Zn(1) - O(4) - C(10)	115.8 (3)	C(1) - C(2) - C(3)	117.3 (5)
Zn(1) - O(2) - C(8)	116.2 (4)	C(1) - C(2) - C(21)	124.8 (5)
Zn(1) - N(1) - C(1)	115.1 (3)	C(3) - C(2) - C(21)	117.9 (5)
Zn(1) - N(1) - C(9)	99.7 (3)	C(6) - C(5) - C(4)	118.8 (7)
C(1) - N(1) - C(9)	111.1 (4)	C(2) - C(3) - C(4)	122.8 (5)
$Z_n(1) = N(1) = C(7)$	100.0 (2)	C(1) - C(6) - C(5)	121.7 (5)
C(1) - N(1) - C(7)	113.3 (4)	C(2) - C(21) - C(22)	113.2 (6)
C(9) - N(1) - C(7)	116.4 (4)	C(5) - C(4) - C(3)	119.9 (6)
O(4) - C(10) - O(3)	123.7 (5)		

Data collection: *DIF4* (Stoe & Cie, 1991*a*). Cell refinement: *DIF4*. Data reduction: *REDU4* (Stoe & Cie, 1991*b*). Program(s) used to solve structure: *SHELXTL-Plus*88 (Sheldrick, 1988). Program(s) used to refine structure: *SHELXTL-Plus*88. Molecular graphics: *SHELXTL-Plus*88.

Lists of structure factors, anisotropic displacement parameters, Hatom coordinates and complete geometry have been deposited with the IUCr (Reference: DE1012). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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# Trimethyloxosulfonium Salts. IX. Study of some Mixed Compounds, (CH<sub>3</sub>)<sub>3</sub>SOCdCl<sub>3-x</sub>Br<sub>x</sub>

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#### Abstract

Crystal structures of six  $(CH_3)_3SOCdCl_{3-x}Br_x$  mixed compounds [(1) x = 2.116, (2) x = 1.787, (3) x = 1.183, (4) x = 0.962, (5) x = 0.607, (6) x = 0.286]

have been determined. Each has space group *Pnma* and is a structural analogue of  $(CH_3)_3SOCdCl_3$  and  $(CH_3)_3SOCdBr_3$ , reported previously. The distribution of Br and Cl atoms among the two anionic sites was especially studied. We have shown that the occupation probabilities are related to the x value but do not vary with it linearly: the Cl atoms showed a preference for the most symmetric site (*m* symmetry), while the Br atoms were better located on a general position more distant from the Cd ion. It is therefore not possible to describe these mixed compounds in terms of continuous solid-solution series.

#### Comment

In a previous paper (Puget, Jannin, de Brauer & Perret, 1991) we described the structures of the isostructural *catena*-trichlorocadmate and *catena*-tribromocadmate salts of  $(CH_3)_3SO$ . As a continuation, the crystal structures of six compositional analogues  $(CH_3)_3SOCdCl_{3-x}Br_x$  are reported here. The precision of the results is very good and the crystal growth process leads to homogeneous bromine and chlorine composition in the whole crystal. Therefore, this study allows us to examine the influence of the site type on the kind of anionic substitution and the modifications resulting from it. No papers in the literature seem to deal with this subject for the Cl–Br couple. We have only found some reports about cationic substitution (Nord, 1983; Thomas, Mayo & Watts, 1992).



As found for the isostructural catena-tribromocadmate salt, the structure of each of the (CH<sub>3</sub>)<sub>3</sub>SOCd- $Cl_{3-x}Br_x$  compounds exhibits two crystallographically non-equivalent anionic sites where Br- and Cl- ions may both be located. The first shared (Br,Cl) site, labelled  $(Br,Cl)_{(1)}$ , is situated on the mirror y = 0.25. Its multiplicity is 4 and its occupation factor is 0.5. The second site, named (Br,Cl)(2), is in a general position. Its multiplicity is 8 and its total occupancy is 1. The occupation rates of Br and Cl atoms in each of the two available sites were refined with the only constraint that the total occupancy should be 0.5 on site (Br,Cl)(1) and 1 on site (Br,Cl)(2). The resulting values for each of the six compounds are listed in Table 3. Figs. 1 and 2, respectively, show the variations of the occupancies of the sites (Br,Cl)(1) and (Br,Cl)(2) versus the composition (x). These figures clearly show that these variations are effectively related to the composition but are not proportional to it: Br and Cl atoms are not equally distributed on the two anionic sites. Cl atoms exhibit a higher affinity for the most symmetric site while Br atoms preferably occupy the other site, which is more distant from the Cd atom. In each  $(CH_3)_3SOCdCl_{3-x}Br_x$ compound, the Cd atoms are coordinated to six halogen atoms defining quasi-regular octahedra, as shown in Fig. 3. Two of the halogen atoms are located on opposed apexes in  $(Br,Cl)_{(1)}$  sites while the other four halogens are in  $(Br,Cl)_{(2)}$  sites at general positions.

The Cd—X bond lengths become progressively longer when the bromine rate increases, and are intermediate between those found for  $(CH_3)_3$ SOCdCl<sub>3</sub> and  $(CH_3)_3$ SOCdBr<sub>3</sub>. Fig. 4 shows the variation with x for each kind of Cd—X bond length, where X is the Br,Cl site: Cd—X(1) bond lengths range from 2.6065 (3) or 2.6279 (3) Å for (6), and 2.6824 (3) or 2.7009 (3) Å for



Fig. 1. Cl and Br atom occupancy in the site  $(Cl,Br)_{(1)}$  versus the composition x.



Fig. 2. Cl and Br atom occupancy in the site  $(Cl,Br)_{(2)}$  versus the composition x.



Fig. 3. Projection of the  $(CH_3)_3SOCdCl_{3-x}Br_x$  structure along the *a* axis. Ellipsoids are shown at the 50% probability level.



Fig. 4. Cd—X bond lengths versus the composition x. (Symmetry code: as given in Table 2.)

(1). Cd—X(2) bond lengths vary from 2.6780(2) or 2.6878(2) Å in (6) to 2.7712(2) or 2.7748(2) Å in (1) (see Table 2).

X-atom angles change little across the range of compounds considered. In all compounds, X—Cd—X angles between two opposite X atoms are equal to  $180^{\circ}$  when the halogens are in  $(Br,Cl)_{(1)}$  sites. If X atoms are in  $(Br,Cl)_{(2)}$  sites, these angles are  $180^{\circ}$  only for (1) and (2) but are very near for the others. The angles between adjacent halogens reflect the weak distortion of the octahedron: some of them range between 83.5 and 86° and the others between 93.5 and 97.5°. Fig. 5 clearly shows that the differences between the largest and the smallest X(1)—Cd—X(2) and X(2)—Cd—X(2) for adjacent X atoms are more important in (6) than in (1). The deformations of the octahedra are therefore more marked for the compounds rich in chlorine.



Fig. 5. X—Cd—X angle values versus the composition x. (Symmetry codes: as given in Table 2.)

The distribution of the halogen atoms on the two sites is the consequence of the properties of the Br<sup>-</sup> and Cl<sup>-</sup> ions relating to bulkiness and polarizability. The Cl<sup>-</sup> ion radius is smaller (Shannon & Prewitt, 1969) and it is less polarizable than the Br<sup>-</sup> ion ( $\alpha_{Cl} = 2.96$  and  $\alpha_{Br} =$ 4.16; Gready, Backskay & Huch, 1970).

It is therefore not possible to describe all these mixed compounds in terms of continuous solid solution series in spite of the fact that the substitution of Cl by Br leads to smooth linear expansions of the a, b and c lattice parameters. As in an ideal solution, the existence of a continuous series of solid solutions imposes the equal distribution of the substituted atoms in the host sites. This condition can only be realised in particular cases. The crystal-field influence and the individual properties of the substituted atoms modify the occupancies of sites of different types. To have the chance to lead to continuous solid solution series, the substitution must involve only one site and ions showing very similar properties. For example, the mixed compounds  $[(CH_3)_4N]M_{1-x}M'_xCl_4$  (M = Mn, Co, Zn), studied in our laboratory by Perret, Godefroy & Arend (1985), exhibit the particular properties of solid solutions.

