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Crystal and Molecular Structure of Cadmium Trihydrogenhexaoxoiodate(VII) Trihydrate

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Crystals of $Cd[H_3IO_6] \cdot 3H_2O$ are monoclinic, space group $P2_1/c$. The unit-cell constants are $a = 5{\cdot}957\ (7)$, $b = 14{\cdot}380\ (11)$, $c = 9{\cdot}715\ (7)$ Å, $\beta = 120{\cdot}8\ (2)°$. The structure has been determined from three-dimensional data. The anion is single and nearly octahedral; the iodine–oxygen bonds can be subdivided into two groups: $I–O^*_{av} = 1{\cdot}95$ Å and $I–O_{av} = 1{\cdot}86$ Å. The cadmium atoms bridge two anions, forming bonds $Cd–O(2) = 2{\cdot}25$ and $Cd–O(5') = 2{\cdot}23$ Å; other short bonds are $Cd–OH_2(2) = 2{\cdot}27$ and $Cd–OH_2(3) = 2{\cdot}41$ Å. Other interactions between cations and a water molecule or anion range from 2·49 to 2·79 Å. Besides the bridging cadmium cations, the anions are bound to one another or to water molecules by several hydrogen bonds, some of which are fairly strong (2·62, 2·65, 2·70, 2·72 Å).

Introduction

Iodine(VII) can form several periodic acids, and the corresponding salts, namely hexaoxoiodic(VII), H_5IO_6, pentaoxoiodic(VII), H_3IO_5, tetraoxoiodic(VII), HIO_4, hendecaoxodiiodic(VII), $H_8I_2O_{11}$, decaoxodiiodic(VII), $H_6I_2O_{10}$, enneaoxodiiodic(VII), $H_4I_2O_9$, and tetracaidecaoxotriiodic(VII), $H_7I_3O_{14}$. Two iso structural hydrates of the cadmium and calcium periodates have been prepared in this laboratory (Biagini Cingi, Emiliani & Guastini, 1967) to which, according to Siebert (1967), the formula $Ca_2H_2I_2O_{10} \cdot 8H_2O$ or $Cd_2H_2I_2O_{10} \cdot 8H_2O$ should have been assigned. This assignment was made by Siebert on the basis of the infrared spectra. However, other formulae could be assigned to these compounds, derived from some of the acids mentioned above. In order to assess which is the proper formula, we have undertaken the study of the crystal structure of the cadmium compound.

Experimental

Preparation

Crystals of the cadmium compound were prepared from aqueous solutions obtained by dissolving cadmium carbonate in periodic acid.

Crystal data

Compound: cadmium trihydrogenhexaoxoiodate(VII) trihydrate, $Cd[H_3IO_6] \cdot 3H_2O$, F.W. 392·39. Crystal class: monoclinic, prismatic. Unit cell (Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å), from rotation and Weissenberg photographs around [100] and [010]: $a = 5{\cdot}957\ (7)$, $b = 14{\cdot}380\ (11)$, $c = 9{\cdot}715\ (7)$ Å, $\beta = 120{\cdot}8\ (2)°$, $V = 714{\cdot}8$ Å^3, $Z = 4$, $D_x = 3{\cdot}65$, $D_m = 3{\cdot}61$ g.cm^{-3}. Space group $P2_1/c$ (No. 14–C^5_{2h}) from systematic absences. μ(Cu $K\alpha$) = 602·4 cm^{-1}.

Intensity measurement

Integrated reflexions $0kl$, $1kl$ ... $5kl$ and $h0l$, $h1l$ ... $h11l$ were recorded by an integrating camera; the intensities of 1447 observed independent reflexions out of the 1673 possible were measured by a microdensitometer. Absorption corrections were applied as for cylindrical specimens ($\mu\bar{R}_{[010]} = 9{\cdot}04$, $\mu\bar{R}_{[100]} = 10{\cdot}84$). The atomic form factors of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) were used for O, and those of Thomas & Umeda (1957) for Cd^{2+} and I.

The calculations were performed on the computer Olivetti Elea 6001/S of Centro di Calcolo Elettronico of the University of Parma.

Determination and refinement of the structure

The structure was solved by standard Patterson and Fourier procedures. The interpretation of the electron density map permits us to assign to the anion the octahedral structure of a hexaoxoiodate(VII) group. The refinement was carried out by differential syntheses; anisotropic thermal parameters were refined by the method of Nardelli & Fava (1960). Due to the high absorption power of the substance, the temperature factors are greatly affected by systematic errors. The physical meaning of the temperature factors is therefore very doubtful and the quoted values are those introduced in the calculation of the structure factors. Assesment of their accuracy is meaningless. Refinement converged to $R=10{\cdot}9\%$ (observed reflexions only). The final results are given in Tables 1–5.

Table 1. *Fractional atomic coordinates (with e.s.d.'s)* $\times 10^4$

	x	*y*	*z*
I	2197 (5)	2411 (1)	0510 (3)
Cd	2426 (7)	0804 (1)	3236 (4)
O(1)	0414 (106)	3214 (9)	1250 (61)
O(2)	0529 (118)	1378 (19)	0733 (80)
O(3)	4817 (54)	2202 (9)	2753 (22)
O(4)	4161 (86)	1576 (10)	−0088 (49)
O(5)	4248 (95)	3388 (14)	0524 (63)
O(6)	−0295 (63)	2650 (13)	−1627 (29)
$H_2O(1)$	2879 (78)	−0356 (8)	5295 (37)
$H_2O(2)$	2822 (141)	−0484 (37)	2044 (88)
$H_2O(3)$	−2000 (132)	0264 (16)	2133 (76)

Discussion

The octahedral anions are clearly recognizable in the structure (Fig. 1). Each cadmium cation is bound to two anions and bridges them. Disregarding the standard deviations which are probably affected by systematic absorption errors, the iodine–oxygen distances in the anion (Fig. 2) can be interpreted on the

Table 2. *Anisotropic thermal parameters* (Å^2)

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
I	2·354	1·544	1·144	−0·026	0·894	−0·017
Cd	2·894	1·969	1·323	−0·116	0·962	−0·047
O(1)	3·268	3·242	1·148	1·983	1·750	1·405
O(2)	4·397	2·493	1·024	−0·290	1·392	−0·366
O(3)	2·420	2·421	0·595	−0·335	0·270	−0·011
O(4)	3·078	3·234	2·220	1·229	2·015	0·332
O(5)	4·389	3·121	1·249	−0·350	1·655	0·064
O(6)	2·074	2·828	0·627	−0·476	0·044	0·334
$H_2O(1)$	3·483	2·020	1·852	0·322	1·102	0·128
$H_2O(2)$	3·632	3·708	2·231	0·001	0·955	−0·017
$H_2O(3)$	3·956	3·294	2·258	0·119	1·781	−0·656

Shifts in the last cycle:
$|\Delta B_{ij}|_{av}=0{\cdot}005$, $|\Delta B_{ij}|_{max}=0{\cdot}020$ for heavy atoms,
$|\Delta B_{ij}|_{av}=0{\cdot}023$, $|\Delta B_{ij}|_{max}=0{\cdot}075$ for light atoms.

