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catena-Poly[[bis(μ_2-1,4,7,10,13,16-hexaoxacyclooctadecane)dipotassium]-μ_2-iodido-(iodidocadmium)-di-μ_2-iodido-(iodidocadmium)-μ_2-iodido]

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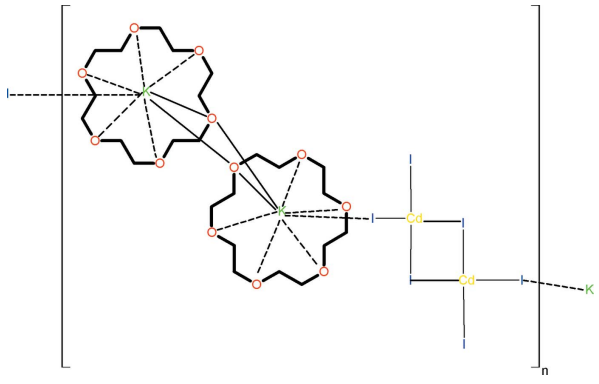
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.028; wR factor = 0.067; data-to-parameter ratio = 18.9.

The reaction of $CdCl_2$, 18-crown-6 and KI in water yields the title coordination polymer, $[\{K(C_{12}H_{24}O_6)\}_2Cd_2I_6]_n$. The potassium ion lies approximately in the plane of the crown ether, coordinated by all six crown ether O atoms and also by an iodide anion bound to a cadmium atom. A C atom of the crown ether is disordered over two positions with site occupancies of 0.77 (2) and 0.23 (2). Two K(18-crown-6)$^+$ units are linked by inversion symmetry, forming a [bis(μ_2-18-crown-6)dipottasium] system with approximately square-planar K_2O_2 units. Inversion symmetry also generates the Cd_2I_6 fragment and the polymeric system is extended along the c axis by the formation of K—I—Cd bridges.

Related literature

For applications of polyiodides, see: Yang *et al.* (2011). For the properties of cadmium compounds, see: Ramesh *et al.* (2012). For related structures, see: Park *et al.* (2010); Guo *et al.* (2006); Kunz *et al.* (2009).



Experimental

Crystal data

$[Cd_2K_2I_6(C_{12}H_{24}O_6)_2]$
M_r = 796.51
Monoclinic, $P2_1/c$
a = 10.627 (2) Å
b = 14.986 (2) Å
c = 15.190 (3) Å
β = 103.959 (1)°
V = 2347.7 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.07 mm^{-1}
T = 293 K
0.20 × 0.15 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.430, T_{max} = 0.631
21969 measured reflections
4129 independent reflections
3585 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.067
S = 1.03
4129 reflections
219 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.53 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5295).

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supporting information

Acta Cryst. (2013). E**69**, m125 [doi:10.1107/S1600536813002274]

catena-Poly[[bis(μ_2-1,4,7,10,13,16-hexaoxacyclooctadecane)dipotassium]-μ_2-iodido-(iodidocadmium)-di-μ_2-iodido-(iodidocadmium)-μ_2-iodido]

K. Rajarajan, A. Pugazhenthi and M. NizamMohideen

S1. Comment

There is a general interest in polyiodides as they are well known for having a significant influence on the redox chemistry in dye-sensitized solar cells (Yang *et al.*, 2011).

In a recent paper, we reported the synthesis and crystal structure of *catena*-Poly[ammonium (cadmium-tri-lthiocyanato-κ^4S:*N*;κ^2N:*S*)-1,4,10,13,16- hexaoxacyclooctadecane (1/1)] (Ramesh *et al.*, 2012). As part of our ongoing investigation of Cd and 18-crown-6 derivatives, we report here the synthesis and structure of the title compound.

The reaction of $CdCl_2$ with 18-crown-6 and KI in de-ionized water yields the title coordination polymer $[\{K(C_{12}H_{24}O_6)\}_2Cd_2I_6]_n$ (Fig.1). The carbon atom (C2) of the crown ether is disordered, as detectable from the large displacement parameters for the C atom and short C-O bond lengths. The disorder over two positions was modelled and the site occupancies refined to 0.77 (2) and 0.23 (2). The geometry was regularized by soft restraints.

The potassium ion lies close to the plane of the crown ether deviating by 0.1257 (2)Å from the mean plane of the six crown ether oxygen atoms (Kunz *et al.,* 2009). The K-O (K1, O1-O6) distances range from 2.686 (4) to 3.011 (4)Å and compare well to those of similar complexes (Kunz *et al.*, 2009). K1 is coordinated by all six oxygen atoms of the crown ether and also by the I3 iodide anion bound to the Cd(II) cation forming a K1—I3—Cd1 bridge. The mean Cd-I (Cd1, I1-I3) bond lengths [2.764 (2)Å] and angles around the Cd1 atom range from 95.0 (2)° to 115.5 (2)° and are similar to those reported for comparable complexes (Park *et al.,* 2010; Guo *et al.,* 2006).

Fig. 2. shows a view of the crystal structure down the *a* axis. The title compound is stabilized by van der Waals forces only, and no classical intra- or intermolecular hydrogen bonds are found.

S2. Experimental

A mixture of 18-crown-6 ($C_{12}H_{24}O_6$), $CdCl_2$ and KI (molar ratio 1:1:3) was thoroughly dissolved in de-ionized water and stirred for 4 h to obtain a homogeneous mixture. Colorless single crystals were obtained after the filtrate had been allowed to stand at room temperature for two weeks.

