0.0150 (9) | -0.0004 (7) | -0.0016 (7) | -0.0003 (7) |
| C35 | 0.0165 (9) | 0.0185 (10) | 0.0151 (9) | -0.0014 (7) | -0.0019 (7) | -0.0023 (7) |
| C36 | 0.0185 (9) | 0.0146 (10) | 0.0185 (9) | -0.0003 (7) | -0.0001 (8) | -0.0024 (8) |
| C37 | 0.0279 (11) | 0.0175 (11) | 0.0168 (10) | -0.0024 (9) | -0.0049 (9) | 0.0008 (8) |
| C38 | 0.0210 (10) | 0.0282 (13) | 0.0196 (10) | -0.0005 (9) | -0.0058 (9) | -0.0009 (9) |
| O5 | 0.0260 (9) | 0.0240 (10) | 0.0300 (10) | -0.0015 (7) | -0.0094 (8) | 0.0014 (8) |
| C39 | 0.0382 (16) | 0.0235 (14) | 0.0330 (15) | 0.0020 (11) | 0.0005 (13) | -0.0007 (11) |

Geometric parameters (Å, °)

| | | | |
|----------|------------|----------|-----------|
| Zn1—I3 | 2.6035 (3) | O3—H1O3 | 0.8200 |
| Zn1—I2 | 2.6135 (3) | O4—C34 | 1.351 (3) |
| Zn1—I1 | 2.6406 (3) | O4—C38 | 1.434 (3) |
| Zn1—I4 | 2.6409 (3) | N2—C28 | 1.354 (3) |
| O1—C14 | 1.364 (3) | N2—C20 | 1.403 (3) |
| O1—H1O1 | 0.8200 | N2—C37 | 1.480 (3) |
| O2—C15 | 1.356 (3) | C20—C21 | 1.408 (3) |
| O2—C19 | 1.426 (3) | C20—C25 | 1.415 (3) |
| N1—C9 | 1.347 (3) | C21—C22 | 1.375 (3) |
| N1—C1 | 1.401 (3) | C21—H21A | 0.9300 |
| N1—C18 | 1.478 (3) | C22—C23 | 1.407 (4) |
| C1—C2 | 1.405 (3) | C22—H22A | 0.9300 |
| C1—C6 | 1.413 (3) | C23—C24 | 1.368 (4) |
| C2—C3 | 1.380 (3) | C23—H23A | 0.9300 |
| C2—H2A | 0.9300 | C24—C25 | 1.412 (3) |
| C3—C4 | 1.399 (4) | C24—H24A | 0.9300 |
| C3—H3A | 0.9300 | C25—C26 | 1.404 (4) |
| C4—C5 | 1.366 (4) | C26—C27 | 1.370 (3) |
| C4—H4A | 0.9300 | C26—H26A | 0.9300 |
| C5—C6 | 1.420 (3) | C27—C28 | 1.415 (3) |
| C5—H5A | 0.9300 | C27—H27A | 0.9300 |
| C6—C7 | 1.413 (4) | C28—C29 | 1.450 (3) |
| C7—C8 | 1.359 (4) | C29—C30 | 1.351 (3) |
| C7—H7A | 0.9300 | C29—H29A | 0.9300 |
| C8—C9 | 1.422 (3) | C30—C31 | 1.450 (3) |
| C8—H8A | 0.9300 | C30—H30A | 0.9300 |
| C9—C10 | 1.455 (3) | C31—C36 | 1.398 (3) |
| C10—C11 | 1.344 (3) | C31—C32 | 1.409 (3) |
| C10—H10A | 0.9300 | C32—C33 | 1.384 (3) |
| C11—C12 | 1.459 (3) | C32—H32A | 0.9300 |
| C11—H11A | 0.9300 | C33—C34 | 1.412 (3) |
| C12—C17 | 1.397 (3) | C34—C35 | 1.389 (3) |
| C12—C13 | 1.408 (3) | C35—C36 | 1.393 (3) |
| C13—C14 | 1.383 (3) | C35—H35A | 0.9300 |
| C13—H13A | 0.9300 | C36—H36A | 0.9300 |
| C14—C15 | 1.405 (3) | C37—H37A | 0.9600 |
| C15—C16 | 1.389 (3) | C37—H37B | 0.9600 |
| C16—C17 | 1.393 (3) | C37—H37C | 0.9600 |
| C16—H16A | 0.9300 | C38—H38A | 0.9600 |

