and Witte & Wölfel (1958), are given in Table 2. Here F'_o and F_o are respectively the observed structure factors before and after correcting for extinction. The values have been scaled so that $F_o(400)$, which has been found to have negligible extinction, is equal to the absolute value given by Renninger.

Concluding remarks

The results indicate that this method of correcting for extinction will work in practice. The main advantage of the method is that it accounts for both primary and secondary extinction in a crystal of any shape. It is applicable to a good accuracy when the extinction is not greater than 25%, but is unsatisfactory for low Bragg angles, say for $2\theta < 20^\circ$, depending upon the accuracy of the intensity measurements.

The present experimental arrangement is defective in one respect. The axis of oscillation remaining vertical for all angles of φ prevents ϱ_{φ} from being measured over the whole range from $\varphi = 90^{\circ}$ to 0°. (The Cox-Shaw factor becomes zero for $\varphi = 0^{\circ}$). The most sensitive portion of the curve connecting $\varrho'_{\varphi}/\varrho'_{\perp}$ versus φ is between $\varphi = 20^{\circ}$ and 0°, and hence the inability to make measurements in this range is a disadvantage. This can be overcome either by rotating the entire diffractometer about the polarized beam or by rotating the plane of polarization. An apparatus for accomplishing the latter, designed with a view to making the experimental procedure as efficient as possible, is now under construction at the Royal Institution. for provision of facilities and for many helpful suggestions. I am also grateful to Dr H. J. Milledge for the loan of the diamonds and for discussions. Thanks are due to Mr E. Nave for his valuable help in setting up the apparatus. The work was carried out during the tenure of a D.S.I.R. Special Research Grant.

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The Crystal Structure of bis-Biuret-Cadmium Chloride

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Bis-biuret-cadmium chloride, $CdCl_2 \cdot 2 C_2H_5N_3O_2$, is monoclinic $(P2_1/c)$ with

$$a = 3.704, b = 19.96, c = 8.20 \text{ Å}; \beta = 111.1^{\circ}; Z = 2.$$

The crystal structure has been determined by Fourier methods using 0kl, 1kl and 2kl reflections. The cadmium atom coordinates octahedrally with four Cl and two O atoms of two different biuret molecules (Cd-Cl = 2.55 and 2.62 Å, Cd-O = 2.34 Å). The biuret molecule is planar and has a 'trans' configuration.

1. Introduction

Biuret, $NH(CONH_2)_2 = Bu$, forms two kinds of coordination compounds with divalent metals. Among those which can be obtained in an alkaline medium, the potassium *bis*-biuret-cuprate tetrahydrate has recently been studied by Freeman, Smith & Taylor (1959), who found that two biuret molecules are coordinated as bidentate ligands, through the nitrogen atoms of the amino-groups, by a copper atom.

In a neutral medium, coordination compounds of

the kind $M^{II}X_2.2Bu$, in which $M^{II}X_2=\text{CuCl}_2$, CuSO₄, Cu(NO₃)₂, NiCl₂, NiSO₄ (Schiff, 1898), CdCl₂ (Schenck, 1904), are formed. The crystal structure of *bis*-biuretcupric chloride has also been determined by Freeman, Smith & Taylor (1959); in this compound the biuret is already a bidentate ligand but the coordination probably occurs through the two oxygen atoms.

In this paper the results of the study of the crystal structure of $CdCl_2.2Bu$ (isostructural with the corresponding Hg-compound (Nardelli & Chierici, 1960)) are reported. The complete structural study has showed that in this case the biuret is a mono-dentate ligand and its configuration is *trans*:



2. Experimental

Bis-biuret-cadmium chloride forms very slender and flattened colourless needles, which are optically biaxial and usually twinned on (001). The unit cell constants are:

$$a=3.704\pm0.005, b=19.96\pm0.03, c=8.20\pm0.01 \text{ Å}, \beta=111.1^{\circ}\pm0.2^{\circ}, Z=2, \text{ space group } P2_1/c.$$

The intensity data were obtained photometrically from 0kl, 1kl and 2kl integrated and non-integrated Weissenberg photographs (Cu $K\alpha$ radiation) using the multiple-film technique. An untwinned sample, cut from a twinned crystal was used. The cross-section was rectangular (0.12 mm. along z^* , 0.008 mm. along y^*) and the relative intensities were corrected for absorption by Albrecht's (1939) method. The variation in size of spots on non-equatorial Weissenberg photographs was taken into account following Scouloudi (1953).

After correction for Lorentz, polarization and velocity factors, the $F_o^2(0kl)$ values were put on an absolute scale by Wilson's (1942) method. This gave a scale factor and an isotropic temperature factor which were in quite good agreement with the final ones (scale factor for F_o 's, from Wilson 2.571, final value 2.502; B from Wilson 2.1 Å², final value 1.8 Å²). The 1kl and 2kl structure factors were successively put on an absolute scale by comparison with the calculated values.

123 0kl (possible 196), 237 1kl (possible 372), and 213 2kl (possible 325) reflections were observed. The majority of the unobserved reflections had k+l odd; this is because the Cd atom lies on a symmetry centre.

3. The structure determination

Locating the Cd atom at the origin of the unit cell allowed us to solve the 'phase problem' in a straightforward way. A first $\rho_0(Y, Z)$ was calculated using the $F_o(0kl)$'s with k+l even, which are influenced strongly by the Cd atom, taken with positive signs. This projection was sufficient to obtain the y and z coordinates of the Cl atom. A succeeding projection, calculated with all the $F_o(0kl)$'s and the signs determined by the contributions of the heavy atoms alone, showed wellresolved peaks corresponding to the light atoms. On examining the resultant projection it was evident that the coordination around the Cd was of the same kind as that previously found in bis-acetamide-cadmium chloride, CdCl₂.2 OCNH₂CH₃, (Cavalca, Nardelli & Coghi, 1957) and in *bis*-urea-cadmium chloride. CdCl₂.2 OC(NH₂)₂, (Nardelli, Cavalca & Fava, 1957). It was therefore easy to calculate the x coordinate of the Cl atom.



Fig. 1. Projection along [100] of: (a) ϱ_0 , (b) S_1 , (c) C_1 , calculated without the Cd contributions. Contours at intervals of 2 e.Å⁻². The zero contour is broken, and the negative contours are dotted.

