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Sodium [*N*,*N*′-ethylenebis(D-penicillaminato)]-indate(III) tetrahydrate

Nobuto Yoshinari* and Takumi Konno

Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan. *Correspondence e-mail: nobuto@chem.sci.osaka-u.ac.jp

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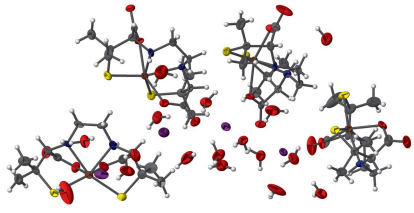
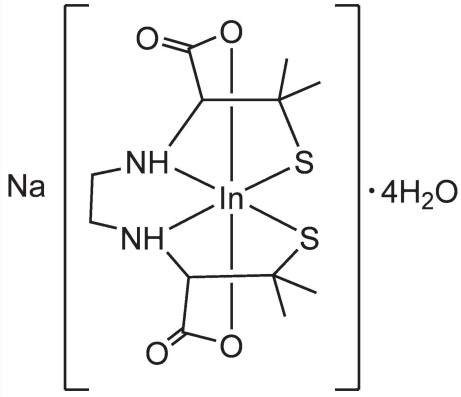
The asymmetric unit of the title compound {systematic name: sodium [2-({2-[(1-carboxylato-2-methyl-2-sulfanidylpropyl)amino]ethyl}amino)-3-methyl-3-sulfanidylbutanoato-κ^4S,N,N',S']indate(III) tetrahydrate}, $Na[In(C_{12}H_{20}N_2O_4S_2)]\cdot 4H_2O$, contains four indate(III) complex anions {$[In(D\text{-ebp})]^-$; D-H_4ebp = *N*,*N*′-ethyelenebis(D-penicillamine)], four sodium(I) cations and sixteen water molecules. The indate(III) anions and sodium cations are alternately connected through coordination bonds between Na^+ ions and the carboxylate groups of the complex anions, forming an infinite sixfold right-handed helix along the *c*-axis direction. In the crystal, the helices are linked by O—H···O hydrogen bonds between water molecules bound to Na^+ ions and carboxylate groups. The crystal studied was twinned *via* a twofold axis about [001].

3D view



Chemical scheme



Structure description

N,*N*′-ethylenebis(D-penicillamine) (D-H_4ebp) (Blondeau *et al.*, 1967) is known as a hexadentate chelating ligand with two thiolate S, two carboxylate O, and amine N donor atoms. Its cobaltate(III) and oxorhenate(V) complexes, $[Co(D\text{-ebp})]^-$ and $[ReO(D\text{-ebp})]^-$ have been synthesized and their chemical reactivity toward alkyl halides and pH response have been reported (Okamoto *et al.*, 1991; Hansen *et al.*, 2000). As part of our ongoing studies on the stepwise synthesis of S-bridged multinuclear metal complexes with D-penicillamine and its derivatives (Yoshinari & Konno, 2018), we recently reported the first multinuclear metal complexes with D-H_4ebp (Hayashi *et al.*, 2019). To create S-bridged multinuclear complexes with main-group metal ions, we designed a new iridium(III) complex with D-H_4ebp. We report herein the crystal structure of the title compound (**1**). This is the first main-group metal complex with D-ebp, although a similar indate(III) complex with a related hexadentate-S_2,N_2,O_2 ligand, $Na[In^{III}(L\text{-ebc})]\cdot 2H_2O$ (L-H_4ebc = *N*,*N*′-ethylenebis-L-cysteine) (**2**), has been reported (Li *et al.*, 1996).

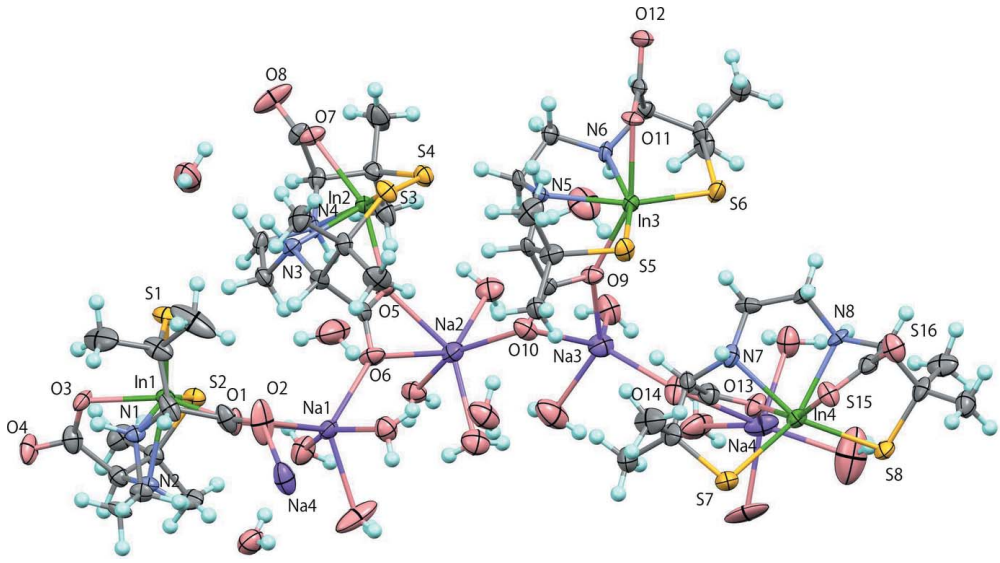


Figure 1
A perspective view of the asymmetric unit of **1** with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

A displacement ellipsoid plot with the atom-numbering scheme of **1** is given in Fig. 1. In each of the four crystallographically independent $[In(D\text{-ebp})]^-$ anions, the central In^{III} atom is surrounded by a hexadentate D-ebp ligand. The coordination geometry of each central In^{III} atom is highly distorted from a regular octahedron with large *cis* S—In—S angles of 120.52 (10), 121.30 (10), 119.79 (10) and 120.31 (10)°. The angles are slightly larger than those in **2** [S—In—S = 115.87 (14)°], most likely as a result of the steric hindrance of the four methyl groups on the D-ebp ligand. In **1**, the $[In(D\text{-ebp})]^-$ anions are linked infinitely by Na^+ ions through Na—O coordination bonds [Na—O = 2.289 (10)–2.796 (11) Å] so as to form a sixfold righthanded helical chain along the *c*-axis direction (Fig. 2). This is distinct from the straight Na—In chain formed for **2**. In the crystal, the helices are linked by O—H···O hydrogen bonds (Table 1) between water molecules bound to Na^+ ions and carboxylate groups. There are also several N—H···O hydrogen bonds between amino groups and water molecules, supporting the crystal lattice.

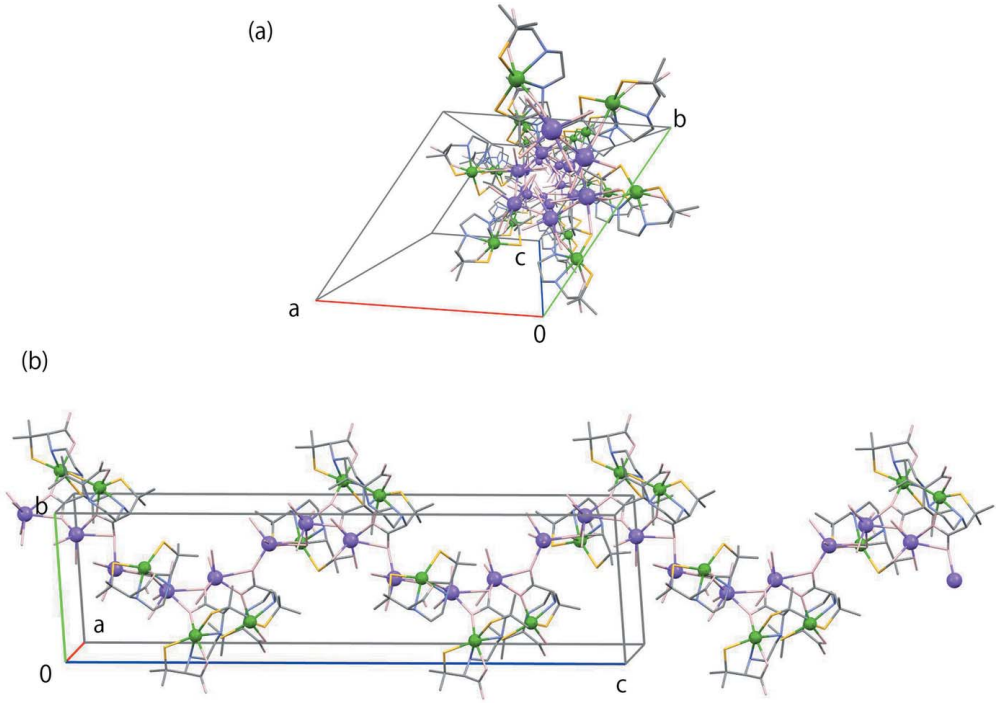


Figure 2
(*a*) Top and (*b*) side views of the helical chain structure along the *c*-axis direction in **1**. Hydrogen atoms are omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O32	1.00	2.04	3.003 (13)	160
N3—H21···O28	1.00	2.36	3.302 (15)	156
N4—H22···O29	1.00	2.08	3.007 (15)	154
N5—H41···O32^{i}	1.00	2.29	3.246 (13)	160
N6—H42···O31	1.00	2.12	3.045 (13)	154
N7—H61···O29^{ii}	1.00	2.52	3.495 (17)	164
N8—H62···O28^{iii}	1.00	2.23	3.143 (14)	151

Symmetry codes: (i) $x-1, y-1, z$; (ii) $x-1, y, z$; (iii) $-y, x-y, z-\frac{1}{3}$.

Synthesis and crystallization

A solution containing D-H_4ebp (50 mg, 0.15 mmol) in water (5 ml) was added to a 3.0 *M* aqueous NaOH solution (210 ml, 0.63 mmol) and $InCl_3$ (34 mg, 0.15 mmol). The mixture was stirred at 70°C for 1 h under an N_2 atmosphere, which gave a colourless solution. After slow evaporation of the solution under aerobic conditions, colourless needle-shaped crystals of the title compound appeared almost quantitatively.

^{1}H NMR (400 MHz, D_2O, p.p.m. from DSS): δ 1.45 (6*H*, *s*, CH_3), 1.49 (6*H*, *s*, CH_3), 2.30 (2*H*, *d*, *J* = 9.3 Hz, CH_2), 3.23 (2*H*, *d*, *J* = 9.3 Hz, CH_2), 3.52 p.p.m. (2*H*, *s*, C*H*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. 24 H atoms (H81, H82, H83, H84, H85, H87, H89, H89, H90, H92, H93, H95, H96, H97, H98, H99, H100, H102, H103, H104, H108, H109, H110 and H111) were refined with intermolecular H···S distance restraints or H···Na antibumping restraints so as to form reasonable hydrogen bonds. The crystal data were refined under consideration of twinning *via* a twofold axis about [001] using the matrix ($\bar{1}00$, $0\bar{1}0$, 001).

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Table 2
Experimental details.