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|--------------|--------------|--------------|-----------|
| C17—H17A | 0.9300 | C38—H38B | 0.9600 |
| C18—H18A | 0.9600 | C38—H38C | 0.9600 |
| C18—H18B | 0.9600 | O5—C39 | 1.429 (4) |
| C18—H18C | 0.9600 | O5—H1O5 | 0.8200 |
| C19—H19A | 0.9600 | C39—H39A | 0.9600 |
| C19—H19B | 0.9600 | C39—H39B | 0.9600 |
| C19—H19C | 0.9600 | C39—H39C | 0.9600 |
| O3—C33 | 1.353 (3) | | |
| I3—Zn1—I2 | 106.804 (12) | C34—O4—C38 | 118.0 (2) |
| I3—Zn1—I1 | 111.295 (11) | C28—N2—C20 | 122.0 (2) |
| I2—Zn1—I1 | 106.985 (11) | C28—N2—C37 | 120.7 (2) |
| I3—Zn1—I4 | 110.977 (11) | C20—N2—C37 | 117.3 (2) |
| I2—Zn1—I4 | 114.187 (11) | N2—C20—C21 | 121.8 (2) |
| I1—Zn1—I4 | 106.583 (11) | N2—C20—C25 | 118.4 (2) |
| C14—O1—H1O1 | 109.5 | C21—C20—C25 | 119.8 (2) |
| C15—O2—C19 | 118.2 (2) | C22—C21—C20 | 119.1 (2) |
| C9—N1—C1 | 122.09 (19) | C22—C21—H21A | 120.4 |
| C9—N1—C18 | 119.8 (2) | C20—C21—H21A | 120.4 |
| C1—N1—C18 | 118.1 (2) | C21—C22—C23 | 121.8 (2) |
| N1—C1—C2 | 121.6 (2) | C21—C22—H22A | 119.1 |
| N1—C1—C6 | 118.6 (2) | C23—C22—H22A | 119.1 |
| C2—C1—C6 | 119.8 (2) | C24—C23—C22 | 119.2 (2) |
| C3—C2—C1 | 119.0 (2) | C24—C23—H23A | 120.4 |
| C3—C2—H2A | 120.5 | C22—C23—H23A | 120.4 |
| C1—C2—H2A | 120.5 | C23—C24—C25 | 120.9 (2) |
| C2—C3—C4 | 121.9 (3) | C23—C24—H24A | 119.5 |
| C2—C3—H3A | 119.0 | C25—C24—H24A | 119.5 |
| C4—C3—H3A | 119.0 | C26—C25—C24 | 121.5 (2) |
| C5—C4—C3 | 119.6 (2) | C26—C25—C20 | 119.5 (2) |
| C5—C4—H4A | 120.2 | C24—C25—C20 | 119.0 (2) |
| C3—C4—H4A | 120.2 | C27—C26—C25 | 119.8 (2) |
| C4—C5—C6 | 120.4 (2) | C27—C26—H26A | 120.1 |
| C4—C5—H5A | 119.8 | C25—C26—H26A | 120.1 |
| C6—C5—H5A | 119.8 | C26—C27—C28 | 121.0 (2) |
| C1—C6—C7 | 119.3 (2) | C26—C27—H27A | 119.5 |
| C1—C6—C5 | 119.1 (2) | C28—C27—H27A | 119.5 |
| C7—C6—C5 | 121.5 (2) | N2—C28—C27 | 118.9 (2) |
| C8—C7—C6 | 119.9 (2) | N2—C28—C29 | 120.1 (2) |
| C8—C7—H7A | 120.0 | C27—C28—C29 | 121.0 (2) |
| C6—C7—H7A | 120.0 | C30—C29—C28 | 124.5 (2) |
| C7—C8—C9 | 120.9 (2) | C30—C29—H29A | 117.7 |
| C7—C8—H8A | 119.6 | C28—C29—H29A | 117.7 |
| C9—C8—H8A | 119.6 | C29—C30—C31 | 124.6 (2) |
| N1—C9—C8 | 119.1 (2) | C29—C30—H30A | 117.7 |
| N1—C9—C10 | 119.9 (2) | C31—C30—H30A | 117.7 |
| C8—C9—C10 | 121.0 (2) | C36—C31—C32 | 118.7 (2) |
| C11—C10—C9 | 125.2 (2) | C36—C31—C30 | 122.2 (2) |
| C11—C10—H10A | 117.4 | C32—C31—C30 | 119.1 (2) |
| C9—C10—H10A | 117.4 | C33—C32—C31 | 121.1 (2) |