Table 1. Atomic coordinates and their standard deviations

	x a	y/b	z/c	x'	y'	z'	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
Cd	0	0	0	0	0	0		_	
Cl	0.3234	0.0446	-0.2053	1.803	0.890	-1.570	0.005	0.005	0.011
Or	0.104	0.105	0.132	-0.014	2.096	1.033	0.007	0.017	0.029
OT	0.842	0.214	0.543	1.511	4.271	4.154	0.020	0.025	0.031
NT	0.572	0.092	0.400	0.934	1.836	3.060	0.024	0.022	0.039
NII	0.354	0.197	0.284	0.472	3.932	2.173	0.022	0.023	0.029
NIII	0.510	0.304	0.393	0.726	6.068	3.007	0.023	0.033	0.024
Cr	0.337	0.130	0.268	0.456	2.595	2.050	0.031	0.038	0.048
$\bar{c_{II}}$	0.579	0.238	0.410	0.934	4.750	3.136	0.017	0.023	0.045

A series of projections of $\varrho_0, C_1, S_1, \varrho_1, C_2, S_2, \varrho_2$ (the suffixes 0, 1, 2 refer to the 0kl, 1kl and 2kl reflections used for calculating the indicated functions respectively) along [100], calculated using the $F_o - F_{Cd}$ values and the signs determined by the heavy atoms, was useful in getting an improved distribution of the light atoms. The ϱ_0, C_1 , and S_1 projections obtained at this stage are shown in Fig. 1.

The values of the ϱ_0 , C_1 , S_1 , C_2 , and S_2 functions at the *i* points near the projections of the atomic centres were used to calculate the $\varrho(X, Y_i, Z_i)$ function. This function is specially influenced by series-termination errors because of the neglect of 3kl and 4kl reflections; nevertheless, it was valuable in giving the *x* coordinates of the light atoms and in improving the other coordinates. To correct the series-termination errors. the $\{\varrho_o - \varrho_c\}(X, Y_i, Z_i)$ function was calculated several times until nearly stationary coordinates were obtained. At the end of these refinement operations the atomic coordinates were those reported in Table 1; in this table are also given the x', y', z' (Å) coordinates referred to orthogonal axes a, b, c', with c' perpendicular to the a and b crystal axes.

The standard deviations $\sigma(y)$ and $\sigma(z)$ reported (Å) are the mean values of those estimated by Cruickshank's (1949) method from $\varrho_0(Y, Z)$, $\varrho_1(Y, Z)$, and $\varrho_2(Y, Z)$; $\sigma(x)$ was calculated by the same method from $\varrho(X, Y, Z)$. The standard deviations of the electron density in the three projections along [100] are: $\sigma(\varrho_0) = 0.51$, $\sigma(\varrho_1) = 0.69$, $\sigma(\varrho_2) = 0.68$ e.Å⁻² and for the three-dimensional data $\sigma(\varrho) = 0.30$ e.Å⁻³.

In Table 2 are given the final values of F_o and F_c .



Fig. 2. A chain of coordination octahedra seen in clinographic projection.

Table 2. Calculated and observed structure factors

A negative sign after an $|F_o|$ must be interpretated as 'less than'