#### Experimental

Homogeneous composition in the whole crystal is the essential condition that allows a study of halogenide-ion distribution in our mixed compounds. The monocrystals we have used

were therefore grown by the procedure described by Arend, Perret, Wüest & Kerkoc (1986) based on a temperaturedifference growth with thermally enforced convection and the use of saturated solutions in equilibrium with precipitated solid phase. This method enables a constant concentration of the solution to be maintained just around the crystal during its growth process. Monocrystals were all grown under the same conditions of temperature: T = 294 K,  $\Delta T = 3$  K. The supersaturated solutions were obtained by dissolution of weighted amounts of (CH<sub>3</sub>)<sub>3</sub>SOCl, CdCl<sub>2</sub>, (CH<sub>3</sub>)<sub>3</sub>SOBr and CdBr<sub>2</sub> in a constant volume of warm water [molar ratio (3 x':(3 - x'):x':x']. The composition of the mother solution near the growing crystal is different from that of the solid mixture initially solved. Chemical analysis was therefore necessary for each composition. It shows that the bromine ratio value (x) of the mixed compounds strongly depends on the composition of the starting mixture of solids and is always a little higher. The analysis results have been systematically verified at the end of each structure refinement by comparison with the x value calculated from the occupation probabilities of Cl and Br in the two anionic sites.

#### Compound (1)

Crystal data

C3H9OS+.Cd2+.-Mo  $K\alpha$  radiation  $(Br_{2.116}Cl_{0.884})^{3-1}$  $\lambda = 0.71073 \text{ Å}$  $M_r = 405.79$ Cell parameters from 25 Orthorhombic reflections  $\theta = 5 - 15^{\circ}$ Pnma  $\mu = 11.24 \text{ mm}^{-1}$ a = 6.847(1) Å T = 293 Kb = 10.429(2) Å c = 13.655(2) Å Prismatic  $V = 975.1 \text{ Å}^{-1}$  $0.2 \times 0.2 \times 0.2$  mm Z = 4Colourless  $D_x = 2.767 \text{ Mg m}^{-3}$ 

Data collection

Enraf-Nonius CAD-4 diffractometer  $\omega/2\theta$  scans Absorption correction:  $\psi$  scans (*MolEN*; Fair, 1990)  $T_{min} = 0.9409$ ,  $T_{max} =$ 0.9995 8949 measured reflections 2057 independent reflections 1087 observed reflections  $[I > 3\sigma(I)]$ *Refinement* Refinement on F

Remember on T R = 0.0113 wR = 0.0133 S = 1.051087 reflections 71 parameters Only H-atom U's refined  $w = 1/\sigma^2(F)$  $(\Delta/\sigma)_{max} = 0.003$   $R_{int} = 0.016$   $\theta_{max} = 30^{\circ}$   $h = -9 \rightarrow 9$   $k = -14 \rightarrow 14$   $l = -5 \rightarrow 19$ 4 standard reflections frequency: 120 min intensity decay: 3.1%

 $\Delta \rho_{max} = 0.201 \text{ e } \text{\AA}^{-3}$  $\Delta \rho_{min} = -0.196 \text{ e } \text{\AA}^{-3}$ Extinction correction: Stout & Jensen (1968) Extinction coefficient: 7.144 × 10<sup>-6</sup> Atomic scattering factors from International Tables for X-ray Crystallography (1974, Vol. IV)

#### Compound (2)

Crystal data C<sub>3</sub>H<sub>9</sub>OS<sup>+</sup>.Cd<sup>2+</sup>.-(Br<sub>1.787</sub>Cl<sub>1.213</sub>)<sup>3-</sup>  $M_r = 391.1$ Orthorhombic *Pnma*  a = 6.825 (1) Å b = 10.415 (2) Å c = 13.630 (2) Å V = 968.9 Å<sup>3</sup> Z = 4 $D_x = 2.684$  Mg m<sup>-3</sup>

#### Data collection

Enraf-Nonius CAD-4 diffractometer  $\omega/2\theta$  scans Absorption correction:  $\psi$  scans (*MolEN*; Fair, 1990)  $T_{min} = 0.8789$ ,  $T_{max} =$ 0.9997 5228 measured reflections 1481 independent reflections 939 observed reflections  $[I > 3\sigma(I)]$ 

#### Refinement

Refinement on F R = 0.015 wR = 0.017 S = 1.29 939 reflections 71 parameters Only H-atom U's refined w =  $1/\sigma^2(F)$  $(\Delta/\sigma)_{max} = 0.003$ 

#### Compound (3)

Crystal data  $C_3H_9OS^*.Cd^{2*}. (Br_{1.183}Cl_{1.817})^{3-}$   $M_r = 364.5$ Orthorhombic *Pnma*  a = 6.782 (1) Å b = 10.335 (2) Å c = 13.572 (2) Å V = 951.3 Å<sup>3</sup> Z = 4 $D_x = 2.546$  Mg m<sup>-3</sup>

### Data collection

Enraf-Nonius CAD-4 diffractometer Mo  $K\alpha$  radiation  $\lambda = 0.71073$  Å Cell parameters from 25 reflections  $\theta = 5-15^{\circ}$   $\mu = 10.03$  mm<sup>-1</sup> T = 293 K Prismatic  $0.2 \times 0.2 \times 0.2$  mm Colourless

 $R_{int} = 0.014$   $\theta_{max} = 30^{\circ}$   $h = -10 \rightarrow 10$   $k = -15 \rightarrow 15$   $l = -5 \rightarrow 20$ 4 standard reflections frequency: 120 min intensity decay: 3.0%

 $\Delta \rho_{\text{max}} = 0.913 \text{ e } \text{\AA}^{-3}$  $\Delta \rho_{\text{min}} = -0.521 \text{ e } \text{\AA}^{-3}$ Extinction correction: Stout & Jensen (1968) Extinction coefficient: 9.613 × 10<sup>-6</sup> Atomic scattering factors from *International Tables* for X-ray Crystallography (1974, Vol. IV)

Mo  $K\alpha$  radiation  $\lambda = 0.71073$  Å Cell parameters from 25 reflections  $\theta = 5-15^{\circ}$   $\mu = 7.88$  mm<sup>-1</sup> T = 293 K Prismatic  $0.2 \times 0.2 \times 0.2$  mm Colourless

 $R_{\rm int} = 0.018$  $\theta_{\rm max} = 30^{\circ}$   $\omega/2\theta$  scans Absorption correction:  $\psi$  scans (*MolEN*; Fair, 1990)  $T_{min} = 0.9206$ ,  $T_{max} =$ 0.9997 8657 measured reflections 1738 independent reflections 957 observed reflections  $[I > 3\sigma(I)]$ 

#### Refinement

Refinement on F R = 0.0109 wR = 0.0126 S = 0.82 957 reflections 71 parameters Only H-atom U's refined w =  $1/\sigma^2(F)$  $(\Delta/\sigma)_{max} = 0.003$ 

#### Compound (4)

Crystal data  $C_3H_9OS^*.Cd^{2+}. (Br_{0.962}Cl_{2.038})^{3-}$   $M_r = 354.7$ Orthorhombic Pnma a = 6.765 (1) Å b = 10.304 (2) Å c = 13.544 (2) Å  $V = 944.1 Å^3$  Z = 4 $D_x = 2.496 Mg m^{-3}$ 

#### Data collection

Enraf-Nonius CAD-4 diffractometer  $\omega/2\theta$  scans Absorption correction:  $\psi$  scans (*MolEN*; Fair, 1990)  $T_{min} = 0.8573$ ,  $T_{max} =$ 0.9987 7311 measured reflections 1444 independent reflections 899 observed reflections  $[I > 3\sigma(I)]$ 

#### Refinement

Refinement on F R = 0.0107 wR = 0.0120 S = 0.88 899 reflections 71 parameters Only H-atom U's refined w =  $1/\sigma^2(F)$  $(\Delta/\sigma)_{max} = 0.003$   $h = -10 \rightarrow 10$   $k = -15 \rightarrow 15$   $l = -5 \rightarrow 20$ 4 standard reflections frequency: 120 min intensity decay: 11.7%

