Acta Cryst. (1971). B27, 1871

Structural Relations between Pumpellyite and Ardennite

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(*Received* 17 *November* 1970)

The valence summation procedure of Donnay & Allmann is used to assign hydrogen to the proper oxygen atoms in the pumpellyite structure determined by Galli & Alberti. The resulting ideal formula can be compared with that of ardennite:

$$Ca_2Al_2(OH)_2M(OH,O)SiO_4\,.\,\tfrac{1}{2}[Si_4O_{12}(OH,O)_2] \text{ (pumpellyite)}$$
$$A_2Al_2(OH)_2M'(OH)\ SiO_4\,.\,\tfrac{1}{2}[Si_3O_{10}\,.\,AsO_4] \text{ (ardennite),}$$

where A_2 = Mn (Mn, Ca), M = Al, Mg, Fe, M' = Mg, Al, Fe. Shifting the origin of ardennite to $\frac{1}{4},\frac{1}{4},0$ and superposing the two structures with a and b in common, shows near coincidences of corresponding atoms in the two similar asymmetric units, which are nearly the same in size and shape. Nonetheless, different symmetry elements in pumpellyite ($A2/m$) and ardennite ($Pnmm$), acting on the respective asymmetric units, produce quite distinct structure types.

Pumpellyite and ardennite are both structurally related to epidote (Table 1). In epidote, chains of AlO_6 and $AlO_4(OH)_2$ octahedra run parallel to the y axis and are bridged by SiO_4 and Si_2O_7 groups. Thus, in a (010) projection, the structure may be described as being composed of five-membered 'mixed rings' (3 tetrahedra, 2 octahedra), with the aluminum octahedra linking the rings into chains along the longest axis c. Whereas the ardennite formula is again that of an oxy–hydroxy silicate, pumpellyite was reported to be an oxy–hydroxy silicate hydrate, $Ca_2Al_2(OH)_2(Al,Mg,Fe)(H_2O,OH)SiO_4\cdot Si_2O_7$. The presence of molecular water in pumpellyite appears questionable in view of the fact that this mineral does not lose any water on heating up to 740°C (Coombs, 1953). Therefore, we decided to check the assignment of protons in the pumpellyite crystal structure by valence summation (Donnay & Allmann, 1970).

For any coordination polyhedron in a given crystal structure, an empirical curve expressing formal bond valence v in terms of bond length L is constructed as follows:

(1) for $L \le \bar{L}$, $v = v_i(\bar{L}/L)^p$;

(2) for $\bar{L} \le L \le L_{\max}$, $v = v_i(L_{\max} - L)/(L_{\max} - \bar{L})$,

where v_i is the ratio of formal cation valence to coordination number, $L_{\max}$ is the sum of the 'maximum radii' for cation and anion, obtained by extrapolating v_i [curve of 'effective ionic radii' (Shannon & Prewitt, 1969) *versus* v_i] to zero, and $\bar{L}$ is the mean of the observed cation–anion distances in the given polyhedron. The coordination number of each cation is uniquely determined as the number of neighboring anions closer than $L_{\max}$. The exponent p is set equal to $\bar{L}/(L_{\max}-\bar{L})$, so that the two segments of the curve have equal slope at their common point: $L=\bar{L}$, $v=v_i$.

First we applied the procedure to ardennite (Table 2), where it confirms that O(10), O(11) and O(12) are hydroxyl groups and indicates hydrogen bonding from O(10)H to O(9). The observed oxygen separation O(10)···O(9) is 2·69 Å, from which we infer (Table 4 in Donnay & Allmann, 1970) a valence transfer from $O(10)H^{1-}$ to $O(9)^{2-}$ of 0·21 v.u. Other possible H bonds, leading to nearly tetrahedral bond angles at the effected oxygen atoms, are: O(12)–H···O(11)–H···O(10)–H with oxygen–oxygen separations of 2·80 and 2·69 Å corresponding to 0·17 and 0·21 v.u. respectively. The short separation O(12)···O(1) of 2·87 Å has a direction unfavorable for an H bond.