S3. Refinement

The C2 atom of the crown ether is disordered over two positions with refined occupancies of 0.77 (2) and 0.23 (2). The corresponding bond distances involving the disordered atoms were restrained to be equal. Carbon H atoms were placed geometrically (C—H = 0.97 Å) and treated as riding with U_{iso}(H) = 1.2U_{eq}(C).

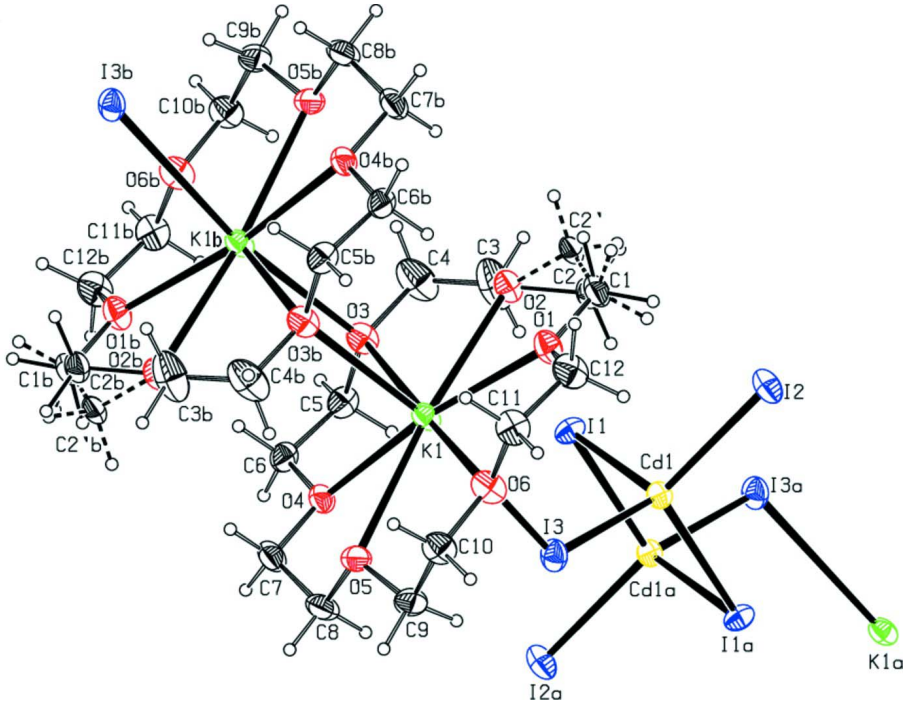

Figure 1

View of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms are presented as a small spheres of arbitrary radius.

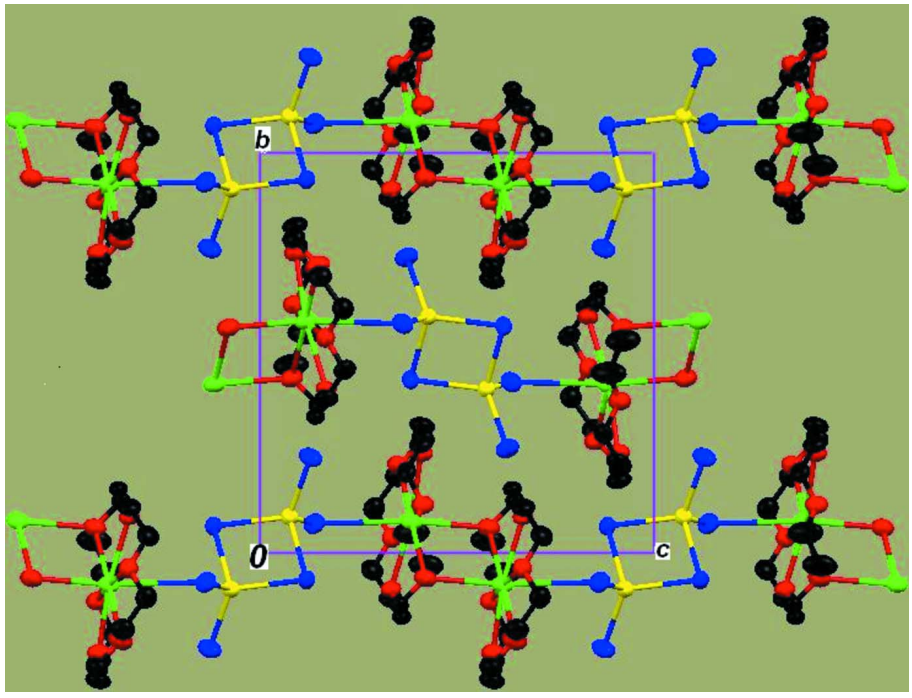

Figure 2

Molecular packing viewed along the *a* axis.