 $\Delta \rho_{max} = 0.246 \text{ e } \text{\AA}^{-3}$  $\Delta \rho_{min} = -0.297 \text{ e } \text{\AA}^{-3}$ Extinction correction: Stout & Jensen (1968) Extinction coefficient: 5.269 × 10<sup>-6</sup> Atomic scattering factors from *International Tables* for X-ray Crystallography (1974, Vol. IV)

Mo  $K\alpha$  radiation  $\lambda = 0.71073 \text{ Å}$ Cell parameters from 25 reflections  $\theta = 5-15^{\circ}$   $\mu = 7.07 \text{ mm}^{-1}$  T = 293 KPrismatic  $0.2 \times 0.2 \times 0.2 \text{ mm}$ Colourless

 $R_{int} = 0.015$   $\theta_{max} = 30^{\circ}$   $h = -9 \rightarrow 9$   $k = -14 \rightarrow 14$   $l = -5 \rightarrow 19$ 4 standard reflections frequency: 120 min intensity decay: 0.9%

 $\Delta \rho_{max} = 0.330 \text{ e} \text{ Å}^{-3}$   $\Delta \rho_{min} = -0.202 \text{ e} \text{ Å}^{-3}$ Extinction correction: Stout & Jensen (1968) Extinction coefficient: 9.247 × 10<sup>-6</sup> Atomic scattering factors from International Tables for X-ray Crystallography (1974, Vol. IV)

#### Compound (5)

Crystal data  $C_{3}H_{9}OS^{+}.Cd^{2+}. (Br_{0.607}Cl_{2.393})^{3-}$   $M_{r} = 339.2$ Orthorhombic Pnma a = 6.744 (1) Å b = 10.253 (2) Å c = 13.517 (2) Å V = 934.6 Å<sup>3</sup> Z = 4 $D_{x} = 2.409$  Mg m<sup>-3</sup>

#### Data collection

Enraf-Nonius CAD-4 diffractometer  $\omega/2\theta$  scans Absorption correction:  $\psi$  scans (*MolEN*; Fair, 1990)  $T_{min} = 0.9311$ ,  $T_{max} =$ 0.9997 8466 measured reflections 1696 independent reflections 1045 observed reflections  $[I > 3\sigma(I)]$ 

#### Refinement

Refinement on F R = 0.0100 wR = 0.0113 S = 0.84 1045 reflections 71 parameters Only H-atom U's refined w =  $1/\sigma^2(F)$  $(\Delta/\sigma)_{max} = 0.003$ 

#### **Compound (6)**

Crystal data C<sub>3</sub>H<sub>9</sub>OS<sup>+</sup>.Cd<sup>2+</sup>.-(Br<sub>0.286</sub>Cl<sub>2.714</sub>)<sup>3-</sup>  $M_r = 324.5$ Orthorhombic *Pnma*  a = 6.716 (1) Å b = 10.192 (2) Å c = 13.476 (2) Å V = 922.4 Å<sup>3</sup> Z = 4 $D_x = 2.339$  Mg m<sup>-3</sup>

#### Data collection

Enraf-Nonius CAD-4 diffractometer

# $C_{3}H_{9}OS^{+}.Cd^{2+}.(Br_{x}Cl_{3-x})^{3-}$

Mo  $K\alpha$  radiation

 $\lambda = 0.71073 \text{ Å}$ Cell parameters from 25

reflections

 $\mu = 5.74 \text{ mm}^{-1}$ 

 $0.2\,\times\,0.2\,\times\,0.2$  mm

 $\theta = 5 - 15^{\circ}$ 

T = 293 K

Colourless

 $R_{\rm int} = 0.015$ 

 $\theta_{\rm max} = 30^\circ$  $h = -10 \rightarrow 10$ 

 $k = -15 \rightarrow 15$ 

4 standard reflections

frequency: 120 min

intensity decay: 6.8%

 $l = -5 \rightarrow 20$ 

Prismatic

$\omega/2\theta$ scans	$h = -10 \rightarrow 10$
Absorption correction:	$k = -15 \rightarrow 15$
$\psi$ scans ( <i>MolEN</i> ; Fair,	$l = -5 \rightarrow 20$
1990)	4 standard reflections
$T_{\min} = 0.8440, T_{\max} = 0.0000$	frequency: 120 min
0.9999	intensity decay: 1.4%
/15/ measured reflections	
1415 independent reflections	
$[I > 3\sigma(I)]$	
Refinement	
Refinement on F	$\Delta \rho_{\rm max} = 0.189 \ {\rm e} \ {\rm \AA}^{-3}$
R = 0.0106	$\Delta \rho_{\rm min} = -0.172 \ {\rm e} \ {\rm \AA}^{-3}$
wR = 0.0130	Extinction correction: Stout
S = 1.13	& Jensen (1968)
1103 reflections	Extinction coefficient:
71 parameters	$0.229 \times 10^{-3}$
Only H-atom $U$ 's refined	Atomic scattering factors
$w = 1/\sigma^2(F)$	from International Tables
$(\Delta/\sigma)_{\rm max} = 0.003$	for X-ray Crystallography (1974, Vol. IV)

# Table 1. Fractional atomic coordinates and equivalentisotropic displacement parameters ( $\mathring{A}^2$ ) for (1)-(6)

## $B_{\rm eq} = (4/3) \sum_i \sum_j \beta_{ij} \mathbf{a}_i . \mathbf{a}_j.$

		x	у	ĩ	$B_{eq}$
	(1) Cd	0 40357 (2)	1/4	0.25034 (1)	2 120 (4)
	s	0.40357(2) 0.2236(1)	1/4	0.23034(1) 0.64161(4)	2.139(4)
	0	0.2250(1) 0.1850(3)	1/4	0.7451(1)	3 18 (4)
$h = 0.070 + h^{-3}$	CUL	0.0108(4)	1/4	0.5715(2)	2.91 (5)
$\Delta \rho_{\rm max} = 0.2/0 \ {\rm e} \ {\rm A}$	C(2)	() 3545(3)	01152(2)	0.6037(1)	2.95 (4)
$\Delta \rho_{\min} = -0.229 \text{ e A}^{-3}$	Cl.Br(1)	0.65227 (5)	1/4	0.40212(2)	2.405 (8)
Extinction correction: Stout	$Cl_Br(2)$	0.65354 (3)	0.42701 (2)	0.16486(1)	2.304 (4)
& Jensen (1968)	(2)				
Extinction coefficient	(2)	0.40226 (4)	1.14	0.25027 (2)	2174 (5)
$4.610 \times 10^{-6}$	Ca	0.40236(4)	1/4	0.25057(2)	2.174 (5)
4.010 × 10	3	0.2232(1)	1/4	0.04099(0)	2.19(2)
Atomic scattering factors	CU	0.1855(4) 0.0094(7)	1/4	0.7449(2) 0.5711(4)	2.06(0)
from International Tables	C(1)	0.0094 (7)	0.1145 (3)	0.5711(4)	2.90(9)
for X-ray Crystallography	C(2)	0.5545(5)	1/4	0.0027(2) 0.40139(4)	251(1)
(1974  Vol  IV)	C   Br(2)	0.05105(9) 0.65248(5)	0.42697 (3)	(16493(2))	2.31(1)
(1), (, (0), 17)	(3)	0.03210(5)	0.12077 (17)		2
	Cd	0.40003(2)	1/4	0.25054(1)	2.077 (3)
	S	0.2220(1)	1/4	0.64047 (4)	2.132 (9)
	Ō	0.1848 (3)	1/4	0.7448(1)	3.08 (4)
	Č(1)	0.0048 (4)	1/4	0.5703 (2)	3.00 (6)
Ma Ka radiation	C(2)	0.3555 (4)	0.1140(2)	0.6021(1)	2.98 (4)
	Cl,Br(1)	0.64893(1)	1/4	0.40013 (3)	2.410 (9)
x = 0.71073  A	Cl,Br(2)	0.65030(4)	0.42666 (2)	0.16556(2)	2.364 (4)
Cell parameters from 25	(4)				
reflections	Cd	0 39917 (2)	1/4	0.25056(1)	2 106 (4)
$\theta = 5 - 15^{\circ}$	S	0.2215(1)	1/4	0.64025(4)	2.14(1)
$u = 4.53 \text{ mm}^{-1}$	õ	0.1833(3)	1/4	0.7446(1)	3.04 (4)
T = 203 V	$\tilde{C}(1)$	0.0052 (4)	1/4	0.5697 (2)	3.11 (6)
I = 295  K	C(2)	0.3552 (4)	0.1136(2)	0.6014(1)	3.04 (4)
Prismatic	Cl.Br(1)	0.64803 (8)	1/4	0.39975 (3)	2.44(1)
$0.2 \times 0.2 \times 0.2$ mm	Cl,Br(2)	0.64944 (4)	0.42628 (3)	0.16582(2)	2.409 (5
Colourless	(5)				
	Cd	0 39755 (2)	1/4	0 25064 (1)	2.015 (3)
	Š	0.22055 (8)	1/4	0.64010 (3)	2.061 (8)
	õ	0.1830(2)	1/4	0.7450(1)	2.94 (3)
	Č(1)	0.0023 (3)	1/4	0.5698 (2)	2.95 (5)
	C(2)	0.3535 (3)	0.1127 (2)	0.6012(1)	2.92 (3)
$R_{\rm int} = 0.012$	Cl,Br(1)	0.64674 (7)	1/4	0.39908 (3)	2.350 (4)
$\theta_{max} = 30^{\circ}$	Cl.Br(2)	0.64787 (4)	0.42545 (2)	0.16652 (2)	2.317 (9)