Crystal data	
Chemical formula	Na[In($C_{12}H_{20}N_2O_4S_2$)]·4H_2O
M_r	530.30
Crystal system, space group	Trigonal, $P3_2$
Temperature (K)	200
a, *c* (Å)	13.3725 (17), 40.840 (5)
V (Å^3)	6324.7 (18)
Z	12
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.38
Crystal size (mm)	0.20 × 0.05 × 0.02
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.508, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	55488, 18807, 17163
R_{int}	0.070
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.076, 1.04
No. of reflections	18807
No. of parameters	1050
No. of restraints	77
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.66, −0.67
Absolute structure	Flack *x* determined using 6790 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.006 (10)

Computer programs: *PROCESS-AUTO* (Rigaku, 1998), *CrystalStructure* (Rigaku/MSC, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) nd *publCIF* (Westrip, 2010).

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full crystallographic data

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Sodium [*N*,*N*′-ethylenebis(D-penicillaminato)]indate(III) tetrahydrate

Nobuto Yoshinari and Takumi Konno

Sodium [2-({2-[(1-carboxylato-2-methyl-2-sulfanidylpropyl)amino]ethyl}amino)-3-methyl-\ 3-sulfanidylbutanoato-κ^4S,N,N',S']indate(III) tetrahydrate

Crystal data

$Na[In(C_{12}H_{20}N_2O_4S_2)]\cdot 4H_2O$
M_r = 530.30
Trigonal, $P3_2$
a = 13.3725 (17) Å
c = 40.840 (5) Å
V = 6324.7 (18) Å^3
Z = 12
$F(000)$ = 3240
D_x = 1.671 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 50136 reflections
θ = 3.0–27.5°
μ = 1.38 mm^{-1}
T = 200 K
Needle, colorless
0.20 × 0.05 × 0.02 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.508, T_{max} = 0.960
55488 measured reflections
18807 independent reflections
17163 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −17→17
k = −17→17
l = −52→50

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.076
S = 1.04
18807 reflections
1050 parameters
77 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0175P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}
Absolute structure: Flack x determined using 6790 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.006 (10)

Special details

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

Refinement. H atoms bound to C and N atoms were placed at calculated positions [C—H = 0.99 (CH_2), 1.00 (CH), or 0.98 Å (CH_3) and N—H = 0.88 Å (NH)] and refined as riding models with U_{iso}(H) = 1.2U_{eq}(C,*N*) for CH_2, CH, and NH and U_{iso}(H) = 1.5U_{eq}(C) for CH_3. H atoms of water molecules were placed so as to form reasonable hydrogen bonding, and were refined with restrained geometric and displacement parameters [O—H = 0.85 (5) Å, H···H = 1.38 (5) Å andU_{iso}(H) = 1.2U_{eq}(O)]. Refined as a two-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
In1	0.80767 (8)	0.71885 (8)	0.90524 (2)	0.02286 (15)
S1	0.6551 (3)	0.5616 (2)	0.93765 (8)	0.0386 (7)
S2	0.8712 (2)	0.6776 (2)	0.85256 (6)	0.0276 (6)
O1	0.6758 (7)	0.7673 (7)	0.89224 (19)	0.0315 (19)
O2	0.5385 (9)	0.7901 (11)	0.9165 (2)	0.071 (4)
O3	0.9686 (6)	0.7406 (7)	0.92835 (18)	0.0316 (18)
O4	1.1578 (7)	0.8447 (8)	0.9248 (2)	0.042 (2)
N1	0.8045 (8)	0.8345 (7)	0.9470 (2)	0.025 (2)
H1	0.842441	0.826949	0.967189	0.029*
N2	0.9546 (7)	0.9032 (7)	0.8918 (2)	0.0235 (19)
H2	0.934263	0.931918	0.871732	0.028*
C1	0.6303 (11)	0.6583 (11)	0.9648 (3)	0.040 (3)
C2	0.6801 (9)	0.7807 (10)	0.9514 (3)	0.032 (3)
H3	0.663814	0.827554	0.967301	0.038*
C3	0.6265 (11)	0.7813 (11)	0.9182 (3)	0.038 (3)
C4	0.6863 (16)	0.6609 (12)	0.9977 (3)	0.068 (5)
H4	0.686247	0.720291	1.011702	0.102*
H5	0.765992	0.678641	0.994050	0.102*
H6	0.642562	0.585382	1.008324	0.102*
C5	0.4999 (12)	0.6031 (14)	0.9708 (4)	0.085 (7)
H7	0.465824	0.628965	0.953965	0.128*
H8	0.486859	0.626377	0.992455	0.128*
H9	0.463946	0.518855	0.970008	0.128*
C6	1.0209 (9)	0.8055 (9)	0.8532 (3)	0.027 (2)
C7	1.0471 (10)	0.8778 (10)	0.8849 (3)	0.029 (3)
H10	1.120632	0.952524	0.881675	0.035*
C8	1.0601 (10)	0.8176 (12)	0.9153 (3)	0.037 (3)
C9	1.0377 (10)	0.8831 (10)	0.8228 (3)	0.035 (3)
H11	1.009751	0.834877	0.803134	0.052*
H12	1.119818	0.939956	0.820246	0.052*
H13	0.993979	0.923305	0.825958	0.052*
C10	1.1063 (11)	0.7607 (12)	0.8494 (3)	0.042 (3)
H14	1.102012	0.715417	0.868823	0.062*
H15	1.184923	0.826245	0.847218	0.062*
H16	1.086407	0.711801	0.829912	0.062*
C11	0.8638 (9)	0.9573 (9)	0.9350 (3)	0.026 (2)
H17	0.878655	1.010728	0.953557	0.032*
H18	0.814863	0.967750	0.918794	0.032*
C12	0.9770 (9)	0.9818 (9)	0.9194 (3)	0.027 (2)

H19	1.019502	1.062701	0.911646	0.033*
H20	1.025490	0.971550	0.935900	0.033*
In2	0.34944 (6)	0.22759 (7)	0.82384 (2)	0.02266 (15)
S3	0.1940 (2)	0.2254 (3)	0.85610 (7)	0.0323 (6)
S4	0.3096 (2)	0.1226 (2)	0.77141 (7)	0.0306 (6)
O5	0.4002 (7)	0.4056 (6)	0.80704 (17)	0.0271 (17)
O6	0.4370 (7)	0.5739 (6)	0.82628 (19)	0.0348 (18)
O7	0.3722 (7)	0.0880 (6)	0.84732 (18)	0.0313 (18)
O8	0.4689 (10)	−0.0044 (9)	0.8399 (2)	0.063 (3)
N3	0.4638 (7)	0.3538 (7)	0.8655 (2)	0.0229 (19)
H21	0.451572	0.312942	0.886897	0.027*
N4	0.5322 (7)	0.2652 (8)	0.8117 (2)	0.0242 (19)
H22	0.562013	0.316957	0.792149	0.029*
C13	0.2865 (10)	0.3614 (10)	0.8788 (2)	0.028 (2)
C14	0.4140 (9)	0.4287 (9)	0.8654 (2)	0.023 (2)
H23	0.461017	0.495837	0.880143	0.027*
C15	0.4158 (9)	0.4756 (9)	0.8300 (3)	0.027 (2)
C16	0.2322 (11)	0.4381 (11)	0.8759 (3)	0.045 (3)
H24	0.282744	0.512744	0.886372	0.067*
H25	0.156812	0.400525	0.886813	0.067*
H26	0.222369	0.450132	0.852761	0.067*
C17	0.2885 (12)	0.3313 (12)	0.9145 (3)	0.046 (3)
H27	0.210882	0.298994	0.923740	0.069*
H28	0.342075	0.401185	0.926555	0.069*
H29	0.314021	0.274389	0.916126	0.069*
C18	0.4420 (9)	0.1085 (9)	0.7708 (3)	0.028 (2)
C19	0.5108 (9)	0.1489 (9)	0.8030 (2)	0.025 (2)
H30	0.586346	0.151408	0.800223	0.030*
C20	0.4461 (10)	0.0713 (10)	0.8322 (3)	0.028 (3)
C21	0.5170 (10)	0.1775 (11)	0.7428 (3)	0.043 (3)
H31	0.480582	0.139642	0.722148	0.064*
H32	0.592557	0.182916	0.744730	0.064*
H33	0.526838	0.255237	0.743285	0.064*
C22	0.4031 (12)	−0.0186 (12)	0.7649 (4)	0.051 (4)
H34	0.469973	−0.029856	0.766225	0.077*
H35	0.367886	−0.041476	0.743185	0.077*
H36	0.346407	−0.066009	0.781630	0.077*
C23	0.5872 (9)	0.4109 (10)	0.8548 (3)	0.029 (3)
H37	0.638691	0.447520	0.873822	0.035*
H38	0.602681	0.471723	0.838469	0.035*
C24	0.6097 (10)	0.3215 (10)	0.8401 (3)	0.029 (3)
H39	0.691178	0.358266	0.832825	0.035*
H40	0.596894	0.262602	0.856765	0.035*
In3	−0.13343 (6)	0.17065 (8)	0.73892 (2)	0.02185 (14)
S5	−0.1703 (2)	0.3022 (2)	0.77206 (7)	0.0308 (6)
S6	−0.2282 (3)	0.1041 (3)	0.68549 (7)	0.0351 (7)
O9	0.0452 (7)	0.3234 (6)	0.73069 (17)	0.0289 (17)
O10	0.1861 (7)	0.4659 (6)	0.75994 (19)	0.0347 (18)

O11	−0.2611 (6)	−0.0034 (6)	0.76053 (17)	0.0261 (17)
O12	−0.3270 (7)	−0.1895 (6)	0.75325 (19)	0.036 (2)
N5	−0.0180 (7)	0.1818 (7)	0.78292 (19)	0.0194 (18)
H41	−0.066650	0.135336	0.801817	0.023*
N6	−0.0708 (7)	0.0411 (7)	0.7257 (2)	0.0221 (19)
H42	−0.016880	0.070319	0.706603	0.026*
C25	−0.0551 (10)	0.3344 (10)	0.8029 (2)	0.030 (3)
C26	0.0370 (9)	0.3050 (8)	0.7900 (2)	0.021 (2)
H43	0.097303	0.325151	0.807223	0.025*
C27	0.0946 (9)	0.3704 (9)	0.7587 (2)	0.022 (2)
C28	−0.2273 (9)	−0.0331 (9)	0.6844 (2)	0.026 (2)
C29	−0.1800 (10)	−0.0591 (10)	0.7162 (3)	0.028 (2)
H44	−0.167937	−0.126154	0.712289	0.033*
C30	−0.2618 (9)	−0.0860 (9)	0.7457 (2)	0.024 (2)
C31	−0.1144 (12)	0.2625 (11)	0.8339 (3)	0.044 (3)
H45	−0.165375	0.288046	0.843306	0.065*
H46	−0.055518	0.273357	0.850047	0.065*
H47	−0.159927	0.180604	0.828078	0.065*
C32	0.0022 (10)	0.4622 (10)	0.8117 (3)	0.034 (3)
H48	0.069281	0.483261	0.825701	0.051*
H49	−0.053199	0.476967	0.823348	0.051*
H50	0.027173	0.508517	0.791598	0.051*
C33	−0.1499 (10)	−0.0291 (11)	0.6550 (3)	0.038 (3)
H51	−0.169047	0.000816	0.635522	0.057*
H52	−0.163971	−0.107060	0.650567	0.057*
H53	−0.068425	0.021585	0.660578	0.057*
C34	−0.3502 (11)	−0.1318 (11)	0.6782 (3)	0.037 (3)
H54	−0.401065	−0.133609	0.695701	0.056*
H55	−0.350599	−0.205282	0.677704	0.056*
H56	−0.377681	−0.119792	0.657087	0.056*
C35	0.0593 (9)	0.1384 (9)	0.7720 (2)	0.024 (2)
H57	0.098280	0.127573	0.791194	0.029*
H58	0.119188	0.194980	0.757107	0.029*
C36	−0.0134 (9)	0.0227 (10)	0.7542 (3)	0.027 (2)
H59	0.036840	−0.007621	0.746796	0.032*
H60	−0.072109	−0.034405	0.769331	0.032*
In4	−0.18314 (6)	0.59570 (7)	0.65354 (2)	0.02535 (16)
S7	−0.0320 (3)	0.7584 (3)	0.68434 (7)	0.0351 (7)
S8	−0.2528 (3)	0.6289 (3)	0.60124 (7)	0.0321 (6)
O13	−0.0478 (7)	0.5516 (7)	0.63979 (19)	0.0339 (19)
O14	0.0914 (7)	0.5306 (9)	0.6622 (2)	0.047 (2)
O15	−0.3502 (6)	0.5629 (7)	0.67759 (18)	0.0310 (18)
O16	−0.5409 (7)	0.4567 (8)	0.6707 (2)	0.043 (2)
N7	−0.1691 (8)	0.4860 (8)	0.6964 (2)	0.029 (2)
H61	−0.203082	0.497552	0.716836	0.035*
N8	−0.3235 (8)	0.4063 (7)	0.6420 (2)	0.024 (2)
H62	−0.299978	0.377320	0.622589	0.029*
C37	0.0075 (12)	0.6721 (11)	0.7113 (3)	0.038 (3)

