Discussion. The structure determination was undertaken since the estimations of the Al coordination which could be derived from the $Sc_2(WO_4)_3$ structure (Abrahams & Bernstein, 1966) were not sufficiently precise. It was only after the refinement was started that we learned of the work of C & S based on Weissenberg data. Since diffractometer data are likely to yield more precise results than photographic data, it was decided to continue the calculations.

The cell dimensions calculated agree within experimental error with those obtained by C & S and those found by Trunov, Lutsenko & Kovba (1967). A comparison of the atomic parameters of the two structure determinations shows that the e.s.d.'s obtained in this work are about half those reported by C & S. Furthermore, all atomic coordinates do not differ by more than three times the e.s.d.'s obtained by C & S except for O(1) [this work: $z=0{\cdot}091$ (2), C & S: $z=0{\cdot}058$ (7)]. This difference could be due to some disorder in the crystal used by C & S, which would also be consistent with the high temperature factor of 2·7 (8) Å^2 found by them for this atom. The O(1) position determined in the present structure results in a much smaller spread in the comparable interatomic distances and angles (see Tables 2 and 3).

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Cadmium(II) Formate Dihydrate

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Abstract. $C_4H_{12}O_{12}\ Cd_2$, monoclinic, $P2_1/c$, $a=8{\cdot}982$ (4), $b=7{\cdot}391(6)$, $c=9{\cdot}760(3)$ Å, $\beta=97{\cdot}32(3)°$, $Z=2$, $D_x=2{\cdot}44$ g cm^{-3}. As previously reported [Osaki, Nakai & Watanabé (1964). *J. Phys. Soc. Japan*, **19**, 717–723] the structure is isomorphous with the formates of manganese, zinc and copper, and forms a three-dimensional polymer. There are two formate ligands, exhibiting *anti–anti* and *anti–syn* configurations, linking together cadmium atoms which are arranged in face-centred positions in the cell. The polymer is further strengthened by hydrogen bonds between coordinated water molecules and formate oxygen atoms. Cd–O distances vary between 2·243(5) and 2·326(5) Å.

Introduction. Cadmium(II) formate was prepared by dissolving finely divided $CdCO_3$ in a slight excess of aqueous formic acid, and crystallized from aqueous solution as colourless parallelepipeds. Accurate cell dimensions were obtained from a least-squares treatment of the 2θ values of 16 reflexions measured on a General Electric XRD 6 diffractometer. Systematic absences were $h0l$ with l odd, $0k0$ with k odd; space group $P2_1/c$. For data collection, a crystal of size approximately $0{\cdot}20\times0{\cdot}20\times0{\cdot}15$ mm was mounted with **b** coincident with the instrument φ axis and all reflexions with $2\theta\le55°$ measured with Zr-filtered Mo $K\alpha$ radiation and the θ–2θ scan technique at a speed of 2° min^{-1} in 2θ. Of a total 1456 observations, 890 had $I>3\sigma$ where $\sigma^2(I)=S+B+(0{\cdot}06S)^2$ (S=scan count, B=background) and were used in the structural refinement. Initial coordinates for the refinement were those of the isomorphous manganous formate dihydrate (Osaki, Nakai & Watanabé, 1964), and after three cycles with isotropic thermal parameters R was 0·099. Refinement was continued with anisotropic thermal parameters, and after two cycles R was 0·065. At this stage a difference synthesis indicated sites for all the hydrogen

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atoms and their contributions were included in subsequent stages with fixed parameters. One reflexion (113) appeared to be suffering from secondary extinction and was excluded from the calculations. With a weighting scheme: $w=1{\cdot}0$ if $|F_o|<F^*$; $w^{1/2}=F^*/|F_o|$ if $|F_o|\geq F^*$, with $F^*=18{\cdot}0$, convergence was attained at R 0·047 (R 0·070 for all reflexions). Final positional and thermal parameters are presented in Tables 1 and 2†.

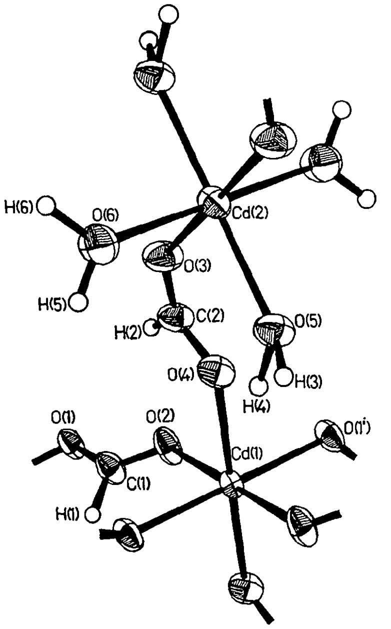

Fig. 1. Perspective view of cadmium(II) formate dihydrate showing slightly more than the asymmetric unit.