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b = 14.986 (2) Å
c = 15.190 (3) Å
β = 103.959 (1)°
V = 2347.7 (7) Å^3
Z = 4
$F(000)$ = 1480
D_x = 2.254 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5995 reflections
θ = 2.4–31.1°
μ = 5.07 mm^{-1}
T = 293 K
Block, colorless
0.20 × 0.15 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.430, T_{max} = 0.631
21969 measured reflections
4129 independent reflections
3585 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −12→12
k = −17→17
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.067
S = 1.03
4129 reflections
219 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 7.1196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.53 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00235 (8)

Special details

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

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

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3249 (6)	0.2719 (4)	0.4090 (5)	0.0679 (16)	

H1A	0.3011	0.3261	0.3740	0.081*	0.772 (18)
H1B	0.3200	0.2840	0.4708	0.081*	0.772 (18)
H1C	0.2860	0.2977	0.3501	0.081*	0.228 (18)
H1D	0.3298	0.3192	0.4533	0.081*	0.228 (18)
C2	0.2332 (7)	0.2020 (6)	0.3714 (8)	0.060 (2)	0.772 (18)
H2A	0.1481	0.2182	0.3790	0.072*	0.772 (18)
H2B	0.2275	0.1966	0.3070	0.072*	0.772 (18)
C2′	0.238 (3)	0.2087 (18)	0.426 (3)	0.055 (5)	0.228 (18)
H2′1	0.1528	0.2214	0.3879	0.066*	0.228 (18)
H2′2	0.2320	0.2155	0.4889	0.066*	0.228 (18)
C3	0.1840 (7)	0.0503 (5)	0.3846 (7)	0.110 (3)	
H3A	0.1013	0.0665	0.3965	0.131*	
H3B	0.1705	0.0449	0.3193	0.131*	
C4	0.2172 (7)	−0.0310 (5)	0.4214 (7)	0.104 (3)	
H4A	0.1537	−0.0738	0.3898	0.125*	
H4B	0.2110	−0.0294	0.4840	0.125*	
C5	0.3433 (6)	−0.1295 (4)	0.3525 (4)	0.0606 (14)	
H5A	0.3073	−0.1049	0.2927	0.073*	
H5B	0.2900	−0.1796	0.3614	0.073*	
C6	0.4776 (6)	−0.1597 (3)	0.3595 (4)	0.0577 (14)	
H6A	0.5175	−0.1768	0.4216	0.069*	
H6B	0.4772	−0.2115	0.3210	0.069*	
C7	0.6773 (6)	−0.1139 (4)	0.3315 (4)	0.0660 (16)	
H7A	0.6775	−0.1703	0.3001	0.079*	
H7B	0.7289	−0.1208	0.3932	0.079*	
C8	0.7332 (6)	−0.0427 (4)	0.2846 (4)	0.0678 (16)	
H8A	0.8191	−0.0600	0.2795	0.081*	
H8B	0.6792	−0.0342	0.2238	0.081*	
C9	0.7834 (6)	0.1110 (4)	0.2893 (4)	0.0642 (15)	
H9A	0.7216	0.1224	0.2321	0.077*	
H9B	0.8665	0.0970	0.2767	0.077*	
C10	0.7961 (5)	0.1915 (4)	0.3483 (5)	0.0684 (16)	
H10A	0.8492	0.1779	0.4082	0.082*	
H10B	0.8373	0.2394	0.3226	0.082*	
C11	0.6678 (6)	0.2865 (4)	0.4144 (5)	0.0721 (17)	
H11A	0.7194	0.3358	0.4010	0.087*	
H11B	0.7072	0.2660	0.4754	0.087*	
C12	0.5374 (6)	0.3184 (4)	0.4112 (5)	0.0760 (18)	
H12A	0.5394	0.3550	0.4642	0.091*	
H12B	0.5081	0.3555	0.3579	0.091*	
O1	0.4507 (4)	0.2494 (2)	0.4086 (3)	0.0636 (10)	
O2	0.2691 (3)	0.1203 (2)	0.4130 (3)	0.0595 (9)	
O3	0.3430 (4)	−0.0632 (2)	0.4197 (3)	0.0616 (10)	
O4	0.5494 (4)	−0.0901 (2)	0.3323 (2)	0.0539 (9)	
O5	0.7407 (4)	0.0380 (2)	0.3341 (2)	0.0568 (9)	
O6	0.6704 (4)	0.2180 (3)	0.3542 (3)	0.0680 (11)	
K1	0.51194 (11)	0.07876 (7)	0.38443 (8)	0.0520 (3)	
Cd1	0.10508 (3)	0.09039 (2)	0.07415 (2)	0.04486 (11)	