	10 F	10 F	1 10 F	10 F	1	10 F	10 F	1	10 F	10 F	1	10 F	10 F	1	10 F	10 F	1	10 F	10 F
	001		08	1		0 16 1		-10	71-	-44		151		-1	1141	1133	-5	348	360
2	397	354	0 389	427	0	330	344				0	157	-120	2	265	2 30	6	97-	72
4	583	590	1 637	540	1	189	-187		111		1	300	318	-2	160	-104	-6	117-	-215
6	277	266	2 866	8 36	2	354	309	0	105	-142	-1	335	284	3	430	394	7	69-	85
8	187	263	3 98	113	3	386	345	1	980	1059	2	78-	109	-3	181	187	-7	253	308
			4 439	426	4	411	383	-1	674	688	-2	547	532	4	113-	2	-8	88-	-19
1	002	1005	5 122	110	5	216	-02	_2	70-	-81	ز 1-	960	800	-4	179	-199		1 14 1	
2	401	390	7 128	57	7	~	-76		393	436	4	105-	-57	-5	526	549	0	570	548
3	307	314	8 307	352	•		• -	-3	986	860	-4	84-	-100	6	112-	-74	1	111-	66
4	94-	-157	9 74	118		0 17 1		4	100-	-144	5	425	444	-6	117-	125	-1	107-	-141
5	735	759			1	459	443	_4	76-	3	-5	802	872	7	94-	143	2	489	461
6	125-	33	09	1	2	131-	61	5	314	309	6	117-	-152	-7	311	385	-2	459	434
7	280	299	1 453	409	3	381	352	-5	214	337	-6	110-	17	8	59 -	30	3	118-	102
8	122-	-202	2 94	- 8 61h	4	154	163	6 4	119-	-22	7	188	218	8	106-	45	-3	188	-212
,	-,,	~ 7 5	4 114	120	6	102-	-122	-0	103-	423	-/	78-	139	-9	225	~95	-4	344	288
	021		5 207	221	7	175	202	-7	387	420	8	114-	32		1 10 1		5	108-	87
0	563	735	6 181	168	-			8	86-	70	-9	161	204	0	700	691	-5	118-	1 34
1	269	-266	7 542	564		0 18 1		-8	117-	-149	-10	62-	-122	1	92-	-132	6	168	1 50
2	323	296	8 106	- 6	0	391	361	-9	361	434				-1	86-	-1 38	-6	381	376
3	79-	-68	9 67	- 151	1	212	-197	-10	71-	20		161		2.	332	290	7	57-	-69
4	654	679			2	427	377				0	661	707	-2	745	685	-7	102-	30
5	571	71	0 10	1 824	3	129-	121	•	121		1	283	= 302	3	108-	60 hh	-8	80-	78
7	112-	151	1 93	- 17		111-	اعر 117-	1	306	~308	-1	850	=30 812	ر- ي	700	648		1 15 7	
8	235	239	2 883	876	6	311	318	-1	229	-238	-2	655	612	-4	325	329	0	335	323
9	95-	-79	3 108	- 9				2	737	749	3	208	152	5	118-	14	1	114-	75
			4 221	236		0 19 1		-2	846	744	-3	75-	-61	-5	111-	-135	-1	510	479
	031		5 128	- 54	1	438	397	3	87-	81	4	451	460	6	259	300	2	117-	-57
1	972	1042	6 326	313	2	216	-214	-3	235	182	-4	548	540	-6	441	515	-2	210	-192
2	66-	0	7 123	- 107	3	169	135	4	189	158	5	188	-217	7	90-	23	3	492	467
3	591	578	8 314	383	4	119	83	-4	753	700	-5	306	-278	-7	115-	51	-3	323	304
5	97- 867	-90 894	9 50	29	5	200	-109	-5	200	-179	ہ ہے	373	428	-0	77-	-3	-4	244	219
6	317	321	0 11	1		70-	,	6	344	368	-0	201	198	-,	11-	-,	5	361	360
7	132-	109	1 706	659		0201		6	291	320	-7	173	159		1 11 1		-5	660	670
8	121-	-70	2 105	61	0	569	588	7	109-	-2	8	75 -	171	0	190	-116	6	82-	30
9	262	298	3 728	725	1	127-	-47	-7	117-	29	-8	256	313	1	412	387	-6	110-	-24
			4 122	126	2	220	181	8	86-	200	-9	94-	-120	-1	892	920	-7	185	185
~	041	1000	5 219	156	3	149	110	-8	468	550	-10	141	248	2	103-	-7	-8	70-	-4
1	346	384	ازا ہ مکن 7	- 39 454	4	91_	80	-9	101-	278		171		-2	447 404	300 404		1 16 1	
2	848	885	8 95	98	6	175	206	-10	.40		0	434	- 346	-3	253	220	0	362	307
з	749	-766		•	-				131		1	630	596	4	117-	34	1	254	219
4	741	753	0 12	1		0 21 1		0	535	-626	-1	932	874	-4	106-	4	-1	115-	-53
5	113-											333	299						
6		83	0 103	- 41	1	348	354	1	1198	1293	2			5	415	461	2	421	363
7	394	83 426	0 103 1 232	- 41 -179	1 2	348 117-	354 -65	1 _1	1198 240	1293 225	2 -2	154	136	5 -5	415 231	461 470	2 -2	421 421	363 389
	394 131-	83 426 106	0 103 1 232 2 910	- 41 -179 840	1 2 3	348 117- 196	354 -65 194	1 -1 2	1198 240 73 -	1293 225 21	2 -2 3	154 653	136 656	5 -5 6	415 231 106-	461 470 19	2 -2 3	421 421 329	363 389 -314
8 0	394 131- 120-	83 426 106 153	0 103 1 232 2 910 3 117 4 226	- 41 -179 840 - 35	1 2 3 4	348 117- 196 97-	354 -65 194 54 358	1 -1 -2 -2	1198 240 73- 359 564	1293 225 21 297 545	2 -2 3 -3	154 653 523	136 656 512	5 -5 6 -6 7	415 231 106- 118- 84-	461 470 19 19	2 -2 3 -3	421 421 329 118-	363 389 -314 -94 258
8 9	394 131- 120- 92-	83 426 106 153 -139	0 103 1 232 2 910 3 117 4 224 5 131	- 41 -179 840 - 35 183 - 22	1 2 3 4 5	348 117- 196 97- 327	354 -65 194 54 358	1 -1 -2 -2 3 -3	1198 240 73- 359 564 1234	1293 225 21 297 545 1171	2 -2 3 -3 4 -4	154 653 523 109-	136 656 512 22 -334	5 -5 6 -6 7	415 231 106- 118- 84- 305	461 470 19 154 319	2 -2 -3 4 -4	421 421 329 118- 275 386	363 389 -314 -94 258 379
8 9	394 131- 120- 92- 0 5 1	83 426 106 153 -139	0 103 1 232 2 910 3 117 4 224 5 131 6 331	- 41 -179 840 - 35 183 - 22 311	1 2 3 4 5	348 117- 196 97- 327 0 22 1	354 -65 194 54 358	1 -1 -2 -2 3 -3 4	1198 240 73- 359 564 1234 102-	1 293 225 21 297 545 1171 82	2 -2 3 -3 4 -4 5	154 653 523 109- 359 448	136 656 512 22 -334 467	5 -5 6 -6 7 -7 -8	415 231 106- 118- 84- 305 98-	461 470 19 154 319 -40	2 -2 3 -3 4 -4 5	421 421 329 118- 275 386 162	363 389 -314 -94 258 379 141
8 9 1	394 131- 120- 92- 0 5 1 726	83 426 106 153 -139 695	0 103 1 232 2 910 3 117 4 224 5 131 6 331 7 115	- 41 -179 840 - 35 183 - 22 311 56	1 2 3 4 5	348 117- 196 97- 327 0 22 1 413	354 -65 194 54 358 441	1 -1 -2 -3 -3 4 -4	1198 240 73- 359 564 1234 102- 312	1 293 225 21 297 545 1171 82 -302	2 -2 3 -3 4 -4 5 -5	1 54 6 5 3 5 2 3 1 0 9 - 3 5 9 4 4 8 5 0 6	136 656 512 22 -334 467 516	5 -5 6 -6 7 -7 -8 -9	415 231 106- 118- 84- 305 98- 114	461 470 19 154 319 -40 130	2 -2 3 -3 -4 -4 5 -5	421 421 329 118- 275 386 162 114-	363 389 -314 -94 258 379 141 151
8 9 1 2	394 131- 120- 92- 0 5 1 726 365	83 426 106 153 -139 695 342	0 103 1 232 2 910 3 117 4 224 5 131 6 331 7 115 8 270	- 41 -179 840 - 35 183 - 22 311 - 56 310	1 2 3 4 5 0	348 117- 196 97- 327 0 22 1 413 112-	354 -65 194 54 358 441 -70	1 -1 -2 -3 -3 -4 -4 5	1198 240 73- 359 564 1234 102- 312 360	1293 225 21 297 545 1171 82 -302 393	2 -2 3 -3 4 -4 5 -5 6	154 653 523 109- 359 448 506 115-	136 656 512 22 -334 467 516 -115	5 -5 6 -6 7 -7 -8 -9	415 231 106- 118- 84- 305 98- 114	461 470 19 154 319 -40 130	2 -2 3 -3 4 -4 5 -5 6	421 421 329 118 275 386 162 114- 161	363 389 -314 -94 258 379 141 151 189
8 9 1 2 3	394 131- 120- 92- 0 5 1 726 365 623	83 426 106 153 -139 695 342 619	0 103 1 232 2 910 3 117 4 224 5 131 6 331 7 115 8 270	- 41 -179 840 - 35 183 - 22 311 56 310	1 2 3 4 5 0 1 2	348 117- 196 97- 327 0 22 1 413 112- 156	354 -65 194 54 358 441 -70 134	1 -1 -2 -2 -3 -3 -4 -4 5 -5	1198 240 73- 359 564 1234 102- 312 360 236	1293 225 21 297 545 1171 82 	2 -2 3 -3 4 -4 5 -5 6 -6	154 653 523 109– 359 448 506 115– 174	136 656 512 22 -334 467 516 -115 208	5 -5 6 -6 7 -7 -8 -9	415 231 106- 118- 84- 305 98- 114 1 12 1	461 470 19 19 154 319 -40 130	2 -2 3 -3 4 -4 5 -5 6 -6	421 421 329 118- 275 386 162 114- 161 305	363 389 -314 -94 258 379 141 151 189 350