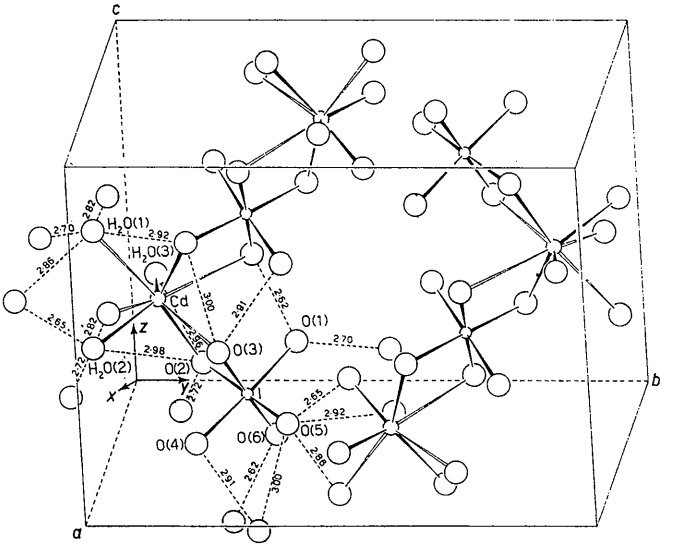

Fig. 1. Clinographic view of the structure with possible hydrogen bonds.

basis of an acceptable model. They can be subdivided into two groups, one group containing the longest distances ($I–O^{*}_{av}=1{\cdot}95$ Å) and the other the shortest distances ($I–O_{av}=186$ Å). It seems reasonable to consider the former as I–OH bonds and the latter as I–O bonds. These distances are comparable to those found in $K_4H_2I_2O_{10}$ (Ferrari, Braibanti & Tiripicchio, 1965) where $I–O^{*}_{av}=1{\cdot}996$ and $I–O_{av}=1{\cdot}807$ Å, in $K_4I_2O_9$ (Brehler, Jacobi & Siebert, 1968) where $I–O^{*}_{av}=2{\cdot}01$ and $I–O_{av}=1{\cdot}77$ Å and in $[Mg(OH_2)]_6[H_3IO_6]$ (Bigoli, Manotti Lanfredi, Tiripicchio & Tiripicchio Camellini, 1970) where $I–O^{*}=2{\cdot}01$ and $1{\cdot}97$ and $I–O=1{\cdot}78$ and $1{\cdot}87$ Å. The resulting octahedron is in a *trans*-configuration (Jones, 1964) which means that the hydrogen atoms lie approximately in one plane passing through the centre of the octahedron. The angles between the

Table 3. *Observed and calculated structure factors*

The $10F_o$ followed by = were not observed.

