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

Suchada Chantrapromma,[a]§ Hoong-Kun Fun,[b]* Kullapa Chanawanno[a] and Pumsak Ruanwas[a]

[a]Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, and [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

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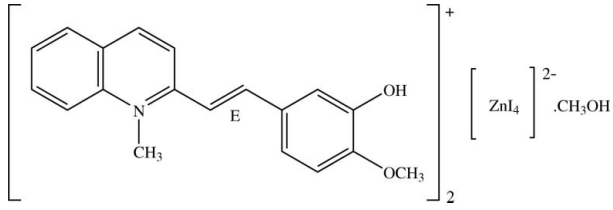
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 40.8.

In the title compound, $(C_{19}H_{18}NO_2)_2[ZnI_4]\cdot CH_3OH$, 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 $[ZnI_4]^{2-}$ 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

$(C_{19}H_{18}NO_2)_2[ZnI_4]\cdot CH_4O$
M_r = 1189.72
Monoclinic, $P2_1/c$
a = 8.6449 (1) Å
b = 23.4312 (4) Å
c = 19.7763 (3) Å
β = 91.724 (1)°
V = 4004.08 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.74 mm^{-1}
T = 100.0 (1) K
0.43 × 0.28 × 0.13 mm

Data collection

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

Refinement

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

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*1···O2	0.82	2.15	2.611 (3)	116
O3—H1*O*3···O4	0.82	2.23	2.673 (3)	114
O3—H1*O*3···O5^{i}	0.82	1.92	2.693 (3)	156
O5—H1*O*5···I1^{ii}	0.82	2.82	3.6161 (17)	163
C2—H2*A*···O3^{iii}	0.93	2.56	3.476 (3)	167
C18—H18*B*···O3^{iii}	0.96	2.60	3.355 (3)	136
C27—H27*A*···I4^{iv}	0.93	3.02	3.899 (3)	158
C19—H19*B*···*Cg*4	0.96	2.99	3.944 (3)	172
C38—H38*B*···*Cg*2	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) $x-1, y, z-1$. *Cg*2 and *Cg*4 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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§ Additional correspondence author, email: suchada.c@psu.ac.th

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

Suchada Chantrapromma, Hoong-Kun Fun, Kullapa Chanawanno and Pumsak Ruanwas

S1. Comment

There is considerable interest in the synthesis of new materials with large second-order nonlinear properties because of their potential usage in a varity 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 systhesize 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···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···O hydrogen bonds and weak C—H···O interactions (Table 1). The cations are also linked to the ZnI_4^{2-} anions through weak C27—H27A···I4 interactions (symmetry code: -1 + *x*, *y*, -1 + *z*). The methanol molecule links with the cation by an O3—H1O3···O5 hydrogen bond

(symmetry code: 1 - *x*, -1/2 + *y*, 1/2 - *z*) and with the ZnI_4^{2-} anion by an O5—H1O5···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 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···π interactions (Table 1); Cg_2 and Cg_4 are the centroids of the C12–C17 and C31–C36 benzene rings, respectively.

S2. Experimental

The title compound was synthesized by mixing a solution of 2-[(*E*)-2-(3-Hydroxy-4-methoxyphenyl)ethynyl]-1-methyl-quinolinium iodide (Chantrapromma *et al.*, 2006*a*) (0.20 g, 0.48 mmol) in hot methanol (50 ml) and a solution of ZnI_2 (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.

S3. 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.