8 9 1 2 3 4 5	394 131- 120- 92- 0 5 1 726 365 623 215 438	83 426 106 153 -139 695 342 619 -244	0 103 1 232 2 910 3 117 4 224 5 131 6 331 7 115 8 270 0 13	- 41 -179 840 - 35 183 - 22 311 56 310	1 2 3 4 5 0 1 2 3	348 117- 196 97- 327 0 22 1 413 112- 156 98- 28h	354 -65 194 54 358 441 -70 134 -49	1 -1 2 -2 3 -3 -3 -4 -5 -5 6 -5	1198 240 73- 359 564 1234 102- 312 360 236 118- 106-	1293 225 21 297 545 1171 82 -302 393 224 0	2 -2 3 -3 4 -4 5 -5 6 -6 7	154 653 523 109– 359 448 506 115– 174 248	136 656 512 22 -334 467 516 -115 208 308	5 -5 6 -6 7 -7 -8 -9	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102-	461 470 19 154 319 -40 130	2 -2 -3 -4 -4 5 -5 -6 -7	421 421 329 118- 275 386 162 114- 161 305 181	363 389 -314 -94 258 379 141 151 189 350 -193 225
9 1 2 3 4 5 6	394 131- 120- 92- 0 5 1 726 365 623 215 438 128-	83 426 106 153 -139 695 342 619 -244 370 133	0 103 1 232 2 910 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 2 3 4 5 0 1 2 3 4	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284	354 -65 194 54 358 441 -70 134 -49 278	1 -1 2 -2 -3 -3 -4 -5 -5 -5 -5 -6 -7	1198 240 73- 359 564 1234 102- 312 360 236 118- 106- 340	1293 225 21 297 545 1171 82 -302 393 224 0 -50 404	2 -2 -3 -4 -4 -5 -5 -6 -6 7 -7 8	154 653 523 109- 359 448 506 115- 174 248 259 71-	136 656 512 22 -334 467 516 -115 208 308 278 135	5 -5 6 -6 7 -7 -8 -9 0 1	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 97-	461 470 19 154 319 -40 130 608 -40 97	2 -2 -3 -4 -4 -5 -5 -6 -7 -8	421 421 329 118 275 386 162 114- 161 305 181 152	363 389 -314 -94 258 379 141 151 189 350 -193 225
8 9 1 2 3 4 5 6 7	94 131- 120- 92- 0 5 1 726 365 623 215 438 128- 287	83 426 106 153 -139 695 342 619 -244 370 133 304	0 103 1 232 2 910 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 2 3 4 5 0 1 2 3 4	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284 0 23 1	354 -65 194 54 358 441 -70 134 -49 278	1 -1 2 -2 3 -3 4 -4 5 -5 6 -6 7 -7	1198 240 73- 359 564 1234 102- 312 360 236 118- 106- 340 380	1293 225 21 297 545 1171 82 -302 393 224 0 -50 404 420	2 -2 3 -3 4 -4 5 -5 6 7 7 7 8 -8	154 653 523 109- 359 448 506 115- 174 248 259 71- 111-	136 656 512 22 -334 467 516 -115 208 308 278 135 85	5 -5 6 -6 7 -7 -8 -9 0 1 -1 2	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 97- 108-	461 470 19 154 319 -40 130 608 -40 97	2 -2 3 -3 4 -4 5 -5 6 -6 -7 -8	421 421 329 118- 275 386 162 114- 161 305 181 152	363 389 -314 -94 258 379 141 151 189 350 -193 225
8 9 1 2 3 4 5 6 7 8	394 131- 120- 92- 0 5 1 726 365 623 215 438 128- 287 118-	83 426 106 153 -139 695 342 619 -244 370 133 304 -156	0 103 1 222 2 910 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649 4 322	- 41 -179 840 - 35 183 - 22 311 56 310 - 1 - 242 - 42 660 - 287	1 2 3 4 5 0 1 2 3 4 4	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284 0 23 1 237	354 -65 194 54 358 441 -70 134 -49 278 209	1 -1 2 -2 3 -3 4 -4 5 -5 6 -6 7 7 -7 8	1198 240 73- 359 564 1234 102- 312 360 236 118- 106- 340 380 84-	1293 225 21 297 545 1171 82 -302 393 224 0 -50 404 420 69	2 -2 3 -3 4 -4 5 -5 6 7 7 8 -8 -8 -9	154 653 523 109- 359 448 506 115- 174 248 259 71- 111- 164	136 656 512 22 -334 467 516 -115 208 278 308 278 135 85 184	5 -5 6 -6 7 -7 -8 -9 0 1 -1 2 -2	415 231 106- 118- 84- 305 98- 114 1 12 I 660 102- 97- 108- 536	461 470 19 19 154 319 -40 130 608 -40 97 16 520	2 -2 3 -3 4 -5 -5 6 -6 -6 -7 -8	421 421 329 118- 275 386 162 114- 161 305 181 152 1 17 1 118-	363 389 -314 -94 258 379 141 151 189 350 -193 225 106
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8 9 1 2 3 4 5 6 7 8 9	0 5 1 726 365 623 215 438 128- 287 118- 271	83 426 106 153 -139 695 342 619 -244 370 133 304 -156 303	0 103 1 232 2 9100 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649 4 322 5 487 6 126	- 41 -179 840 - 35 183 - 22 311 56 310 - 242 - 422 - 422 - 660 287 - 367 54	1 2 3 4 5 0 1 2 3 4 4 . 1 2 3 3	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284 0 23 1 237 95- 117	254 -65 194 54 258 441 -70 134 -49 278 209 22 141	1 -1 2 -2 3 -3 4 -4 5 -5 6 -6 7 7 8 -8 -8	1198 240 73- 359 564 1234 102- 312 260 236 118- 106- 380 84- 115- 215	1293 225 21 297 545 1171 82 -302 393 224 0 -50 404 420 69 32 262	2 -2 3 -3 4 -4 5 -5 6 -6 7 -7 8 8 -8 -9	154 653 523 109- 359 448 506 115- 174 248 259 71- 111- 164	136 656 512 22 -334 467 516 -115 208 308 278 135 85 184	5 -5 6 -6 7 -7 -8 -9 0 1 -1 2 -2 3 -3	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 597- 108- 536 114- 175	461 470 19 154 319 -40 130 608 -40 97 16 520 -122 187	2 -2 -3 -4 -5 -5 -6 -6 -7 -7 -8 0 1	421 421 329 118- 275 386 162 114- 161 305 181 152 1 17 1 118- 478 431	363 389 -314 258 379 141 151 189 350 -193 225 106 435 392
89 123456789	994 131- 120- 92- 0 5 1 726 365 623 215 438 128- 287 118- 271 0 6 1	83 426 106 153 -139 695 342 619 -244 370 133 304 -156 303	0 103 1 222 2 9100 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649 4 322 5 487 6 126 7 3200 8	$\begin{array}{c} - & 41 \\ -179 \\ 840 \\ - & 35 \\ 183 \\ - & 22 \\ 311 \\ - & -56 \\ 310 \\ 1 \\ 242 \\ - & -42 \\ 660 \\ 287 \\ - & -54 \\ 346 \\ \end{array}$	1 2 3 4 5 5 0 1 2 3 4 1 2 3 4	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284 0 23 1 237 95- 117 64-	254 -65 194 54 258 441 -70 134 -49 278 209 22 141 24	1 -1 2 -2 3 -3 4 -4 5 -5 6 -6 7 7 -7 8 -8 -9 -10	1198 240 73- 359 564 1234 102- 312 360 236 118- 106- 340 84- 115- 215 68-	1293 225 21 297 545 1171 82 -302 393 224 0 -50 404 420 69 32 262 6	2 -2 3 -4 -4 5 -5 6 -6 7 -7 8 -8 -9 0	154 653 523 109- 359 448 506 115- 174 248 259 71- 111- 164 1 8 1 913	136 656 512 22 -334 467 516 -115 208 308 278 135 85 184 882	5 -5 6 -7 -7 -8 -9 0 1 -1 2 -2 3 -3 4	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 97- 108- 536 114- 175 561	461 470 19 154 319 -40 130 608 -40 97 16 520 -122 187 590	2 -2 -3 -4 -4 -5 -5 -6 -6 -6 -7 -8 0 1 -1 2	421 421 329 118- 275 386 162 161 305 181 152 1 17 1 118- 478 431 117- 27-	363 389 -314 258 379 141 151 189 350 -193 225 106 435 392 -64