h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$
1	0	0	607	450	1	1	1	1198	-1113	0	9	1	515	675	0	1	2	755	-627	0	9	2	1185	-1395	2	2	-3	180	-183	3	10	3	208	-171
2	0	0	2149	-2431	1	1	-1	1644	1415	1	9	1	193	137	1	1	2	1198	-1338	1	9	2	1231	-1501	3	2	3	463	603	3	10	-3	385	-382
3	0	0	508	-626	2	1	1	447	539	1	9	-1	115=	111	1	1	-2	931	-939	1	9	-2	1222	-1403	3	2	-3	987	1091	4	10	3	144	-126
4	0	0	1442	1650	2	1	-1	426	553	2	9	1	477	-561	2	1	2	111=	-65	2	9	2	726	762	4	2	3	143	122	4	10	-3	393	422
5	0	0	602	681	3	1	1	593	754	2	9	-1	463	-514	2	1	-2	482	-568	2	9	-2	1573	-1697	4	2	-3	119	107	5	10	-3	538	545
6	0	0	317	-525	3	1	-1	834	-963	3	9	1	299	-268	3	1	2	468	573	3	9	2	1059	1104	5	2	3	452	-330	6	10	-3	140	-168
1	1	0	2596	-2845	4	1	1	166	-235	3	9	-1	145	-119	3	1	-2	65=	-15	3	9	-2	416	459	5	2	-3	494	-637	0	11	3	350	311
2	1	0	360	-446	4	1	-1	274	-339	4	9	1	359	352	4	1	2	228	331	4	9	2	236	-158	6	2	-3	176=	-95	1	11	3	475	448
3	1	0	935	1139	5	1	1	331	-346	4	9	-1	144	156	4	1	-2	516	624	4	9	-2	1104	1186	7	2	-3	210	201	1	11	-3	505	-572
4	1	0	699	813	5	1	-1	413	472	5	9	1	149	152	5	1	2	485	-392	5	9	2	498	-584	0	3	3	976	-782	2	11	3	185	-106
5	1	0	560	-696	6	1	1	49=	62	5	9	-1	214	185	5	1	-2	91	90	5	9	-2	212	-190	1	3	3	135=	66	2	11	-3	635	-702
6	1	0	447	-443	6	1	-1	140	156	6	9	-1	54=	-63	6	1	-2	395	-430	6	9	-2	767	-713	1	3	-3	393	-298	3	11	3	200	-185
0	2	0	1465	-1333	0	2	1	1550	-1362	0	10	1	239	246	7	1	-2	180	-181	0	10	2	1004	-1090	2	3	3	189	133	3	11	-3	396	425
1	2	0	421	-351	1	2	1	298	203	1	10	1	854	-1074	0	2	2	2063	-2026	1	10	2	741	792	2	3	-3	115=	-78	4	11	3	49=	11
2	2	0	410	-336	1	2	-1	587	440	1	10	-1	845	-995	1	2	2	1161	1238	1	10	-2	832	-918	3	3	3	200	-208	4	11	-3	426	440
3	2	0	428	560	2	2	1	800	922	2	10	1	755	-860	1	2	-2	1995	-2149	2	10	2	760	820	3	3	-3	275	266	5	11	-3	376	-318
4	2	0	249	-311	2	2	-1	904	-1062	2	10	-1	415	448	2	2	2	1830	2004	2	10	-2	448	505	4	3	3	109=	-45	6	11	-3	366	-385
5	2	0	493	-524	3	2	1	116	-75	3	10	1	544	562	2	2	-2	1288	1293	3	10	2	173	-117	4	3	-3	318	-255	0	12	3	526	489
6	2	0	135=	-13	3	2	-1	431	-597	3	10	-1	503	574	3	2	2	228	-235	3	10	-2	791	899	5	3	3	54=	-8	1	12	3	640	631
1	3	0	632	449	4	2	1	443	-558	4	10	1	482	379	3	2	-2	1453	1617	4	10	2	618	-512	5	3	-3	91	-110	1	12	-3	242	180
2	3	0	291	264	4	2	-1	430	608	4	10	-1	124	-106	4	2	2	690	-865	4	10	-2	187	-183	6	3	-3	133=	-14	2	12	3	289	-270
3	3	0	214	-242	5	2	1	93=	23	5	10	1	311	-307	4	2	-2	210	-291	5	10	-2	717	-656	7	3	-3	74=	52	2	12	-3	383	445
4	3	0	416	-520	5	2	-1	253	264	5	10	-1	412	-345	5	2	2	80=	-42	6	10	-2	54=	-19	0	4	3	68=	73	3	12	3	421	-369
5	3	0	171	-118	6	2	1	225	193	0	11	1	818	-920	5	2	-2	1004	-1210	0	11	2	137	62	1	4	3	868	-839	3	12	-3	205	-191
6	3	0	290	232	6	2	-1	274	-259	1	11	1	471	-525	6	2	-2	171=	-73	1	11	2	397	360	1	4	-3	1465	-1671	4	12	-3	417	-443
0	4	0	1304	1309	0	3	1	479	-420	1	11	-1	120=	115	7	2	-2	430	413	1	11	-2	357	382	2	4	3	388	-429	5	12	-3	89	-84
1	4	0	377	328	1	3	1	135=	46	2	11	1	555	583	0	3	2	2342	2064	2	11	2	106	57	2	4	-3	612	619	0	13	3	1171	1108
2	4	0	890	-973	1	3	-1	53=	-48	2	11	-1	571	662	1	3	2	1822	1938	2	11	-2	116=	42	3	4	3	503	534	1	13	3	262	-226
3	4	0	474	-574	2	3	1	468	452	3	11	1	536	495	1	3	-2	1942	2116	3	11	2	227	-254	3	4	-3	1309	1297	1	13	-3	408	424
4	4	0	475	500	2	3	-1	225	241	3	11	-1	100	-74	2	3	-2	1129	-1326	3	11	-2	130	103	4	4	3	186	99	2	13	3	895	-844
5	4	0	430	405	3	3	1	53=	-30	4	11	1	384	-340	2	3	-2	2840	2865	4	11	2	295	-257	4	4	-3	210	-185	2	13	-3	620	-721
6	4	0	105=	29	3	3	-1	127	125	4	11	-1	435	-403	3	3	2	1234	-1568	4	11	-2	236	-216	5	4	3	190	-150	3	13	3	105	84
1	5	0	1383	-1514	4	3	1	201	-205	5	11	1	284	-349	3	3	-2	892	-1028	5	11	-2	79=	-38	5	4	-3	601	-629	3	13	-3	395	-464
2	5	0	485	-622	4	3	-1	119=	51	5	11	-1	144	-129	4	3	2	322	334	0	12	2	289	222	6	4	-3	148=	95	4	13	-3	499	473
3	5	0	1360	1559	5	3	1	79=	-84	0	12	1	342	409	4	3	-2	1459	-1586	1	12	2	113=	112	7	4	-3	360	311	5	13	-3	265	295
4	5	0	664	716	5	3	-1	84=	-22	1	12	-1	478	543	5	3	2	869	756	1	12	-2	268	-247	0	5	3	883	-718	0	14	3	298	-237
5	5	0	513	-464	6	3	1	60=	65	2	12	1	376	390	5	3	-2	236	237	2	12	2	193	-138	1	5	3	366	-368	1	14	3	812	-754
6	5	0	421	-372	6	3	-1	115=	47	2	12	-1	181	127	6	3	-2	871	901	2	12	-2	125	83	1	-5	3	468	572	1	14	-3	615	-594
0	6	0	2018	-2405	0	4	1	1054	-1080	2	12	-1	319	339	7	3	-2	49=	45	3	12	2	439	-414	2	5	3	605	631	2	14	3	144	144
1	6	0	451	-441	1	4	1	554	594	3	12	1	263	-248	0	4	2	1140	994	3	12	-2	89=	-68	2	5	-3	1233	1276	2	14	-3	431	-464
2	6	0	2064	2303	1	4	-1	1357	1141	3	12	-1	184	-196	1	4	2	969	-941	4	12	2	140	121	3	5	3	360	374	3	14	3	434	512
3	6	0	555	649	2	4	1	966	1047	4	12	1	35=	12	1	4	-2	1567	1800	4	12	-2	162	-147	3	5	-3	469	-478	3	14	-3	362	383
4	6	0	1155	-1248	2	4	-1	697	-776	4	12	-1	459	-440	2	4	2	1447	-1647	5	12	-2	135	100	4	5	3	179	-137	4	14	-3	457	432
5	6	0	535	-500	3	4	1	414	-461	5	12	1	54	85	2	4	-2	1530	-1480	0	13	2	338	-271	4	5	-3	685	-698	5	14	-3	82	-99
6	6	0	441	383	3	4	-1	511	-671	0	13	1	290	300	3	4	2	390	430	1	13	2	394	-377	5	5	3	70	-69	0	15	3	217	-144
1	7	0	1865	2012	4	4	1	550	-604	1	13	1	572	-664	3	4	-2	1429	-1565	1	13	-2	333	-366	5	5	-3	96	92	1	15	3	331	271
2	7	0	408	470	4	4	-1	228	231	1	13	-1	725	849	4	4	2	760	800	2	13	2	84=	43	6	5	-3	458	414	1	15	-3	528	-487
3	7	0	1278	-1403	5	4	1	122	114	2	13	1	334	-318	4	4	-2	298	307	2	13	-2	319	-352	7	5	-3	54=	-71	2	15	3	185	153
4	7	0	511	-524	5	4	-1	442	416	2	13	-1	136	-112	5	4	2	79=	12	3	13	2	365	328	0	6	3	201	-164	2	15	-3	162	-137