Cd	0.39586 (2)	1/4	0.25073(1)	1.938 (3)	Cd— <i>X</i> (2) Cd— <i>X</i> (2 <sup>'</sup> )	2.6878 (2) 2.6780 (2)	S—C(2)		1.7468 (8)
0 0	0.21934(7) 0.1822(2)	1/4	0.03758 (3)	2 84 (2)	X(1)—Cd— $X(1')$	180.0	X(2')—Cd-	$-X(2^{n})$	179.63 (1)
Č(1)	0.0002 (3)	1/4	0.5698 (1)	2.80 (4)	X(1) - Cd - X(2)	85.30(1)	X(2')—Cd-	$-X(2^{m})$	82.93 (1)
C(2)	0.3524 (2)	0.1120 (	1) 0.6011 (1)	2.81 (3)	X(1) = Cd = X(2)	93.00(1)	0 = s = C(1)	1) 7)	112.74 (8)
Cl,Br(1)	0.64513 (6)	1/4	0.39899 (3)	2.240 (9)	X(1) - Cd - X(2)	85.08(1)	C(1)-S-	C(2)	105 56 (5)
Cl,Br(2)	0.64605 (4)	0.42399	0.16755 (2)	2.290 (4)	X(2')—Cd— $X(2')$	) 97.25(1)	C(2)—S—	C(2")	107.26 (6)
	~ · ·		, <b>e</b>	a	$X(2)$ —Cd— $X(2^n)$	82.56(2)			
Table 2. Selected geometric parameters $(A, \circ)$ for $(1)$ – $(6)$			Symmetry code	s: (i) $x - \frac{1}{2}, y, \frac{1}{2} - z$	$x;$ (ii) $x, \frac{1}{2} - y, z$	$z; (iii) x - \frac{1}{2}$	$, \frac{1}{2} - y, \frac{1}{2} - z.$		
Cd—X(1)		2.6824 (3)	S—0	1.437 (1)	<b>TIL 2 0</b>		• .• .	1.00	
Cd - X(1')		2.7009 (3)	S = C(1)	1.743 (3)	Table 3. Occ	supation rates	in the two i	lifferent	sites of the
Cd = X(2) Cd = X(2')		2.7712(2)	S-C(2)	1.740(1)	( <i>C</i> .	$(H_3)_3 SOCdCl_3$	_xBrx mixed	d crystal.	S
X(1)-Cd-	$X(1^{\prime})$	180.0	$X(2^{1}) = Cd = X(2^{11})$	180.0		Site (Cl Br)(1)	Site (	CI Briva	
X(1) - Cd	X(2)	86.18(1)	$X(2^{1})$ —Cd— $X(2^{11})$	83.53 (1)	C	$\Gamma(1)$ $Pr(1)$	CI(2)	Dr(2)	
X(1)—Cd—	$X(2^{1})$	93.98 (1)	0-S-C(1)	112.7(1)		(1) = a $(1) = a$	(1 - b)	bi(2) h	x = 2(a + b)
X(1')—Cd—	-X(2)	93.94 (1)	O - S - C(2)	112.70(7)	(1) 0	0.484 0.516	0.200	0.800	2.116
$X(\Gamma) \rightarrow Cd$	-X(2')	85.90(1)	C(1) = S = C(2)	105.44 (8)	(2) 0	0.635 0.365	0.289	0.711	1.787
$X(2) \rightarrow Cd \rightarrow X(2) \rightarrow X(2)$	$X(2^{n})$	90.33(1) 83.41(1)	C(2) = 3 = C(2)	107.27 (8)	(3) 0	0.809 0.191	0.504	0.496	1.183
(2)	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	0			(4) (5)	0.864 0.136	0.586	0.413	0.962
(2)		2 6677 (6)	S0	1 442 (3)	(5) 0	0.065 0.065	0.729	0.271	0.607
Cd - X(1')		2.6871 (6)	S = C(1)	1.742 (5)	(0) 0		0.074	0.120	0.200
Cd - X(2)		2.7689 (3)	S—C(2)	1.751(2)	Heavy-atom	coordinates fro	m the assur	ned isost	ructural tri-
Cd - X(2')		2.7637 (3)			bromocadmat	e (Puget Jannir	de Brauer	& Perret	1991) were
X(1)—Cd—.	X(1')	180.0	$X(2^{1})$ —Cd— $X(2^{1})$	180.0	used in an in	uitial model to	solve the st	ructure of	F(1) Then
X(1)—Cd—.	X(2)	86.12(1)	$X(2^{1})$ —Cd— $X(2^{11})$	83.66(1)	the structure	of each other	compound w	vac colve	d using the
X(1)—Cd—	$X(2^{1})$	94.03 (1)	O - S - C(1)	112.3 (2)	hoosus atom o	or each other	d for the ear	vas sulve	u using me
X(1') = Cd =	-X(2) -Y(2)	94.00(1)	0-S-C(2)	112.8(1)	high act. Dr. ac	noontration Th		npouna w	the next
X(1) - Cd - X(2) - X	$X(2^{1})$	96.44 (1)	C(1)=3=C(2) $C(2)=S=C(2^{n})$	107.3(1)	nignest br co	incentration. In		es of the	snared (CI,
X(2)—Cd—	X(2")	83.46 (1)		10/12/17	Br) sites wer	re renned using	g the PROM	METHEU.	S programs
(3)					(Zucker, Pere	ninaler, Kuns, r		SCRUIZ,	1985).
Cd—X(1)		2.6403 (5)	S—0	1.438(1)	For all com	pounds, data co	flection: Mo	IEN (Fair,	(1990); cell
Cd = X(1')		2.6611 (5)	S = C(1)	1.754 (3)	rennement: M	ioiciv; data red	uction: Mol	EN; progi	am(s) used
Cd = X(2)		2.7467(2)	S = C(2)	1.751(1)	to solve struc	cture: <i>MolEN</i> ;	program(s)	used to r	enne struc-
$Cu = \lambda(2)$	14/11	2.7585(2)			ture: PROME	<i>THEUS</i> ; molect	llar graphics	: ORIEP	ll (Johnson,
		1 1 1 2 3 2 3							
X(1) - Cd - X(1)	X(1)	180.0	X(2')—Cd— $X(2'')$	179.74 (1)	1976).				
X(1) = Cd = X X(1) = Cd = X	X(1) X(2) $X(2^{1})$	180.0 85.86 (1) 94.34 (1)	X(2')—Cd— $X(2'')X(2')$ —Cd— $X(2''')O—S—C(1)$	179.74 (1) 83.63 (1) 112.78 (1)	1976).				
X(1)—Cd X(1)—Cd X(1)—Cd X(1)—Cd	X(1) X(2) $X(2^{1})$ -X(2)	180.0 85.86 (1) 94.34 (1) 94.17 (1)	$\begin{array}{l} X(2') \longrightarrow Cd \longrightarrow X(2'') \\ X(2') \longrightarrow Cd \longrightarrow X(2'') \\ O \longrightarrow S \longrightarrow C(1) \\ O \longrightarrow S \longrightarrow C(2) \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6)	1976).				
X(1) - Cd - Z X(1) - Cd - Z X(1) - Cd - Z X(1') - Cd - Z X(1') - Cd - Z	X(1) X(2) X(2 <sup>i</sup> ) -X(2) -X(2 <sup>i</sup> )	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1)	$\begin{array}{l} X(2') - Cd - X(2'') \\ X(2') - Cd - X(2'') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9)	Lists of structu	ure factors, anisc	ptropic displac	cement pa	rameters, H-
X(1)—Cd X(1)—Cd X(1)—Cd X(1)—Cd X(1')—Cd X(1')—Cd X(2)—Cd X(2)—Cd X(2)—Cd	X(1) X(2) $X(2^{1})$ -X(2) -X(2') X(2') X(2')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1)	$\begin{array}{l} X(2^{*}) \longrightarrow Cd \longrightarrow X(2^{*}) \\ X(2^{*}) \longrightarrow Cd \longrightarrow X(2^{**}) \\ O \longrightarrow S \longrightarrow C(1) \\ O \longrightarrow S \longrightarrow C(2) \\ C(1) \longrightarrow S \longrightarrow C(2) \\ C(2) \longrightarrow S \longrightarrow C(2^{**}) \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9)	Lists of structu atom coordinate	ure factors, aniso es and complete	tropic displace geometry hav	cement par ve been de	rameters, H- posited with
X(1) = Cd = 2 X(1) = Cd = 2 X(1) = Cd = 2 X(1) = Cd = 2 X(1) = Cd = 2 X(2) = Cd = 2 X(2) = Cd = 2	X(1) X(2) X(2') -X(2) -X(2) X(2') X(2')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1)	$\begin{array}{l} \chi(2^{\circ}) \longrightarrow Cd \longrightarrow \chi(2^{\circ}) \\ \chi(2^{\circ}) \longrightarrow Cd \longrightarrow \chi(2^{\circ}) \\ O \longrightarrow S \longrightarrow C(1) \\ O \longrightarrow S \longrightarrow C(2) \\ C(1) \longrightarrow S \longrightarrow C(2) \\ C(2) \longrightarrow S \longrightarrow C(2^{\circ}) \\ C(2) \longrightarrow S \longrightarrow C(2^{\circ}) \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9)	Lists of structu atom coordinate the IUCr (Refer Managing Edit	ure factors, aniso es and complete rence: PA1189). (	ptropic displac geometry hav Copies may be	cement par ve been de e obtained	rameters, H- posited with through The
$\begin{array}{c} X(1) - Cd - z \\ X(2) - Cd - z \\ X(3) - $	X(1) X(2) -X(2) -X(2) -X(2') X(2') X(2'')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1)	$\begin{array}{l} \chi(2^{\circ}) \longrightarrow Cd \longrightarrow \chi(2^{\circ}) \\ \chi(2^{\circ}) \longrightarrow Cd \longrightarrow \chi(2^{\circ}) \\ O \longrightarrow S \longrightarrow C(1) \\ O \longrightarrow S \longrightarrow C(2) \\ C(1) \longrightarrow S \longrightarrow C(2) \\ C(2) \longrightarrow S \longrightarrow C(2^{\circ}) \\ \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Scurge Chester	ure factors, anisc es and complete rence: PA1189). ( or, International CH12HULEng	tropic displac geometry hav Copies may be Union of Cry and	cement pa ve been de e obtained vstallograph	rameters, H- posited with through The ny, 5 Abbey
$\begin{array}{c} X(1) - Cd - J \\ X(1) - Cd - J \\ X(1) - Cd - J \\ X(1') - Cd - J \\ X(1') - Cd - J \\ X(2) $	X(1)  X(2)  -X(2)  -X(2)  -X(2')  X(2')  X(2'')  X(2'')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5)	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2''') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9)	1976). Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl	etropic displac geometry hav Copies may be Union of Cry and.	cement pa ve been de e obtained vstallograph	rameters, H- posited with through The ny, 5 Abbey