| | | | |
|---------------|------------|-----------------|------------|
| C10—C11—C12 | 125.0 (2) | C33—C32—H32A | 119.4 |
| C10—C11—H11A | 117.5 | C31—C32—H32A | 119.4 |
| C12—C11—H11A | 117.5 | O3—C33—C32 | 119.5 (2) |
| C17—C12—C13 | 119.0 (2) | O3—C33—C34 | 121.2 (2) |
| C17—C12—C11 | 122.4 (2) | C32—C33—C34 | 119.3 (2) |
| C13—C12—C11 | 118.5 (2) | O4—C34—C35 | 125.3 (2) |
| C14—C13—C12 | 120.0 (2) | O4—C34—C33 | 114.5 (2) |
| C14—C13—H13A | 120.0 | C35—C34—C33 | 120.2 (2) |
| C12—C13—H13A | 120.0 | C34—C35—C36 | 119.9 (2) |
| O1—C14—C13 | 120.5 (2) | C34—C35—H35A | 120.0 |
| O1—C14—C15 | 119.3 (2) | C36—C35—H35A | 120.0 |
| C13—C14—C15 | 120.2 (2) | C35—C36—C31 | 120.8 (2) |
| O2—C15—C16 | 126.4 (2) | C35—C36—H36A | 119.6 |
| O2—C15—C14 | 113.4 (2) | C31—C36—H36A | 119.6 |
| C16—C15—C14 | 120.2 (2) | N2—C37—H37A | 109.5 |
| C15—C16—C17 | 119.4 (2) | N2—C37—H37B | 109.5 |
| C15—C16—H16A | 120.3 | H37A—C37—H37B | 109.5 |
| C17—C16—H16A | 120.3 | N2—C37—H37C | 109.5 |
| C16—C17—C12 | 121.1 (2) | H37A—C37—H37C | 109.5 |
| C16—C17—H17A | 119.4 | H37B—C37—H37C | 109.5 |
| C12—C17—H17A | 119.4 | O4—C38—H38A | 109.5 |
| N1—C18—H18A | 109.5 | O4—C38—H38B | 109.5 |
| N1—C18—H18B | 109.5 | H38A—C38—H38B | 109.5 |
| H18A—C18—H18B | 109.5 | O4—C38—H38C | 109.5 |
| N1—C18—H18C | 109.5 | H38A—C38—H38C | 109.5 |
| H18A—C18—H18C | 109.5 | H38B—C38—H38C | 109.5 |
| H18B—C18—H18C | 109.5 | C39—O5—H1O5 | 109.5 |
| O2—C19—H19A | 109.5 | O5—C39—H39A | 109.5 |
| O2—C19—H19B | 109.5 | O5—C39—H39B | 109.5 |
| H19A—C19—H19B | 109.5 | H39A—C39—H39B | 109.5 |
| O2—C19—H19C | 109.5 | O5—C39—H39C | 109.5 |
| H19A—C19—H19C | 109.5 | H39A—C39—H39C | 109.5 |
| H19B—C19—H19C | 109.5 | H39B—C39—H39C | 109.5 |
| C33—O3—H1O3 | 109.5 | | |
| C9—N1—C1—C2 | -177.6 (2) | C28—N2—C20—C21 | -173.4 (2) |
| C18—N1—C1—C2 | 2.9 (3) | C37—N2—C20—C21 | 8.6 (3) |
| C9—N1—C1—C6 | 2.0 (3) | C28—N2—C20—C25 | 6.4 (3) |
| C18—N1—C1—C6 | -177.6 (2) | C37—N2—C20—C25 | -171.7 (2) |
| N1—C1—C2—C3 | -178.9 (2) | N2—C20—C21—C22 | -177.8 (2) |
| C6—C1—C2—C3 | 1.6 (4) | C25—C20—C21—C22 | 2.5 (4) |
| C1—C2—C3—C4 | 0.7 (4) | C20—C21—C22—C23 | 1.1 (4) |
| C2—C3—C4—C5 | -1.9 (4) | C21—C22—C23—C24 | -3.1 (4) |
| C3—C4—C5—C6 | 0.8 (4) | C22—C23—C24—C25 | 1.5 (4) |
| N1—C1—C6—C7 | -3.1 (3) | C23—C24—C25—C26 | -176.3 (2) |
| C2—C1—C6—C7 | 176.4 (2) | C23—C24—C25—C20 | 2.1 (4) |
| N1—C1—C6—C5 | 177.9 (2) | N2—C20—C25—C26 | -5.4 (3) |
| C2—C1—C6—C5 | -2.6 (3) | C21—C20—C25—C26 | 174.4 (2) |
| C4—C5—C6—C1 | 1.4 (4) | N2—C20—C25—C24 | 176.2 (2) |
| C4—C5—C6—C7 | -177.6 (2) | C21—C20—C25—C24 | -4.0 (3) |