C38	−0.0429 (9)	0.5446 (10)	0.6992 (3)	0.029 (2)
H63	−0.020233	0.501190	0.714597	0.035*
C39	0.0036 (10)	0.5445 (10)	0.6642 (3)	0.033 (3)
C40	−0.0394 (14)	0.6701 (12)	0.7462 (3)	0.057 (4)
H64	0.006629	0.746191	0.756382	0.086*
H65	−0.034226	0.611835	0.759493	0.086*
H66	−0.120161	0.651083	0.744763	0.086*
C41	0.1398 (11)	0.7278 (12)	0.7128 (4)	0.055 (4)
H67	0.160570	0.687976	0.729279	0.082*
H68	0.174052	0.809434	0.718795	0.082*
H69	0.168956	0.721533	0.691366	0.082*
C42	−0.3958 (11)	0.4935 (11)	0.6007 (3)	0.033 (3)
C43	−0.4215 (10)	0.4229 (10)	0.6334 (3)	0.026 (2)
H70	−0.492496	0.345801	0.630512	0.032*
C44	−0.4385 (10)	0.4851 (10)	0.6624 (3)	0.028 (3)
C45	−0.3969 (12)	0.4173 (11)	0.5730 (3)	0.046 (3)
H71	−0.400051	0.450866	0.551965	0.069*
H72	−0.464694	0.340040	0.575175	0.069*
H73	−0.326606	0.411685	0.573966	0.069*
C46	−0.4874 (10)	0.5252 (12)	0.5951 (3)	0.042 (3)
H74	−0.563671	0.455367	0.595757	0.063*
H75	−0.475810	0.562283	0.573634	0.063*
H76	−0.482690	0.578770	0.612224	0.063*
C47	−0.2303 (10)	0.3659 (9)	0.6871 (3)	0.032 (3)
H77	−0.244749	0.318052	0.706984	0.038*
H78	−0.181155	0.350620	0.672214	0.038*
C48	−0.3431 (11)	0.3307 (10)	0.6706 (3)	0.033 (3)
H79	−0.378877	0.249331	0.663362	0.039*
H80	−0.396364	0.337027	0.686189	0.039*
Na1	0.5474 (4)	0.7552 (4)	0.84934 (10)	0.0300 (10)
Na2	0.3897 (4)	0.5160 (4)	0.76279 (11)	0.0357 (11)
Na3	0.1789 (4)	0.4514 (4)	0.69228 (12)	0.0394 (11)
Na4	0.0712 (5)	0.5601 (5)	0.59539 (13)	0.0503 (14)
O17	0.7134 (8)	0.7753 (9)	0.8184 (2)	0.049 (2)
H81	0.734 (10)	0.724 (8)	0.819 (2)	0.059*
H82	0.705 (12)	0.786 (10)	0.7979 (10)	0.059*
O18	0.6165 (11)	0.9304 (11)	0.8206 (3)	0.079 (4)
H83	0.640 (12)	0.938 (12)	0.8008 (15)	0.095*
H84	0.576 (12)	0.964 (13)	0.822 (3)	0.095*
O19	0.3735 (8)	0.7639 (8)	0.8570 (2)	0.040 (2)
H85	0.386 (9)	0.831 (3)	0.855 (3)	0.047*
H86	0.316 (7)	0.715 (6)	0.847 (3)	0.047*
O20	0.5833 (7)	0.5857 (7)	0.7402 (2)	0.0376 (19)
H87	0.595 (10)	0.590 (8)	0.7194 (8)	0.045*
H88	0.601 (6)	0.653 (3)	0.747 (2)	0.045*
O21	0.4313 (8)	0.7105 (8)	0.7502 (2)	0.049 (2)
H89	0.504 (3)	0.741 (6)	0.753 (2)	0.058*
H90	0.414 (9)	0.697 (6)	0.7301 (10)	0.058*

O22	0.3332 (8)	0.3489 (8)	0.7291 (2)	0.046 (2)
H91	0.373 (9)	0.377 (10)	0.7118 (18)	0.056*
H92	0.361 (8)	0.310 (8)	0.739 (2)	0.056*
O23	0.3678 (9)	0.6011 (10)	0.6896 (3)	0.068 (3)
H93	0.354 (6)	0.630 (8)	0.673 (2)	0.082*
H94	0.422 (10)	0.586 (13)	0.685 (3)	0.082*
O24	0.2237 (8)	0.3419 (8)	0.6576 (2)	0.051 (2)
H95	0.231 (9)	0.375 (7)	0.6385 (12)	0.061*
H96	0.293 (4)	0.347 (8)	0.659 (3)	0.061*
O25	0.2531 (10)	0.5569 (9)	0.5924 (3)	0.071 (3)
H97	0.260 (15)	0.574 (10)	0.5718 (11)	0.086*
H98	0.227 (14)	0.485 (3)	0.594 (3)	0.086*
O26	−0.0207 (8)	0.3605 (9)	0.5793 (2)	0.050 (2)
H99	−0.053 (6)	0.346 (9)	0.5593 (9)	0.060*
H100	0.036 (7)	0.347 (11)	0.576 (2)	0.060*
O27	−0.0495 (14)	0.6058 (17)	0.5599 (3)	0.117 (6)
H101	−0.117 (6)	0.591 (16)	0.565 (4)	0.140*
H102	−0.055 (13)	0.564 (15)	0.543 (3)	0.140*
O28	0.5054 (9)	0.2466 (9)	0.9336 (3)	0.069 (3)
H103	0.454 (7)	0.179 (3)	0.9274 (18)	0.082*
H104	0.475 (10)	0.267 (8)	0.949 (2)	0.082*
O29	0.6791 (10)	0.4671 (10)	0.7679 (4)	0.082 (4)
H105	0.653 (14)	0.513 (11)	0.764 (4)	0.098*
H106	0.726 (12)	0.494 (12)	0.784 (3)	0.098*
O30	0.2701 (9)	0.6871 (9)	0.7946 (2)	0.057 (3)
H107	0.228 (10)	0.612 (3)	0.792 (3)	0.068*
H108	0.308 (9)	0.710 (9)	0.7759 (17)	0.068*
O31	0.1417 (9)	0.1217 (10)	0.6826 (3)	0.068 (3)
H109	0.140 (10)	0.176 (6)	0.671 (3)	0.082*
H110	0.201 (9)	0.161 (7)	0.696 (3)	0.082*
O32	0.8588 (8)	0.9988 (8)	0.8422 (3)	0.052 (2)
H111	0.798 (5)	1.006 (9)	0.848 (2)	0.062*
H112	0.826 (7)	0.932 (6)	0.833 (3)	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.0240 (4)	0.0217 (4)	0.0228 (3)	0.0113 (3)	0.0008 (3)	−0.0008 (3)
S1	0.0443 (19)	0.0238 (15)	0.0333 (15)	0.0062 (14)	0.0101 (14)	0.0011 (12)
S2	0.0306 (15)	0.0251 (14)	0.0267 (12)	0.0135 (12)	0.0037 (11)	−0.0023 (11)
O1	0.028 (4)	0.049 (5)	0.028 (4)	0.028 (4)	−0.007 (3)	−0.007 (4)
O2	0.052 (6)	0.130 (10)	0.070 (7)	0.074 (7)	−0.019 (5)	−0.039 (7)
O3	0.028 (4)	0.039 (5)	0.033 (4)	0.021 (4)	0.004 (3)	0.017 (4)
O4	0.021 (4)	0.070 (6)	0.041 (5)	0.026 (4)	0.001 (4)	0.010 (4)
N1	0.023 (5)	0.024 (5)	0.025 (5)	0.011 (4)	0.006 (4)	0.004 (4)
N2	0.022 (5)	0.016 (4)	0.027 (5)	0.006 (4)	0.004 (4)	0.001 (4)
C1	0.037 (7)	0.038 (7)	0.031 (6)	0.007 (6)	0.016 (5)	−0.006 (5)
C2	0.017 (5)	0.046 (7)	0.025 (6)	0.010 (5)	0.004 (4)	−0.014 (5)