Before proceeding with the valence summation for pumpellyite, we must re-examine the formula $Ca_2Al_2(OH)_2(Al_{0.5}Mg_{0.35}Fe_{0.15})(OH,H_2O)SiO_4Si_2O_7$, used by Galli & Alberti (1969) in their refinement. The detailed chemical formula they give first is derived from a chemical analysis (by A. Alietti) whose weight percentages of oxides are, unfortunately, not to be found in the literature. It shows an excess of 0·15 cations over the available sites in the cell, as well as 0·39 excess positive charges. Let us omit 0·15 Fe^{3+}, the chemical species which is present in minimal amount. The total positive charge contributed by the corrected number of cations, 97·23, is to be neutralized by the 56 anions in the cell. Anticipating the absence of water indicated by the valence summation (Table 3), OH^{1-} and O^{2-} jointly must balance this charge. The structural formula thus obtained reads:

$(Ca_{0.90}Fe^{2+}_{0.10})CaAl_{2.0}(OH)_{2.0}$
$(Al_{0.50}Mg_{0.40}Fe^{2+}_{0.09}Fe^{3+}_{0.01})\,[(OH)_{0.84}O_{0.16}]$
$(Si_{0.90}Al_{0.10})O_4(Si_{1.90}Al_{0.10})O_6[(OH)_{0.85}O_{0.15}]$,

where the assignment of $0{\cdot}10Fe^{2+}$ to the first calcium position is based on size considerations and on the comparison with epidote and ardennite, in both of

Table 1. *Crystal data*

	Epidote	Ardennite†	Pumpellyite‡
a	8·96 Å	8·71 Å	8·83 Å
b	5·63	5·81	5·90
c	10·30	18·52	19·17 $19{\cdot}02 = c \sin\beta = c'$
β	115°24′	90°	97°7′
Z	2	4	4
Space group	$P2_1/m$	*Pnmm*	$A2/m$
Formula	(Fe^{3+}, Al)	(Mn^{2+}, Ca)	(Ca, Fe^{2+})
	Ca	—	—
	Ca	Mn^{2+}	Ca
	Al(OH)	Al(OH)	Al(OH)
	—	Al(OH)	Al(OH)
	AlO	(Mg, Al, Fe^{3+}) (OH)	(Al, Mg, Fe) (OH, O)
	SiO_4	SiO_4	SiO_4
	Si_2O_7	$\frac{1}{2}(Si_3O_{10}.AsO_4)$	$Si_2O_6(OH, O)$

* Data from Ito, Morimoto & Sadanaga, 1954.
† Data from Donnay & Allmann, 1968.
‡ Data from Galli & Alberti, 1969, except for formula which comes from present study.

Table 2. *Ardennite*: *bond lengths* (Å, *upper value*) *and estimated bond valences* (v.u. *lower value*)

Anions	Cations: Mn, Ca[(a)]	Mn	Al(1)	Al(2)	Mg, Al, Fe[(b)]	Si(1)	Si(2)	Si(3)	As, V[(c)]	Anion chem. $\sum_c v$	$\sum_c v$ corrected for H-bonds
O(1)	2·189* 0·36		1·904* 0·53			1·623* 1·03				O^{2-} 1·92	
O(2)		2·127* 0·44		1·888* 0·52			1·604* 1·04			O^{2-} 2·00	
O(3)	2·403 0·21		†2·006* 0·37				1·631 0·98			O^{2-} 1·93	
O(4)		(2·921) —		†1·934* 0·46		1·644 0·99				O^{2-} 1·91	
O(5)	†2·305* 0·28				2·189 0·28				1·721* 1·20	O^{2-} 2·04	
O(6)		†2·305* 0·29			2·055 0·36			1·631* 1·02		O^{2-} 1·96	
O(7)		2·514 0·11			†1·970* 0·41	1·657 0·96				O^{2-} 1·89	
O(8)	2·473 0·17						1·649 0·95	1·647* 0·98		O^{2-} 2·10	
O(9)		2·127 0·44							1·675* 1·30	O^{2-} 1·74	+0·21 1·95
O(10)			†1·853* 0·61							OH^{1-} 1·22	−0·21 1·01
O(11)				†1·883* 0·53						OH^{1-} 1·06	
O(12)	2·207 0·35				†1·940* 0·43					OH^{1-} 1·21	
L	2·296	2·251	1·921	1·902	2·011	1·637	1·622	1·639	1·698		
L_{max}	2·72	2·65	2·26	2·26	2·67	2·13	2·13	2·13	2·29		
P	5·42	5·63	5·67	5·31	3·05	3·32	3·19	3·34	2·87		
v_i	2/7	2/6	3/6	3/6	2·33/6	4/4	4/4	4/4	5/4		
$\sum_A v$	2·01	2·01	3·02	3·02	2·32	4·01	4·01	4·00	5·00		