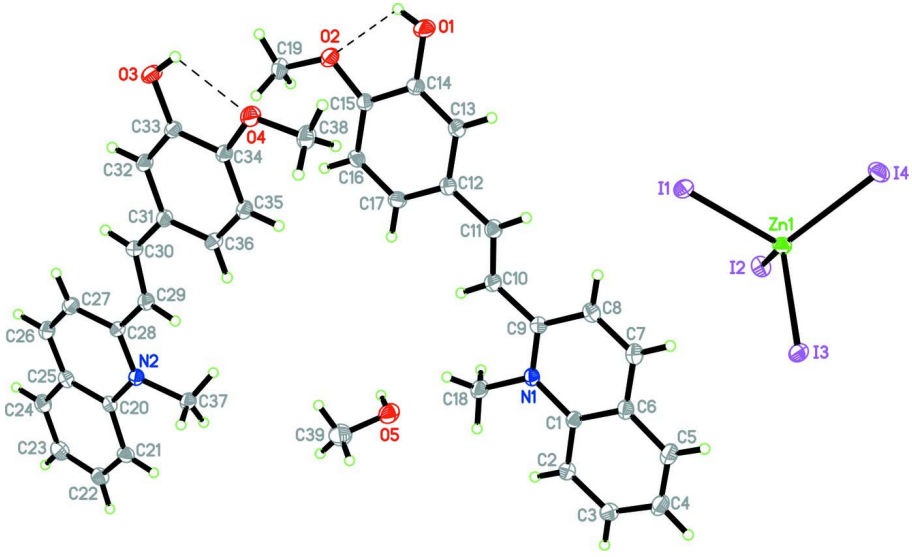

Figure 1

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

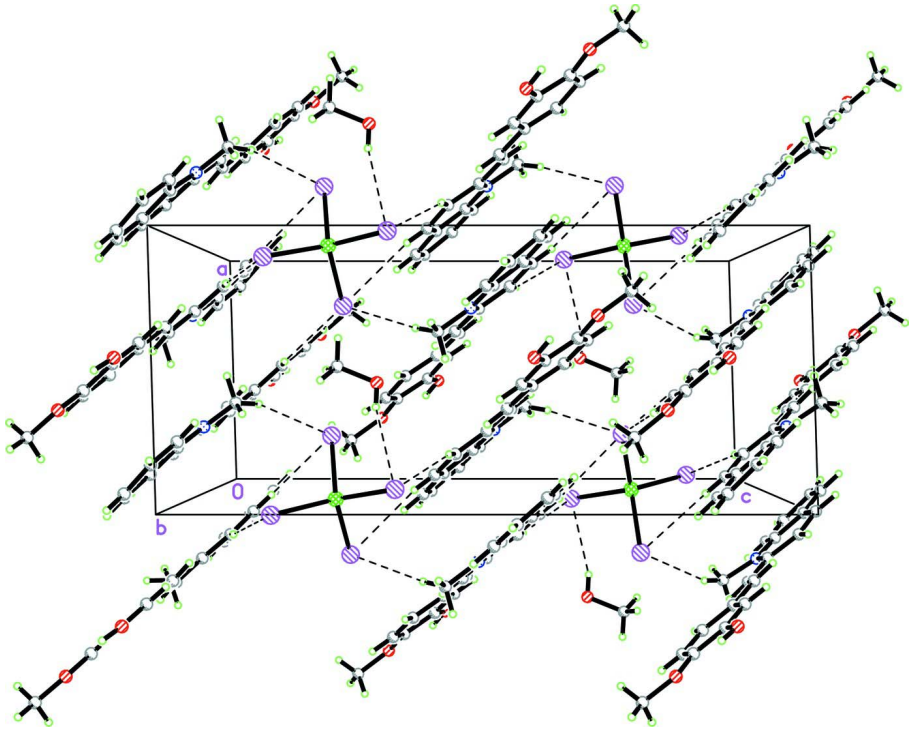

Figure 2

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

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

Crystal data

$(C_{19}H_{18}NO_2)_2[ZnI_4]\cdot CH_4O$
$M_r = 1189.72$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.6449\ (1)$ Å
$b = 23.4312\ (4)$ Å
$c = 19.7763\ (3)$ Å
$\beta = 91.724\ (1)°$
$V = 4004.08\ (10)$ Å^3
$Z = 4$
$F(000) = 2280$
$D_x = 1.974$ Mg m^{-3}
Melting point = 493–494 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 18959 reflections
$\theta = 1.4$–$36.0°$
$\mu = 3.74$ mm^{-1}
$T = 100$ K
Plate, orange
0.43 × 0.28 × 0.13 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.295$, $T_{max} = 0.646$
100181 measured reflections
18959 independent reflections
15305 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 36.0°$, $\theta_{min} = 1.4°$
$h = -14\rightarrow14$
$k = -38\rightarrow38$
$l = -32\rightarrow32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.091$
$S = 1.10$
18959 reflections
465 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
$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 5.8575P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 4.98$ e Å^{-3}
$\Delta\rho_{min} = -1.46$ e Å^{-3}

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem 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 $F^2 > \sigma(F^2)$ 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}
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*

Atomic displacement parameters (Å²)

	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, º)

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
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)
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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*1···O2	0.82	2.15	2.611 (3)	116
O3—H1*O*3···O4	0.82	2.23	2.673 (3)	114
O3—H1*O*3···O5^{i}	0.82	1.92	2.693 (3)	156
O5—H1*O*5···I1^{ii}	0.82	2.82	3.6161 (17)	163
C2—H2*A*···O3^{iii}	0.93	2.56	3.476 (3)	167
C18—H18*B*···O3^{iii}	0.96	2.60	3.355 (3)	136
C27—H27*A*···I4^{iv}	0.93	3.02	3.899 (3)	158
C19—H19*B*···*Cg*4	0.96	2.99	3.944 (3)	172
C38—H38*B*···*Cg*2	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.