Table 2. *Final hydrogen atom positional parameters* ($\times 10^3$)

$U_{\text{iso}}=0{\cdot}063$ Å^2 throughout.

	x	y	z
H(1)	−58	271	233
H(2)	322	484	391
H(3)	176	1108	564
H(4)	171	922	538
H(5)	311	1085	248
H(6)	470	1153	217

Discussion. The crystal structures of formate dihydrates of the divalent metals Mg, Zn, Mn, Cu and Cd have been shown to be isomorphous (Osaki, Nakai & Watanabé, 1963). The Mg and Mn salts have been solved (Osaki, Nakai & Watanabé, 1964) two-dimensionally. The present work yields more accurate structural parameters than found in the isomorphs, and will also facilitate a recent e.s.r. study of Cu(II) doped cadmium formate dihydrate crystals (Herring & Booth, 1974).

A view of slightly more than the asymmetric unit is shown in Fig. 1 while the mode of extension into a three-dimensional polymer is indicated in the packing

Table 1. *Final positional* ($\times 10^4$) *and thermal parameters* (Å$^2\times 10^3$) *with standard deviations in parentheses*

The anisotropic thermal parameters are defined by:

$$T=\exp\left[-2\pi^2(U_{11}a^{*2}h^2+U_{22}b^{*2}k^2+U_{33}c^{*2}l^2+2U_{12}a^*b^*hk+2U_{13}a^*c^*hl+2U_{23}b^*c^*kl)\right]$$

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	0	5000	5000	29·0 (5)	21·8 (4)	19·5 (4)	−0·6 (2)	−2·1 (3)	0·0 (2)
Cd(2)	5000	10000	5000	30·5 (5)	32·2 (5)	28·8 (5)	−3·1 (3)	−2·4 (3)	1·1 (3)
O(1)	1010 (5)	964 (7)	2117 (5)	37 (2)	39 (3)	26 (2)	7 (2)	−8 (2)	−11 (2)
O(2)	882 (6)	2532 (6)	4025 (4)	54 (3)	33 (3)	29 (2)	13 (2)	−9 (2)	−11 (2)
O(3)	4387 (5)	7104 (7)	4182 (5)	34 (3)	43 (3)	56 (3)	−11 (2)	7 (2)	−12 (3)
O(4)	2178 (5)	6601 (6)	4892 (5)	37 (3)	31 (3)	47 (3)	−8 (2)	1 (2)	−5 (2)
O(5)	2654 (6)	10139 (6)	5698 (5)	29 (3)	40 (3)	47 (3)	4 (2)	0 (2)	−3 (2)
O(6)	4078 (6)	11140 (11)	2936 (6)	41 (3)	109 (6)	39 (3)	−5 (4)	−4 (2)	35 (4)
C(1)	440 (8)	2081 (10)	2829 (7)	42 (4)	33 (4)	34 (3)	6 (3)	−8 (3)	−10 (3)
C(2)	3296 (7)	6163 (10)	4321 (7)	28 (3)	33 (4)	46 (4)	−3 (3)	2 (3)	−10 (3)

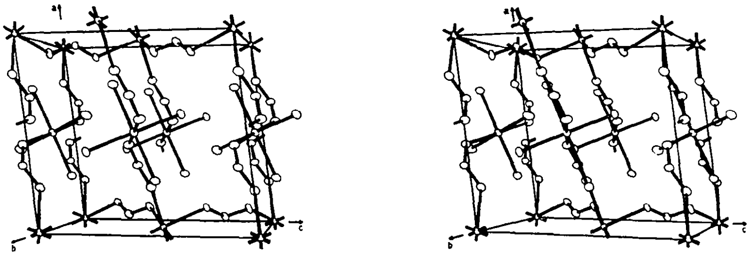

Fig. 2. Stereoscopic view of the polymeric lattice.

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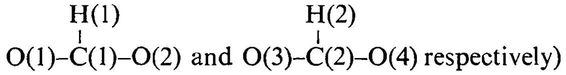
† A table of structure factors has been deposited with the British Library Lending Division, as Supplementary Publication No. SUP 30435 (15 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

diagram, Fig. 2. Bond distances and angles for the structure are presented in Table 3. Atoms of the type Cd(1) and Cd(2) occupy centres of symmetry, on the space group special positions (*a*) and (*d*) respectively, to form a face-centred array which the formate ligands *A* and *B* (*A* and *B* refer to