* Two bonds per cation
† Two bonds per anion

(*a*) $Mn_{0.88}Ca_{0.12}$
(*b*) $Mg_{0.67}Al_{0.20}Fe_{0.13}{}^{3+}$
(*c*) $As_{0.905}V_{0.095}$

Table 3. *Pumpellyite*: *bond lengths* (Å, *upper value*) *and estimated bond valences* (v.u., *lower value*)

Anions	Cations: Ca(1)[(a)]	Ca(2)	Al	Al, Mg,[(b)] Fe	Si(1)	Si(2)[(c)]	Si(3)[(c)]	Anion chem. / $\sum_C v$
		2·34*	1·84		1·60*			O^{2-}
O(1)		0·33	0·63		1·07			2·03
	2·43*	2·37*		2·04*		1·63*		O^{2-}
O(2)	0·28	0·31		0·37		0·99		1·95
	2·41*		1·87				1·63*	O^{2-}
O(3)	0·29		0·58				1·00	1·87
	2·39		†2·04		1·64			O^{2-}
O(4)	0·30		0·32		0·98			1·92
			†1·93					$(OH)^{1-}$
O(5)			0·49					0·98
		2·80	†1·94				1·67	O^{2-}
O(6)		0·16	0·47				0·93	2·03
			†1·89					$(OH)^{1-}$
O(7)			0·55					1·10
	2·52				1·69	1·66		O^{2-}
O(8)	0·25				0·88	0·94		2·07
		2·50		†2·03*			1·65	O^{2-}
O(9)		0·27		0·38			0·97	2·00
		2·40				1·65		$(OH)^{1-}_{0.85}O^{2-}_{0.15}$
O(10)		0·30				0·96		1·26
	2·32			†1·90*				$(OH)^{1-}_{0.84}O^{2-}_{0.16}$
O(11)	0·33			0·49				1·31
L	2·42	2·45	1·92	1·99	1·63	1·64	1·64$_5$	
L_{max}	3·18	3·25	2·26	2·52	2·13	2·14	2·14	
p	3·18	3·06	5·65	3·75	3·26	3·28	3·32	
v_i	2/7	2/7	3/6	2.51/6	4/4	3·9/4	3·9/4	
$\sum_A v$	2·02	2·01	3·04	2·48	4·00	3·88	3·90	

* Two bonds per cation
† Two bonds per anion

(*a*) $Ca_{0.9}Fe^{2+}_{0.1}$
(*b*) $Al_{0.50}Mg_{0.40}Fe^{2+}_{0.09}Fe^{3+}_{9.01}$
(*c*) $Si_{0.9}Al_{0.1}$

Table 4. *Comparison of atomic coordinates of ardennite* (*A*) *and pumpellyite* (*P*)*

Ardennite	X_A	ΔX	Y_A	ΔY	Z_A	ΔZ	Pumpellyite	Δ(Å)
4(*f*)Mn, Ca	0·694	+0·013	0	±0	0·155	+0·005	4(*i*)Ca(1)	0·15
4(*f*)Mn	0·146	+0·002	½	±0	0·160	−0·005	4(*i*)Ca(2)	0·10
4(*c*)Al(1)	¾	−0·005	¾	−0·005	0	+0·004	8(*j*)Al	0·09
4(*d*)Al(2)	¼	+0·005	¾	−0·005	0	−0·004	8(*j*)Al″	0·09
4(*e*)Mg, Al, Fe	0·429	+0·004	0·748	+0·002	¼	±0	4(*f*)Al, Mg, Fe	0·04
4(*f*)Si(1)	0·514	−0·006	½	±0	0·097	+0·001	4(*i*)Si(3)	0·06
4(*f*)Si(2)	0·027	−0·004	0	±0	0·095	−0·004	4(*i*)Si(1)	0·08
2(*a*)Si(3)	0·091	+0·009	0	±0	¼	−0·002	4(*i*)Si(2)	0·09
2(*b*)As, V	0·793	−0·028	½	±0	¼	+0·002	4(*i*)Si(2‴)	0·25
8(*g*)O(1′)	0·622	−0·011	0·723	−0·001	0·083	−0·004	8(*j*)O(3)	0·12
8(*g*)O(2′)	0·126	−0·009	0·771	+0·007	0·083	−0·014	8(*j*)O(1)	0·28
4(*f*)O(3)	0·863	−0·008	0	±0	0·053	+0·002	4(*i*)O(4‴)	0·08
4(*f*)O(4)	0·367	−0·009	½	±0	0·042	+0·003	4(*i*)O(6)	0·10
4(*e*)O(5)	0·680	−0·016	0·743	−0·011	¼	+0·006	8(*j*)O(2′)	0·19
4(*e*)O(6)	0·193	+0·008	0·765	−0·003	¼	−0·006	8(*j*)O(2)	0·13
4(*f*)O(7)	0·432	−0·004	½	±0	0·178	−0·002	4(*i*)O(9)	0·05
4(*f*)O(8)	0·973	+0·017	0	±0	0·181	−0·003	4(*i*)O(8)	0·16
4(*f*)O(9)	0·904	−0·021	½	±0	0·176	+0·009	4(*i*)O(10‴)$H_{0.85}$	0·25
4(*f*)O(10)H	0·863	−0·003	½	±0	0·032	+0·012	4(*i*)O(5‴)H	0·23
4(*f*)O(11)H	0·365	−0·007	0	±0	0·036	−0·002	4(*i*)O(7)H	0·07
4(*f*)O(12)H	0·447	+0·004	0	±0	0·182	+0·005	4(*i*)O(11)$H_{0.84}$	0·10