$\begin{array}{c} X(1) - Cd \\ X(1) - Cd \\ X(1) - Cd \\ X(1') - Cd \\ X(1') - Cd \\ X(2) - Cd$	X(1) X(2) X(2') -X(2) -X(2') X(2') X(2'')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2)	$\begin{array}{l} \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(1) \\ S - C(2) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1)	1976). Lists of structu atom coordinate the IUCr (Refen Managing Edite Square, Chester	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl	etropic displac geometry hav Copies may be Union of Cry and.	cement pa ve been de e obtained vstallograpi	rameters, H- posited with through The ny, 5 Abbey
$\begin{array}{l} \chi(1) = Cd = -, \\ \chi(2) = $	X(1) X(2) X(2') -X(2) -X(2') X(2') X(2')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2)	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2''') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl	etropic displac geometry hav Copies may be Union of Cry and.	cement pa ve been de e obtained vstallograph	rameters, H- posited with through The ny, 5 Abbey
$\begin{array}{l} \chi(1) = Cd = 0, \\ \chi(2) = 0$	X(1) X(2) X(2) -X(2) -X(2) X(2') X(2') X(2'')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0	$\begin{array}{l} \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester References	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl	etropic displac geometry hav Copies may be Union of Cry and.	cement pa ve been de e obtained vstallograph	rameters, H- posited with through The ny, 5 Abbey
$\begin{array}{l} \chi(1) = Cd = 0, \\ \chi(2) = 0, $	X(1) X(2) X(2') -X(2) X(2') X(2') X(2') X(2') X(2'') X(2'')	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1)	$\begin{array}{l} \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(2) \\ S - C(1) \\ S - C(2) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester <b>References</b> Arend, H., Per	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl Tet, R., Wüest,	tropic displac geometry hav Copies may be Union of Cry and. H. & Kerkoo	cement par ve been de e obtained vstallograph	rameters, H- posited with through The ny, 5 Abbey 5). J. Cryst.
$\begin{array}{l} \chi(1) = Cd = , \\ \chi(2) = Cd = , \\ \chi(1) = $	X(1) X(2) X(2') -X(2) -X(2') X(2') X(2') X(2') $X(1^{1})$ X(2) X(2) X(2')	180.0 85.86 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.17 (1)	$\begin{array}{l} \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(2) \\ S - C(1) \\ S - C(2) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ Q - S - C(1) \\ S - C(2) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 2	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl Tet, R., Wüest, 321–325.	tropic displac geometry hav Copies may be Union of Cry and. H. & Kerkoo	cement par ve been de e obtained vstallograph	rameters, H- posited with through The ny, 5 Abbey
$\begin{array}{c} \chi(1) - Cd - , \\ \chi(2) - Cd - , \\ \chi(1) - , \\ \chi($	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  X(2)  X(2)  X(2)  X(2)  X(2)  X(2)  -X(2)	180.0 85.86 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1)	$\begin{array}{l} \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(2) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ Q - S - C(1) \\ O - S - C(2) \\ \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105 54 (0)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 5 Fair, C. K. (19	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl Tet, R., Wüest, 321–325. 990). <i>MolEN</i> . Au	tropic displac geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>Interactive</i>	cement par ve been de e obtained vstallograph c, P. (1986 Intelligent	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. System for
$\begin{array}{c} \chi(1) - Cd - , \\ \chi(2) - Cd - , \\ \chi(1) - Cd - , \\ \chi(2) -$	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -	180.0 85.86 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1) 96.63 (1)	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2''') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105.54 (9) 106.6 (1)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 5 Fair, C. K. (1) <i>Crystal Struc</i>	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl Tet, R., Wüest, 321–325. 990). <i>MolEN</i> . As <i>ture Analysis</i> . En	tropic displat geometry hav Copies may be Union of Cry and. H. & Kerkoc <i>n Interactive</i> raf-Nonius, D	cement par ve been de e obtained stallograph c, P. (1980 Intelligent Delft, The f	ameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5): J. Cryst. System for Netherlands.
$\begin{array}{c} x(1) - Cd - \\ x(2) - Cd - \\ x(1) - Cd - \\ x(2) $	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -X(2)  -X(2)  X(2)  -X(2)  -X	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.427 (1) 85.52 (1) 96.63 (1) 83.21 (1)	$\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ \end{array}$ $\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.75 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105.54 (9) 106.6 (1)	Lists of structu atom coordinate the IUCr (Refei Managing Editt Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 1 Fair, C. K. (1 <sup>th</sup> <i>Crystal Struc</i> Gready, J. E., B 467, 473	ure factors, anisc es and complete rence: PA1189). ( or, International - CH1 2HU, Engl ret, R., Wüest, 321–325. 990). <i>MolEN. As</i> <i>ture Analysis.</i> En Bacskay, G. B. &	tropic displac geometry hav Copies may be Union of Cry and. H. & Kerkoc <i>n Interactive</i> raf–Nonius, E Huch, N. S. (	cement pai ve been de e obtained stallograph s, P. (1980 Intelligent belft, The I 1970). Che	<ul> <li>rameters, H-posited with through The hy, 5 Abbey</li> <li>5). J. Cryst.</li> <li>5): System for Netherlands.</li> <li>m. Phys. 33,</li> </ul>
$\begin{array}{c} \chi(1) - Cd - , \\ \chi(2) - Cd - , \\ \chi(1) - Cd - , \\ \chi(2) - , \\ \chi($	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1) 96.63 (1) 83.21 (1)	$\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105.54 (9) 106.6 (1)	Lists of structu atom coordinate the IUCr (Refei Managing Editt Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 3 Fair, C. K. (19 <i>Crystal Struc</i> Gready, J. E., B 467–473. Iobnson, C. K.	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	tropic displat geometry hav Copies may be Union of Cry and. H. & Kerkoc <i>n Interactive</i> raf–Nonius, E Huch, N. S. (	cement pai ve been de e obtained stallograph s, P. (1980 <i>Intelligent</i> Delft, The I 1970). Che RNL 5138	<ul> <li>rameters, H-posited with through The 19, 5 Abbey</li> <li>5). J. Cryst.</li> <li>5). J. Cryst.</li> <li>5) System for Netherlands.</li> <li>m. Phys. 33,</li> <li>Oak Bidge</li> </ul>