I1	−0.01908 (3)	−0.06719 (2)	0.11826 (2)	0.05110 (11)
I2	−0.00034 (4)	0.23919 (3)	0.12810 (3)	0.06725 (14)
I3	0.36601 (3)	0.07316 (3)	0.13778 (3)	0.05971 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.070 (4)	0.049 (3)	0.089 (4)	0.022 (3)	0.030 (3)	0.009 (3)
C2	0.050 (4)	0.066 (5)	0.059 (6)	0.019 (3)	0.004 (4)	0.005 (5)
C2′	0.048 (8)	0.060 (9)	0.058 (10)	0.024 (8)	0.012 (10)	0.002 (10)
C3	0.045 (4)	0.076 (5)	0.198 (10)	−0.006 (4)	0.009 (5)	0.005 (6)
C4	0.063 (4)	0.074 (5)	0.186 (9)	−0.012 (4)	0.052 (5)	−0.010 (5)
C5	0.071 (4)	0.050 (3)	0.059 (3)	−0.012 (3)	0.013 (3)	−0.002 (3)
C6	0.082 (4)	0.038 (3)	0.055 (3)	0.000 (3)	0.019 (3)	0.000 (2)
C7	0.069 (4)	0.049 (3)	0.085 (4)	0.018 (3)	0.028 (3)	−0.001 (3)
C8	0.072 (4)	0.065 (4)	0.076 (4)	0.011 (3)	0.038 (3)	−0.011 (3)
C9	0.053 (3)	0.076 (4)	0.070 (4)	−0.003 (3)	0.028 (3)	0.004 (3)
C10	0.050 (3)	0.070 (4)	0.089 (4)	−0.011 (3)	0.024 (3)	−0.002 (3)
C11	0.068 (4)	0.065 (4)	0.079 (4)	−0.010 (3)	0.009 (3)	−0.011 (3)
C12	0.086 (5)	0.046 (3)	0.100 (5)	−0.010 (3)	0.031 (4)	−0.013 (3)
O1	0.058 (2)	0.045 (2)	0.088 (3)	0.0044 (18)	0.018 (2)	−0.0001 (19)
O2	0.049 (2)	0.051 (2)	0.078 (3)	0.0035 (17)	0.0144 (19)	0.0012 (18)
O3	0.060 (2)	0.049 (2)	0.078 (3)	−0.0065 (18)	0.022 (2)	−0.0076 (18)
O4	0.061 (2)	0.0392 (18)	0.065 (2)	0.0083 (16)	0.0214 (18)	0.0028 (16)
O5	0.062 (2)	0.059 (2)	0.056 (2)	0.0023 (18)	0.0263 (18)	−0.0008 (17)
O6	0.058 (2)	0.058 (2)	0.092 (3)	−0.0112 (19)	0.024 (2)	−0.013 (2)
K1	0.0499 (6)	0.0392 (6)	0.0724 (8)	−0.0007 (5)	0.0256 (6)	−0.0059 (5)
Cd1	0.0438 (2)	0.0415 (2)	0.0481 (2)	−0.00042 (15)	0.00872 (15)	−0.00202 (15)
I1	0.0600 (2)	0.0530 (2)	0.04247 (19)	−0.01331 (16)	0.01657 (15)	0.00179 (14)
I2	0.0590 (2)	0.0554 (2)	0.0825 (3)	0.01439 (18)	0.0077 (2)	−0.01480 (19)
I3	0.0436 (2)	0.0646 (2)	0.0658 (2)	0.00437 (16)	0.00337 (16)	0.00944 (17)

Geometric parameters (Å, º)

C1—O1	1.380 (7)	C8—O5	1.416 (6)
C1—C2′	1.39 (3)	C8—H8A	0.9700
C1—C2	1.451 (11)	C8—H8B	0.9700
C1—H1A	0.9700	C9—O5	1.419 (7)
C1—H1B	0.9700	C9—C10	1.489 (8)
C1—H1C	0.9700	C9—H9A	0.9700
C1—H1D	0.9700	C9—H9B	0.9700
C2—O2	1.388 (9)	C10—O6	1.417 (7)
C2—K1	3.456 (8)	C10—H10A	0.9700
C2—H2A	0.9700	C10—H10B	0.9700
C2—H2B	0.9700	C11—O6	1.379 (7)
C2′—O2	1.39 (3)	C11—C12	1.455 (8)
C2′—H2′1	0.9700	C11—K1	3.504 (6)
C2′—H2′2	0.9700	C11—H11A	0.9700

C3—C4	1.352 (10)	C11—H11B	0.9700
C3—O2	1.383 (8)	C12—O1	1.380 (7)
C3—H3A	0.9700	C12—H12A	0.9700
C3—H3B	0.9700	C12—H12B	0.9700
C4—O3	1.427 (8)	O1—K1	2.686 (4)
C4—H4A	0.9700	O2—K1	2.788 (4)
C4—H4B	0.9700	O3—K1	2.916 (4)
C5—O3	1.424 (6)	O3—K1^{i}	3.011 (4)
C5—C6	1.477 (8)	O4—K1	2.709 (3)
C5—H5A	0.9700	O5—K1	2.786 (4)
C5—H5B	0.9700	O6—K1	2.788 (4)
C6—O4	1.413 (6)	K1—O3^{i}	3.011 (4)
C6—H6A	0.9700	Cd1—I2	2.7097 (6)
C6—H6B	0.9700	Cd1—I3	2.7197 (7)
C7—O4	1.408 (6)	Cd1—I1	2.8624 (6)
C7—C8	1.485 (8)	Cd1—I1^{ii}	2.8652 (7)
C7—H7A	0.9700	I1—Cd1^{ii}	2.8652 (7)
C7—H7B	0.9700		