C3	0.031 (7)	0.047 (8)	0.037 (7)	0.020 (6)	−0.007 (5)	−0.022 (6)
C4	0.109 (14)	0.044 (9)	0.022 (7)	0.016 (9)	0.005 (7)	0.004 (6)
C5	0.041 (9)	0.067 (11)	0.102 (13)	−0.007 (8)	0.041 (9)	−0.035 (10)
C6	0.030 (6)	0.028 (6)	0.022 (5)	0.013 (5)	0.001 (5)	−0.003 (4)
C7	0.026 (6)	0.031 (6)	0.028 (6)	0.011 (5)	0.001 (5)	−0.002 (5)
C8	0.026 (6)	0.053 (8)	0.037 (7)	0.023 (6)	0.000 (5)	−0.004 (6)
C9	0.042 (7)	0.033 (6)	0.022 (6)	0.013 (6)	0.010 (5)	0.006 (5)
C10	0.045 (8)	0.049 (8)	0.042 (7)	0.032 (7)	0.012 (6)	0.005 (6)
C11	0.032 (6)	0.022 (6)	0.026 (6)	0.015 (5)	0.005 (5)	−0.006 (4)
C12	0.027 (6)	0.017 (5)	0.028 (6)	0.003 (5)	0.007 (5)	−0.006 (4)
In2	0.0236 (4)	0.0210 (4)	0.0236 (3)	0.0113 (4)	−0.0019 (3)	−0.0007 (3)
S3	0.0221 (14)	0.0349 (16)	0.0361 (15)	0.0114 (12)	0.0026 (12)	−0.0049 (13)
S4	0.0315 (15)	0.0310 (16)	0.0272 (13)	0.0141 (13)	−0.0054 (12)	−0.0055 (11)
O5	0.040 (5)	0.017 (4)	0.025 (4)	0.015 (4)	−0.002 (3)	0.004 (3)
O6	0.049 (5)	0.023 (4)	0.037 (4)	0.021 (4)	0.004 (4)	0.001 (3)
O7	0.042 (5)	0.030 (4)	0.032 (4)	0.025 (4)	0.012 (4)	0.006 (3)
O8	0.101 (9)	0.074 (7)	0.059 (6)	0.078 (8)	0.040 (6)	0.032 (5)
N3	0.029 (5)	0.022 (5)	0.020 (4)	0.015 (4)	0.001 (4)	−0.002 (4)
N4	0.025 (5)	0.030 (5)	0.018 (4)	0.013 (4)	−0.014 (4)	−0.007 (4)
C13	0.028 (6)	0.035 (6)	0.020 (5)	0.016 (5)	−0.003 (4)	−0.004 (4)
C14	0.032 (6)	0.022 (5)	0.019 (5)	0.017 (5)	−0.003 (4)	−0.011 (4)
C15	0.018 (5)	0.026 (6)	0.034 (6)	0.009 (5)	−0.008 (4)	0.000 (5)
C16	0.047 (8)	0.038 (7)	0.057 (8)	0.027 (7)	0.001 (7)	−0.011 (6)
C17	0.060 (9)	0.053 (9)	0.024 (6)	0.028 (7)	−0.003 (6)	0.003 (5)
C18	0.026 (6)	0.026 (6)	0.025 (5)	0.008 (5)	0.000 (5)	0.001 (4)
C19	0.027 (6)	0.035 (6)	0.016 (5)	0.017 (5)	0.001 (4)	0.000 (4)
C20	0.039 (7)	0.033 (6)	0.023 (5)	0.027 (6)	0.002 (5)	−0.003 (5)
C21	0.034 (7)	0.054 (8)	0.030 (6)	0.014 (6)	−0.004 (6)	−0.013 (6)
C22	0.053 (9)	0.044 (8)	0.059 (9)	0.026 (7)	−0.022 (7)	−0.025 (7)
C23	0.020 (6)	0.027 (6)	0.035 (6)	0.008 (5)	−0.005 (5)	−0.004 (5)
C24	0.029 (6)	0.037 (7)	0.031 (6)	0.023 (6)	−0.008 (5)	−0.001 (5)
In3	0.0224 (3)	0.0218 (4)	0.0234 (3)	0.0126 (4)	−0.0014 (4)	0.0008 (3)
S5	0.0300 (15)	0.0350 (16)	0.0371 (14)	0.0234 (13)	−0.0037 (12)	−0.0072 (12)
S6	0.0481 (18)	0.0346 (17)	0.0293 (13)	0.0258 (16)	−0.0126 (13)	−0.0018 (12)
O9	0.034 (4)	0.026 (4)	0.025 (4)	0.013 (4)	0.005 (3)	0.002 (3)
O10	0.027 (4)	0.030 (4)	0.046 (5)	0.013 (4)	0.002 (4)	−0.007 (4)
O11	0.022 (4)	0.016 (4)	0.030 (4)	0.002 (3)	0.007 (3)	0.005 (3)
O12	0.042 (5)	0.020 (4)	0.033 (4)	0.006 (4)	−0.004 (4)	0.003 (3)
N5	0.022 (4)	0.015 (4)	0.019 (4)	0.007 (4)	−0.002 (3)	0.000 (3)
N6	0.018 (4)	0.031 (5)	0.022 (4)	0.015 (4)	−0.003 (3)	0.003 (4)
C25	0.041 (7)	0.029 (6)	0.021 (5)	0.019 (6)	0.007 (5)	−0.001 (5)
C26	0.019 (5)	0.021 (5)	0.026 (5)	0.013 (4)	−0.008 (4)	−0.009 (4)
C27	0.023 (5)	0.021 (5)	0.023 (5)	0.013 (5)	−0.005 (4)	0.000 (4)
C28	0.027 (6)	0.030 (6)	0.018 (5)	0.013 (5)	−0.006 (4)	−0.006 (4)
C29	0.030 (6)	0.024 (6)	0.033 (6)	0.016 (5)	0.000 (5)	−0.002 (5)
C30	0.028 (6)	0.021 (6)	0.015 (5)	0.007 (5)	−0.005 (4)	0.000 (4)
C31	0.068 (9)	0.055 (8)	0.019 (5)	0.039 (8)	0.006 (5)	−0.002 (5)
C32	0.031 (6)	0.033 (7)	0.038 (6)	0.016 (6)	−0.007 (5)	−0.003 (5)

C33	0.034 (6)	0.058 (8)	0.021 (6)	0.022 (6)	0.001 (5)	−0.007 (6)
C34	0.041 (7)	0.044 (8)	0.033 (6)	0.025 (6)	−0.008 (5)	−0.004 (6)
C35	0.023 (6)	0.028 (6)	0.021 (5)	0.013 (5)	−0.012 (4)	−0.009 (5)
C36	0.021 (6)	0.030 (6)	0.032 (6)	0.015 (5)	−0.002 (5)	0.000 (5)
In4	0.0291 (4)	0.0262 (5)	0.0233 (4)	0.0157 (3)	0.0023 (4)	0.0032 (4)
S7	0.0376 (17)	0.0266 (15)	0.0382 (16)	0.0137 (13)	−0.0018 (13)	0.0051 (13)
S8	0.0339 (16)	0.0318 (16)	0.0274 (14)	0.0141 (13)	0.0001 (12)	0.0105 (12)
O13	0.037 (5)	0.043 (5)	0.026 (4)	0.023 (4)	0.007 (4)	0.010 (4)
O14	0.037 (5)	0.074 (7)	0.032 (4)	0.030 (5)	0.009 (4)	0.012 (4)
O15	0.023 (4)	0.040 (5)	0.027 (4)	0.014 (4)	0.003 (3)	−0.007 (3)
O16	0.038 (5)	0.053 (6)	0.038 (5)	0.023 (5)	−0.003 (4)	−0.014 (4)
N7	0.029 (5)	0.040 (6)	0.022 (5)	0.019 (5)	0.001 (4)	0.005 (4)
N8	0.032 (5)	0.025 (5)	0.020 (4)	0.018 (4)	0.008 (4)	0.012 (4)
C37	0.051 (8)	0.037 (7)	0.015 (5)	0.014 (6)	−0.004 (5)	0.001 (5)
C38	0.023 (6)	0.033 (6)	0.026 (5)	0.011 (5)	−0.007 (5)	0.001 (5)
C39	0.027 (6)	0.035 (7)	0.034 (6)	0.014 (5)	0.002 (5)	0.001 (5)
C40	0.099 (12)	0.045 (8)	0.017 (6)	0.028 (8)	0.001 (6)	−0.008 (6)
C41	0.040 (8)	0.049 (9)	0.064 (9)	0.013 (7)	−0.021 (7)	0.010 (7)
C42	0.040 (7)	0.046 (7)	0.017 (5)	0.025 (6)	0.001 (5)	0.009 (5)
C43	0.031 (6)	0.030 (6)	0.021 (6)	0.017 (5)	0.001 (5)	0.006 (5)
C44	0.028 (6)	0.031 (6)	0.025 (6)	0.015 (5)	0.005 (5)	0.008 (5)
C45	0.061 (9)	0.040 (7)	0.033 (7)	0.023 (7)	0.017 (7)	0.007 (6)
C46	0.030 (7)	0.054 (8)	0.041 (7)	0.020 (6)	−0.003 (6)	0.006 (6)
C47	0.042 (7)	0.017 (6)	0.032 (6)	0.011 (5)	0.008 (5)	0.001 (5)
C48	0.044 (7)	0.029 (6)	0.030 (6)	0.021 (6)	0.002 (5)	0.012 (5)
Na1	0.037 (3)	0.027 (2)	0.029 (2)	0.019 (2)	−0.0046 (19)	0.0011 (18)
Na2	0.038 (3)	0.034 (3)	0.035 (3)	0.018 (2)	0.000 (2)	0.007 (2)
Na3	0.031 (3)	0.041 (3)	0.047 (3)	0.019 (2)	0.011 (2)	0.008 (2)
Na4	0.065 (4)	0.040 (3)	0.056 (3)	0.034 (3)	0.023 (3)	0.009 (2)
O17	0.049 (6)	0.063 (7)	0.047 (5)	0.036 (5)	0.000 (5)	0.007 (5)
O18	0.097 (9)	0.097 (9)	0.084 (8)	0.078 (8)	0.059 (8)	0.066 (8)
O19	0.036 (5)	0.041 (5)	0.043 (5)	0.021 (4)	−0.003 (4)	−0.005 (4)
O20	0.042 (5)	0.031 (4)	0.035 (5)	0.015 (4)	0.001 (4)	−0.005 (4)
O21	0.041 (5)	0.048 (6)	0.054 (6)	0.020 (5)	0.008 (4)	0.002 (5)
O22	0.049 (6)	0.045 (6)	0.042 (5)	0.022 (5)	0.010 (4)	0.007 (4)
O23	0.036 (6)	0.054 (7)	0.112 (9)	0.020 (5)	−0.004 (6)	−0.018 (6)
O24	0.045 (5)	0.060 (6)	0.045 (5)	0.024 (5)	−0.007 (5)	−0.011 (5)
O25	0.056 (7)	0.058 (7)	0.113 (9)	0.038 (6)	0.012 (7)	0.032 (7)
O26	0.048 (6)	0.066 (6)	0.046 (5)	0.036 (5)	−0.009 (4)	−0.007 (5)
O27	0.142 (14)	0.221 (19)	0.065 (8)	0.149 (15)	−0.012 (8)	−0.029 (10)
O28	0.071 (8)	0.054 (7)	0.086 (8)	0.035 (6)	−0.030 (6)	−0.022 (6)
O29	0.051 (7)	0.057 (7)	0.133 (12)	0.024 (6)	0.006 (7)	0.038 (7)
O30	0.038 (6)	0.048 (6)	0.081 (7)	0.019 (5)	0.003 (5)	−0.013 (5)
O31	0.047 (6)	0.079 (8)	0.069 (8)	0.023 (6)	0.014 (5)	0.003 (6)
O32	0.055 (6)	0.047 (6)	0.060 (6)	0.031 (5)	−0.001 (5)	0.009 (5)

Geometric parameters (Å, º)