$\begin{array}{c} x(1) - Cd - z \\ x(2) - Cd - z \\ x(1) - Cd - z \\ x(2) - $	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2')  -X(	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1) 96.63 (1) 83.21 (1) 2.6172 (2)	$\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ \circ}) \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1)	Lists of structu atom coordinate the IUCr (Refei Managing Editt Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 3 Fair, C. K. (19 <i>Crystal Struct</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab	ure factors, aniso es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	tropic displat geometry hav Copies may be Union of Cry and. H. & Kerkoc <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e. USA	cement pai ve been de e obtained stallograph s, P. (1980 <i>Intelligent</i> Delft, The I 1970). Che RNL-5138.	<ul> <li>rameters, H-posited with through The 19, 5 Abbey</li> <li>5). J. Cryst.</li> <li>5). J. Cryst.</li> <li>5) System for Netherlands.</li> <li>m. Phys. 33,</li> <li>Oak Ridge</li> </ul>
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ x($	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2')  X(2')  -X(2')  -X(2')  -X(2')  -X(2')  -X(2')  -X(2')  -X(2')  -X(2')  -X(2)	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1) 96.63 (1) 83.21 (1) 2.6172 (2) 2.6375 (2)	$\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \hline X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - O \\ S - C(1) \\ \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1) 1.752 (2)	Lists of structu atom coordinate the IUCr (Refei Managing Editu Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 3 Fair, C. K. (19 <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19	ure factors, aniso es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	tropic displat geometry hav Copies may be Union of Cry and. H. & Kerkot <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report OI e, USA. <i>Bull.</i> <b>18</b> , 765	cement pai ve been de e obtained vstallograph c, P. (1980 Intelligent Delft, The I 1970). Che RNL-5138. –773.	<ul> <li>rameters, H-posited with through The 19, 5 Abbey</li> <li>5). J. Cryst.</li> <li>5). J. Cryst.</li> <li>5). System for Netherlands.</li> <li>m. Phys. 33,</li> <li>Oak Ridge</li> </ul>
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ x(2$	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2')  X(2')  -X(2')  -X(	180.0 85.86 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1) 96.63 (1) 83.21 (1) 2.6172 (2) 2.6375 (2) 2.7164 (4) 7.766 (4)	$\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - O \\ S - C(1) \\ S - C(2) \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.7 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1) 1.752 (2) 1.750 (1)	Lists of structu atom coordinate the IUCr (Refei Managing Editt Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 3 Fair, C. K. (19 <i>Crystal Struct</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19 Perret, R., Go	ure factors, aniso es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	tropic displat geometry hav Copies may be Union of Cry and. H. & Kerkoc <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report OI e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985	cement pai ve been de e obtained stallograph s, P. (1980 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J.	rameters, H- posited with through The iy, 5 Abbey 5). J. Cryst. 5). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 00ak Ridge Appl. Phys.
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ x(2$	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)	180.0           85.86 (1)           94.34 (1)           94.34 (1)           94.17 (1)           85.63 (1)           96.53 (1)           83.32 (1)           2.6300 (5)           2.6516 (5)           2.7355 (2)           2.7269 (2)           180.0           85.77 (1)           94.44 (1)           94.27 (1)           85.52 (1)           96.63 (1)           83.21 (1)           2.6172 (2)           2.6375 (2)           2.7164 (4)           2.7065 (4)           90.02	$\begin{array}{l} X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \hline X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ X(2^{\circ}) - Cd - X(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \hline S - O \\ S - C(1) \\ S - C(2) \\ \hline \end{array}$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1) 1.752 (2) 1.750 (1)	Lists of structu atom coordinate the IUCr (Refei Managing Editu Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 3 Fair, C. K. (19 <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (15) Perret, R., Goo <i>Suppl.</i> 24, 75	Tret, R., Wüest, 321–325. 990). <i>MolEN. Alture Analysis</i> . En Bacskay, G. B. & (1976). <i>ORTEP</i> oratory, Tennesse 83). <i>Mater. Res.</i> defroy, G. & Arc 56–764.	tropic displat geometry hav Copies may be Union of Cry and. H. & Kerkot <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report OI <i>e</i> , USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985)	cement pai ve been de e obtained vstallograph c, P. (1980 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J.	rameters, H- posited with through The iy, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0 Oak Ridge Appl. Phys.
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - Cd - , \\ x(2) - , \\ x(1) - , \\ x(2) - , \\$	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)	180.0           85.86 (1)           94.34 (1)           94.34 (1)           94.17 (1)           85.63 (1)           96.53 (1)           83.32 (1)           2.6300 (5)           2.6516 (5)           2.7355 (2)           2.7269 (2)           180.0           85.77 (1)           94.44 (1)           94.27 (1)           85.52 (1)           96.63 (1)           83.21 (1)           2.6172 (2)           2.6375 (2)           2.7164 (4)           2.7065 (4)           180.0           85.57 (1)	$\begin{array}{l} \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \chi(2^{\circ}) - Cd - \chi(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{\circ}) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179.69 (1) 83.24 (1)	1976). Lists of structu atom coordinate the IUCr (Refer Managing Editu Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 3 Fair, C. K. (19 <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19 Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni	ure factors, aniso es and complete rence: PA1189). ( or, International · CH1 2HU, Engl · CH1 2	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoce <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret,	cement pai ve been de obtained stallograph c, P. (1980 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J. R. (1991)	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0. Oak Ridge Appl. Phys. Acta Cryst.
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - , \\ $	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  X(2)  -X(2)  -X(	180.0           85.86 (1)           94.34 (1)           94.34 (1)           94.17 (1)           85.63 (1)           96.53 (1)           83.32 (1)           2.6300 (5)           2.6516 (5)           2.7355 (2)           2.7269 (2)           180.0           85.77 (1)           94.44 (1)           94.27 (1)           85.52 (1)           96.63 (1)           83.21 (1)           2.6172 (2)           2.6375 (2)           2.7164 (4)           2.7065 (4)           180.0           85.52 (1)           94.72 (1)	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - \chi(2'') \\ \chi(2'') \chi$	179,74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179.69 (1) 83.31 (1) 112.77 (9)	Lists of structu atom coordinate the IUCr (Refer Managing Editu Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 2 Fair, C. K. (19 <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19 Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni C47, 1803–13	ure factors, aniso es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	Here the transformed to the transformation of transformation of the transformation of the transformation of the transformation of transformation	cement pai ve been de e obtained stallograph c, P. (1980 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J. R. (1991)	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0. Oak Ridge Appl. Phys. . Acta Cryst.