O1—C1—C2′	121.5 (11)	C11—C12—H12B	109.2
O1—C1—C2	112.4 (5)	H12A—C12—H12B	107.9
O1—C1—H1A	109.1	C12—O1—C1	117.3 (4)
C2′—C1—H1A	125.1	C12—O1—K1	122.4 (3)
C2—C1—H1A	109.1	C1—O1—K1	120.0 (3)
O1—C1—H1B	109.1	C3—O2—C2	116.1 (6)
C2′—C1—H1B	75.5	C3—O2—C2′	127.2 (12)
C2—C1—H1B	109.1	C3—O2—K1	110.0 (4)
H1A—C1—H1B	107.9	C2—O2—K1	106.8 (4)
O1—C1—H1C	107.0	C2′—O2—K1	119.8 (12)
C2′—C1—H1C	107.0	C5—O3—C4	114.3 (5)
C2—C1—H1C	80.2	C5—O3—K1	105.6 (3)
H1B—C1—H1C	135.0	C4—O3—K1	112.2 (4)
O1—C1—H1D	106.9	C5—O3—K1^{i}	124.4 (3)
C2′—C1—H1D	106.9	C4—O3—K1^{i}	105.5 (5)
C2—C1—H1D	136.0	K1—O3—K1^{i}	92.68 (11)
H1A—C1—H1D	74.4	C7—O4—C6	113.9 (4)
H1C—C1—H1D	106.7	C7—O4—K1	116.7 (3)
O2—C2—C1	112.0 (6)	C6—O4—K1	118.5 (3)
O2—C2—K1	50.6 (3)	C8—O5—C9	112.8 (4)
C1—C2—K1	83.0 (4)	C8—O5—K1	113.1 (3)
O2—C2—H2A	109.2	C9—O5—K1	111.4 (3)
C1—C2—H2A	109.2	C11—O6—C10	114.9 (5)
K1—C2—H2A	159.8	C11—O6—K1	109.8 (3)
O2—C2—H2B	109.2	C10—O6—K1	114.6 (3)
C1—C2—H2B	109.2	O1—K1—O4	170.67 (13)
K1—C2—H2B	81.8	O1—K1—O5	120.16 (12)
H2A—C2—H2B	107.9	O4—K1—O5	61.03 (11)
C1—C2′—O2	115 (2)	O1—K1—O6	59.05 (12)

C1—C2′—H2′1	108.5	O4—K1—O6	120.91 (12)
O2—C2′—H2′1	108.5	O5—K1—O6	61.14 (11)
C1—C2′—H2′2	108.5	O1—K1—O2	60.16 (11)
O2—C2′—H2′2	108.5	O4—K1—O2	117.43 (12)
H2′1—C2′—H2′2	107.5	O5—K1—O2	173.22 (12)
C4—C3—O2	117.9 (7)	O6—K1—O2	118.49 (12)
C4—C3—K1	87.1 (4)	O1—K1—O3	119.29 (12)
O2—C3—K1	48.2 (3)	O4—K1—O3	60.85 (11)
C4—C3—H3A	107.8	O5—K1—O3	120.48 (11)
O2—C3—H3A	107.8	O6—K1—O3	178.21 (12)
K1—C3—H3A	156.0	O2—K1—O3	60.01 (11)
C4—C3—H3B	107.8	O1—K1—O3^{i}	91.24 (12)
O2—C3—H3B	107.8	O4—K1—O3^{i}	98.07 (11)
K1—C3—H3B	84.9	O5—K1—O3^{i}	88.95 (11)
H3A—C3—H3B	107.2	O6—K1—O3^{i}	91.99 (12)
C3—C4—O3	116.7 (7)	O2—K1—O3^{i}	97.83 (11)
C3—C4—H4A	108.1	O3—K1—O3^{i}	87.32 (11)
O3—C4—H4A	108.1	O1—K1—C2	42.81 (17)
C3—C4—H4B	108.1	O4—K1—C2	131.82 (18)
O3—C4—H4B	108.1	O5—K1—C2	153.38 (19)
H4A—C4—H4B	107.3	O6—K1—C2	97.71 (17)
O3—C5—C6	109.4 (4)	O2—K1—C2	22.61 (18)
O3—C5—H5A	109.8	O3—K1—C2	80.96 (17)
C6—C5—H5A	109.8	O3^{i}—K1—C2	109.0 (2)
O3—C5—H5B	109.8	O1—K1—C11	42.17 (14)
C6—C5—H5B	109.8	O4—K1—C11	140.31 (14)
H5A—C5—H5B	108.2	O5—K1—C11	79.29 (13)
O4—C6—C5	109.5 (4)	O6—K1—C11	21.74 (13)
O4—C6—H6A	109.8	O2—K1—C11	101.99 (13)
C5—C6—H6A	109.8	O3—K1—C11	156.50 (14)
O4—C6—H6B	109.8	O3^{i}—K1—C11	80.03 (13)
C5—C6—H6B	109.8	C2—K1—C11	84.52 (18)
H6A—C6—H6B	108.2	O1—K1—C3	80.91 (15)
O4—C7—C8	108.6 (5)	O4—K1—C3	95.91 (16)
O4—C7—H7A	110.0	O5—K1—C3	154.87 (17)
C8—C7—H7A	110.0	O6—K1—C3	136.86 (16)
O4—C7—H7B	110.0	O2—K1—C3	21.72 (16)
C8—C7—H7B	110.0	O3—K1—C3	41.94 (15)
H7A—C7—H7B	108.3	O3^{i}—K1—C3	105.17 (19)
O5—C8—C7	109.7 (5)	C2—K1—C3	39.42 (19)
O5—C8—H8A	109.7	C11—K1—C3	123.07 (17)
C7—C8—H8A	109.7	O1—K1—I3	95.98 (9)
O5—C8—H8B	109.7	O4—K1—I3	74.79 (8)
C7—C8—H8B	109.7	O5—K1—I3	84.10 (8)
H8A—C8—H8B	108.2	O6—K1—I3	88.43 (9)
O5—C9—C10	109.2 (5)	O2—K1—I3	89.13 (9)
O5—C9—H9A	109.8	O3—K1—I3	92.49 (9)
C10—C9—H9A	109.8	O3^{i}—K1—I3	171.82 (8)