5	7	0	461	405	6	4	1	387	337	3	13	1	412	385	5	4	-2	798	836	3	13	-2	105	69	1	6	3	411	-506	3	15	-3	508	504
6	7	0	321	312	6	4	-1	127=	-131	3	13	-1	681	-736	6	4	-2	138=	57	4	13	2	130	147	1	6	-3	653	-761	4	15	-3	200	184
0	8	0	365	456	0	5	1	644	621	4	13	1	230	236	7	4	-2	371	-403	4	13	-2	439	401	2	6	3	365	419	0	16	3	582	454
1	8	0	341	339	1	5	1	796	977	4	13	-1	119	-89	0	5	2	537	402	5	13	-2	35=	9	2	6	-3	617	-657	1	16	3	160	-100
2	8	0	264	-260	1	5	-1	1362	-1146	5	13	-1	401	481	1	5	2	497	-512	0	14	2	704	-714	3	6	3	333	348	1	16	-3	278	-217
3	8	0	379	-407	2	5	1	563	-668	0	14	1	599	-684	1	5	-2	759	-717	1	14	2	674	634	3	6	-3	478	461	2	16	3	288	-174
4	8	0	136	94	2	5	-1	1072	-1135	1	14	1	390	-376	2	5	2	202	-146	1	14	-2	642	-695	4	6	3	51=	3	2	16	-3	572	555
5	8	0	416	376	3	5	1	688	-810	1	14	-1	253	-241	7	5	-2	1211	-1176	2	14	2	682	641	4	6	-3	229	213	3	16	-3	360	355
1	9	0	218	150	3	5	-1	259	261	2	14	1	374	347	3	5	2	775	893	2	14	-2	441	504	5	6	3	176	-174	0	17	3	79=	43
2	9	0	214	-225	4	5	1	290	315	2	14	-1	587	-647	3	5	-2	214	177	3	14	2	236	-201	5	6	-3	49=	-42	1	17	3	241	-303
3	9	0	225	-214	4	5	-1	370	375	3	14	1	336	292	4	5	2	338	330	3	14	-2	689	747	6	6	-3	89=	-128	1	17	-3	541	490
4	9	0	362	347	5	5	1	535	453	3	14	-1	121	96	4	5	-2	324	313	4	14	-2	286	-254	7	6	-3	30=	-21	2	17	-3	160	142
5	9	0	165	128	5	5	-1	197	-163	4	14	1	114	-147	5	5	2	295	-269	0	15	2	744	702	0	7	3	1397	-1342	3	17	-3	331	-392
0	10	0	888	-1058	6	5	1	44=	-70	4	14	-1	592	573	5	5	-2	233	229	1	15	2	763	704	1	7	3	140=	0	1	18	-3	253	-284
1	10	0	116=	-132	6	5	-1	335	-270	0	15	1	447	-465	6	5	-2	294	-301	1	15	-2	568	583	1	7	-3	275	-277	0	0	4	406	394
2	10	0	478	519	0	6	1	468	-461	1	15	1	89=	-73	0	6	2	193	127	2	15	2	426	-367	2	7	3	830	875	1	0	4	2626	-2930
3	10	0	198	232	1	6	1	237	-300	1	15	-1	93=	-31	1	6	2	547	-585	2	15	-2	696	763	2	7	-3	1084	1119	1	0	-4	2220	2422
4	10	0	283	-233	1	6	-1	582	-545	2	15	1	528	487	1	6	-2	226	-184	3	15	2	463	-333	3	7	3	114	83	2	0	4	533	-634
5	10	0	336	-304	2	6	1	111=	62	2	15	-1	478	497	2	6	2	541	593	3	15	-2	398	-363	3	7	-3	405	402	2	0	-4	311	320
1	11	0	1270	1564	2	6	-1	213	-190	3	15	1	219	206	2	6	-2	361	334	4	15	-2	577	-609	4	7	3	763	-673	3	0	4	849	1002
2	11	0	213	246	3	6	1	469	522	3	15	-1	336	301	3	6	2	380	419	0	16	2	434	369	4	7	-3	604	-629	3	0	-4	2269	-2505
3	11	0	818	-863	3	6	-1	148	103	4	15	-1	171	-163	3	6	-2	396	381	1	16	2	275	-208	5	7	3	14=	-140	4	0	4	626	539
4	11	0	517	-435	4	6	1	112=	-7	0	16	1	414	-320	4	6	2	265	-224	1	16	-2	484	419	5	7	-3	244	-213	4	0	-4	897	-1057
5	11	0	421	448	4	6	-1	338	330	1	16	1	696	663	4	6	-2	216	217	2	16	2	416	-382	6	7	-3	248	187	5	0	4	422	-491
0	12	0	1264	1480	5	6	1	165	-124	1	16	-1	663	670	5	6	2	416	-375	2	16	-2	219	-191	0	8	3	264	220	5	0	-4	964	1235
1	12	0	221	170	5	6	-1	21=	-11	2	16	1	462	419	5	6	-2	111	-100	3	16	-2	471	-451	1	8	3	804	848	6	0	-4	587	652
2	12	0	940	-1119	6	6	-1	149	-111	2	16	-1	170	-122	6	6	-2	290	-254	0	17	2	89=	18	1	8	-3	672	743	7	0	-4	447	-409
3	12	0	378	-376	0	7	1	303	238	3	16	1	409	-494	0	7	2	217	166	1	17	2	120	-123	2	8	3	171	-94	0	1	4	2286	-2588
4	12	0	727	660	1	7	1	1034	1320	3	16	-1	502	-505	1	7	2	420	501	1	17	-2	65=	-18	2	8	-3	450	458	1	1	4	366	-522
5	12	0	391	405	1	7	-1	1225	-1241	0	17	1	652	559	1	7	-2	682	674	2	17	-2	26=	-43	3	8	3	728	-736	1	1	-4	127=	112
1	13	0	684	-803	2	7	1	202	159	1	17	1	171	131	2	7	2	190	-151	3	17	-2	30=	5	3	8	-3	593	-632	2	1	4	944	1125
2	13	0	192	-196	2	7	-1	122	104	1	17	-1	120	-48	2	7	-2	1001	986	0	18	2	60=	-36	4	8	3	268	-196	2	1	-4	1283	-1433
3	13	0	550	523	3	7	1	533	-569	2	17	1	486	-529	3	7	2	617	-649	1	18	-2	135	103	4	8	-3	338	-341	3	1	4	380	454
4	13	0	336	296	3	7	-1	956	1087	2	17	-1	572	-560	3	7	-2	252	-226	2	18	-2	14=	-49	5	8	-3	129	115	3	1	-4	579	-677
0	14	0	171	-172	4	7	1	187	-137	3	17	-1	123	-164	4	7	2	154	-124	0	1	3	956	1070	6	8	-3	270	215	4	1	4	599	-522
1	14	0	188	-143	4	7	-1	348	317	0	18	1	351	-275	4	7	-2	346	-317	1	1	3	307	361	0	9	3	355	285	4	1	-4	1430	1682
2	14	0	216	168	5	7	1	311	266	1	18	1	272	-356	5	7	2	251	229	1	1	-3	131=	-133	1	9	3	490	-496	5	1	4	345	-411
3	14	0	177	145	5	7	-1	567	-520	1	18	-1	325	-295	5	7	-2	47=	-23	2	1	3	648	-808	1	9	-3	575	644	5	1	-4	575	649
4	14	0	54=	-28	6	7	-1	195	-130	0	0	2	647	549	6	7	-2	351	320	2	1	-3	311	-403	2	9	3	226	-228	6	1	-4	491	-530
1	15	0	169	-117	0	8	1	1079	1205	1	0	2	160=	-36	0	8	2	1199	1338	3	1	3	175	-220	2	9	-3	116	-51	7	1	-4	462	-435
2	15	0	224	183	1	8	1	131=	-7	1	0	-2	155=	151	1	8	2	707	-876	3	1	-3	65=	-26	3	9	3	206	154	0	2	4	340	-348
3	15	0	84	67	1	8	-1	127=	112	2	0	2	427	-487	1	8	-2	1265	1413	4	1	3	438	463	3	9	-3	375	-426	1	2	4	705	817
0	16	0	214	170	2	8	1	364	-367	2	0	-2	283	152	2	8	2	1148	-1304	4	1	-3	486	594	4	9	3	260	209	1	2	-4	311	-286
1	16	0	143	183	2	8	-1	764	846	3	0	2	452	-551	2	8	-2	858	-894	5	1	3	241	175	4	9	-3	38=	-33	2	2	4	436	526
2	16	0	275	-224	3	8	1	162	-150	3	0	-2	201	258	3	8	2	371	339	5	1	-3	79	91	5	9	-3	275	280	2	2	-4	87=	86
3	16	0	109	-98	3	8	-1	141	104	4	0	2	83=	1	3	8	-2	1121	-1216	6	1	-3	228	-303	6	9	-3	251	205	3	2	4	118=	-12
1	17	0	757	-669	4	8	1	325	323	4	0	-2	147	-130	4	8	2	856	732	7	1	-3	95	-57	0	10	3	723	-683	3	2	-4	633	907
2	17	0	185	-169	4	8	-1	717	-753	5	0	2	466	362	4	8	-2	319	297	0	2	3	283	169	1	10	3	254	192	4	2	4	590	-521
0	18	0	788	-658	5	8	1	70=	68	5	0	-2	272	435	5	8	2	49=	-32	1	2	3	1364	-1616	1	10	-3	597	643	4	2	-4	343	412
1	18	0	176	-145	5	8	-1	134	-92	6	0	2	174	209	5	8	-2	822	777	1	2	-3	1497	-1384	2	10	3	403	414	5	2	4	279	-311
0	1	1	849	-656	6	8	-1	401	365	7	0	-2	84=	-5	6	8	-2	114=	8	2	2	3	136=	-30	2	10	-3	420	-475	6	2	-4	310	-243