In1—O1	2.226 (7)	C26—H43	1.0000
In1—O3	2.231 (7)	C27—Na3	2.928 (11)
In1—N1	2.316 (9)	C28—C34	1.529 (16)
In1—N2	2.322 (9)	C28—C29	1.560 (14)
In1—S1	2.459 (3)	C28—C33	1.566 (15)
In1—S2	2.474 (3)	C29—C30	1.541 (15)
S1—C1	1.853 (12)	C29—H44	1.0000
S2—C6	1.873 (12)	C31—H45	0.9800
O1—C3	1.310 (14)	C31—H46	0.9800
O1—Na1	2.402 (8)	C31—H47	0.9800
O2—C3	1.241 (15)	C32—H48	0.9800
O2—Na4^{i}	2.315 (11)	C32—H49	0.9800
O2—Na1	2.796 (11)	C32—H50	0.9800
O3—C8	1.257 (15)	C33—H51	0.9800
O4—C8	1.229 (14)	C33—H52	0.9800
N1—C2	1.457 (13)	C33—H53	0.9800
N1—C11	1.504 (13)	C34—H54	0.9800
N1—H1	1.0000	C34—H55	0.9800
N2—C7	1.465 (14)	C34—H56	0.9800
N2—C12	1.466 (13)	C35—C36	1.537 (15)
N2—H2	1.0000	C35—H57	0.9900
C1—C2	1.528 (17)	C35—H58	0.9900
C1—C4	1.531 (19)	C36—H59	0.9900
C1—C5	1.536 (18)	C36—H60	0.9900
C2—C3	1.534 (17)	In4—O13	2.238 (8)
C2—H3	1.0000	In4—O15	2.273 (7)
C3—Na1	2.963 (13)	In4—N8	2.325 (9)
C4—H4	0.9800	In4—N7	2.349 (9)
C4—H5	0.9800	In4—S7	2.450 (3)
C4—H6	0.9800	In4—S8	2.458 (3)
C5—H7	0.9800	S7—C37	1.854 (12)
C5—H8	0.9800	S8—C42	1.863 (13)
C5—H9	0.9800	O13—C39	1.241 (14)
C6—C10	1.540 (16)	O13—Na4	2.378 (9)
C6—C7	1.547 (14)	O14—C39	1.281 (14)
C6—C9	1.561 (15)	O14—Na3	2.289 (10)
C7—C8	1.539 (16)	O14—Na4	2.788 (10)
C7—H10	1.0000	O15—C44	1.279 (14)
C9—H11	0.9800	O16—C44	1.269 (14)
C9—H12	0.9800	N7—C47	1.441 (13)
C9—H13	0.9800	N7—C38	1.468 (14)
C10—H14	0.9800	N7—H61	1.0000
C10—H15	0.9800	N8—C43	1.477 (14)
C10—H16	0.9800	N8—C48	1.480 (13)
C11—C12	1.519 (15)	N8—H62	1.0000
C11—H17	0.9900	C37—C41	1.539 (18)

C11—H18	0.9900	C37—C40	1.551 (15)
C12—H19	0.9900	C37—C38	1.568 (16)
C12—H20	0.9900	C38—C39	1.557 (15)
In2—O5	2.232 (7)	C38—H63	1.0000
In2—O7	2.250 (7)	C39—Na4	2.928 (12)
In2—N4	2.290 (9)	C40—H64	0.9800
In2—N3	2.345 (8)	C40—H65	0.9800
In2—S3	2.449 (3)	C40—H66	0.9800
In2—S4	2.468 (3)	C41—H67	0.9800
S3—C13	1.857 (11)	C41—H68	0.9800
S4—C18	1.872 (12)	C41—H69	0.9800
O5—C15	1.267 (13)	C42—C46	1.502 (16)
O5—Na2	2.382 (8)	C42—C45	1.518 (17)
O6—C15	1.209 (13)	C42—C43	1.571 (14)
O6—Na1	2.316 (9)	C43—C44	1.527 (16)
O6—Na2	2.690 (9)	C43—H70	1.0000
O7—C20	1.275 (13)	C45—H71	0.9800
O8—C20	1.236 (14)	C45—H72	0.9800
N3—C14	1.454 (12)	C45—H73	0.9800
N3—C23	1.495 (13)	C46—H74	0.9800
N3—H21	1.0000	C46—H75	0.9800
N4—C19	1.478 (14)	C46—H76	0.9800
N4—C24	1.484 (13)	C47—C48	1.497 (16)
N4—H22	1.0000	C47—H77	0.9900
C13—C17	1.513 (15)	C47—H78	0.9900
C13—C16	1.528 (17)	C48—H79	0.9900
C13—C14	1.576 (15)	C48—H80	0.9900
C14—C15	1.571 (15)	Na1—O18	2.357 (11)
C14—H23	1.0000	Na1—O19	2.407 (10)
C15—Na2	2.853 (12)	Na1—O17	2.450 (10)
C16—H24	0.9800	Na2—O22	2.402 (10)
C16—H25	0.9800	Na2—O21	2.428 (11)
C16—H26	0.9800	Na2—O20	2.451 (10)
C17—H27	0.9800	Na2—Na3	3.815 (7)
C17—H28	0.9800	Na2—H88	2.57 (6)
C17—H29	0.9800	Na2—H89	2.63 (7)
C18—C21	1.496 (16)	Na2—H90	2.64 (7)
C18—C22	1.527 (16)	Na3—O23	2.312 (11)
C18—C19	1.540 (15)	Na3—O24	2.322 (11)
C19—C20	1.533 (15)	Na3—H93	2.49 (7)
C19—H30	1.0000	Na3—H95	2.66 (9)
C21—H31	0.9800	Na4—O26	2.405 (11)
C21—H32	0.9800	Na4—O25	2.457 (13)
C21—H33	0.9800	Na4—O27	2.462 (15)
C22—H34	0.9800	Na4—H97	2.62 (18)
C22—H35	0.9800	O17—H81	0.86 (3)
C22—H36	0.9800	O17—H82	0.86 (3)
C23—C24	1.498 (15)	O18—H83	0.86 (3)

C23—H37	0.9900	O18—H84	0.86 (3)
C23—H38	0.9900	O19—H85	0.83 (3)
C24—H39	0.9900	O19—H86	0.83 (3)
C24—H40	0.9900	O20—H87	0.86 (3)
In3—O9	2.261 (8)	O20—H88	0.85 (3)
In3—O11	2.266 (7)	O21—H89	0.86 (3)
In3—N5	2.325 (8)	O21—H90	0.84 (3)
In3—N6	2.333 (9)	O22—H91	0.85 (3)
In3—S6	2.456 (3)	O22—H92	0.87 (3)
In3—S5	2.457 (3)	O23—H93	0.85 (3)
S5—C25	1.867 (12)	O23—H94	0.86 (3)
S6—C28	1.841 (11)	O24—H95	0.87 (3)
O9—C27	1.312 (12)	O24—H96	0.89 (3)
O9—Na3	2.351 (8)	O25—H97	0.86 (3)
O10—C27	1.252 (12)	O25—H98	0.85 (3)
O10—Na2	2.460 (9)	O26—H99	0.90 (3)
O10—Na3	2.768 (9)	O26—H100	0.87 (3)
O11—C30	1.257 (13)	O27—H101	0.85 (3)
O12—C30	1.252 (13)	O27—H102	0.86 (3)
N5—C26	1.459 (12)	O28—H103	0.85 (3)
N5—C35	1.484 (13)	O28—H104	0.86 (3)
N5—H41	1.0000	O29—H105	0.86 (3)
N6—C29	1.457 (14)	O29—H106	0.85 (3)
N6—C36	1.482 (13)	O30—H107	0.88 (3)
N6—H42	1.0000	O30—H108	0.88 (3)
C25—C32	1.526 (16)	O31—H109	0.88 (3)
C25—C31	1.548 (15)	O31—H110	0.88 (3)
C25—C26	1.559 (14)	O32—H111	0.89 (3)
C26—C27	1.525 (14)	O32—H112	0.86 (3)

O1—In1—O3	156.3 (3)	H54—C34—H55	109.5
O1—In1—N1	72.5 (3)	C28—C34—H56	109.5
O3—In1—N1	86.6 (3)	H54—C34—H56	109.5
O1—In1—N2	90.4 (3)	H55—C34—H56	109.5
O3—In1—N2	73.3 (3)	N5—C35—C36	108.8 (8)
N1—In1—N2	75.7 (3)	N5—C35—H57	109.9
O1—In1—S1	86.5 (2)	C36—C35—H57	109.9
O3—In1—S1	102.6 (2)	N5—C35—H58	109.9
N1—In1—S1	83.7 (2)	C36—C35—H58	109.9
N2—In1—S1	159.2 (2)	H57—C35—H58	108.3
O1—In1—S2	105.5 (2)	N6—C36—C35	108.9 (9)
O3—In1—S2	88.9 (2)	N6—C36—H59	109.9
N1—In1—S2	155.7 (2)	C35—C36—H59	109.9
N2—In1—S2	80.2 (2)	N6—C36—H60	109.9
S1—In1—S2	120.52 (10)	C35—C36—H60	109.9
C1—S1—In1	94.9 (4)	H59—C36—H60	108.3
C6—S2—In1	96.5 (3)	O13—In4—O15	154.7 (3)
C3—O1—In1	112.2 (7)	O13—In4—N8	88.9 (3)

C3—O1—Na1	101.9 (7)	O15—In4—N8	72.4 (3)
In1—O1—Na1	143.0 (4)	O13—In4—N7	72.2 (3)
C3—O2—Na4^{i}	136.8 (10)	O15—In4—N7	86.3 (3)
C3—O2—Na1	85.2 (7)	N8—In4—N7	75.1 (3)
Na4^{i}—O2—Na1	113.5 (4)	O13—In4—S7	86.9 (2)
C8—O3—In1	114.1 (7)	O15—In4—S7	104.1 (2)
C2—N1—C11	115.3 (9)	N8—In4—S7	158.3 (2)
C2—N1—In1	99.1 (6)	N7—In4—S7	83.4 (2)
C11—N1—In1	108.4 (6)	O13—In4—S8	105.0 (2)
C2—N1—H1	111.1	O15—In4—S8	89.2 (2)
C11—N1—H1	111.1	N8—In4—S8	81.3 (2)
In1—N1—H1	111.1	N7—In4—S8	156.3 (2)
C7—N2—C12	114.9 (9)	S7—In4—S8	120.31 (10)
C7—N2—In1	99.4 (6)	C37—S7—In4	96.8 (4)
C12—N2—In1	109.9 (6)	C42—S8—In4	97.6 (3)
C7—N2—H2	110.7	C39—O13—In4	111.7 (7)
C12—N2—H2	110.7	C39—O13—Na4	103.5 (7)
In1—N2—H2	110.7	In4—O13—Na4	142.1 (4)
C2—C1—C4	110.1 (10)	C39—O14—Na3	138.6 (8)
C2—C1—C5	110.7 (13)	C39—O14—Na4	83.3 (7)
C4—C1—C5	107.1 (12)	Na3—O14—Na4	134.3 (4)
C2—C1—S1	113.6 (8)	C44—O15—In4	111.5 (7)
C4—C1—S1	106.5 (10)	C47—N7—C38	118.4 (9)
C5—C1—S1	108.5 (9)	C47—N7—In4	108.9 (7)
N1—C2—C1	110.5 (10)	C38—N7—In4	98.9 (6)
N1—C2—C3	108.1 (9)	C47—N7—H61	110.0
C1—C2—C3	111.6 (10)	C38—N7—H61	110.0
N1—C2—H3	108.9	In4—N7—H61	110.0
C1—C2—H3	108.9	C43—N8—C48	115.1 (9)
C3—C2—H3	108.9	C43—N8—In4	100.2 (6)
O2—C3—O1	122.5 (12)	C48—N8—In4	110.8 (7)
O2—C3—C2	121.1 (11)	C43—N8—H62	110.1
O1—C3—C2	116.3 (10)	C48—N8—H62	110.1
O2—C3—Na1	70.1 (7)	In4—N8—H62	110.1
O1—C3—Na1	52.5 (6)	C41—C37—C40	109.2 (11)
C2—C3—Na1	167.8 (8)	C41—C37—C38	107.7 (11)
C1—C4—H4	109.5	C40—C37—C38	108.8 (10)
C1—C4—H5	109.5	C41—C37—S7	109.8 (9)
H4—C4—H5	109.5	C40—C37—S7	108.5 (10)
C1—C4—H6	109.5	C38—C37—S7	112.8 (8)
H4—C4—H6	109.5	N7—C38—C39	106.3 (8)
H5—C4—H6	109.5	N7—C38—C37	111.0 (10)
C1—C5—H7	109.5	C39—C38—C37	109.7 (9)
C1—C5—H8	109.5	N7—C38—H63	109.9
H7—C5—H8	109.5	C39—C38—H63	109.9
C1—C5—H9	109.5	C37—C38—H63	109.9
H7—C5—H9	109.5	O13—C39—O14	122.8 (11)
H8—C5—H9	109.5	O13—C39—C38	120.1 (11)