supplementary materials

| | | | |
|-----------------|------------|-----------------|------------|
| C1—C6—C7—C8 | 1.5 (4) | C24—C25—C26—C27 | 179.1 (2) |
| C5—C6—C7—C8 | -179.4 (2) | C20—C25—C26—C27 | 0.8 (4) |
| C6—C7—C8—C9 | 1.2 (4) | C25—C26—C27—C28 | 3.2 (4) |
| C1—N1—C9—C8 | 0.8 (3) | C20—N2—C28—C27 | -2.5 (3) |
| C18—N1—C9—C8 | -179.7 (2) | C37—N2—C28—C27 | 175.4 (2) |
| C1—N1—C9—C10 | -179.0 (2) | C20—N2—C28—C29 | 177.5 (2) |
| C18—N1—C9—C10 | 0.5 (3) | C37—N2—C28—C29 | -4.6 (3) |
| C7—C8—C9—N1 | -2.4 (4) | C26—C27—C28—N2 | -2.4 (4) |
| C7—C8—C9—C10 | 177.4 (2) | C26—C27—C28—C29 | 177.7 (2) |
| N1—C9—C10—C11 | 178.1 (3) | N2—C28—C29—C30 | 172.1 (2) |
| C8—C9—C10—C11 | -1.7 (4) | C27—C28—C29—C30 | -7.9 (4) |
| C9—C10—C11—C12 | 179.1 (2) | C28—C29—C30—C31 | -179.3 (2) |
| C10—C11—C12—C17 | 4.9 (4) | C29—C30—C31—C36 | 5.7 (4) |
| C10—C11—C12—C13 | -173.1 (3) | C29—C30—C31—C32 | -174.6 (2) |
| C17—C12—C13—C14 | -0.7 (4) | C36—C31—C32—C33 | -0.2 (4) |
| C11—C12—C13—C14 | 177.4 (2) | C30—C31—C32—C33 | -180.0 (2) |
| C12—C13—C14—O1 | -178.3 (2) | C31—C32—C33—O3 | -179.5 (2) |
| C12—C13—C14—C15 | 1.0 (4) | C31—C32—C33—C34 | -0.2 (4) |
| C19—O2—C15—C16 | -0.4 (4) | C38—O4—C34—C35 | 1.2 (4) |
| C19—O2—C15—C14 | 178.4 (2) | C38—O4—C34—C33 | -178.3 (2) |
| O1—C14—C15—O2 | -0.5 (3) | O3—C33—C34—O4 | -0.4 (3) |
| C13—C14—C15—O2 | -179.8 (2) | C32—C33—C34—O4 | -179.7 (2) |
| O1—C14—C15—C16 | 178.3 (2) | O3—C33—C34—C35 | -180.0 (2) |
| C13—C14—C15—C16 | -1.0 (4) | C32—C33—C34—C35 | 0.7 (4) |
| O2—C15—C16—C17 | 179.2 (2) | O4—C34—C35—C36 | 179.6 (2) |
| C14—C15—C16—C17 | 0.5 (4) | C33—C34—C35—C36 | -0.9 (4) |
| C15—C16—C17—C12 | -0.2 (4) | C34—C35—C36—C31 | 0.5 (4) |
| C13—C12—C17—C16 | 0.2 (4) | C32—C31—C36—C35 | 0.0 (4) |
| C11—C12—C17—C16 | -177.7 (2) | C30—C31—C36—C35 | 179.8 (2) |