iodine–oxygen bonds show some distortions with maximum deviation +6·3° from 90° and average deviation +2·2°.

Each cadmium cation (Fig. 3) is bound to two different anions with bonds Cd–O(2) = 2·25 and Cd–O(5^{i}) = 2·23 Å; these bonds, together with Cd–OH_2(2) = 2·27 and Cd–OH_2(3) = 2·41 Å, form the first coordination sphere in a distorted tetrahedral arrangement. These bonds are comparable to those obtained in cadmium bis(hydrazinecarboxylates) where Cd–O = 2·34, 2·28 (Braibanti, Manotti Lanfredi, Tiripicchio & Bigoli, 1969), 2·24, 2·26 Å (Braibanti, Tiripicchio, Manotti Lanfredi & Bigoli, 1968). The environment of the cadmium atom is completed by the interactions Cd–OH_2(1) = 2·51, Cd–OH_2(1^{i}) = 2·49, Cd–O(3) = 2·64 and Cd–O(6^{i}) = 2·79 Å. Altogether

Table 3 (*cont.*)

h	k	l	10F$_o$	10F$_c$	h	k	l	10F$_o$	10F$_c$	h	k	l	10F$_o$	10F$_c$	h	k	l	10F$_o$	10F$_c$	h	k	l	10F$_o$	10F$_c$	h	k	l	10F$_o$	10F$_c$
7	2	-4	176	112	4	11	-4	819	-909	4	5	-5	228	246	1	17	-5	564	638	0	9	6	1109	-1033	0	5	7	122	-97	2	1	8	421	382
0	3	4	345	296	5	11	-4	472	-423	5	5	-5	644	643	2	17	-5	24=	2	1	9	6	639	621	1	5	7	273	267	2	1	-8	81=	39
1	3	4	903	972	6	11	-4	396	392	6	5	-5	128=	-24	0	0	6	479	589	1	9	-6	1396	1292	1	5	-7	750	-727	3	1	-8	1315	-1528
1	3	-4	895	777	0	12	4	156=	-71	7	5	-5	251	-194	1	0	6	597	-679	2	9	6	785	725	2	5	7	116	80	4	1	-8	330	-437
2	3	4	157	171	1	12	4	1156	-1109	0	6	5	493	-395	1	0	-6	771	876	2	9	-6	713	-667	2	5	-7	283	298	5	1	-8	930	785
2	3	-4	174	128	1	12	-4	1273	1269	1	6	5	254	258	2	0	6	522	-550	3	9	-6	1301	-1322	3	5	7	184	-227	6	1	-8	449	470
3	3	4	624	-694	2	12	4	185	-166	1	6	-5	43=	51	2	0	-6	477	-551	4	9	-6	543	525	3	5	-7	521	509	7	1	-8	502	-479
3	3	-4	139	-83	2	12	-4	284	268	2	6	5	225	198	3	0	6	525	496	5	9	-6	1135	1138	4	5	-7	87=	-53	0	2	8	379	334
4	3	4	161	-101	3	12	4	603	625	2	6	-5	495	-454	3	0	-6	407	-459	6	9	-6	100=	-29	5	5	-7	563	-525	1	2	8	665	661
4	3	-4	194	-191	3	12	-4	981	-1124	3	6	5	98	75	4	0	-6	25=	-11	0	10	6	462	362	6	5	-7	123=	56	1	2	-8	545	-564
5	3	-4	163	-152	4	12	-4	544	-542	3	6	-5	409	-446	5	0	-6	133	191	1	10	6	837	757	7	5	-7	286	275	2	2	8	160	-106
6	3	-4	135=	-58	5	12	-4	692	674	4	6	5	176	-157	6	0	-6	190=	-1	1	10	-6	848	-785	0	6	7	427	-418	2	2	-8	571	-608
7	3	-4	275	227	0	13	4	723	-619	4	6	-5	112=	50	7	0	-6	144=	72	2	10	6	190	-158	1	6	7	95=	-39	3	2	-8	183	165
0	4	4	728	657	*1	13	4	181	-171	5	6	-5	253	196	0	1	6	637	-800	2	10	-6	731	-689	1	6	-7	255	196	4	2	-8	486	513
1	4	4	660	-630	1	13	-4	98=	-11	6	6	-5	95=	-39	1	1	6	187	-198	3	10	-6	471	463	2	6	7	275	215	5	2	-8	101=	0
1	4	-4	961	923	2	13	4	551	486	7	6	-5	176	-152	1	1	-6	214	197	4	10	-6	674	674	2	6	-7	384	-342	6	2	-8	406	-340
2	4	4	662	-688	2	13	-4	665	-677	0	7	5	835	716	2	1	6	673	754	5	10	-6	196	-218	3	6	-7	192	-161	7	2	-8	219	-207
2	4	-4	263	-254	3	13	4	212	269	1	7	5	221	-208	2	1	-6	690	-776	6	10	-6	517	-471	4	6	-7	117=	82	0	3	8	913	896
3	4	4	264	240	3	13	-4	234	-211	1	7	-5	140=	-34	3	1	6	406	374	0	11	6	539	473	5	6	-7	232	205	1	3	8	95=	-104
3	4	-4	956	-1084	4	13	-4	467	488	2	7	5	374	-387	3	1	-6	361	-432	1	11	6	248	200	6	6	-7	93=	-4	1	3	-8	121=	-97
4	4	4	708	579	5	13	-4	306	314	2	7	-5	575	-579	4	1	-6	355	407	1	11	-6	228	173	7	6	-7	160	-149	2	3	8	723	-677
4	4	-4	344	-317	0	14	4	295	-235	3	7	5	35=	20	5	1	-6	607	650	2	11	-6	281	-315	0	7	7	294	233	2	3	-8	740	785
5	4	-4	222	184	1	14	4	77=	82	3	7	-5	431	-458	6	1	-6	99=	-28	2	11	-6	257	276	1	7	7	795	801	3	3	-8	506	574
6	4	-4	380	309	1	14	-4	226	-156	4	7	-5	707	720	7	1	-6	186	-226	3	11	-6	142	106	1	7	-7	1111	-1066	4	3	-8	294	-293
7	4	-4	195	-152	2	14	4	365	368	5	7	-5	307	268	0	2	6	779	886	4	11	-6	232	-209	2	7	7	144	-149	5	3	-8	230	-189
0	5	4	1903	-1776	2	14	-4	277	214	6	7	-5	395	-379	1	2	6	810	940	5	11	-6	183	-136	2	7	-7	478	-464	6	3	-8	122=	27
1	5	4	227	-221	3	14	-4	199	166	7	7	-5	180	-197	1	2	-6	1214	-1350	6	11	-6	79=	-35	3	7	-7	898	847	7	3	-8	225	188
1	5	-4	394	332	4	14	-4	120	88	0	8	5	112	-75	2	2	6	305	-295	0	12	6	469	393	4	7	-7	483	438	0	4	8	461	-408
2	5	4	948	1004	5	14	-4	24=	-8	1	8	5	598	-612	2	2	-6	1266	-1601	1	12	6	270	-214	5	7	-7	410	-360	1	4	8	724	-685
2	5	-4	1806	-2173	0	15	4	92=	-59	1	8	-5	340	-287	3	2	6	846	-760	1	12	-6	341	306	6	7	-7	449	-367	1	4	-8	674	651
3	5	4	395	382	1	15	4	290	276	2	8	5	117	101	3	2	-6	591	740	2	12	6	242	-279	7	7	-7	256	258	2	4	8	171	139
3	5	-4	619	-600	1	15	-4	202	149	2	8	-5	30=	-30	4	2	-6	1258	1587	2	12	-6	140	-77	0	8	7	908	821	2	4	-8	754	771
4	5	4	723	-594	2	15	4	24=	80	3	8	5	79	42	5	2	-6	272	-279	3	12	-6	218	-173	1	8	7	272	-210	3	4	-8	221	-216
4	5	-4	1129	1183	2	15	-4	113	74	3	8	-5	625	661	6	2	-6	968	-916	4	12	-6	154	-80	1	8	-7	533	-492	4	4	-8	606	-585
5	5	-4	539	535	3	15	-4	125	-128	4	8	-5	319	255	7	2	-6	57=	-31	5	12	-6	79	50	2	8	7	532	-495	5	4	-8	73	-47
6	5	-4	603	-574	4	15	-4	60=	5	5	8	-5	512	-509	0	3	6	1291	1380	0	13	6	528	-431	2	8	-7	918	830	6	4	-8	472	414
7	5	-4	476	-448	0	16	4	89=	14	6	8	-5	157	-111	1	3	-6	795	-884	1	13	6	54=	12	3	8	-7	566	541	7	4	-8	270	222
0	6	4	92=	39	1	16	4	140	-131	0	9	5	187	-138	1	3	-6	1550	-1650	1	13	-6	21=	5	4	8	-7	337	-303	0	5	8	239	-164
1	6	4	1559	1642	1	16	-4	351	262	1	9	5	458	-473	2	3	6	1066	-1171	2	13	-6	494	-420	5	8	-7	509	-475	1	5	8	874	803
2	6	-4	2044	-2323	2	16	-4	60=	-12	1	9	-5	732	704	2	3	-6	1259	1428	3	13	-6	403	-361	6	8	-7	341	263	2	5	-8	1051	1040
3	6	-4	372	360	3	16	-4	236	-230	2	9	5	228	-193	3	3	6	432	323	4	13	-6	210	192	0	9	7	252	-189	2	5	8	311	303
2	6	-4	568	-569	0	17	4	592	-567	2	9	-5	171	-130	3	3	-6	1410	1638	5	13	-6	214	222	1	9	7	237	-213	2	5	-8	163	136
3	6	4	1000	-1038	1	17	-4	171	132	3	9	5	251	246	4	3	-6	523	-533	0	14	6	506	381	1	9	-7	261	181	3	5	-8	1249	-1272
3	6	-4	1728	1955	2	17	-4	562	-589	3	9	-5	381	-375	5	3	-6	1205	-1361	1	14	6	406	480	2	9	7	89	97	4	5	-8	516	-449
4	6	4	541	-434	0	1	5	465	-568	4	9	-5	317	-309	6	3	-6	132	95	1	14	-6	677	-540	2	9	-7	279	239	5	5	-8	826	787
4	6	-4	712	704	1	1	5	426	569	5	9	-5	291	279	7	3	-6	813	677	2	14	-6	678	-610	3	9	-7	101=	-38	6	5	-8	544	466