C10—C6—C7	110.3 (10)	O14—C39—C38	117.1 (10)
C10—C6—C9	106.9 (9)	O13—C39—Na4	52.1 (6)
C7—C6—C9	109.7 (9)	O14—C39—Na4	71.0 (6)
C10—C6—S2	107.8 (8)	C38—C39—Na4	171.6 (8)
C7—C6—S2	112.8 (8)	C37—C40—H64	109.5
C9—C6—S2	109.2 (8)	C37—C40—H65	109.5
N2—C7—C8	107.2 (9)	H64—C40—H65	109.5
N2—C7—C6	110.7 (9)	C37—C40—H66	109.5
C8—C7—C6	113.4 (10)	H64—C40—H66	109.5
N2—C7—H10	108.5	H65—C40—H66	109.5
C8—C7—H10	108.5	C37—C41—H67	109.5
C6—C7—H10	108.5	C37—C41—H68	109.5
O4—C8—O3	124.5 (12)	H67—C41—H68	109.5
O4—C8—C7	118.7 (12)	C37—C41—H69	109.5
O3—C8—C7	116.8 (10)	H67—C41—H69	109.5
C6—C9—H11	109.5	H68—C41—H69	109.5
C6—C9—H12	109.5	C46—C42—C45	109.9 (10)
H11—C9—H12	109.5	C46—C42—C43	109.6 (9)
C6—C9—H13	109.5	C45—C42—C43	107.7 (10)
H11—C9—H13	109.5	C46—C42—S8	108.3 (9)
H12—C9—H13	109.5	C45—C42—S8	108.8 (8)
C6—C10—H14	109.5	C43—C42—S8	112.6 (8)
C6—C10—H15	109.5	N8—C43—C44	106.4 (9)
H14—C10—H15	109.5	N8—C43—C42	110.4 (9)
C6—C10—H16	109.5	C44—C43—C42	112.3 (9)
H14—C10—H16	109.5	N8—C43—H70	109.2
H15—C10—H16	109.5	C44—C43—H70	109.2
N1—C11—C12	107.2 (8)	C42—C43—H70	109.2
N1—C11—H17	110.3	O16—C44—O15	122.2 (10)
C12—C11—H17	110.3	O16—C44—C43	118.4 (10)
N1—C11—H18	110.3	O15—C44—C43	119.4 (10)
C12—C11—H18	110.3	C42—C45—H71	109.5
H17—C11—H18	108.5	C42—C45—H72	109.5
N2—C12—C11	110.1 (9)	H71—C45—H72	109.5
N2—C12—H19	109.6	C42—C45—H73	109.5
C11—C12—H19	109.6	H71—C45—H73	109.5
N2—C12—H20	109.6	H72—C45—H73	109.5
C11—C12—H20	109.6	C42—C46—H74	109.5
H19—C12—H20	108.2	C42—C46—H75	109.5
O5—In2—O7	157.0 (3)	H74—C46—H75	109.5
O5—In2—N4	88.7 (3)	C42—C46—H76	109.5
O7—In2—N4	72.7 (3)	H74—C46—H76	109.5
O5—In2—N3	73.4 (3)	H75—C46—H76	109.5
O7—In2—N3	88.7 (3)	N7—C47—C48	112.9 (9)
N4—In2—N3	76.0 (3)	N7—C47—H77	109.0
O5—In2—S3	89.0 (2)	C48—C47—H77	109.0
O7—In2—S3	103.1 (2)	N7—C47—H78	109.0
N4—In2—S3	157.7 (2)	C48—C47—H78	109.0

N3—In2—S3	82.1 (2)	H77—C47—H78	107.8
O5—In2—S4	101.8 (2)	N8—C48—C47	109.6 (9)
O7—In2—S4	88.7 (2)	N8—C48—H79	109.8
N4—In2—S4	80.8 (2)	C47—C48—H79	109.8
N3—In2—S4	156.4 (2)	N8—C48—H80	109.8
S3—In2—S4	121.30 (10)	C47—C48—H80	109.8
C13—S3—In2	96.4 (4)	H79—C48—H80	108.2
C18—S4—In2	97.0 (4)	O6—Na1—O18	124.5 (4)
C15—O5—In2	114.2 (7)	O6—Na1—O1	115.3 (3)
C15—O5—Na2	98.2 (6)	O18—Na1—O1	112.6 (5)
In2—O5—Na2	144.5 (4)	O6—Na1—O19	88.7 (3)
C15—O6—Na1	140.2 (8)	O18—Na1—O19	85.7 (4)
C15—O6—Na2	85.1 (7)	O1—Na1—O19	125.3 (3)
Na1—O6—Na2	128.9 (3)	O6—Na1—O17	88.5 (3)
C20—O7—In2	112.1 (7)	O18—Na1—O17	75.6 (4)
C14—N3—C23	114.5 (9)	O1—Na1—O17	77.9 (3)
C14—N3—In2	97.8 (6)	O19—Na1—O17	155.0 (3)
C23—N3—In2	108.2 (6)	O6—Na1—O2	121.1 (4)
C14—N3—H21	111.8	O18—Na1—O2	110.5 (5)
C23—N3—H21	111.8	O1—Na1—O2	50.3 (3)
In2—N3—H21	111.8	O19—Na1—O2	75.0 (3)
C19—N4—C24	116.1 (8)	O17—Na1—O2	126.9 (3)
C19—N4—In2	101.4 (6)	O6—Na1—C3	120.8 (4)
C24—N4—In2	109.9 (6)	O18—Na1—C3	114.6 (5)
C19—N4—H22	109.7	O1—Na1—C3	25.6 (3)
C24—N4—H22	109.7	O19—Na1—C3	99.6 (4)
In2—N4—H22	109.7	O17—Na1—C3	103.1 (4)
C17—C13—C16	109.3 (10)	O2—Na1—C3	24.7 (3)
C17—C13—C14	109.1 (9)	O5—Na2—O22	87.0 (3)
C16—C13—C14	109.4 (10)	O5—Na2—O21	140.6 (3)
C17—C13—S3	108.2 (9)	O22—Na2—O21	132.2 (4)
C16—C13—S3	108.1 (8)	O5—Na2—O20	98.2 (3)
C14—C13—S3	112.7 (7)	O22—Na2—O20	85.4 (3)
N3—C14—C15	110.9 (8)	O21—Na2—O20	83.1 (3)
N3—C14—C13	110.1 (9)	O5—Na2—O10	105.5 (3)
C15—C14—C13	110.1 (8)	O22—Na2—O10	85.9 (3)
N3—C14—H23	108.6	O21—Na2—O10	84.9 (3)
C15—C14—H23	108.6	O20—Na2—O10	154.2 (3)
C13—C14—H23	108.6	O5—Na2—O6	50.9 (2)
O6—C15—O5	125.0 (11)	O22—Na2—O6	137.7 (3)
O6—C15—C14	119.9 (10)	O21—Na2—O6	90.1 (3)
O5—C15—C14	115.0 (9)	O20—Na2—O6	101.6 (3)
O6—C15—Na2	69.9 (6)	O10—Na2—O6	101.1 (3)
O5—C15—Na2	55.7 (5)	O5—Na2—C15	26.1 (3)
C14—C15—Na2	169.1 (7)	O22—Na2—C15	112.8 (3)
C13—C16—H24	109.5	O21—Na2—C15	115.0 (4)
C13—C16—H25	109.5	O20—Na2—C15	103.2 (3)
H24—C16—H25	109.5	O10—Na2—C15	102.6 (3)

C13—C16—H26	109.5	O6—Na2—C15	25.0 (3)
H24—C16—H26	109.5	O5—Na2—Na3	134.3 (3)
H25—C16—H26	109.5	O22—Na2—Na3	60.2 (3)
C13—C17—H27	109.5	O21—Na2—Na3	80.2 (3)
C13—C17—H28	109.5	O20—Na2—Na3	108.8 (3)
H27—C17—H28	109.5	O10—Na2—Na3	46.4 (2)
C13—C17—H29	109.5	O6—Na2—Na3	146.5 (2)
H27—C17—H29	109.5	C15—Na2—Na3	146.1 (3)
H28—C17—H29	109.5	O5—Na2—H88	104 (2)
C21—C18—C22	108.5 (10)	O22—Na2—H88	103.9 (9)
C21—C18—C19	109.7 (9)	O21—Na2—H88	66.5 (16)
C22—C18—C19	109.6 (9)	O20—Na2—H88	19.4 (8)
C21—C18—S4	108.9 (8)	O10—Na2—H88	149 (2)
C22—C18—S4	107.5 (8)	O6—Na2—H88	91.3 (19)
C19—C18—S4	112.5 (8)	C15—Na2—H88	101 (2)
N4—C19—C20	105.8 (8)	Na3—Na2—H88	113 (2)
N4—C19—C18	110.0 (8)	O5—Na2—H89	129.7 (17)
C20—C19—C18	113.0 (9)	O22—Na2—H89	135 (2)
N4—C19—H30	109.3	O21—Na2—H89	18.9 (9)
C20—C19—H30	109.3	O20—Na2—H89	67.0 (16)
C18—C19—H30	109.3	O10—Na2—H89	103.7 (10)
O8—C20—O7	123.4 (11)	O6—Na2—H89	84 (2)
O8—C20—C19	117.7 (10)	C15—Na2—H89	108 (2)
O7—C20—C19	118.9 (10)	Na3—Na2—H89	95.1 (14)
C18—C21—H31	109.5	H88—Na2—H89	49.0 (18)
C18—C21—H32	109.5	O5—Na2—H90	159.0 (10)
H31—C21—H32	109.5	O22—Na2—H90	113.7 (10)
C18—C21—H33	109.5	O21—Na2—H90	18.6 (9)
H31—C21—H33	109.5	O20—Na2—H90	81 (2)
H32—C21—H33	109.5	O10—Na2—H90	81 (2)
C18—C22—H34	109.5	O6—Na2—H90	108.6 (10)
C18—C22—H35	109.5	C15—Na2—H90	133.6 (10)
H34—C22—H35	109.5	Na3—Na2—H90	64.3 (13)
C18—C22—H36	109.5	H88—Na2—H90	68 (3)
H34—C22—H36	109.5	H89—Na2—H90	30.9 (9)
H35—C22—H36	109.5	O14—Na3—O23	99.5 (4)
N3—C23—C24	108.7 (9)	O14—Na3—O24	108.4 (4)
N3—C23—H37	110.0	O23—Na3—O24	90.2 (4)
C24—C23—H37	110.0	O14—Na3—O9	108.5 (3)
N3—C23—H38	110.0	O23—Na3—O9	140.0 (4)
C24—C23—H38	110.0	O24—Na3—O9	106.9 (4)
H37—C23—H38	108.3	O14—Na3—O10	120.8 (3)
N4—C24—C23	110.5 (9)	O23—Na3—O10	90.1 (4)
N4—C24—H39	109.5	O24—Na3—O10	130.0 (4)
C23—C24—H39	109.5	O9—Na3—O10	51.1 (3)
N4—C24—H40	109.5	O14—Na3—C27	118.5 (3)
C23—C24—H40	109.5	O23—Na3—C27	114.5 (4)
H39—C24—H40	108.1	O24—Na3—C27	120.3 (4)