* X_A, Y_A, Z_A designate atomic coordinates of ardennite after shift of origin to ¼, ¼, 0; $X_A = x_A - \frac{1}{4}$, $Y_A = y_A - \frac{1}{4}$, $Z_A = z_A$, where x_A, y_A, z_A are the coordinates before the shift of origin. $\Delta X = X_P - X_A$, with $X_P = x_P - z_P[(c/a)\cos\beta^*]_P = x_P - 0{\cdot}269\, z_P$; $\Delta Y = y_P - Y_A$; $\Delta Z = z_P - Z_A$; where x_P, y_P, z_P refer to the monoclinic cell of pumpellyite; X_P refers to the noncrystallographic set of axes *a*, *b*, *c′* [Fig. 1(*b*)].

Δ: distance in Å between corresponding sites of ardennite and pumpellyite referred to mean orthogonal parallelepiped with edges, $a = \frac{1}{2}(a_A + a_P) = 8{\cdot}77$, $b = \frac{1}{2}(b_A + b_P) = 5{\cdot}855$, $c = \frac{1}{2}(c_A + c'_P) = 18{\cdot}77$ Å.

which the first calcium position shows some substitution.

Interatomic distances of pumpellyite (Galli & Alberti, 1969) are used to calculate the valence sums reaching the anions (Table 3). Column $\sum_{C} v$ indicates hydroxyl groups for O(5), O(7), O(10) and O(11). For the last two, the above formula leads to expected valence sums of 1·15 and 1·16 v.u., which are less than the calculated sums of 1·28 and 1·33 v.u. respectively. Charge equalization between $O(10)^{2-}$ and $O(10)H^{1-}$ and between $O(11)^{2-}$ and $O(11)H^{1-}$ may occur *via* the following chains of hydrogen bonds: O(10)–H···O(5)–H···O(5)–H···O(10) with oxygen–oxygen approaches of 2·69, 2·98 and 2·69 Å in one chain, and O(11)–H···O(7)–H···O(7)–H···O(11) with distances of 3·03, 2·76 and 3·03 Å in the other. These are the only possible H bonds leading to near-tetrahedral bond angles.

The replacement of oxygen by hydroxyl at a corner of a silicon tetrahedron has been considered unlikely by silicate workers in the past. We have, however, good evidence for such partial replacement in many supposedly hydroxyl-free silicates, for example pyroxenes, where infrared spectra confirm the evidence presented by valence summation (Martin & Donnay, 1971).

When comparing the (010) projections of the pumpellyite and ardennite structures [Fig. 1(*a*) and (*b*)], we were struck by the similarities in the atomic positions within properly chosen asymmetric units ($0 \le x \le 1$; $0 \le y \le \frac{1}{2}$, $0 \le z \le \frac{1}{4}$). The mirror planes parallel to (010) permit a comparison of double the asymmetric unit with y ranging from 0 to 1. To permit quantitative comparison of coordinates, the origin of ardennite is shifted to $\frac{1}{4}, \frac{1}{4}, 0$ and the pumpellyite coordinates are referred to orthogonal, noncrystallographic axes a, b, $c' = c \sin \beta$ (Table 1 & Fig. 1). The coordinates thus obtained agree to better than 0·3 Å, with a mean difference of only 0·13 Å when the lengths of the cell edges are taken as the mean values of the two sets (Table 4). As might be expected, the biggest differences result from the replacement of an (As, V) tetrahedron in ardennite by an Si tetrahedron in pumpellyite. Most intriguing is the action of the different symmetry elements in the space groups *Pnmm* and *A*2/*m* acting on their asymmetric units: a 2_1-axis at $z=0$ parallel to **b** in ardennite is replaced by a 2-axis in pumpellyite; a mirror at $z=\frac{1}{4}$ in ardennite is replaced by a 2_1-axis parallel to **b** in pumpellyite. As a result, neither the Si_3O_{10} groups nor the isolated $(As,V)O_4$ tetrahedra of ardennite are to be found in pumpellyite.