5	6	-4	889	-872	1	1	-5	797	-930	6	9	-5	210	170	0	4	6	664	-642	3	14	-6	392	366	4	9	-7	334	-345	7	5	-8	447	-438
6	6	-4	637	-591	2	1	5	305	374	0	10	5	1117	-1044	1	4	6	852	-862	4	14	-6	587	564	5	9	-7	266	-217	0	6	8	1254	1227
7	6	-4	436	452	2	1	-5	704	798	1	10	5	397	-347	1	4	-6	1432	1408	0	15	6	457	440	6	9	-7	286	231	1	6	8	221	202
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1	7	4	652	647	3	1	-5	641	715	2	10	5	711	691	2	4	-6	1236	1276	2	15	-6	441	397	1	10	7	144	102	2	6	-8	541	-649
1	7	-4	140=	-8	4	1	5	401	-309	2	10	-5	989	-988	3	4	6	933	784	3	15	-6	738	742	1	10	-7	219	162	2	6	-8	1446	-1444
2	7	4	808	-834	4	1	-5	239	-375	3	10	5	551	544	3	4	-6	658	-652	4	15	-6	149	-168	2	10	7	24=	-122	3	6	-8	537	-467
2	7	-4	1432	1604	5	1	-5	200	-332	3	10	-5	172	146	4	4	-6	966	-972	1	16	-6	243	291	2	10	-7	362	297	4	6	-8	1194	1211
3	7	4	504	-475	6	1	-5	263	258	4	10	-5	615	662	5	4	-6	202	198	2	16	-6	325	349	3	10	-7	203	-177	5	6	-8	674	606
3	7	-4	381	332	7	1	-5	286	255	5	10	-5	77=	55	6	4	-6	820	760	3	16	-6	201	-233	4	10	-7	485	-456	6	6	-8	860	-732
4	7	4	567	478	0	2	5	412	424	6	10	-5	360	-333	7	4	-6	100=	25	0	1	7	279	-283	5	10	-7	203	177	7	6	-8	441	-489
4	7	-4	860	-890	1	2	5	418	461	0	11	5	414	-256	0	5	6	674	-618	1	1	7	693	-767	6	10	-7	300	284	0	7	8	338	272
5	7	-4	487	-476	1	2	-5	950	1111	1	11	5	766	742	1	5	6	361	-369	1	1	-7	527	593	0	11	7	345	271	1	7	8	748	-693
6	7	-4	474	437	2	2	5	235	-258	1	11	-5	853	-808	1	5	-6	381	310	2	1	7	77=	36	1	11	7	74=	-23	1	7	-8	1001	-941
7	7	-4	374	406	2	2	-5	732	818	2	11	5	602	542	2	5	6	447	496	2	1	-7	355	470	1	11	-7	338	300	2	7	-8	119=	53
0	8	4	526	449	3	2	5	440	-426	2	11	-5	321	278	2	5	-6	766	-751	3	1	-7	401	370	2	11	-7	380	-315	3	7	-8	1086	1051
1	8	4	362	-303	3	2	-5	638	-741	3	11	5	281	-341	3	5	6	430	377	3	1	-7	762	-897	3	11	-7	209	-190	4	7	-8	293	232
1	8	-4	612	586	4	2	5	165	117	3	11	-5	677	706	3	5	-6	430	-367	4	1	-7	309	-340	4	11	-7	371	330	5	7	-8	819	-748
2	8	4	538	-544	4	2	-5	281	-331	4	11	-5	149	125	4	5	-6	274	216	5	1	-7	496	531	5	11	-7	381	337	6	7	-8	522	-417
2	8	-4	72=	-46	5	2	-5	230	280	5	11	-5	522	-488	5	5	-6	503	527	6	1	-7	127	190	6	11	-7	54=	-143	0	8	8	353	-308
3	8	4	130	74	6	2	-5	370	322	6	11	-5	109	-108	6	5	-6	31=	-14	7	1	-7	246	-204	0	12	7	365	359	1	8	8	682	-648
3	8	-4	415	-420	7	2	-5	275	-193	0	12	5	371	313	7	5	-6	316	-282	0	2	7	697	-796	1	12	7	140	-144	1	8	-8	421	412
4	8	4	416	393	0	3	5	34=	3	1	12	5	87=	-57	0	6	6	576	-539	1	2	7	127=	-97	1	12	-7	470	-392	2	8	-8	366	284
4	8	-4	187	-139	1	3	5	348	355	1	12	-5	240	-173	1	6	-6	419	405	1	2	-7	262	273	2	12	-7	323	275	3	8	-8	349	-363
5	8	-4	277	237	1	3	-5	328	-290	2	12	5	290	-261	1	6	-6	842	-821	2	2	7	708	667	3	12	-7	513	484	4	8	-8	452	-440
6	8	-4	273	227	2	3	5	167	146	2	12	-5	353	329	2	6	6	517	563	2	2	-7	618	-680	4	12	-7	198	-146	5	8	-8	83=	-16
0	9	4	170=	-76	2	3	-5	498	-470	3	12	5	404	404	2	6	-6	35=	22	3	2	7	54=	-5	5	12	-7	321	-307	6	8	-8	300	228
1	9	4	561	-572	3	3	5	189	-180	4	12	-5	300	-268	3	6	6	411	-360	3	2	-7	194	-193	0	13	7	225	-221	0	9	8	596	-508
1	9	-4	257	-189	3	3	-5	173	135	5	12	-5	330	-308	3	6	-6	403	365	4	2	-7	861	960	1	13	-7	808	665	1	9	8	54=	-11
2	9	4	218	-183	4	3	5	84	34	0	13	5	571	-463	4	6	-6	133	-74	5	2	-7	248	235	2	13	-7	512	464	1	9	-8	113	72
2	9	-4	186	106	4	3	-5	111=	-50	1	13	5	228	-184	5	6	-6	174	-138	6	2	-7	304	-236	3	13	-7	761	-700	2	9	-8	483	-464
3	9	4	381	361	5	3	-5	225	-224	1	13	-5	96=	46	6	6	-6	270	-226	7	2	-7	180	-139	4	13	-7	476	-453	3	9	-8	219	-173
3	9	-4	108=	50	6	3	-5	135=	-69	2	13	5	149	136	7	6	-6	79	-52	0	3	7	167=	-34	5	13	-7	214	283	4	9	-8	296	268
4	9	4	149	139	7	3	-5	95=	-76	2	13	-5	634	588	0	7	6	896	818	1	3	7	333	316	0	14	7	49=	-585	5	9	-8	263	208
4	9	-4	95=	81	0	4	5	950	870	3	13	-5	25=	-6	1	7	6	234	199	1	3	-7	273	284	1	14	-7	401	384	6	9	-8	79=	-12
5	9	-4	88	101	1	4	5	872	875	4	13	-5	546	-536	1	7	-6	325	-282	2	3	7	130	68	2	14	-7	592	-530	0	10	8	486	393
6	9	-4	100=	-41	1	4	-5	827	723	5	13	-5	74	-71	2	7	6	562	-572	2	3	-7	157	-110	3	14	-7	527	-499	1	10	8	371	433
0	10	4	472	-400	2	4	5	484	-513	0	14	5	223	-174	2	7	-6	653	621	3	3	7	74	-34	4	14	-7	351	375	1	10	-8	366	-293
1	10	4	518	480	2	4	-5	881	887	1	14	5	185	182	3	7	6	219	-204	3	3	-7	298	323	1	15	-7	30=	-57	2	10	-8	498	-433
1	10	-4	533	-522	3	4	5	488	-487	1	14	-5	394	343	3	7	-6	122	91	4	3	-7	21=	17	2	15	-7	360	-414	3	10	-8	208	164
2	10	4	485	447	3	4	-5	379	-371	2	14	-5	203	-192	4	7	-6	369	-373	5	3	-7	61=	-21	3	15	-7	35=	38	4	10	-8	520	483
2	10	-4	102	75	4	4	5	341	288	3	14	-5	563	-550	5	7	-6	369	-386	6	3	-7	133=	-75	0	0	8	1392	-1454	5	10	-8	100	67
3	10	4	209	-171	4	4	-5	739	-832	4	14	-5	24=	11	6	7	-6	146=	13	7	3	-7	165	-122	1	0	8	350	-307	6	10	-8	190	-235
3	10	-4	360	395	5	4	-5	298	288	5	14	-5	272	311	7	7	-6	195	209	0	4	7	633	-622	1	0	-8	142=	-33	0	11	8	165	139
4	10	-4	230	225	6	4	-5	454	388	0	15	5	135	-97	0	8	6	830	-758	1	4	7	116=	18	2	0	8	848	803	1	11	-8	950	-819
5	10	-4	319	-316	7	4	-5	100=	12	1	15	5	392	431	1	8	6	808	-806	1	4	-7	416	-366	2	0	-8	1630	1821	2	11	-8	62=	-27
6	10	-4	225	-195	0	5	5	827	699	1	15	-5	632	-523	1	8	-6	936	878	2	4	7	346	320	3	0	-8	430	514	3	11	-8	914	840
0	11	4	1427	1318	1	5	5	578	-572	2	15	-5	205	-148	2	8	6	284	267	2	4	-7	864	-920	4	0	-8	1403	-1535	4	11	-8	404	321
1	11	4	350	271	1	5	-5	1155	1089	3	15	5	471	454	2	8	-6	1290	1217	3	4	7	39=	119	5	0	-8	455	-638	5	11	-8	622	-577
1	11	-4	129=	0	2	5	5	558	-574	4	15	-5	185	194	3	8	6	522	544	3	4	-7	161	111	6	0	-8	771	831	0	12	8	773	-711
2	11	4	938	-858	2	5	-5	486	-404	0	16	5	687	662	3	8	-6	531	-494	4	4	-7	459	412	7	0	-8	608	625	1	12	-8	95	-53
2	**11**	-4	1041	1172	3	5	5	368	387	1	16	-5	295	237	4	8	-6	925	-992	5	4	-7	92=	-21	0	1	8	332	-263*	2	12	-8	999	909
3	**11**	4	316	-265	3	5	-5	761	-770	2	16	-5	773	779	5	8	-6	280	264	6	4	-7	576	-477	1	1	8	972	956	3	12	-8	441	363
3	**11**	-4	346	347	4	5	5	396	318	3	16	-5	44=	31	6	8	-6	881	767	7	4	-7	100=	-20	1	1	-8	906	1022	4	12	-8	753	-726