O9—In3—O11	154.0 (3)	O9—Na3—C27	26.0 (3)
O9—In3—N5	71.9 (3)	O10—Na3—C27	25.2 (2)
O11—In3—N5	84.2 (3)	O14—Na3—Na2	142.3 (3)
O9—In3—N6	91.6 (3)	O23—Na3—Na2	58.3 (3)
O11—In3—N6	72.1 (3)	O24—Na3—Na2	102.1 (3)
N5—In3—N6	75.7 (3)	O9—Na3—Na2	82.4 (2)
O9—In3—S6	108.4 (2)	O10—Na3—Na2	40.07 (19)
O11—In3—S6	89.2 (2)	C27—Na3—Na2	59.3 (2)
N5—In3—S6	156.3 (2)	O14—Na3—H93	80.7 (13)
N6—In3—S6	80.7 (2)	O23—Na3—H93	20.0 (9)
O9—In3—S5	86.3 (2)	O24—Na3—H93	90 (3)
O11—In3—S5	101.7 (2)	O9—Na3—H93	157 (3)
N5—In3—S5	83.9 (2)	O10—Na3—H93	106 (2)
N6—In3—S5	159.0 (2)	C27—Na3—H93	131 (2)
S6—In3—S5	119.79 (10)	Na2—Na3—H93	77.9 (12)
C25—S5—In3	95.7 (3)	O14—Na3—H95	91.6 (16)
C28—S6—In3	97.1 (3)	O23—Na3—H95	85 (2)
C27—O9—In3	110.8 (6)	O24—Na3—H95	18.7 (14)
C27—O9—Na3	102.4 (6)	O9—Na3—H95	121.3 (17)
In3—O9—Na3	146.3 (4)	O10—Na3—H95	147.6 (16)
C27—O10—Na2	131.6 (7)	C27—Na3—H95	138.4 (14)
C27—O10—Na3	84.5 (6)	Na2—Na3—H95	113.9 (19)
Na2—O10—Na3	93.5 (3)	H93—Na3—H95	79 (4)
C30—O11—In3	112.7 (6)	O2^{ii}—Na4—O13	111.6 (4)
C26—N5—C35	116.4 (8)	O2^{ii}—Na4—O26	146.7 (4)
C26—N5—In3	99.8 (6)	O13—Na4—O26	101.3 (4)
C35—N5—In3	108.3 (6)	O2^{ii}—Na4—O25	75.3 (4)
C26—N5—H41	110.6	O13—Na4—O25	133.0 (4)
C35—N5—H41	110.6	O26—Na4—O25	85.9 (4)
In3—N5—H41	110.6	O2^{ii}—Na4—O27	82.6 (6)
C29—N6—C36	114.9 (8)	O13—Na4—O27	87.4 (4)
C29—N6—In3	100.2 (6)	O26—Na4—O27	94.6 (5)
C36—N6—In3	110.5 (6)	O25—Na4—O27	138.8 (5)
C29—N6—H42	110.3	O2^{ii}—Na4—O14	106.4 (4)
C36—N6—H42	110.3	O13—Na4—O14	50.0 (3)
In3—N6—H42	110.3	O26—Na4—O14	98.1 (3)
C32—C25—C31	108.5 (9)	O25—Na4—O14	83.1 (4)
C32—C25—C26	110.1 (9)	O27—Na4—O14	137.1 (4)
C31—C25—C26	110.1 (9)	O2^{ii}—Na4—C39	109.6 (4)
C32—C25—S5	108.1 (8)	O13—Na4—C39	24.3 (3)
C31—C25—S5	107.6 (8)	O26—Na4—C39	102.4 (4)
C26—C25—S5	112.3 (7)	O25—Na4—C39	108.7 (4)
N5—C26—C27	107.8 (8)	O27—Na4—C39	111.4 (4)
N5—C26—C25	109.6 (9)	O14—Na4—C39	25.7 (3)
C27—C26—C25	112.1 (8)	O2^{ii}—Na4—H97	68 (3)
N5—C26—H43	109.1	O13—Na4—H97	151.9 (18)
C27—C26—H43	109.1	O26—Na4—H97	85 (3)
C25—C26—H43	109.1	O25—Na4—H97	19.2 (15)

O10—C27—O9	121.8 (9)	O27—Na4—H97	119.6 (16)
O10—C27—C26	120.4 (9)	O14—Na4—H97	102.2 (17)
O9—C27—C26	117.9 (9)	C39—Na4—H97	127.6 (17)
O10—C27—Na3	70.3 (6)	Na1—O17—H81	122 (9)
O9—C27—Na3	51.7 (5)	Na1—O17—H82	109 (9)
C26—C27—Na3	168.7 (7)	H81—O17—H82	107 (5)
C34—C28—C29	109.0 (9)	Na1—O18—H83	122 (9)
C34—C28—C33	108.0 (9)	Na1—O18—H84	116 (9)
C29—C28—C33	108.2 (9)	H83—O18—H84	108 (5)
C34—C28—S6	108.9 (8)	Na1—O19—H85	111 (8)
C29—C28—S6	114.0 (7)	Na1—O19—H86	116 (8)
C33—C28—S6	108.5 (8)	H85—O19—H86	114 (5)
N6—C29—C30	106.0 (9)	Na2—O20—H87	121 (8)
N6—C29—C28	110.4 (9)	Na2—O20—H88	88 (4)
C30—C29—C28	112.5 (9)	H87—O20—H88	107 (4)
N6—C29—H44	109.3	Na2—O21—H89	94 (5)
C30—C29—H44	109.3	Na2—O21—H90	95 (5)
C28—C29—H44	109.3	H89—O21—H90	111 (5)
O12—C30—O11	123.2 (10)	Na2—O22—H91	103 (9)
O12—C30—C29	118.2 (10)	Na2—O22—H92	105 (8)
O11—C30—C29	118.6 (9)	H91—O22—H92	106 (5)
C25—C31—H45	109.5	Na3—O23—H93	92 (5)
C25—C31—H46	109.5	Na3—O23—H94	119 (10)
H45—C31—H46	109.5	H93—O23—H94	108 (5)
C25—C31—H47	109.5	Na3—O24—H95	103 (7)
H45—C31—H47	109.5	Na3—O24—H96	119 (7)
H46—C31—H47	109.5	H95—O24—H96	101 (4)
C25—C32—H48	109.5	Na4—O25—H97	91 (10)
C25—C32—H49	109.5	Na4—O25—H98	100 (10)
H48—C32—H49	109.5	H97—O25—H98	107 (5)
C25—C32—H50	109.5	Na4—O26—H99	114 (7)
H48—C32—H50	109.5	Na4—O26—H100	105 (9)
H49—C32—H50	109.5	H99—O26—H100	100 (4)
C28—C33—H51	109.5	Na4—O27—H101	123 (10)
C28—C33—H52	109.5	Na4—O27—H102	99 (10)
H51—C33—H52	109.5	H101—O27—H102	108 (5)
C28—C33—H53	109.5	H103—O28—H104	107 (5)
H51—C33—H53	109.5	H105—O29—H106	108 (5)
H52—C33—H53	109.5	H107—O30—H108	103 (4)
C28—C34—H54	109.5	H109—O31—H110	102 (4)
C28—C34—H55	109.5	H111—O32—H112	101 (4)

In1—S1—C1—C2	16.8 (9)	N3—C23—C24—N4	59.1 (12)
In1—S1—C1—C4	−104.6 (9)	In3—S5—C25—C32	140.8 (7)
In1—S1—C1—C5	140.4 (11)	In3—S5—C25—C31	−102.2 (7)
C11—N1—C2—C1	−177.8 (8)	In3—S5—C25—C26	19.1 (8)
In1—N1—C2—C1	66.8 (9)	C35—N5—C26—C27	60.9 (10)
C11—N1—C2—C3	59.8 (12)	In3—N5—C26—C27	−55.2 (8)