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - $	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2')  X(2)  X	180.0           85.86 (1)           94.34 (1)           94.34 (1)           94.17 (1)           85.63 (1)           96.53 (1)           83.32 (1)           2.6300 (5)           2.6516 (5)           2.7355 (2)           2.7269 (2)           180.0           85.77 (1)           94.44 (1)           94.27 (1)           85.52 (1)           96.63 (1)           83.21 (1)           2.6172 (2)           2.6375 (2)           2.7164 (4)           2.7065 (4)           180.0           85.52 (1)           94.72 (1)           94.72 (1)	$\begin{array}{l} \chi(2^{i}) - Cd - \chi(2^{ii}) \\ \chi(2^{i}) - Cd - \chi(2^{ii}) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{ii}) \\ \chi(2^{i}) - Cd - \chi(2^{ii}) \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2^{ii}) \\ (2^{ii}) - Cd - \chi(2^{ii}) \\ S - C(2) \\ \chi(2^{ii}) - Cd - \chi(2^{ii}) \\ O - S - C(1) \\ O - S - C(2) \\ \end{array}$	179,74 (1) 83.63 (1) 112,78 (1) 112,55 (6) 105,83 (9) 106,77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179,73 (1) 83.54 (1) 112,84 (6) 105,54 (9) 106,6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179,69 (1) 83.31 (1) 112,72 (9) 112,70 (5)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 17 Fair, C. K. (11) <i>Crystal Struce</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (15) Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni C47, 1803–13 Shannon, R. D.	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret, (1969). Acta	cement pai ve been de e obtained stallograph c, P. (1986 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J. R. (1991) Cryst. B2	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0. Oak Ridge Appl. Phys. 6. Acta Cryst. 5, 925–946.
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(2) - Cd - , \\ x(2) - Cd - , \\ x(1) - ,$	X(1)  X(2)  X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2)  X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -X(	180.0           85.86 (1)           94.34 (1)           94.34 (1)           94.17 (1)           85.63 (1)           96.53 (1)           83.32 (1)           2.6300 (5)           2.6516 (5)           2.7355 (2)           2.7269 (2)           180.0           85.77 (1)           94.44 (1)           94.27 (1)           85.52 (1)           96.63 (1)           83.21 (1)           2.6172 (2)           2.6375 (2)           2.7164 (4)           2.7065 (4)           180.0           85.52 (1)           94.72 (1)           94.72 (1)           94.72 (1)           94.72 (1)           94.72 (1)	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ O - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ (1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ \end{array}$	179,74 (1) 83.63 (1) 112,78 (1) 112,55 (6) 105,83 (9) 106,77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179,73 (1) 83.54 (1) 112,84 (6) 105,54 (9) 106,6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179,69 (1) 83.31 (1) 112,72 (9) 112,70 (5) 105,51 (7)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester <b>References</b> Arend, H., Per <i>Growth</i> , 74, 7 Fair, C. K. (1) <i>Crystal Struce</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19 Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni C47, 1803–13 Shannon, R. D. Stout, G. H. &	ure factors, aniso es and complete rence: PA1189). (o or, International CH1 2HU, Engl CH1 2HU, Engl	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret, (1969). <i>Acta</i> 268). X-ray St	cement pai ve been de e obtained stallograph c, P. (1980 Intelligent Delft, The I 1970). Che RNL-5138. -773. 5). Jpn J. R. (1991) Cryst. B29 tructure De	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0. Oak Ridge Appl. Phys. 6. Acta Cryst. 5, 925–946. etermination.
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ x($	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2')  -X(2)	180.0 85.86 (1) 94.34 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 85.52 (1) 94.63 (1) 83.21 (1) 2.6172 (2) 2.7164 (4) 2.7065 (4) 180.0 85.52 (1) 94.42 (1) 85.32 (1) 94.43 (1) 85.32 (1) 94.43 (1) 85.32 (1) 94.43 (1) 85.32 (1) 94.43 (1) 94.43 (1) 85.32 (1) 94.43 (1) 94.44 (1) 94.43 (1) 94.43 (1) 94.44 (1) 94.43 (1) 94.44 (1) 94.43 (1) 94.44 (1) 94.43 (1) 94.44 (1) 94.43 (1) 94.44 (1) 94.43 (1) 94.44 (1) 94.44 (1) 94.43 (1) 94.44 (1) 85.32 (1) 95.44 (1) 85.44	$\begin{array}{l} \chi(2') - \mathbb{C}d - \chi(2'') \\ \chi(2') - \mathbb{C}d - \chi(2'') \\ O - S - \mathbb{C}(1) \\ O - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(2) - S - \mathbb{C}(2'') \\ \end{array}$ $\begin{array}{l} S - 0 \\ S - \mathbb{C}(2) \\ \chi(2') - \mathbb{C}d - \chi(2'') \\ \chi(2') - \mathbb{C}d - \chi(2'') \\ O - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2'') \\ \end{array}$ $\begin{array}{l} S - 0 \\ S - \mathbb{C}(2) \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2'') \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2'') \\ \end{array}$	179,74 (1) 83.63 (1) 112,78 (1) 112,75 (6) 105,83 (9) 106,77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179,73 (1) 83.54 (1) 112,84 (6) 105,54 (9) 106,6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179,69 (1) 83.31 (1) 112,72 (9) 112,70 (5) 105,51 (7) 107,12 (7)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester References Arend, H., Per <i>Growth</i> , 74, 7 Fair, C. K. (1 <sup>11</sup> <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19 Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni C47, 1803–13 Shannon, R. D. Stout, G. H. & New York: M	ure factors, anisc es and complete rence: PA1189). ( or, International CH1 2HU, Engl CH1 2HU, Engl C	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret, (1969). <i>Acta</i> 968). X-ray St	cement pai ve been de e obtained stallograph c, P. (1986 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J. R. (1991) Cryst. B29 tructure De	<ul> <li>rameters, H-posited with through The ny, 5 Abbey</li> <li>5). J. Cryst.</li> <li>5). J. Cryst.</li> <li>5). System for Netherlands.</li> <li>m. Phys. 33,</li> <li>Oak Ridge</li> <li>Appl. Phys.</li> <li>Acta Cryst.</li> <li>5, 925–946.</li> <li>etermination.</li> </ul>