Table 3 (*cont.*)

h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$	h	k	l	$10F_o$	$10F_c$
5	12	-8	356	-381	0	4	9	345	218	0	8	9	113	-98	4	0	-10	418	-473	6	4	-10	190	134	3	10	-10	382	-361	6	5	-11	201	-230
1	13	-8	541	535	1	4	9	506	-474	1	8	-9	91=	39	5	0	-10	100	-91	0	5	10	316	-272	4	10	-10	286	330	2	6	-11	130	131
2	13	-8	49=	-38	1	4	-9	679	-661	2	8	-9	288	-262	6	0	-10	255	243	1	5	-10	812	755	5	10	-10	478	520	3	6	-11	230	-201
3	13	-8	551	-546	2	4	-9	197	159	3	8	-9	262	-232	7	0	-10	70=	142	2	5	-10	24=	5	3	11	-10	255	339	4	6	-11	205	-195
4	13	-8	255	-248	3	4	-9	831	868	4	8	-9	430	393	0	1	10	270	-186	3	5	-10	669	-670	4	11	-10	35=	0	5	6	-11	84	71
2	14	-8	164	-200	4	4	-9	257	-226	5	8	-9	79=	7	1	1	-10	864	892	4	5	-10	303	-262	1	1	-11	270	-282	2	7	-11	522	-592
3	14	-8	135	157	5	4	-9	755	-625	6	8	-9	200	-173	2	1	-10	29=	-14	5	5	-10	524	436	2	1	-11	517	510	3	7	-11	376	-396
0	1	9	593	517	6	4	-9	147	-86	0	9	9	452	-418	3	1	-10	530	-590	6	5	-10	246	229	3	1	-11	309	307	4	7	-11	356	347
1	1	9	336	278	7	4	-9	286	291	1	9	-9	392	287	4	1	-10	309	-291	0	6	10	567	523	4	1	-11	485	-441	5	7	-11	365	412
1	1	-9	457	-490	0	5	9	738	-604	2	9	-9	409	363	5	1	-10	453	452	1	6	-10	421	-364	5	1	-11	376	-309	2	8	-11	317	-367
2	1	-9	483	-608	1	5	9	306	-253	3	9	-9	178	179	6	1	-10	316	335	2	6	-10	627	-598	6	1	-11	200	171	3	8	-11	351	389
3	1	-9	198	210	1	5	-9	349	292	4	9	-9	349	-317	7	1	-10	35=	-117	3	6	-10	219	205	1	2	-11	376	361	4	8	-11	387	478
4	1	-9	279	358	2	5	-9	730	705	5	9	-9	125	-87	0	2	10	739	765	4	6	-10	625	597	2	2	-11	265	225	3	9	-11	158	181
5	1	-9	156	-192	3	5	-9	214	-158	6	9	-9	171	213	1	2	-10	631	592	5	6	-10	176	121	3	2	-11	663	-701	2	0	-12	39=	-43
6	1	-9	319	-357	4	5	-9	774	-745	0	10	9	300	-343	2	2	-10	732	-799	6	6	-10	241	-212	4	2	-11	328	-302	3	0	-12	713	821
7	1	-9	89	109	5	5	-9	62=	37	1	10	-9	873	810	3	2	-10	725	-806	0	7	10	102	142	5	2	-11	346	232	4	0	-12	341	309
0	2	9	404	342	6	5	-9	465	371	2	10	-9	241	-184	4	2	-10	580	562	1	7	-10	517	-485	6	2	-11	251	244	5	0	-12	848	-802
1	2	9	316	-245	7	5	-9	49=	55	3	10	-9	749	-697	5	2	-10	1004	911	2	7	-10	35=	6	1	3	-11	54=	71	2	1	-12	611	736
1	2	-9	505	-524	0	6	9	129	-144	4	10	-9	84=	-47	6	2	-10	281	-228	3	7	-10	517	507	2	3	-11	185	-145	3	1	-12	44=	31
2	2	-9	334	311	1	6	9	176	173	5	10	-9	627	601	7	2	-10	556	-591	4	7	-10	320	258	3	3	-11	41=	23	4	1	-12	637	-651
3	2	-9	376	389	1	6	-9	316	278	1	11	-9	230	-232	0	3	10	507	-523	5	7	-10	311	-263	4	3	-11	134	99	5	1	-12	260	-221
4	2	-9	115	-55	2	6	-9	91=	38	2	11	-9	692	-692	1	3	-10	826	-816	6	7	-10	251	-257	5	3	-11	65=	68	2	2	-12	374	-449
5	2	-9	433	-431	3	6	-9	134	-83	3	11	-9	114	-71	2	3	-10	940	-985	1	8	-10	551	-542	6	3	-11	149	111	3	2	-12	441	-495
6	2	-9	279	233	4	6	-9	192	-150	4	11	-9	652	651	3	3	-10	469	650	2	8	-10	566	484	1	4	-11	396	435	4	2	-12	295	271
7	2	-9	341	313	5	6	-9	105	98	5	11	-9	70	78	4	3	-10	1144	1150	3	8	-10	668	594	2	4	-11	149	117	5	2	-12	671	657
0	3	9	266	198	6	6	-9	205	140	1	12	-9	223	-249	5	3	-10	307	-265	4	8	-10	522	-484	3	4	-11	241	-188	3	3	-12	481	573
1	3	9	195	125	0	7	9	120	-117	2	12	-9	114	-103	6	3	-10	964	-858	5	8	-10	818	-768	4	4	-11	130	-90	4	3	-12	251	254
1	3	-9	108=	112	1	7	9	193	-252	3	12	-9	265	263	7	3	-10	35=	-3	6	8	-10	30=	40	5	4	-11	486	447	5	3	-12	336	-361
2	3	-9	157	-140	1	7	-9	102	84	4	12	-9	105	125	0	4	10	748	-638	1	9	-10	471	523	6	4	-11	74=	83	3	4	-12	406	553
3	3	-9	186	149	2	7	-9	289	264	3	13	-9	231	273	1	4	-10	508	-449	2	9	-10	733	726	1	5	-11	39=	-8	4	4	-12	225	-249
4	3	-9	273	277	3	7	-9	552	-523	0	0	10	762	-643	2	4	-10	606	628	3	9	-10	541	-523	2	5	-11	214	-188	5	4	-12	329	-381
5	3	-9	83=	73	4	7	-9	322	-262	1	0	-10	409	406	3	4	-10	703	707	4	9	-10	863	-865	3	5	-11	62=	-46	3	5	-12	76	109
6	3	-9	192	111	5	7	-9	347	299	2	0	-10	528	609	4	4	-10	460	-407	5	9	-10	210	219	4	5	-11	360	315	4	5	-12	596	-693
7	3	-9	160	-107	6	7	-9	195	164	3	0	-10	301	-339	5	4	-10	907	-755	2	10	-10	336	-382	5	5	-11	33=	18					