Hydrogen-bond 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> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| O1—H1O1...O2 | 0.82 | 2.15 | 2.611 (3) | 116 |
| O3—H1O3...O4 | 0.82 | 2.23 | 2.673 (3) | 114 |
| O3—H1O3...O5 ⁱ | 0.82 | 1.92 | 2.693 (3) | 156 |
| O5—H1O5...I1 ⁱⁱ | 0.82 | 2.82 | 3.6161 (17) | 163 |
| C2—H2A...O3 ⁱⁱⁱ | 0.93 | 2.56 | 3.476 (3) | 167 |
| C18—H18B...O3 ⁱⁱⁱ | 0.96 | 2.60 | 3.355 (3) | 136 |
| C27—H27A...I4 ^{iv} | 0.93 | 3.02 | 3.899 (3) | 158 |
| C19—H19B...Cg4 | 0.96 | 2.99 | 3.944 (3) | 172 |
| C38—H38B...Cg2 | 0.96 | 2.94 | 3.871 (3) | 165 |

Symmetry codes: (i) $-x+1, y-1/2, -z+1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y+1/2, -z+1/2$; (iv) $x-1, y, z-1$.

Fig. 1

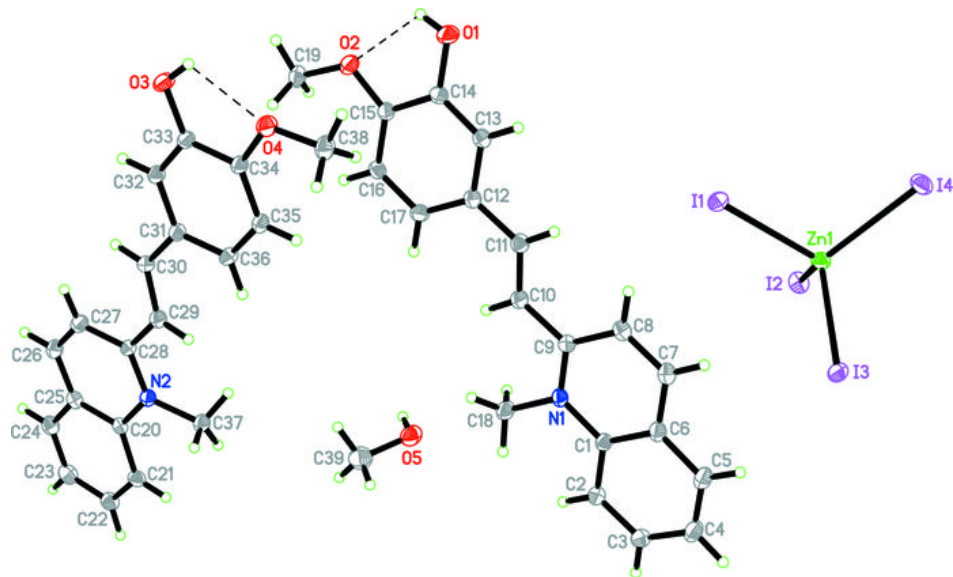


Fig. 2

