4 × 2·163 (5) and 2·041 (5) Å. The structure of ε-TaN described above is thus different from that arrived at previously (Brauer & Zapp, 1954).

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Cadmium Diiodate

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Abstract. $Cd(IO_3)_2$, orthorhombic, $P2_12_12_1$, $a = 5 \cdot 856$ (1), $b = 17 \cdot 470$ (3), $c = 5 \cdot 582$ (1) Å, $Z = 4$, $D_m = 5 \cdot 31$, $D_x = 5 \cdot 373$ g cm^{-3}. The structure was solved by Patterson methods and refined to an R of 0·038 for 1876 independent reflexions. The coordination number of Cd is seven, the surrounding O atoms form a distorted pentagonal bipyramid, and the Cd–O distances range between 2·262 and 2·510 Å. The I atoms are closely bonded to three O atoms at distances between 1·81 and 1·83 Å and weakly bonded to three further O atoms at distances between 2·58 and 2·77 Å. Thus, a distorted octahedral coordination is achieved. The O atoms link neighbouring Cd and I atoms in a nearly planar trigonal configuration.

Introduction. Recently attention was drawn to different salts of iodic acid in view of their piezoelectric and electrooptical applications. Single crystals of $Cd(IO_3)_2$ with a size of several mm in all directions were grown by Bach (1976) at a temperature of 70°C by evaporation of an aqueous solution containing 60% HNO_3. A small sample was ground in a Bond chamber to an approximately spherical shape of 0·140 mm diameter. Intensities were collected with an automated Stoe two-circle diffractometer STADI 2. With Mo $K\alpha$ radiation 1876 independent reflexions (hkl, $l = 0$ to 7) were recorded in the range $2 \cdot 3° < \theta < 35 \cdot 0°$. With respect to anomalous dispersion, hkl and $\bar{h}kl$ were averaged separately from the group of $\bar{h}kl$ and $hk\bar{l}$ reflexions. The 46 weakest reflexions with $F_o < 10$ were not considered. An absorption correction was applied ($\mu_{MoK} = 146 \cdot 1$ cm^{-1}), assuming spherical shape.

Computations were carried out with the XRAY system (Stewart, Kundell & Baldwin, 1970). Approxi-

Table 1. *Fractional atomic coordinates and thermal parameters* U_{ij} (Å$^2 \times 10^2$)

Standard deviations given in parentheses refer to the last significant digits in the parameter values. The temperature factor is of the form
$$T = \exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)].$$

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd	0·17191 (7)	0·09346 (2)	0·70714 (13)	1·14 (2)	1·18 (2)	1·28 (19)	−0·05 (1)	−0·03 (2)	0·11 (2)
I(1)	0·21417 (6)	0·20870 (2)	0·25443 (11)	1·02 (2)	0·90 (2)	1·07 (18)	−0·05 (1)	0·02 (2)	−0·06 (2)
I(2)	0·63699 (6)	0·07754 (2)	0·02919 (11)	0·93 (2)	0·88 (2)	1·32 (18)	0·02 (1)	−0·01 (2)	0·07 (2)

	x	y	z	U		x	y	z	U
O(1)	0·0203 (11)	0·1650 (4)	0·0417 (19)	1·81 (12)	O(4)	0·8169 (8)	0·0482 (3)	−0·2196 (15)	0·80 (9)
O(2)	0·3694 (10)	0·1249 (4)	0·3645 (16)	1·27 (10)	O(5)	0·5057 (8)	0·1613 (3)	−0·1070 (14)	0·72 (9)
O(3)	0·0327 (10)	0·2081 (4)	0·5185 (18)	1·52 (11)	O(6)	0·3977 (8)	0·0148 (3)	−0·0456 (14)	0·80 (9)

mate positions of all atoms were easily detected by Patterson methods. Full-matrix least-squares refinement yielded an R value of 0·038. Cd and I were refined anisotropically and O isotropically. Reciprocal standard deviations were used as weights and anomalous dispersion was considered. Atomic scattering factors and anomalous dispersion coefficients were taken from *International Tables for X-ray Crystallography* (1962). The final positional and thermal parameters are given in Table 1.*

The anomalous dispersion of the I and Cd scattering makes it possible to determine the absolute configuration. Assuming the enantiomorphous configuration, which is obtained by reversing appropriate signs of the parameters in Table 1, yielded after refinement an R value of 0·041. The ratio of the R values is about 1·08.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33028 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Therefore, the parameters given in Table 1 represent the correct absolute configuration of the sample under investigation.