In conclusion, let us note that in other widely different mineral groups we can also observe near-identical, energetically stable assemblies of cation polyhedra which can be considered macro building blocks. The ditrigonal rings composed of six silicon tetrahedra all pointing the same way and sharing their apical oxygen atoms with edge-sharing octahedra may serve as an example; they are found in tourmalines as well as in micas. Such large groups of polyhedra invite comparison with prefabricated structural units that builders assemble into houses of different types.

Note added in proof: According to a personal communication by E. Galli, the chemical analysis given by Galli & Alberti (1969, p. 2276) contains a printing error: $Mg_{1.20}$ should read $Mg_{1.02}$. The remaining excess of 0.03 positive charges is due to rounding errors. Omitting 0.03 H^+ per cell for charge balancing, the structural formula of pumpellyite as given above must be slightly changed to:
$(Ca_{0.90}Fe^{2+}_{0.10})\,Ca_{1.0}Al_{2.0}(OH)_{2.0}(Al_{0.50}Mg_{0.35}Fe^{2+}_{0.09}Fe^{3+}_{0.05})$ $[(OH)_{0.83}O_{0.17}]\,(Si_{0.90}Al_{0.10})O_4\,(Si_{1.90}Al_{0.10})O_6\,[(OH)_{0.84}O_{0.16}]$. The resulting alterations in Table 3 will be only minor (≤ 0.02 v.u.) and will not influence our conclusions.

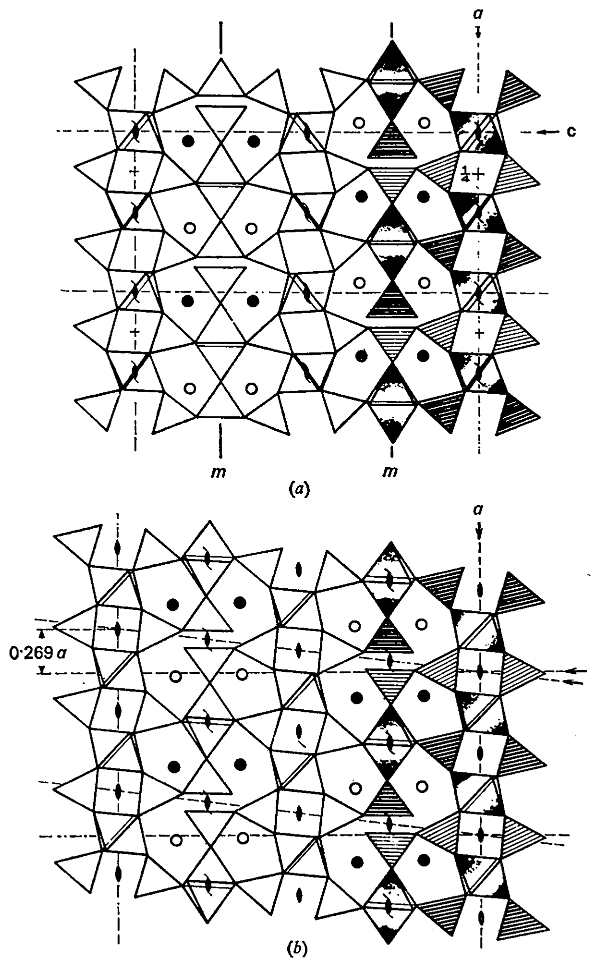

Fig. 1. Projection comparison. (*a*) Ardennite projection on (010). The part similar to pumpellyite is shaded. Dark circles: Mn at $y=\frac{3}{4}$ ($Y=\frac{1}{2}$), light circles: Mn at $y=\frac{1}{4}$ ($Y=0$). Dark tetrahedra have $y_{Si}=\frac{3}{4}$ ($Y_{Si}=\frac{1}{2}$), light tetrahedra have $y_{Si}=\frac{1}{4}$ ($Y_{Si}=0$). (*b*) Pumpellyite projection on (010). Shading as in (*a*) at $y=\frac{1}{2}$ (dark) and at $y=0$ (light). Circles represent Ca.