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8 9 1 2 3 4 5 6 7 8 9 0 1 2	394 394 131- 120- 92- 0 5 1 726 365 623 215 438 128- 287 118- 271 0 6 1 378 756	83 426 106 153 -139 695 342 619 -244 370 133 304 -156 303 372 764 568	0 103 1 222 2 9100 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649 4 322 5 487 6 126 7 320 8 79 0 14	$\begin{array}{c} - & 41 \\ -179 \\ 840 \\ - & 35 \\ 183 \\ - & 22 \\ 311 \\ - & -56 \\ 310 \\ 1 \\ 242 \\ - & 420 \\ 287 \\ - & 420 \\ 287 \\ 367 \\ - & -54 \\ 346 \\ - & 63 \end{array}$	1 2 3 4 5 5 1 2 3 4 4 1 2 3 4 2 3 4 2 3 4 2 3 4 3 4 3 4 5 3 4 5 3 4 5 3 4 5 3 4 5 5 4 5 5 4 5 5 4 5 5	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284 0 23 1 237 95- 117 64- 0 24 1 356	254 -65 194 54 258 441 -70 134 -49 278 209 227 141 24	1 -1 2 -2 3 -3 4 -4 5 -5 6 -6 7 7 -7 8 8 -9 -10	1198 240 73- 359 564 1234 102- 312 360 236 236 236 236 236 240 380 84- 115- 215 68- 1 4 1	1293 225 21 297 545 1171 82 -302 224 0 -50 404 420 69 32 262 6 585	2 -2 -3 -4 -4 -5 -6 -6 -7 -7 -7 -8 -9 0 1 -1 2	154 653 523 109- 359 448 506 115- 174 248 259 71- 111- 164 1 8 1 913 81- 355 278	136 656 512 22 -334 467 516 -115 208 308 278 135 184 882 22 352 264	5 -5 -6 -7 -7 -8 -9 0 1 -1 2 2 3 -3 -4 -4 5 -5 -5 -6 -7 -7 -8 -9 0 1 -1 2 2 3 -4 -5 -4 -5 -5 -5 -6 -7 -7 -7 -8 -9 -9 -12 -9 -12 -12 -12 -12 -12 -12 -12 -12 -12 -12	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 97- 108- 536 114- 175 561 385 714- 172-	461 470 19 154 319 -40 130 608 -40 97 16 520 -122 187 590 384 106	2 -2 -3 -3 -4 -5 -5 -5 -6 -7 -8 0 1 -1 2 -2 3 -2 3	421 421 329 118- 275 386 162 114- 161 305 181 152 1 17 1 118- 478 431 117- 231 384	363 389 -314 258 379 141 151 189 350 -193 225 106 435 392 -64 -197 332
8 9 1 2 3 4 5 6 7 8 9 0 1 2 3	994 131- 120- 92- 0 5 1 726 365 623 215 438 128- 287 118- 271 0 6 1 378 754 576 91-	83 426 105 153 -139 695 342 619 -244 370 133 304 -156 303 372 764 568 51	0 103 1 222 2 9100 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649 4 322 5 487 6 126 7 320 8 79 0 14 0 0 14 0 0 14 0 0 14 0 0 14 0 0 0 0 0	- 41 -179 -35 183 -22 311 56 310 -242 -42 660 287 -54 -54 -63 1 277	1 2 3 4 5 5 1 2 3 4 4 1 2 3 4 4 0 1	348 117- 196 97- 327 0 22 1 413 112- 156 98- 284 0 23 1 237 95- 117 64- 0 24 1 356 87-	254 -65 194 54 258 441 -70 134 -49 278 209 22 278 209 22 141 24 24 55	1 -1 2 -3 -3 -4 -5 -5 -5 -6 -6 -6 -7 -7 -7 -8 -9 -10 0 1	1198 240 73- 359 564 1234 102- 312 360 236 118- 106- 340 884- 115- 215 68- 1 4 1 531 297	1293 225 21 297 545 1171 82 -302 393 224 0 -50 404 420 69 32 262 6 585 -285	2 -2 -3 -4 -4 -5 -5 -5 -6 -6 -6 -7 -7 8 -9 -9 0 1 -1 2 2 -2 -3 -3 -5 -5 -5 -5 -6 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7	154 653 523 109- 359 448 506 115- 174 248 259 71- 111- 164 1 8 1 913 81- 355 278 730	136 656 512 22 -334 467 516 -115 208 208 278 135 85 184 882 22 352 264 730	5 -5 -6 -7 -7 -8 -9 0 1 -1 -2 -3 -3 -4 -5 -5 -5 -5 -7 -7 -8 -9 0 1 -1 -2 -3 -3 -4 -5 -5 -5 -6 -6 -7 -7 -8 -9 -5 -6 -6 -6 -7 -7 -8 -9 -5 -6 -6 -7 -7 -8 -9 -5 -6 -6 -7 -7 -8 -9 -5 -6 -6 -7 -7 -8 -9 -5 -6 -7 -7 -8 -9 -7 -7 -8 -9 -5 -6 -6 -7 -7 -7 -8 -9 -7 -7 -7 -8 -9 -7 -7 -8 -9 -7 -7 -7 -8 -9 -7 -7 -7 -7 -7 -7 -7 -8 -9 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 97- 108- 536 114- 175 561 385 114- 177- 102-	461 470 19 154 319 -40 130 608 -40 97 16 520 -122 187 590 384 106 485	2 -2 -3 -4 -4 -5 -5 -6 -6 -7 -8 0 1 -1 2 -2 -3 -3	421 421 329 118 275 386 162 114- 161 305 181 152 1 17 1 118- 478 431 117- 231 384 333 104-	363 389 -314 258 379 141 151 189 350 -193 225 392 -64 -197 332 370 -71
8 9 1 2 3 4 5 6 7 8 9 0 1 2 3 4	394 394 131- 120- 92- 0 5 1 726 365 623 215 438 128- 287 118- 271 0 6 1 378 754 576 91- 772	83 426 106 153 -139 695 342 619 -244 370 133 304 -156 303 372 764 568 51 756	0 103 1 222 2 9100 3 117 4 224 5 131 6 331 7 115 8 270 0 13 1 305 2 116 3 649 4 322 5 483 6 126 7 320 8 79 0 14 0 301 1 180	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 2 3 4 5 5 1 2 3 4 1 2 3 4 0 1 2 3 4 0 1 2 3 4 0 1 2 3 4 0 1 2 3 4 0 1 2 1 3 4 1 3 4 5 5 5 5 5 5 5 5 5	348 117 196 97 327 0 22 1 413 112- 156 98 284 0 23 1 237 95 117 64 0 24 1 356 87 123	254 -65 194 358 441 -70 134 -49 278 209 22 141 24 351 55 124	1 -1 2 -3 -3 -4 -5 -5 -5 -6 7 -7 8 -9 -10 0 1 -1	1198 240 73- 359 564 1234 102- 312 260 236 236 236 236 240 380 84- 115- 215 68- 141 531 297 51-	1293 225 211 297 545 1171 82 393 224 0 -50 404 420 69 32 262 6 585 -285 153	2 -2 -3 -4 -4 -5 -5 -6 -6 -7 -7 -8 -8 -9 0 1 -1 2 2 3	154 653 523 109- 359 448 506 115- 174 248 259 71- 164 181 913 81- 355 278 730 220	136 656 512 22 -334 467 516 -115 208 308 278 135 85 184 882 22 352 264 730 164	5 -5 -6 -7 -7 -8 -9 0 1 -1 2 2 3 -3 4 4 5 5 6 -6 -6 -6 -7 -7 -7 -8 -9 0 1 -1 2 2 3 -3 4 4 5 5 6 -6 -6 -6 -7 -7 -7 -8 -9 -6 -6 -7 -7 -7 -7 -7 -6 -6 -6 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7 -7	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- ⁵ 97- 108- 536 114- 175 561 114- 175 565 114- 117- 102- 567	461 470 19 154 519 -40 130 -122 520 -122 187 590 384 106 44 5638	2 -2 -3 -3 -4 -5 -6 -7 -8 0 -1 -1 2 -2 -3 -3 -4 -4 -4	421 421 329 118- 275 386 162 114- 161 305 181 152 1 17 1 118- 478 431 117- 231 384 333 104- 117-	363 389 -94 258 379 141 151 151 225 106 435 392 -64 -197 332 370 -71
8 9 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5	394 394 394 394 31- 22- 0 5 1 726 365 623 215 438 287 118- 271 0 6 1 378 754 576 91- 772 117-	83 426 106 153 -139 695 342 619 -244 370 133 304 133 304 133 304 568 516 568 516 71	0 103 1 222 2 9100 3 117 4 224 5 131 6 331 7 115 8 270 0 12 1 305 2 116 3 649 4 322 5 487 6 126 7 320 8 79 0 14 0 301 1 180 2 747	$\begin{array}{c} - & 41 \\ -179 \\ - & 179 \\ 35 \\ 183 \\ - & 22 \\ 311 \\ - & -56 \\ 310 \\ 1 \\ 242 \\ - & -66 \\ 287 \\ - & -54 \\ 660 \\ 287 \\ - & -54 \\ - & 63 \\ 1 \\ 277 \\ -194 \\ -668 \end{array}$	1 2 3 4 5 5 0 1 2 3 3 4 4 0 1 2 3 3 4 3 2 3 3 3 4 3 3 4 3 3 3 3 4 3 3 4 3 4	348 117 196 97 327 0 22 1 413 112- 156 98 284 0 23 1 237 95 117 64 0 24 1 356 87 123 65	254 -65 194 258 441 -70 134 -49 278 209 22 141 24 351 55 124 -48	1 -1 2 -3 -3 -4 -5 -5 -5 -5 -6 7 -7 8 8 -9 -10 0 1 1 -2	1198 240 73- 359 564 1234 102- 312 360 236 118- 340 380 84- 115- 215 68- 115- 215 68- 141 531 297 51- 873	1293 225 211 297 545 1171 82 393 224 0 -50 404 420 0 932 262 6 585 -285 153 918	2 -2 -3 -4 -4 -5 -5 -6 -7 -7 -7 -8 -9 0 1 -1 2 -2 -3 -3	154 653 523 109- 448 506 115- 174 248 259 71- 164 181 913 81- 355 278 730 220 208	136 656 512 22 -334 467 516 208 308 278 308 278 135 85 184 882 22 352 264 730 164 213	5 -5 6 -6 7 -7 8 -9 0 1 -1 2 2 3 -3 4 4 5 -5 6 6 7 7 -7 8 -9 0 1 -1 2 2 3 -3 4 4 5 -5 6 6 7	415 231 106- 118- 84- 305 98- 114 1 12 1 660 102- 97- 108- 536 114- 175 561 385 714- 117- 102- 567 77-	461 470 19 19 154 319 -40 130 130 608 -40 97 16 520 97 16 520 -122 187 598 4 106 44 85 598 4 45 85 638 -33	2 -2 -3 -3 -4 -5 -5 -6 -7 -8 0 1 -1 2 -2 -3 -4 -4 -5 -5 -5 -7 -8 0 1 -1 -2 -3 -4 -5 -5 -7 -7 -7 -4 -5 -5 -7 -7 -5 -5 -7 -7 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5	421 421 329 118- 275 386 162 114- 161 305 181 152 1 17 1 118- 478 431 117- 231 1084 333 104- 117- 253	363 389 -94 258 379 141 151 189 350 -193 225
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Table 2 (cont.)