Discussion. Fig. 1 shows a stereoscopic view of the unit cell including a complete coordination sphere of one of the Cd atoms, the coordinating O atoms being joined by lines to the central Cd atom. The coordination number of Cd is seven. Distances and angles are given in Table 2. The coordination polyhedron may be regarded as a distorted pentagonal bipyramid, the apices being built by O(3) and O(6). The pentagon is made up by O(1), O(5), O(2), O(6′), and O(4). Angles from Cd to these O atoms are near the ideal value of 72° (Table 2). The apices O(3) and O(6) are turned to O(2) and O(5), respectively, because these two pairs of O atoms belong to the same iodate group. Hence, angles O(2)–Cd–O(3) and O(5)–Cd–O(6) are minimal. O(6) belongs to two adjacent Cd coordination spheres whereas the other six O atoms belong to only one particular Cd atom.
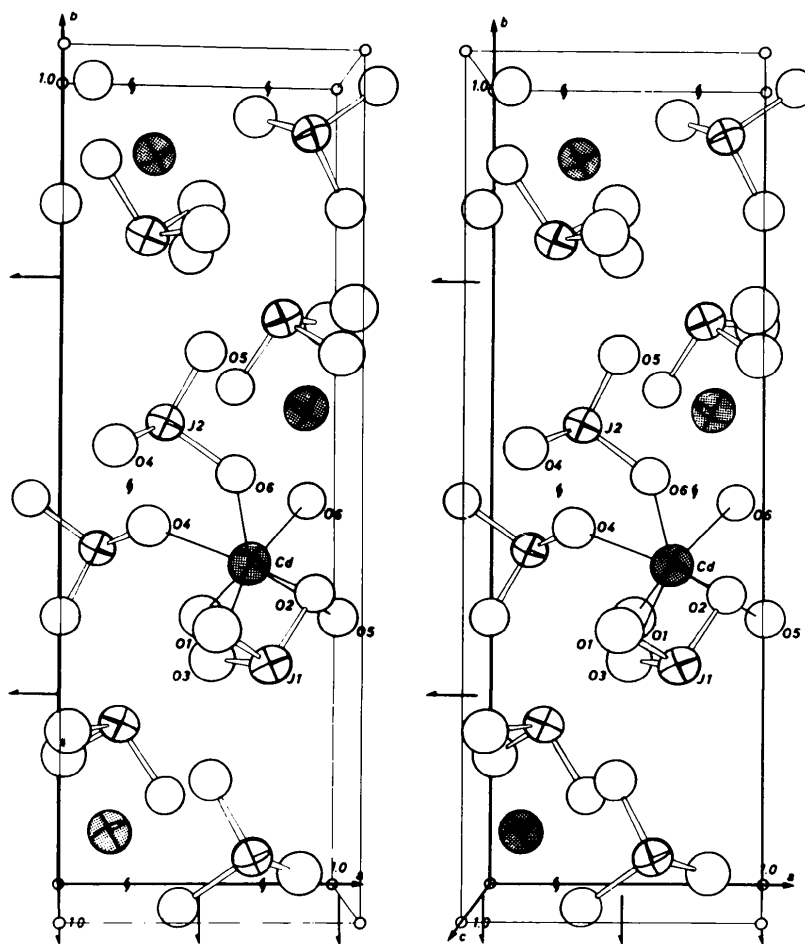

Fig. 1. Stereoscopic view of the unit cell as seen down the c axis [drawn by *ORTEP* (Johnson, 1965)].

Table 2. *Distances* (Å) *and angles* (°) *around the* Cd *atom*

Cd—O(1)	2·416 (9)	Cd—Cd	4·392 (1)
Cd—O(2)	2·301 (8)		
Cd—O(3)	2·405 (7)	O(1)—Cd—O(5)	73·9 (2)
Cd—O(4)	2·262 (5)	O(5)—Cd—O(2)	80·8 (2)
Cd—O(5)	2·510 (6)	O(2)—Cd—O(6')	77·5 (2)
Cd—O(6)	2·355 (6)	O(6')—Cd—O(4)	71·0 (2)
Cd—O(6')	2·394 (6)	O(4)—Cd—O(1)	72·7 (2)
O(3)—Cd—O(1)	77·5 (3)	O(6)—Cd—O(1)	93·2 (3)
O(3)—Cd—O(5)	93·0 (2)	O(6)—Cd—O(5)	66·2 (2)
O(3)—Cd—O(2)	66·9 (2)	O(6)—Cd—O(2)	110·1 (2)
O(3)—Cd—O(6')	110·0 (3)	O(6)—Cd—O(6')	88·9 (2)
O(3)—Cd—O(4)	93·3 (2)	O(6)—Cd—O(4)	101·9 (2)