they form a distorted square antiprism. The position of the cadmium atom seems to be determined by its interactions with the anions and by steric constraints. The isostructural substitution of calcium for cadmium is a consequence of the similar ionic radii of Cd^{2+} and Ca^{2+}, although cadmium generally forms covalent complexes and calcium ionic compounds.

There are eleven independent intermolecular distances $O\cdots O \leq 3{\cdot}00$ Å in the structure (Table 5), which are possible hydrogen bonds. Three of them bind one anion to another, seven bind an anion to a water molecule, and two bind one water molecule to another.

The anions form layers parallel to (010), each layer containing asymmetric units related by glide planes; these anions are held together by the bridging cadmium cations, by short hydrogen bonds $O(1)\cdots O(6^{i}) = 2{\cdot}62$ Å and by bridging water molecules forming hydrogen bonds $O(2)\cdots H_2O(2^{iii}) = 2{\cdot}72$ and $O(5^{vii})\cdots H_2O(2^{iii}) = 2{\cdot}65$ Å.

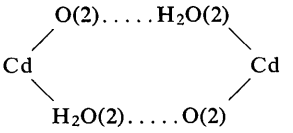
The layers are bound to one another through a chain of bonds forming a hexagonal ring

Table 4. *Main interatomic distances and angles*

I–O(1)	1·94 (6) Å	O(1)–I–O(2)	90·3 (2·4)°
I–O(2)	1·86 (5)	O(1)–I–O(3)	87·4 (1·7)
I–O(3)	1·95 (2)	O(1)–I–O(4)	176·1 (1·8)
I–O(4)	1·96 (5)	O(1)–I–O(5)	91·7 (2·1)
I–O(5)	1·86 (5)	O(1)–I–O(6)	91·6 (1·8)
I–O(6)	1·86 (3)	O(2)–I–O(3)	85·1 (2·2)
		O(2)–I–O(4)	89·0 (2·3)
		O(2)–I–O(5)	172·5 (2·6)
		O(2)–I–O(6)	96·3 (2·3)
		O(3)–I–O(4)	88·8 (1·4)
		O(3)–I–O(5)	87·8 (1·8)
		O(3)–I–O(6)	178·1 (0·6)
		O(4)–I–O(5)	88·5 (1·9)
		O(4)–I–O(6)	92·2 (1·6)
		O(5)–I–O(6)	90·8 (1·9)
Cd–O(5^{i})	2·23 (5)	O(5^{i})–—Cd–$H_2O(2)$	144·2 (2·3)
Cd–O(2)	2·25 (6)	O(5^{i})–—Cd–$H_2O(3)$	118·3 (2·3)
Cd–$OH_2(2)$	2·27 (6)	$H_2O(2)$–Cd–$H_2O(3)$	83·3 (2·6)
Cd–$OH_2(3)$	2·41 (8)	$H_2O(2)$–Cd–O(2)	82·7 (2·2)
Cd–$OH_2(1^{vi})$	2·49 (5)	O(2) –—Cd–O(5^{i})	127·1 (1·2)
Cd–$OH_2(1)$	2·51 (3)	O(2) –—Cd–$H_2O(3)$	78·9 (2·4)
Cd–O(3)	2·64 (3)	$H_2O(1)$–Cd–O(2)	120·7 (2·2)
Cd–O(6^{i})	2·79 (3)		

Asymmetric unit transformations:

i	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$	v	$1-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$
ii	$-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$	vi	$1-x$	$-y$	$1-z$
iii	$-x$	$-y$	$-z$	vii	$-1+x$	$\frac{1}{2}-y$	$-\frac{1}{2}+z$
iv	x	$\frac{1}{2}-y$	$-\frac{1}{2}+z$				



A further hydrogen bond joins O(1) to $H_2O(1^{ii})$ (2·70 Å).

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Table 5. *Possible hydrogen bonds* ($\leq 3{\cdot}0$ Å)

O(1) —O(6^{i})	2·62 (6) Å
O(1) —$H_2O(1^{ii})$	2·70 (5)
O(2) —$H_2O(2)$	2·98 (7)
O(2) —$H_2O(3)$	2·96 (10)
O(2) —$H_2O(2^{iii})$	2·72 (9)
O(3) —O(5^{i})	3·00 (6)
O(4) —O(3^{iv})	2·91 (5)
O(5) —$H_2O(1^{v})$	2·86 (6)
O(5) —$H_2O(1^{iv})$	2·92 (3)
O(5) —$H_2O(2^{v})$	2·65 (8)
$H_2O(2)$–$H_2O(1^{vi})$	2·82 (8)

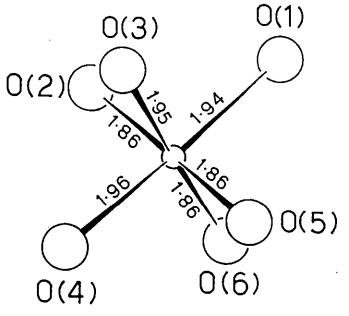

Fig. 2. The trihydrogenhexaoxoiodato(VII) anion. The hydrogen atoms are probably bound to O(1), O(3) and O(4).

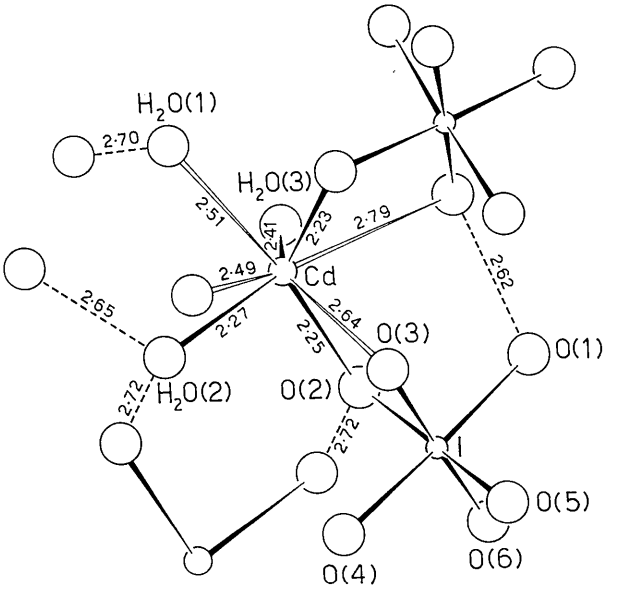

Fig. 3. The environment of cadmium cations and the strongest hydrogen bonds.

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