1	10 F	10 F	1	10 F	10 F	1	10 5	10 F	1	¹⁰ F	10 F	1	10 F	10 F	1	10 F	10 F	1	10 5	10 F
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-5	105-	155	0	145	151	-3	462	365	-5	255	242	0	763	679	-6	91-	11			,
-6	192	159	1	63 -	-44	4	170	159	6	220	252	1	85-	-101	-7	147	148		2 18 1	
-7	68-	-85	-1	71-	-38	-4	62-	89	-6	458	492	-1	77-	-15	-8	68-	94	0	266	211
			-2	193	196	5	193	207	-7	93-	38	2	363	324				1	176	131
	1 19 1		-3	58 .	-33	-5	452	468	-8	200	212	-2	315	308		2 14 1		-1	88-	-88
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1	353	355		201		-6	84-	77	-10	104	182	-3	79-	-28	1	93-	24	-2	307	330
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2	110-	1	2	591	596	-7	441	465		271		-4	445	428	2	445	346	-3	162	162
-2	290	-273	-2	833	992	-8	92 .	-148	0	452	457	5	78-	15	-2	185	148	-4	282	296
3	148	119	4	578	505	-9	100	99	1	692	590	-5	89-	42	3	86-	-80	-5	157	-151
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4	89-	48	6	78-	85				2	235	-209	-6	159	147	4	272	233	-7	47-	68
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2	177	196	-8	272	313	0	470	461	3	454	393	-8	303	338	5	57-	-78		2 19 1	
->	210	189	-10	230	340	1	77	-98	-3	383	356	-9	62-	-6	-5	92-	-112	0	84	-72
-0	-10	12				-1	387	490	4	93-	43				-6	222	229	1	187	149
-/	193	293	•	211		2	625	572	-4	74-	-186		2 11 1		-7	78-	-128	-1	425	430
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	220	197	-1	681	872	-3	248	-172	6	69 -	-104	-1	388	352		2 15 1		3	266	298
	108-	-12	2	74-	-6	4	455	440	-6	89-	146	2	92-	7	0	93-	-89	-3	254	267
-1	101-	220	-2	253	-311	-4	412	385	-7	252	269	-2	81-	-37	1	774	653	-4	77-	11
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_4	369	378	-5	326	302	-7	49- 246	-110	•	- 81		5	386	376	-3	324	311	0	267	245
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-ó	122	133	-6	83-	111	-9	79-	2/0	-1	264	218	6	- UC	->>	-4	93-	222	-1	163	-157
			7	260	259	-10	131	173	-,	423	404	-0	9)- 88-	-41	2	124	244	2	240	215
	1 21 1		-7	516	548			.,,,	-2	432	381	-8	77-	-68	-6	84-	-103	-2	75	409
0	104-	27	-8	92-	-66		251			92-	26	-9	280	-00	-7	100	227	ر ــــــــــــــــــــــــــــــــــــ	75 -	60 41
1	475	451	-9	119	144	0	158	167	-3	307	-312			505	-8	54-	81	-5	61-	0
-1	200	198	-10	60-	-3	1	699	730	4	300	289		2 12 1		-			-6	179	251
2	94-	-84				-1	423	577	-4	558	663	0	689	628		2 16 1				
-2	103-	-18		221		2	1 36	-147	5	149	158	1	91⇒	2	0	385	355		2 21 1	
3	269	260	0	379	384	-2	53 -	-100	-5	210	223	-1	85-	-106	1	89-	95	0	66-	-72
-3	352	332	1	1 30	-120	3	486	448	6	304	347	2	407	387	-1	251	-244	1	127	78
4	63-	43	-1	122	13	-3	480	519	-6	237	276	-2	163	150	2	314	288	-1	310	305
-4	90-	71	2	409	416	4	214	200	-7	93-	-29	3	92-	121	-2	351	395	2	86	61
-5	97	97	-2	759	973	-4	67-	-90	-8	259	326	-3	86-	117	3	77-	38	-2	69-	25
			3	85-	-13	5	129	1 39	-9	70-	-44	4	216	192	-3	93-	127	-3	230	247
	1 22 1		-3	48-	38	-5	525	532				-4	721	714	4	205	187	-4	60-	26
•	179	152	4	390	406	6	74-	-10		291		5	70-	3	-4	375	368	-5	125	125
1	92-	-10	-4	584	579	6	242	228	0	178	117	-5	93-	-44	-5	159	-176			
-1	221	220	2	91-	18	7	45-	143	1	724	574	-6	166	177	-6	313	330		2 22 1	
<u>,</u>	223	الرو البارد	->	14=	101	-7	394	461	-1	515	474	-7	86-	12	-7	155	211	0	146	146
	69-	_9	-6	585	628	-0	101	-104	2	241	-223	-8	312	385	-8	121	172	1	44-	34
-3	89-	66	-0	505	-80	-10	52-	207	-2	72-	26	-9	49-	-10				-1	59-	15
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-1	86-	79	0	86	-50	-2	627	593	-6	92-	33		243	209	-3	318	277			ر ـــ
2	69-	-35	1	202	179	3	89-	-68	-7	200	213	-1	4 50	454	4	87	-113			
-2	82-	44	-1	594	694	-3	409	-485	-8	84-	-61	4	80-	-63	-4	87-	8			
-3	328	354	2	300	-313	4	315	305	-9	267	366	-4	92-	49	-5	263	257			
- 4	63-	-6	-2	41-	-60	-4	599	660	-			5	281	304	-6	74-	-53			
												-			-	•				