O5—C9—H9B	109.8	C2—K1—I3	79.04 (19)
C10—C9—H9B	109.8	C11—K1—I3	102.81 (11)
H9A—C9—H9B	108.3	C3—K1—I3	79.86 (18)
O6—C10—C9	108.4 (5)	O1—K1—K1^{i}	110.35 (10)
O6—C10—H10A	110.0	O4—K1—K1^{i}	76.54 (8)
C9—C10—H10A	110.0	O5—K1—K1^{i}	109.39 (9)
O6—C10—H10B	110.0	O6—K1—K1^{i}	134.75 (10)
C9—C10—H10B	110.0	O2—K1—K1^{i}	75.86 (8)
H10A—C10—H10B	108.4	O3—K1—K1^{i}	44.54 (8)
O6—C11—C12	113.2 (5)	O3^{i}—K1—K1^{i}	42.78 (7)
O6—C11—K1	48.5 (3)	C2—K1—K1^{i}	96.98 (18)
C12—C11—K1	82.6 (3)	C11—K1—K1^{i}	120.13 (12)
O6—C11—H11A	108.9	C3—K1—K1^{i}	71.22 (16)
C12—C11—H11A	108.9	I3—K1—K1^{i}	136.43 (4)
K1—C11—H11A	157.3	I2—Cd1—I3	115.538 (18)
O6—C11—H11B	108.9	I2—Cd1—I1	111.13 (2)
C12—C11—H11B	108.9	I3—Cd1—I1	109.058 (17)
K1—C11—H11B	85.7	I2—Cd1—I1^{ii}	110.792 (17)
H11A—C11—H11B	107.8	I3—Cd1—I1^{ii}	113.455 (17)
O1—C12—C11	112.3 (5)	I1—Cd1—I1^{ii}	94.994 (15)
O1—C12—H12A	109.2	Cd1—I1—Cd1^{ii}	85.006 (15)
C11—C12—H12A	109.2	Cd1—I3—K1	120.06 (2)
O1—C12—H12B	109.2		

O1—C1—C2—O2	52.9 (10)	C3—O2—K1—O4	−8.3 (5)
C2′—C1—C2—O2	−60.7 (19)	C2—O2—K1—O4	−135.1 (5)
O1—C1—C2—K1	10.6 (5)	C2′—O2—K1—O4	−170.4 (18)
C2′—C1—C2—K1	−103 (2)	C3—O2—K1—O6	151.8 (5)
O1—C1—C2′—O2	−21 (3)	C2—O2—K1—O6	25.0 (5)
C2—C1—C2′—O2	63 (2)	C2′—O2—K1—O6	−10.3 (19)
O2—C3—C4—O3	−51.3 (13)	C3—O2—K1—O3	−29.3 (5)
K1—C3—C4—O3	−12.7 (8)	C2—O2—K1—O3	−156.1 (5)
O3—C5—C6—O4	−68.8 (6)	C2′—O2—K1—O3	168.6 (19)
O4—C7—C8—O5	63.5 (6)	C3—O2—K1—O3^{i}	−111.6 (5)
O5—C9—C10—O6	−68.1 (6)	C2—O2—K1—O3^{i}	121.6 (5)
O6—C11—C12—O1	44.6 (8)	C2′—O2—K1—O3^{i}	86.2 (18)
K1—C11—C12—O1	6.1 (5)	C3—O2—K1—C2	126.8 (7)
C11—C12—O1—C1	177.6 (6)	C2′—O2—K1—C2	−35.3 (16)
C11—C12—O1—K1	−9.4 (8)	C3—O2—K1—C11	167.0 (5)
C2′—C1—O1—C12	−166 (2)	C2—O2—K1—C11	40.2 (5)
C2—C1—O1—C12	157.4 (7)	C2′—O2—K1—C11	4.8 (18)
C2′—C1—O1—K1	21 (2)	C2—O2—K1—C3	−126.8 (7)
C2—C1—O1—K1	−15.8 (8)	C2′—O2—K1—C3	−162.1 (19)
C4—C3—O2—C2	178.1 (9)	C3—O2—K1—I3	64.1 (5)
K1—C3—O2—C2	121.4 (7)	C2—O2—K1—I3	−62.7 (5)
C4—C3—O2—C2′	−143 (2)	C2′—O2—K1—I3	−98.1 (18)
K1—C3—O2—C2′	160 (2)	C3—O2—K1—K1^{i}	−74.6 (5)
C4—C3—O2—K1	56.6 (10)	C2—O2—K1—K1^{i}	158.6 (5)

