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CELL DATA OF ORIENTITE AND ITS RELATION TO ARDENNITE AND ZOISITE

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Orientite is an abundant constituent of the manganese ores deposited by the replacement of latite tuffs, Bueycito region, Oriente Province, Cuba.

A single crystal displaying only prismatic and basal pinacoidal faces, and of approximate dimensions .05 × .05 × .10 mm, was selected for this study. The specimen is filed in the University of Chicago collections, No. 3323, and was donated by Hewett who first described it as a new mineral (Hewett & Shannon, 1921).

Oscillation, Weissenberg, precession, and powder photographs were used to determine cell data. The morphological observations agree with point-group $2/m\ 2/m\ 2/m$ established previously (Hewett & Shannon, 1921). The systematic extinctions observed upon inspection of $h0l$, $h1l$, $hk0$ and $hk1$ Weissenberg photographs and $0kl$, $1kl$, $h0l$, and $h1l$ precession

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photographs are consistent with space group *Cmcm*. The cell data are given in Table 1.

TABLE 1. ORIENTITE, ARDENNITE, ZOISITE: STRUCTURE CELL DATA

Orientite	Ardennite	Zoisite
$Ca_4(Mn^3, Mn^2, H_2)_6$ $(Si,H_4)_6O_{24}(OH)_2$	$Mn_4(Mn^3, Al^3)_6$ $(VH, AsH, Si)_6O_{24}(OH)_2$	$Ca_4Al_6Si_6O_{24}(OH)_2$
a 6.08 A	5.80 Å[1]	5.58 Å
b 9.04	8.70[1]	10.10
c 19.14	18.49[1]	16.24
S.G. *Cbnn* (*Cmcm*)	*Pmnm*	*Pbnm*
Z 2	2	2
Ref. this study	Gossner & Strunz in Strunz (1957), [1]this study	Strunz (1957)

The chemical formula given by Hewett is written $H_4Ca_4(Mn^3OH)_4(SiO_4)_5$. The calculated density based on this formula and $Z = 2$ is 2.89, a serious departure from the observed density of 3.05. Furthermore, the minimum equipoint rank of space group Cmcm is 4. This means that atomic species must each be of multiplicity 4 in the cell, unless sites are shared. A discrepancy immediately appears with respect to the silicon, of which there are 10 atoms in the unit cell.

No clear explanation of the two anomalies could be given until Dr. C. Sclar kindly informed the author that he had recast the Shannon analysis (Hewett & Shannon, 1921) into a zoisite-type formula.

The cell formula then becomes,

$$2\{Ca_{4.00}[Mn^3_{.68}, Mn^2_{.02}, Al^3_{.04}, Fe^3_{.03}, (H_3)_{.23}]_6[Si_{.90}, (H_4)_{.10}]_6\, O_{24}\, (OH)_2\}$$

Dr. Sclar's formula resolves the anomalies. This formula, condensed into a general zoisite-type formula, is

$$2[X^2_4\ Y^3_6\ Si_6\ O_{24}\ (OH)_2]$$

where, for orientite,

$$X^2 = Ca; \quad Y^3 = [Mn^3_{.68}, Mn^2_{.02}, Al^3_{.04}, Fe^3_{.03}, (H_3)_{.23}]$$

The numbers of the species, X, Y, Si, and OH in the unit cell are each multiples of rank 4. The calculated density of orientite using the zoisite-type formula is now 3.09, in good agreement with the observed density of 3.05.

Objections may be raised regarding hydrogen assigned to sites of tetrahedral coordination. However, this is evidenced in hydrogrossular, and is

treated in the article by McConnell (1964) on some analcime-type structures in which a proposed ion of type $(H_3O_2)^-$ appears in linked tetrahedra, analogous to $(AlO_2)^-$, $(PO_2)^+$, and $(SiO_2)^\circ$.

Table 1 lists the chemical formulae and cell data for the minerals orientite, ardennite (dewalquite) and zoisite. Both the formulae and cell data have been rearranged from their conventional forms to elucidate the relationship. The data for these minerals show considerable similarities. The most notable difference is in the C-centring of the lattice of orientite. The photographs were carefully checked for violations of C-centring but none were detected.

Further studies were undertaken to clarify these relationships. A small chip of ardennite from Salm Chateau, near Ottrez, Belgium (University of Chicago collections, No. 3741), afforded excellent precession photographs. The structure cell data of Gossner & Strunz (Strunz, 1957) were confirmed, including space group *Pmnm*. It was further noted that for general *hkl* reflections, where $h + k \neq 2n$, the diffractions were relatively weak, and $01l$ were, for the most part, nearly absent. This suggests the super-group *Cbnn*, amplifying the relationship between ardennite and orientite.

The powder data for orientite and Salm Chateau ardennite are presented in Table 2.

Further discussion

Comparison of cell data of orientite to those of kentrolite and melanotekite (Gabrielson, 1962) shows no apparent structural relation as suggested by Hewett & Shannon (1921) on the basis of morphological evidence.

Sclar (1961) presents revised Barker classification angles and morphological axial ratios for orientite. However, the $b:c$ morphological cell ratio is based on a rough microscope determination of the angle $(101) \wedge (\bar{1}01) = 61°00'$ by Hewett. This results in a morphological cell ratio of 0.672:1:0.3958. The axial ratios of the structure cell (this study) are 0.672:1:2.117. Assuming the corrected morphological angle $(101) \wedge (\bar{1}01) = 64°50'$, the transformation matrix from morphological cell to structure cell is (100/010/005).

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TABLE 2. ORIENTITE AND ARDENNITE: *X*-RAY POWDER DATA
Fe/Mn radiation, $\lambda = 1.9360$ Å, NaF internal standard,
I/I_0 visual, camera diameter 114.6 mm.

Orientite				Ardennite			
I/I_0	d_{obs}	d_{calc}	*hkl*	I/I_0	d_{obs}	d_{calc}	*hkl*
7	9.58 Å	9.57 Å	002	2	9.22 Å	9.24 Å	002
9	5.06	5.04	110	2	8.70	8.70	010
3	4.908	4.89	111	1	6.28	6.30	012
1	4.783	4.79	004	2	5.48	5.51	101
5	4.520	4.52	020	3	4.76	4.80	110
9	4.394	4.39	021	3.5	4.59	4.62	004
5	4.080	4.08	022	6	4.21	4.23	021
6	3.290	3.29	024	1	3.90	3.93	022
7	3.059	3.05	115	5	3.76	3.80	113
5	2.914	2.92	025	4	3.52	3.48	120
10	2.704	2.70	116	1	3.39	3.40	015
5	2.679	2.68	130	6	3.15	3.17	024
3	2.606	2.60	132	3	3.00	3.03	123
4	2.578	2.57	204	7	2.911	2.90	200, 030
2	2.537	—	—	6	2.871	2.87	031
4	2.452	2.44	222	2	2.795	2.78	124
2	2.410	2.40	117	4	2.748	2.75	210
6	2.357	2.36	134	3	2.712	2.72	211
3	2.244	2.23	224	10	2.574	2.56	131
3	2.115	2.11	225	3	2.501	2.50	132
2	2.068			4	2.440	2.43	204
2	1.982			2	2.396	2.39	133, 221
1	1.951			4	2.310	2.31	008
2	1.886			5	2.245	2.25	223
3	1.846			1	2.195	2.20	215
4	1.791			3	2.147	2.14	224
1	1.743			3	2.101	2.10	127
				3	2.037	2.04	028
				5	2.011	2.00	232
				About ten lines, less than 4.			
				5	1.604		
				5	1.569		
				6	1.448		

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