$\overset{\mathrm{H(1)}}{\mathrm{O(1)–C(1)–O(2)}}$ and $\overset{\mathrm{H(2)}}{\mathrm{O(3)–C(2)–O(4)}}$ respectively)

bridge in the following manner. Ligand *A* coordinates Cd(1) atoms alone, in *anti–anti* configuration, and links them into two-dimensional layers parallel to *bc*. Ligand B, which exhibits *anti–syn* configuration, bridges Cd(1) and Cd(2) atoms in planes parallel to *ab*, forming the three-dimensional polymeric lattice. Cd(1) is six-coordinate through atoms O(1^{i}) and O(2) of ligand *A* and O(4) of *B* (plus symmetry-related atoms), while Cd(2) completes its coordination sphere with O(3) from ligand *B* and coordinated water molecules O(5) and O(6). The polymer is further strengthened by the formation of hydrogen bonds between the water molecules and each of the formate oxygen atoms (Table 4).

Table 3. *Bond distances* (Å) *and angles* (°) *with standard deviations in parentheses*

Cd(1)–O(2)	2·248 (4)	C(2)–O(3)	1·224 (8)
Cd(1)–O(4)	2·301 (5)	C(2)–O(4)	1·251 (8)
Cd(1)–O(1^{i})	2·263 (4)	C(1)–H(1)	1·09
Cd(2)–O(3)	2·326 (5)	C(2)–H(2)	1·06
Cd(2)–O(5)	2·298 (5)	O(5)–H(3)	1·06
Cd(2)–O(6)	2·243 (5)	O(5)–H(4)	1·09
C(1)–O(1)	1·231 (8)	O(6)–H(5)	0·95
C(1)—O(2)	1·230 (7)	O(6)–H(6)	1·03
O(2)—Cd(1)–O(4)	92·9 (2)	Cd(1)–O(4)–C(2)	128·5 (4)
O(2)—Cd(1)–O(1^{i})	90·5 (2)	O(3)—C(2)–O(4)	127·0 (7)
O(4)—Cd(1)–O(1^{i})	87·7 (2)	Cd(2)–O(3)–C(2)	130·0 (5)
O(3)—Cd(2)–O(5)	87·5 (2)	O(1)—C(1)–H(1)	115
O(3)—Cd(2)–O(6)	89·6 (2)	O(2)—C(1)–H(1)	118
O(5)—Cd(2)–O(6)	90·1 (2)	O(3)—C(2)–H(2)	120
Cd(1^{i})–O(1^{i})–Cd(1)	125·4 (4)	O(4)—C(2)–H(2)	113
O(1)—C(1)—O(2)	127·6 (6)	H(3)—O(5)–H(4)	81
C(1)—O(2)—Cd(1)	122·2 (4)	H(5)—O(6)–H(6)	106

Table 4. *Hydrogen-bond distances* (Å) *and angles* (°)

O(5)–H(3)–O(2^{ii})	128	O(5)···O(2^{ii})	2·769 (7)
O(5)–H(4)–O(4)	118	O(5)···O(4)	2·748 (7)
O(6)–H(5)–O(1^{ii})	157	O(6)···O(1^{ii})	2·773 (8)
O(6)–H(6)–O(3^{iii})	175	O(6)···O(3^{iii})	2·721 (7)

Superscripts refer to the following symmetry-related positions:

(i)	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$
(ii)	x	$1+y$	z
(iii)	$1-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$

Each coordination polyhedron is very close to regular octahedral (Table 3) and the variation in Cd–O distance [2·243(5)–2·326(5) Å] is within the range found with other cadmium carboxylates (Harrison & Trotter, 1972; Post & Trotter, 1974*a*, *b*, *c*). The longer distances Cd(1)–O(4) and Cd(2)–O(3) probably reflect the more sterically restrictive requirements imposed upon ligand *B* in bridging between Cd(1) and Cd(2) layers, although residual charge upon the metal atoms [Cd(1) is coordinated by six formate oxygen atoms and Cd(2) by only two] could be a contributing factor (Post & Trotter, 1974*b*). The residual charge effect could also produce the longer C(2)–O(4) bond (1·251 Å). Cd(2) may be expected to possess slight positive charge and, therefore, necessitate greater electron donation from O(3) than would be the case of donation from O(4) to Cd(1). In ligand *B*, a withdrawal of electrons into the bond C(2)–O(3), to facilitate such a trend toward neutralization of charge, would have a weakening effect upon the bond C(2)–O(4).

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Refinement of the Crystal Structure of $NaInSi_2O_6$

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Abstract. $NaInSi_2O_6$, $C2/c$. Cell constants at 20 °C with Mo $K\alpha$ ($\lambda=0·71069$ Å): $a=9·9023$ (4), $b=9·1307$ (4), $c=5·3589$ (2) Å, $\beta=107·200$ (1)°. The variation in cell dimensions across the Na pyroxene series is linear with