C1—C2—O2—C3	177.0 (7)	C2′—O2—K1—K1^{i}	123.2 (18)
K1—C2—O2—C3	−123.1 (7)	C5—O3—K1—O1	143.2 (3)
C1—C2—O2—C2′	58 (2)	C4—O3—K1—O1	18.0 (5)
K1—C2—O2—C2′	118 (2)	K1^{i}—O3—K1—O1	−89.92 (14)
C1—C2—O2—K1	−59.9 (8)	C5—O3—K1—O4	−26.1 (3)
C1—C2′—O2—C3	−148.2 (16)	C4—O3—K1—O4	−151.3 (5)
C1—C2′—O2—C2	−65 (3)	K1^{i}—O3—K1—O4	100.78 (13)
C1—C2′—O2—K1	11 (3)	C5—O3—K1—O5	−39.7 (4)
C6—C5—O3—C4	−178.0 (5)	C4—O3—K1—O5	−164.9 (5)
C6—C5—O3—K1	58.1 (5)	K1^{i}—O3—K1—O5	87.20 (13)
C6—C5—O3—K1^{i}	−46.3 (5)	C5—O3—K1—O2	132.5 (3)
C3—C4—O3—C5	−103.7 (8)	C4—O3—K1—O2	7.3 (5)
C3—C4—O3—K1	16.6 (10)	K1^{i}—O3—K1—O2	−100.63 (13)
C3—C4—O3—K1^{i}	116.1 (8)	C5—O3—K1—O3^{i}	−126.9 (3)
C8—C7—O4—C6	168.6 (5)	C4—O3—K1—O3^{i}	107.9 (5)
C8—C7—O4—K1	−47.6 (6)	K1^{i}—O3—K1—O3^{i}	0.0
C5—C6—O4—C7	−176.6 (5)	C5—O3—K1—C2	123.4 (4)
C5—C6—O4—K1	40.3 (5)	C4—O3—K1—C2	−1.8 (5)
C7—C8—O5—C9	−175.2 (5)	K1^{i}—O3—K1—C2	−109.7 (2)
C7—C8—O5—K1	−47.7 (6)	C5—O3—K1—C11	175.9 (4)
C10—C9—O5—C8	−176.6 (5)	C4—O3—K1—C11	50.8 (6)
C10—C9—O5—K1	55.0 (5)	K1^{i}—O3—K1—C11	−57.2 (4)
C12—C11—O6—C10	173.5 (5)	C5—O3—K1—C3	116.8 (4)
K1—C11—O6—C10	−130.9 (5)	C4—O3—K1—C3	−8.4 (5)
C12—C11—O6—K1	−55.5 (6)	K1^{i}—O3—K1—C3	−116.4 (3)
C9—C10—O6—C11	173.6 (5)	C5—O3—K1—I3	44.9 (3)
C9—C10—O6—K1	45.0 (6)	C4—O3—K1—I3	−80.3 (5)
C12—O1—K1—O5	−10.5 (5)	K1^{i}—O3—K1—I3	171.81 (8)
C1—O1—K1—O5	162.3 (4)	C5—O3—K1—K1^{i}	−126.9 (3)
C12—O1—K1—O6	−12.6 (4)	C4—O3—K1—K1^{i}	107.9 (5)
C1—O1—K1—O6	160.3 (4)	O2—C2—K1—O1	−133.4 (7)
C12—O1—K1—O2	177.3 (5)	C1—C2—K1—O1	−7.4 (4)
C1—O1—K1—O2	−9.8 (4)	O2—C2—K1—O4	57.3 (6)
C12—O1—K1—O3	166.6 (4)	C1—C2—K1—O4	−176.7 (4)
C1—O1—K1—O3	−20.5 (5)	O2—C2—K1—O5	166.8 (3)
C12—O1—K1—O3^{i}	79.0 (5)	C1—C2—K1—O5	−67.1 (8)
C1—O1—K1—O3^{i}	−108.2 (4)	O2—C2—K1—O6	−158.0 (5)
C12—O1—K1—C2	−163.9 (6)	C1—C2—K1—O6	−31.9 (5)
C1—O1—K1—C2	8.9 (5)	C1—C2—K1—O2	126.0 (9)
C12—O1—K1—C11	5.4 (4)	O2—C2—K1—O3	20.8 (5)
C1—O1—K1—C11	178.2 (5)	C1—C2—K1—O3	146.9 (5)
C12—O1—K1—C3	−175.8 (5)	O2—C2—K1—O3^{i}	−63.2 (5)
C1—O1—K1—C3	−3.0 (4)	C1—C2—K1—O3^{i}	62.9 (5)
C12—O1—K1—I3	−97.1 (5)	O2—C2—K1—C11	−140.6 (5)
C1—O1—K1—I3	75.7 (4)	C1—C2—K1—C11	−14.6 (5)
C12—O1—K1—K1^{i}	118.2 (4)	O2—C2—K1—C3	27.8 (4)
C1—O1—K1—K1^{i}	−69.0 (4)	C1—C2—K1—C3	153.9 (8)
C7—O4—K1—O5	16.9 (3)	O2—C2—K1—I3	115.1 (5)