The conventional R indices (observed reflections only) are:

R(0kl) = 6.60%, R(1kl) = 9.08%, R(2kl) = 11.14%.

The scattering factors of Berghuis *et al.* (1955) were used for C, N, O, Cl⁻, while for Cd^{2+} the values given by Thomas & Umeda (1957) were employed.

An estimate of the accuracy of the coordinates is also given by the R' indices calculated for the observed reflections with k+l odd, in which the cadmium has no influence. These reflections are rather weak and their number is small (24 0kl, 59 1kl, 51 2kl); nevertheless, the R' values are fairly small:

R'(0kl) = 7.76%, R'(1kl) = 11.99%, R'(2kl) = 16.19%.

4. Discussion of the structure

The coordination polyhedron around the Cd atom is octahedral. Fig. 2 shows how these polyhedra are

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linked in chains parallel to [100]. The bond distances and angles concerning Cd are as follows (the coordinates are not given if the atom is at x, y, z):

Cd–Cl	$= 2.55 \pm 0.01$ Å
Cd-Cl(x-1, y, z)	$= 2.62 \pm 0.01$
Cd-O _I	$= 2 \cdot 34 \pm 0 \cdot 02$
Cl-Cd-Cl(x-1, y, z)	$=91.5\pm0.3^{\circ}$
Cd-Cl-Cd(x+1, y, z)	$=91.5\pm0.3$
O _I CdCl	$= 87.9 \pm 0.5$
$O_{I}-Cd-Cl(x-1, y, z)$	$= 88.0 \pm 0.5$

The standard deviations in distances and angles were calculated using the relations of Ahmed & Cruickshank (1953). The distances Cd–Cl are in agreement with the corresponding ones found in the coordination compounds formed by CdCl₂ and *bis*-acetamide (2.58, 2.66 Å; Cavalca, Nardelli & Coghi, 1957), *bis*-urea (2.64 Å; Nardelli, Cavalca & Fava, 1957), *mono*-methylurea, CdCl₂. OC(NH₂)NHCH₃, (2.58, 2.62 Å; Nardelli, Coghi & Azzoni, 1958). The distance Cd–O is a little larger than those found in the other compounds (2.23, 2.28, 2.18 Å respectively).