In1—N1—C2—C3	−55.6 (9)	C35—N5—C26—C25	−176.8 (8)
C4—C1—C2—N1	59.3 (13)	In3—N5—C26—C25	67.0 (8)
C5—C1—C2—N1	177.5 (10)	C32—C25—C26—N5	177.8 (8)
S1—C1—C2—N1	−60.1 (11)	C31—C25—C26—N5	58.1 (11)
C4—C1—C2—C3	179.6 (11)	S5—C25—C26—N5	−61.7 (10)
C5—C1—C2—C3	−62.2 (13)	C32—C25—C26—C27	−62.5 (11)
S1—C1—C2—C3	60.2 (12)	C31—C25—C26—C27	177.8 (9)
Na4^{i}—O2—C3—O1	−117.1 (13)	S5—C25—C26—C27	58.0 (10)
Na1—O2—C3—O1	2.5 (13)	Na2—O10—C27—O9	−94.2 (11)
Na4^{i}—O2—C3—C2	66 (2)	Na3—O10—C27—O9	−4.3 (9)
Na1—O2—C3—C2	−174.6 (11)	Na2—O10—C27—C26	85.9 (11)
Na4^{i}—O2—C3—Na1	−119.7 (13)	Na3—O10—C27—C26	175.8 (9)
In1—O1—C3—O2	−168.1 (12)	Na2—O10—C27—Na3	−89.9 (7)
Na1—O1—C3—O2	−3.0 (15)	In3—O9—C27—O10	−169.0 (8)
In1—O1—C3—C2	9.1 (13)	Na3—O9—C27—O10	5.2 (11)
Na1—O1—C3—C2	174.2 (9)	In3—O9—C27—C26	10.8 (10)
In1—O1—C3—Na1	−165.1 (8)	Na3—O9—C27—C26	−174.9 (7)
N1—C2—C3—O2	−147.8 (13)	In3—O9—C27—Na3	−174.2 (7)
C1—C2—C3—O2	90.4 (15)	N5—C26—C27—O10	−147.1 (9)
N1—C2—C3—O1	34.9 (14)	C25—C26—C27—O10	92.2 (11)
C1—C2—C3—O1	−86.8 (13)	N5—C26—C27—O9	33.1 (12)
N1—C2—C3—Na1	57 (4)	C25—C26—C27—O9	−87.7 (11)
C1—C2—C3—Na1	−65 (4)	N5—C26—C27—Na3	12 (4)
In1—S2—C6—C10	125.0 (7)	C25—C26—C27—Na3	−108 (3)
In1—S2—C6—C7	3.0 (8)	In3—S6—C28—C34	126.4 (7)
In1—S2—C6—C9	−119.2 (7)	In3—S6—C28—C29	4.4 (8)
C12—N2—C7—C8	62.0 (12)	In3—S6—C28—C33	−116.2 (7)
In1—N2—C7—C8	−55.2 (9)	C36—N6—C29—C30	62.6 (11)
C12—N2—C7—C6	−173.8 (9)	In3—N6—C29—C30	−55.8 (8)
In1—N2—C7—C6	68.9 (9)	C36—N6—C29—C28	−175.3 (8)
C10—C6—C7—N2	−169.8 (9)	In3—N6—C29—C28	66.3 (8)
C9—C6—C7—N2	72.7 (12)	C34—C28—C29—N6	−171.0 (9)
S2—C6—C7—N2	−49.2 (11)	C33—C28—C29—N6	71.8 (11)
C10—C6—C7—C8	−49.3 (13)	S6—C28—C29—N6	−49.0 (11)
C9—C6—C7—C8	−166.8 (10)	C34—C28—C29—C30	−52.8 (12)
S2—C6—C7—C8	71.3 (11)	C33—C28—C29—C30	−170.0 (9)
In1—O3—C8—O4	178.5 (10)	S6—C28—C29—C30	69.1 (11)
In1—O3—C8—C7	−3.7 (14)	In3—O11—C30—O12	−179.0 (8)
N2—C7—C8—O4	−138.2 (11)	In3—O11—C30—C29	0.0 (12)
C6—C7—C8—O4	99.3 (14)	N6—C29—C30—O12	−139.6 (10)
N2—C7—C8—O3	43.8 (14)	C28—C29—C30—O12	99.7 (11)
C6—C7—C8—O3	−78.6 (13)	N6—C29—C30—O11	41.4 (13)
C2—N1—C11—C12	−158.0 (9)	C28—C29—C30—O11	−79.3 (12)
In1—N1—C11—C12	−48.0 (9)	C26—N5—C35—C36	−159.8 (8)
C7—N2—C12—C11	−152.0 (9)	In3—N5—C35—C36	−48.5 (9)
In1—N2—C12—C11	−40.9 (10)	C29—N6—C36—C35	−151.5 (9)
N1—C11—C12—N2	60.5 (11)	In3—N6—C36—C35	−39.0 (9)
In2—S3—C13—C17	−112.2 (8)	N5—C35—C36—N6	59.6 (11)

In2—S3—C13—C16	129.5 (8)	In4—S7—C37—C41	133.9 (9)
In2—S3—C13—C14	8.5 (8)	In4—S7—C37—C40	−106.8 (9)
C23—N3—C14—C15	60.9 (11)	In4—S7—C37—C38	13.8 (9)
In2—N3—C14—C15	−53.2 (8)	C47—N7—C38—C39	64.1 (12)
C23—N3—C14—C13	−177.0 (8)	In4—N7—C38—C39	−53.1 (9)
In2—N3—C14—C13	68.9 (7)	C47—N7—C38—C37	−176.7 (9)
C17—C13—C14—N3	65.1 (11)	In4—N7—C38—C37	66.1 (9)
C16—C13—C14—N3	−175.4 (8)	C41—C37—C38—N7	−178.7 (9)
S3—C13—C14—N3	−55.1 (10)	C40—C37—C38—N7	63.1 (12)
C17—C13—C14—C15	−172.3 (9)	S7—C37—C38—N7	−57.4 (11)
C16—C13—C14—C15	−52.8 (11)	C41—C37—C38—C39	−61.5 (12)
S3—C13—C14—C15	67.5 (10)	C40—C37—C38—C39	−179.8 (10)
Na1—O6—C15—O5	−142.7 (9)	S7—C37—C38—C39	59.8 (12)
Na2—O6—C15—O5	9.1 (11)	In4—O13—C39—O14	−173.4 (9)
Na1—O6—C15—C14	33.2 (17)	Na4—O13—C39—O14	−7.7 (14)
Na2—O6—C15—C14	−175.0 (9)	In4—O13—C39—C38	10.5 (14)
Na1—O6—C15—Na2	−151.8 (11)	Na4—O13—C39—C38	176.2 (9)
In2—O5—C15—O6	−175.5 (9)	In4—O13—C39—Na4	−165.8 (8)
Na2—O5—C15—O6	−10.4 (13)	Na3—O14—C39—O13	−152.1 (10)
In2—O5—C15—C14	8.4 (11)	Na4—O14—C39—O13	6.4 (12)
Na2—O5—C15—C14	173.5 (7)	Na3—O14—C39—C38	24.1 (18)
In2—O5—C15—Na2	−165.1 (7)	Na4—O14—C39—C38	−177.4 (10)
N3—C14—C15—O6	−141.5 (10)	Na3—O14—C39—Na4	−158.5 (12)
C13—C14—C15—O6	96.4 (12)	N7—C38—C39—O13	33.2 (15)
N3—C14—C15—O5	34.9 (13)	C37—C38—C39—O13	−86.9 (13)
C13—C14—C15—O5	−87.3 (11)	N7—C38—C39—O14	−143.1 (11)
N3—C14—C15—Na2	65 (4)	C37—C38—C39—O14	96.8 (13)
C13—C14—C15—Na2	−58 (4)	In4—S8—C42—C46	127.9 (7)
In2—S4—C18—C21	−114.2 (7)	In4—S8—C42—C45	−112.6 (8)
In2—S4—C18—C22	128.5 (8)	In4—S8—C42—C43	6.7 (8)
In2—S4—C18—C19	7.6 (8)	C48—N8—C43—C44	63.8 (12)
C24—N4—C19—C20	64.7 (11)	In4—N8—C43—C44	−55.0 (8)
In2—N4—C19—C20	−54.3 (8)	C48—N8—C43—C42	−174.1 (9)
C24—N4—C19—C18	−172.9 (9)	In4—N8—C43—C42	67.0 (9)
In2—N4—C19—C18	68.0 (8)	C46—C42—C43—N8	−171.3 (10)
C21—C18—C19—N4	70.3 (12)	C45—C42—C43—N8	69.1 (12)
C22—C18—C19—N4	−170.7 (10)	S8—C42—C43—N8	−50.8 (11)
S4—C18—C19—N4	−51.1 (10)	C46—C42—C43—C44	−52.8 (13)
C21—C18—C19—C20	−171.8 (10)	C45—C42—C43—C44	−172.3 (11)
C22—C18—C19—C20	−52.8 (13)	S8—C42—C43—C44	67.8 (11)
S4—C18—C19—C20	66.9 (11)	In4—O15—C44—O16	−176.7 (9)
In2—O7—C20—O8	−176.8 (11)	In4—O15—C44—C43	3.8 (12)
In2—O7—C20—C19	3.3 (13)	N8—C43—C44—O16	−141.7 (10)
N4—C19—C20—O8	−142.8 (11)	C42—C43—C44—O16	97.4 (12)
C18—C19—C20—O8	96.9 (14)	N8—C43—C44—O15	37.8 (13)
N4—C19—C20—O7	37.1 (13)	C42—C43—C44—O15	−83.1 (12)
C18—C19—C20—O7	−83.3 (13)	C38—N7—C47—C48	−153.8 (9)
C14—N3—C23—C24	−151.9 (9)	In4—N7—C47—C48	−42.0 (11)

In2—N3—C23—C24	−44.1 (10)	C43—N8—C48—C47	−151.2 (10)
C19—N4—C24—C23	−156.7 (10)	In4—N8—C48—C47	−38.4 (11)
In2—N4—C24—C23	−42.5 (11)	N7—C47—C48—N8	55.3 (13)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O32	1.00	2.04	3.003 (13)	160
C5—H7···O2	0.98	2.41	3.19 (2)	135
C9—H13···O32	0.98	2.56	3.528 (15)	169
N3—H21···O28	1.00	2.36	3.302 (15)	156
N4—H22···O29	1.00	2.08	3.007 (15)	154
N5—H41···O32^{iii}	1.00	2.29	3.246 (13)	160
N6—H42···O31	1.00	2.12	3.045 (13)	154
C33—H53···O31	0.98	2.60	3.561 (16)	169
N7—H61···O29^{iv}	1.00	2.52	3.495 (17)	164
N8—H62···O28^{v}	1.00	2.23	3.143 (14)	151
C41—H69···O14	0.98	2.52	3.154 (18)	122
C47—H77···S5	0.99	2.88	3.752 (12)	147
O17—H81···S2	0.86 (3)	2.60 (5)	3.296 (9)	139 (8)
O17—H82···O12^{vi}	0.86 (3)	1.94 (3)	2.800 (12)	175 (12)
O18—H83···O11^{vi}	0.86 (3)	2.01 (5)	2.835 (12)	162 (14)
O18—H84···O8^{vii}	0.86 (3)	1.83 (5)	2.646 (14)	157 (12)
O19—H85···O8^{vii}	0.83 (3)	2.00 (5)	2.785 (13)	157 (11)
O19—H86···O30	0.83 (3)	2.21 (9)	2.838 (13)	133 (11)
O20—H87···O15^{viii}	0.86 (3)	1.97 (4)	2.775 (10)	156 (10)
O22—H91···O16^{viii}	0.85 (3)	2.02 (3)	2.860 (12)	173 (10)
O22—H92···S4	0.87 (3)	2.61 (5)	3.360 (10)	145 (8)
O23—H94···O16^{viii}	0.86 (3)	2.11 (9)	2.860 (14)	145 (15)
O24—H96···O16^{viii}	0.89 (3)	2.02 (6)	2.779 (12)	142 (9)
O25—H98···O4^{ix}	0.85 (3)	2.00 (3)	2.842 (13)	172 (13)
O26—H99···O7^{v}	0.90 (3)	1.99 (4)	2.838 (11)	158 (8)
O26—H100···O4^{ix}	0.87 (3)	1.97 (4)	2.771 (12)	152 (8)
O27—H101···S8	0.85 (3)	2.58 (7)	3.343 (14)	150 (13)
O27—H102···O8^{v}	0.86 (3)	2.30 (5)	3.111 (18)	157 (13)
O28—H103···O26^{x}	0.85 (3)	1.93 (4)	2.756 (14)	161 (10)
O29—H105···O20	0.86 (3)	1.92 (6)	2.732 (14)	157 (14)
O30—H107···O10	0.88 (3)	2.18 (7)	2.948 (12)	146 (10)
O30—H108···O21	0.88 (3)	1.95 (6)	2.713 (12)	143 (9)
O31—H109···O24	0.88 (3)	2.00 (5)	2.774 (15)	147 (8)
O32—H111···O18	0.89 (3)	2.39 (6)	3.025 (16)	129 (6)
O32—H112···O17	0.86 (3)	1.96 (4)	2.802 (14)	164 (9)

Symmetry codes: (iii) *x*−1, *y*−1, *z*; (iv) *x*−1, *y*, *z*; (v) −*y*, *x*−*y*, *z*−1/3; (vi) *x*+1, *y*+1, *z*; (vii) *x*, *y*+1, *z*; (viii) *x*+1, *y*, *z*; (ix) −*y*+1, *x*−*y*, *z*−1/3; (x) −*x*+*y*, −*x*, *z*+1/3.