C6—O4—K1—O5	159.0 (4)	C1—C2—K1—I3	−118.8 (5)
C7—O4—K1—O6	29.8 (4)	O2—C2—K1—K1^{i}	−20.9 (5)
C6—O4—K1—O6	172.0 (3)	C1—C2—K1—K1^{i}	105.1 (5)
C7—O4—K1—O2	−170.6 (3)	O6—C11—K1—O1	−134.5 (5)
C6—O4—K1—O2	−28.5 (4)	C12—C11—K1—O1	−4.3 (4)
C7—O4—K1—O3	−149.8 (4)	O6—C11—K1—O4	31.8 (5)
C6—O4—K1—O3	−7.6 (3)	C12—C11—K1—O4	161.9 (4)
C7—O4—K1—O3^{i}	−67.4 (4)	O6—C11—K1—O5	31.6 (4)
C6—O4—K1—O3^{i}	74.7 (4)	C12—C11—K1—O5	161.7 (4)
C7—O4—K1—C2	168.0 (4)	C12—C11—K1—O6	130.1 (6)
C6—O4—K1—C2	−49.8 (5)	O6—C11—K1—O2	−141.6 (4)
C7—O4—K1—C11	16.7 (5)	C12—C11—K1—O2	−11.5 (4)
C6—O4—K1—C11	158.8 (4)	O6—C11—K1—O3	−179.1 (3)
C7—O4—K1—C3	−173.7 (4)	C12—C11—K1—O3	−49.0 (6)
C6—O4—K1—C3	−31.5 (4)	O6—C11—K1—O3^{i}	122.4 (4)
C7—O4—K1—I3	108.5 (4)	C12—C11—K1—O3^{i}	−107.4 (4)
C6—O4—K1—I3	−109.3 (3)	O6—C11—K1—C2	−127.2 (4)
C7—O4—K1—K1^{i}	−104.6 (4)	C12—C11—K1—C2	3.0 (4)
C6—O4—K1—K1^{i}	37.5 (3)	O6—C11—K1—C3	−135.9 (4)
C8—O5—K1—O1	−152.3 (3)	C12—C11—K1—C3	−5.7 (5)
C9—O5—K1—O1	−24.1 (4)	O6—C11—K1—I3	−49.8 (4)
C8—O5—K1—O4	17.0 (3)	C12—C11—K1—I3	80.4 (4)
C9—O5—K1—O4	145.2 (4)	O6—C11—K1—K1^{i}	137.9 (3)
C8—O5—K1—O6	−150.3 (4)	C12—C11—K1—K1^{i}	−91.9 (4)
C9—O5—K1—O6	−22.1 (3)	C4—C3—K1—O1	−148.6 (6)
C8—O5—K1—O3	30.6 (4)	O2—C3—K1—O1	−16.2 (5)
C9—O5—K1—O3	158.8 (3)	C4—C3—K1—O4	40.3 (6)
C8—O5—K1—O3^{i}	116.9 (4)	O2—C3—K1—O4	172.6 (5)
C9—O5—K1—O3^{i}	−114.9 (3)	C4—C3—K1—O5	62.4 (9)
C8—O5—K1—C2	−109.6 (5)	O2—C3—K1—O5	−165.2 (3)
C9—O5—K1—C2	18.6 (6)	C4—C3—K1—O6	−169.8 (5)
C8—O5—K1—C11	−163.1 (4)	O2—C3—K1—O6	−37.4 (6)
C9—O5—K1—C11	−34.9 (3)	C4—C3—K1—O2	−132.4 (10)
C8—O5—K1—C3	−8.4 (6)	C4—C3—K1—O3	8.2 (5)
C9—O5—K1—C3	119.8 (5)	O2—C3—K1—O3	140.6 (6)
C8—O5—K1—I3	−58.8 (3)	C4—C3—K1—O3^{i}	−59.8 (6)
C9—O5—K1—I3	69.4 (3)	O2—C3—K1—O3^{i}	72.6 (5)
C8—O5—K1—K1^{i}	78.6 (4)	C4—C3—K1—C2	−161.4 (8)
C9—O5—K1—K1^{i}	−153.3 (3)	O2—C3—K1—C2	−29.0 (4)
C11—O6—K1—O1	33.9 (4)	C4—C3—K1—C11	−147.6 (6)
C10—O6—K1—O1	165.0 (4)	O2—C3—K1—C11	−15.3 (6)
C11—O6—K1—O4	−156.9 (4)	C4—C3—K1—I3	113.6 (6)
C10—O6—K1—O4	−25.9 (4)	O2—C3—K1—I3	−114.0 (5)
C11—O6—K1—O5	−144.0 (4)	C4—C3—K1—K1^{i}	−33.3 (6)
C10—O6—K1—O5	−12.9 (4)	O2—C3—K1—K1^{i}	99.0 (5)
C11—O6—K1—O2	43.7 (4)	I2—Cd1—I1—Cd1^{ii}	114.57 (2)
C10—O6—K1—O2	174.8 (4)	I3—Cd1—I1—Cd1^{ii}	−116.930 (19)
C11—O6—K1—O3^{i}	−56.3 (4)	I1^{ii}—Cd1—I1—Cd1^{ii}	0.0

C10—O6—K1—O3^{i}	74.8 (4)	I2—Cd1—I3—K1	55.85 (3)
C11—O6—K1—C2	53.2 (4)	I1—Cd1—I3—K1	−70.15 (3)
C10—O6—K1—C2	−175.8 (4)	I1^{ii}—Cd1—I3—K1	−174.64 (2)
C10—O6—K1—C11	131.1 (6)	O1—K1—I3—Cd1	−65.72 (9)
C11—O6—K1—C3	58.5 (5)	O4—K1—I3—Cd1	112.93 (8)
C10—O6—K1—C3	−170.4 (4)	O5—K1—I3—Cd1	174.47 (8)
C11—O6—K1—I3	131.9 (4)	O6—K1—I3—Cd1	−124.39 (9)
C10—O6—K1—I3	−97.0 (4)	O2—K1—I3—Cd1	−5.86 (8)
C11—O6—K1—K1^{i}	−54.7 (4)	O3—K1—I3—Cd1	54.07 (8)
C10—O6—K1—K1^{i}	76.4 (4)	C2—K1—I3—Cd1	−26.22 (15)
C3—O2—K1—O1	161.4 (5)	C11—K1—I3—Cd1	−107.96 (11)
C2—O2—K1—O1	34.7 (5)	C3—K1—I3—Cd1	13.90 (13)
C2′—O2—K1—O1	−0.7 (18)	K1^{i}—K1—I3—Cd1	62.41 (7)

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