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(2) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ x(2) - Cd - , \\ x(2) - Cd - , \\ x(2) - , \\ x(2$	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2')  X(2')  X(2')  X(2)  -X(2)  -	$\begin{array}{l} 180.0\\ 85.86 (1)\\ 94.34 (1)\\ 94.34 (1)\\ 94.7 (1)\\ 85.63 (1)\\ 96.53 (1)\\ 83.32 (1)\\ 2.6300 (5)\\ 2.6516 (5)\\ 2.7355 (2)\\ 2.7269 (2)\\ 180.0\\ 85.77 (1)\\ 94.44 (1)\\ 94.27 (1)\\ 85.52 (1)\\ 94.44 (1)\\ 94.27 (1)\\ 85.52 (1)\\ 94.63 (1)\\ 83.21 (1)\\ 2.6172 (2)\\ 2.7164 (4)\\ 2.7065 (4)\\ 180.0\\ 85.52 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.72 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.32 (1)\\ 94.74 (1)\\ 85.94 (1)\\ 82.94 (1)\\ 82.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\ 85.94 (1)\\$	$\begin{array}{l} \chi(2') - \mathbb{C}d - \chi(2'') \\ \chi(2') - \mathbb{C}d - \chi(2'') \\ O - S - \mathbb{C}(1) \\ O - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(2) - S - \mathbb{C}(2'') \\ \end{array}$ $\begin{array}{l} S - 0 \\ S - \mathbb{C}(2) \\ \chi(2') - \mathbb{C}d - \chi(2'') \\ \chi(2') - \mathbb{C}d - \chi(2'') \\ O - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(1) - S - \mathbb{C}(2) \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2'') \\ \end{array}$ $\begin{array}{l} S - 0 \\ S - \mathbb{C}(2) \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2'') \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2) \\ \mathbb{C}(1) - \mathbb{C}d - \mathbb{C}(2) \\ \mathbb{C}(2) - \mathbb{C}d - \mathbb{C}(2'') \\ \end{array}$	179,74 (1) 83.63 (1) 112,78 (1) 112,55 (6) 105,83 (9) 106,77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179,73 (1) 83.54 (1) 112,84 (6) 105,54 (9) 106,6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179,69 (1) 83.31 (1) 112,72 (9) 112,70 (5) 105,51 (7) 107,12 (7)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester References Arend, H., Per <i>Growth</i> , 74, 7 Fair, C. K. (1 <sup>11</sup> <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (19 Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni C47, 1803–13 Shannon, R. D. Stout, G. H. & New York: M	ure factors, aniso es and complete rence: PA1189). (o or, International CH1 2HU, Engl CH1 2HU, Engl	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret, (1969). <i>Acta</i> 968). <i>X-ray Si</i> Vatts, B. E. (1	cement pai ve been de e obtained /stallograph c, P. (1986 <i>Intelligent</i> Delft, The N 1970). <i>Che</i> RNL-5138. –773. 5). <i>Jpn J.</i> R. (1991) <i>Cryst.</i> B29 tructure De 992). Acta	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0 Oak Ridge Appl. Phys. 6, Acta Cryst. 5, 925–946. etermination. 6 Cryst. B48,
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - , \\ $	X(1)  X(2)  X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2)  -X(2)  -X(2)  -X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2')  -X(2)	180.0 85.86 (1) 94.34 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 85.52 (1) 94.63 (1) 83.21 (1) 2.6172 (2) 2.7164 (4) 2.7065 (4) 180.0 85.52 (1) 94.42 (1) 85.32 (1) 94.43 (1) 85.32 (1) 94.44 (1) 85.52 (1) 94.44 (1) 85.52 (1) 94.44 (1) 85.52 (1) 94.44 (1) 85.52 (1) 94.44 (1) 85.52 (1) 94.44 (1) 85.54	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ (1) - S - C(2) \\ \chi(2') - Cd - \chi(2'') \\ (2) - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$	179.74 (1) 83.63 (1) 112.78 (1) 112.55 (6) 105.83 (9) 106.77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179.73 (1) 83.54 (1) 112.84 (6) 105.54 (9) 106.6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179.69 (1) 83.31 (1) 112.72 (9) 112.70 (5) 105.51 (7) 107.12 (7)	Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester References Arend, H., Per <i>Growth</i> , 74, 7 Fair, C. K. (11 <i>Crystal Struc</i> Gready, J. E., B 467–473. Johnson, C. K. National Lab Nord, A. G. (15 Perret, R., Goo <i>Suppl.</i> 24, 75 Puget, R., Janni C47, 1803–13 Shannon, R. D. Stout, G. H. & New York: M Thomas, P. A., 401–407. Zucker, 11 H	ure factors, aniso es and complete rence: PA1189). (o or, International CH1 2HU, Engl CH1 2HU, Engl	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret, (1969). <i>Acta</i> 968). <i>X-ray Si</i> Vatts, B. E. (1 uhs W F Pat	cement pai ve been de e obtained stallograph c, P. (1986 Intelligent Delft, The I 1970). Che RNL-5138. –773. 5). Jpn J. R. (1991) Cryst. B29 tructure De 992). Acta	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0 Oak Ridge Appl. Phys. 6, 925–946. etermination. 6 Cryst. B48, 8 & Schulz
$\begin{array}{c} x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - Cd - , \\ x(2) - Cd - , \\ x(1) - $	X(1)  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2)  X(2)  -X(2)  -X(2)  X(2')  X(2')  X(2')  X(2')  X(2')  X(2')  X(2')  X(2)  -X(2)  X(2')  X(2)  -X(2)  -X(	180.0 85.86 (1) 94.34 (1) 94.34 (1) 94.17 (1) 85.63 (1) 96.53 (1) 83.32 (1) 2.6300 (5) 2.6516 (5) 2.7355 (2) 2.7269 (2) 180.0 85.77 (1) 94.44 (1) 94.27 (1) 85.52 (1) 94.63 (1) 83.21 (1) 2.6172 (2) 2.7164 (4) 2.7065 (4) 180.0 85.52 (1) 94.44 (1) 85.52 (1) 94.44 (1) 94.74 (1) 85.52 (1) 94.74 (1) 85.52 (1) 94.74 (1) 85.52 (1) 94.74 (1) 94.74 (1) 85.75 (2) 2.7164 (4) 2.7065 (3) 2.6065 (3) 2.60279 (3)	$\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \chi(2') - Cd - \chi(2'') \\ O - S - C(1) \\ O - S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ S - C(2) \\ \end{array}$ $\begin{array}{l} \chi(2') - Cd - \chi(2'') \\ \end{array}$ $\begin{array}{l} S - O \\ S - C(1) \\ O - S - C(2) \\ C(1) - S - C(2) \\ C(1) - S - C(2) \\ C(2) - S - C(2'') \\ \end{array}$	179,74 (1) 83.63 (1) 112,78 (1) 112,75 (6) 105,83 (9) 106,77 (9) 1.437 (1) 1.748 (3) 1.752 (1) 179,73 (1) 83.54 (1) 112,84 (6) 105,54 (9) 106,6 (1) 1.440 (1) 1.752 (2) 1.750 (1) 179,69 (1) 83.31 (1) 112,72 (9) 112,70 (5) 105,51 (7) 107,12 (7) 1.439 (1) 1.749 (2)	<ul> <li>1976).</li> <li>Lists of structu atom coordinate the IUCr (Refer Managing Edite Square, Chester</li> <li>References</li> <li>Arend, H., Per <i>Growth</i>, 74, 7</li> <li>Fair, C. K. (1<sup>1</sup> <i>Crystal Struc</i></li> <li>Gready, J. E., B 467–473.</li> <li>Johnson, C. K. National Lab</li> <li>Nord, A. G. (19)</li> <li>Perret, R., Goo <i>Suppl.</i> 24, 75</li> <li>Puget, R., Janni C47, 1803–13</li> <li>Shannon, R. D.</li> <li>Stout, G. H. &amp; New York: M</li> <li>Thomas, P. A., 401–407.</li> <li>Zucker, U. H., H</li> <li>H. (1983) 1</li> </ul>	ure factors, aniso es and complete rence: PA1189). (o or, International CH1 2HU, Engl CH1 2HU, Engl Tet, R., Wüest, 321-325. 990). MolEN. An ture Analysis. En Bacskay, G. B. & . (1976). ORTEP oratory, Tennesse 983). Mater. Res. defroy, G. & Aro 56-764. in, M., de Brauer 805. & Prewitt, C. T. Jensen, L. M. (19 facmillan. Mayo, S. C. & W Perenthaler, E., K Appl. Cryst 16	tropic displace geometry hav Copies may be Union of Cry and. H. & Kerkoo <i>n Interactive</i> raf–Nonius, E Huch, N. S. ( II. Report Ol e, USA. <i>Bull.</i> <b>18</b> , 765 end, H. (1985) , C. & Perret, (1969). <i>Acta</i> 968). <i>X-ray Si</i> Vatts, B. E. (1 uhs, W. F., Ba 358.	cement pai ve been de e obtained /stallograph c, P. (1986 Intelligent Delft, The N 1970). Che RNL-5138. –773. 5). Jpn J. R. (1991) Cryst. B29 tructure De 992). Acta achmann, J	rameters, H- posited with through The ny, 5 Abbey 6). J. Cryst. 5). J. Cryst. 5). System for Netherlands. m. Phys. 33, 0 Oak Ridge Appl. Phys. 6, Acta Cryst. 5, 925–946. etermination. 6 Cryst. B48, R. & Schulz,