Table 3. *Distances* (Å) *and angles* (°) *around the* I *atoms*

I(1)—O(1)	1·811 (9)	I(2)—O(4)	1·817 (7)
I(1)—O(2)	1·830 (7)	I(2)—O(5)	1·819 (6)
I(1)—O(3)	1·817 (9)	I(2)—O(6)	1·828 (5)
O(1)—O(2)	2·814 (11)	O(4)—O(5)	2·760 (7)
O(1)—O(3)	2·767 (14)	O(4)—O(6)	2·704 (8)
O(2)—O(3)	2·596 (9)	O(5)—O(6)	2·659 (7)
O(1)—I(1)—O(2)	101·1 (3)	O(4)—I(2)—O(5)	98·7 (3)
O(1)—I(1)—O(3)	99·4 (4)	O(4)—I(2)—O(6)	95·8 (3)
O(2)—I(1)—O(3)	90·8 (3)	O(5)—I(2)—O(6)	93·6 (2)
I(1)—O(3')	2·683 (7)	I(2)—O(1)	2·717 (7)
I(1)—O(5)	2·707 (6)	I(2)—O(2)	2·577 (8)
I(1)—O(5')	2·770 (7)	I(2)—O(4')	2·620 (6)
I(1)—I(2)	3·600 (1)	I(1)—Cd	3·241 (1)
I(1)—I(1')	4·263 (1)	I(2)—Cd	3·275 (1)
I(2)—I(2')	4·109 (1)		

Table 4. *Distances, Δ, of the* O *atoms from the plane defined by three ligands and angles,* φ, *around the* O *atoms*

	Δ(Å)		φ (°)
I(1)—O(1) ·Cd ··I(2)	0·38	I(1)—O(1)···Cd	119·6
		I(1)—O(1)···I(2)	140·5
		Cd···O(1)···I(2)	89·6
I(1)—O(2) ·Cd ··I(2)	0·20	I(1)—O(2)···Cd	102·7
		I(1)—O(2)···I(2)	108·4
		Cd···O(2)···I(2)	146·4
I(1)—O(3) ·Cd ··I(1')	0·05	I(1)—O(3)···Cd	118·7
		I(1)—O(3)···I(1')	141·8
		Cd···O(3)···I(1')	99·3
I(2)—O(4) ·Cd ··I(2')	0·25	I(2)—O(4)···Cd	124·9
		I(2)—O(4)···I(2')	134·8
		Cd···O(4)···I(2')	95·8
I(2)—O(5) ·Cd ··I(1)	0·34	I(2)—O(5)···Cd	97·0
		I(2)—O(5)···I(1)	127·7
		Cd···O(5)···I(1)	128·4
I(2)—O(6) ·Cd ··Cd'	0·26	I(2)—O(6)···Cd	118·0
		I(2)—O(6)···Cd'	102·4
		Cd···O(6)···Cd'	135·3

The two different iodate groups are built up in the usual way by a triangle of O atoms with I displaced from this plane by a certain amount Δ, which is 0·908 Å for I(1) and 0·933 Å for I(2). The bond distances and angles around the I atoms are listed in Table 3. The I atoms are strongly bonded to the three O atoms of the iodate group (distances 1·81 to 1·83 Å) and linked by weaker forces to three further remote O atoms (distances 2·58 to 2·77 Å). The coordination polyhedron is a distorted octahedron. This configuration is found in most of the iodates investigated so far [see review of Ghose & Wan (1974)].

Each O atom of a particular iodate group connects two further atoms in a nearly planar trigonal configuration. In Table 4 the environments of the six O atoms are indicated and the distances, Δ, of the O atoms from a plane defined by the three ligands are listed (in Å). These values give a measure of the planarity of the trigonal arrangement. The angles φ (Table 4) at the O atoms range around the value 120° for an ideal trigonal geometry. This configuration suggests an sp^2-type bonding where two pairs of electrons of the O atoms are directed towards the neighbouring I and Cd atoms.

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