We thank Professor J. D. H. Donnay for many helpful suggestions and our two anonymous referees for their constructive critique.

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Acta Cryst. (1971). B**27**, 1875

The Crystal Structure of YCd_6*

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(*Received* 2 *November* 1970)

YCd_6 is cubic, $a=15{\cdot}482$ (3) Å with 24 formula units in space group *Im*3. The structure was solved by direct methods from counter data and is isomorphous with Ru_3Be_{17}, but with an additional Cd atom in a 24-fold 0*yz* position which is ⅓ occupied. This fractional atom occupies the large void at the origin of the otherwise ordered structure. Least-squares refinement with anisotropic thermal parameters gave $R=3{\cdot}1$ and $R_w=2{\cdot}8$ %; with the fractional atom excluded, $R=6{\cdot}4$ and $R_w=5{\cdot}5$ %.

Introduction

A large number of MCd_6 compounds have been reported by Johnson, Schablaske, Tani & Anderson (1964) where M is yttrium or any of the rare earths except lanthanum and promethium. The compounds are cubic with *a* about 15·5 Å. This compound was accidentally prepared during an attempted preparation of $Y_2Cd_{\sim 9}$ (Cromer & Larson, 1970) and, because it was an unknown structure type, we decided to study it. Also, we hoped that this structure might help in solving the superstructure of $Y_2Cd_{\sim 9}$.

Experimental

Crystals of YCd_6 were formed by slowly cooling a melt of nominal composition $YCd_{4{\cdot}5}$. A second phase, YCd_3 was presumably present although all single-crystal fragments examined were YCd_6. Crystals of $Y_2Cd_{\sim 9}$ are produced by rapidly cooling a melt of this composition. Preliminary precession photographs showed the crystals to be cubic, space group *Im*3, if centric.

Lattice constants and intensities were measured using graphite monochromated Mo $K\alpha$ radiation and a Picker four-circle goniometer interfaced with a PDP-8 computer. The orientation, least-squares, and data-collection programs were obtained from Busing, Ellison, Levy, King & Roseberry (1968). The lattice constant that was found, $a=15{\cdot}482$ (3) Å ($\lambda=0{\cdot}70926$ Å), is in good agreement with $a=15{\cdot}479$ (2) Å reported by Johnson *et al.* (1964). The θ–2θ scan mode was used for intensity measurements with steps of 0·05° 2θ over a scan range of 2° plus the α_1–α_2 dispersion. Two-second counts were taken at each step. The background was counted for 20 seconds at each extreme and assumed to vary linearly over the scan range. A total of 4462 reflections with $2\theta \le 55°$ was measured in one

* Work performed under the auspices of the U.S. Atomic Energy Commission.

Table 1. *Least-squares parameters for* YCd_6

Position and thermal parameters are multiplied by 10^5.

	Set	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Y	24(*g*)	0	29966 (7)	18985 (6)	75 (3)	102 (4)	100 (4)	0	0	18 (6)
Cd(1)	48(*h*)	11835 (4)	20031 (4)	34049 (4)	189 (2)	132 (2)	121 (2)	82 (4)	−51 (4)	−24 (4)
Cd(2)	24(*g*)	0	09227 (6)	24069 (8)	117 (3)	117 (3)	559 (6)	0	0	179 (8)
Cd(3)	24(*g*)	0	34603 (5)	40438 (5)	136 (3)	115 (3)	102 (3)	0	0	49 (5)
Cd(4)	16(*f*)	16081 (4)	—	—	191 (2)	β_{11}	β_{11}	179 (5)	β_{12}	β_{12}
Cd(5)	12(*e*)	0	19018 (7)	½	103 (4)	103 (4)	210 (5)	0	0	0
Cd(6)	12(*d*)	0	0	40551 (8)	140 (5)	473 (8)	124 (5)	0	0	0
Cd(7)	24(*g*)	0	0832 (3)	0741 (4)	1640 (45)	405 (25)	578 (30)	0	0	−667 (41)

Occupancy of Cd(7) = 0·331 (4).
$g=1{\cdot}78\ (10)\times 10^{-8}$.
The temperature factor is $\exp\left[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})\right]$.