A diagrammatic projection of a part of a unit cell along [100] is given in Fig. 3.



Fig. 3. Diagrammatic projection along [100] of a part of a unit cell.

The results confirm the *trans* configuration of the biuret molecule, and so an intramolecular hydrogen bond is possible, as suggested by Kogon (1957) from the study of infrared absorption spectra of some alkyland aryl-alkyl-biurets. The *trans* configuration with the indicated hydrogen bonding is present in dioxane solution of biuret too, as Kumler (1959) deduced from the dipole moment (3.27 Debyes) which is considerably less than that of urea (4.56 D.) and that of acetamide (3.90 D.). Because of this hydrogen bonding, the two oxygen atoms (O_I and O_{II}) are not equivalent and only O_I can be coordinated by the metal atom. The

biuret molecule has the following bond lengths and angles:

O _I -C _I	$= 1.23 \pm 0.05 \text{ Å}$
$C_{I}-N_{I}$	$= 1.35 \pm 0.05$
$C_{I}-N_{II}$	$= 1.35 \pm 0.04$
N _{II} –C _{II}	$= 1.34 \pm 0.04$
$C_{II} - O_{II}$	$= 1.26 \pm 0.05$
C_{II} – N_{III}	$= 1.35 \pm 0.04$
$N_1 \cdots O_{11}$	$= 2.73 \pm 0.04$
$O_{I} - C_{I} - N_{I}$	$= 121.6 \pm 2.9^{\circ}$
O_{I} - C_{I} - N_{II}	$=119\cdot3\pm2\cdot7$
N_{I} – C_{I} – N_{II}	$= 119 \cdot 1 \pm 2 \cdot 8$
C_{I} – N_{II} – C_{II}	$= 131.9 \pm 3.0$
$N_{II} - C_{II} - O_{II}$	$= 121 \cdot 1 \pm 2 \cdot 3$
N _{II} -C _{II} -N _{III}	$= 118.0 \pm 2.5$
$O_{II} - C_{II} - N_{III}$	$= 120.9 \pm 2.5$
$O_{II} \cdots N_{I-C_{I}}$	$= 82.8 \pm 2.1$
$N_1 \cdots O_{11} - C_{11}$	= 85.0 + 2.0

The configuration assumed for the organic molecule is based on the following considerations:

(a) The values of the electron density at the maxima of the peaks attributed to the oxygen atoms are higher than those of the nitrogen atoms, e.g. the values for $\rho_{\text{max.}}$ in $\rho_0(Y, Z)$ projection are:

$$\begin{array}{ccccc} O_{I} & O_{II} & N_{I} & N_{II} & N_{III} \\ \varrho_{max.} & \left\{ \begin{array}{ccccc} {\rm obs.} & 10\cdot 1 & 9\cdot 2 & 8\cdot 4 & 8\cdot 1 & 7\cdot 6 & e. {\rm \AA}^{-2} \\ {\rm calc.} & 9\cdot 9 & 9\cdot 8 & 8\cdot 6 & 7\cdot 9 & 7\cdot 1 \end{array} \right. \end{array}$$

(b) The interatomic distances O–C and N–C agree with those expected.

(c) The trans configuration and the interatomic distances correspond to what has been found for the biuret hydrate by Hughes, Yakel & Freeman (1959). (d) The two cis configurations



can be ruled out because with (I) the biuret molecule should behave as a bidentate ligand, and with (II) the steric hindrance between the hydrogen atoms of the NH_2 -groups should push these out of the plane of the molecule. The *trans* configuration is stabilized by a strong intramolecular hydrogen-bond.

The planarity of the molecule is indicated by the values of the angles at C_{I} and C_{II} , which in both cases add up to 360°, and by the sum of the angles in the pentagon $N_{I}C_{I}N_{II}C_{II}O_{II}$, which is 539.9°. The equation of the least-squares plane of the molecule is:

$$\cdot 9288x' + 0.0782y' - 1.0000z' + 1 = 0$$

1

using the orthogonal coordinates of the atoms. The average deviation of all atoms from this plane is 0.04 Å, the greatest deviation being 0.06 Å for N_{III}. It is easy to calculate from this that the contribution to the structure factor from the organic molecule is a maximum for the $20\overline{2}$ reflection.

The distances and angles found in the organic molecule are in good agreement with those reported in the literature for the amide groups (Tomiie, Koo & Nitta, 1958). The angle $C_{I}-N_{II}-C_{II}$ is considerably larger than that required by trigonal sp^2 hybridization on nitrogen atom; the increased value can be justified by steric hindrance between N_I and O_{II}.

The angle $Cd-O_I-C_I = 136\cdot3^\circ \pm 2\cdot8^\circ$ is similar to the corresponding ones found in *bis*-urea- (134°), in *bis*-acetamide- (134°) and in *mono*-methylurea- (128°) cadmium chlorides.

Interaction of the different parallel chains occurs through the atoms of the organic molecules, which form hydrogen bonds of $NH \cdots O$ type. The most significant intermolecular distances are:

The distance between the planes of molecules separated by one unit cell translation along the x axis is 3.29 Å.



Fig. 4. Hydrogen-bonding around N_{III} .

An intermolecular hydrogen bond occurs between $N_{II} (1+x, \frac{1}{2}-y, \frac{1}{2}+z)$ and O_{II} ; this is indicated by the short value of the interatomic distance (2.82 Å),

by the small distance (0.12 Å) of O_{II} from the plane of the molecule containing the nitrogen donor-atom and by the angles

$$\begin{array}{l} C_{II} (1+x, \frac{1}{2}-y, \frac{1}{2}+z) - N_{II} (1+x, \frac{1}{2}-y, \frac{1}{2}+z) - O_{II} \\ = 103 \cdot 5^{\circ} \\ C_{I} (1+x, \frac{1}{2}-y, \frac{1}{2}+z) - N_{II} (1+x, \frac{1}{2}-y, \frac{1}{2}+z) - O_{II} \end{array}$$

 $= 123.9^{\circ}$.

The nearest neighbours of the N_{III} atom are represented diagrammatically in Fig. 4, in which the values in brackets indicate the distances of these atoms from the plane containing $C_{II}N_{III}H_2$. The positions of the two H-atoms are deduced assuming that they lie in the plane of the molecule and form trigonal angles. From this diagram one can deduce that hydrogen bonding with O_I is probable, because this atom is not very far from the plane of the molecule containing the H-donor. The angular values indicate that the other H-atom is more probably bound to O_{II} than to Cl, but it may be bound to both of them.

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