

Significance and possible implications of the results of these experiments to diagenesis of carbonates and to the formation of dolomite are discussed.

THE CRYSTAL STRUCTURES OF LAUEITE AND METASTRENGITE AND A CRYSTALLOCHEMICAL CLASSIFICATION OF Fe-Mn ORTHOPHOSPHATE HYDRATES¹

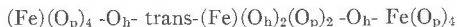
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The crystal structures of laueite and metastrengite were determined by means of vector interpretations of Patterson projections; Fourier projections, and three-dimensional refinements. The intensities were gathered on film, using Zr-filtered MoK α radiation, and corrected for the standard geometric factors as well as crystal shape. 637 independent intensities were collected for laueite and 678 for metastrengite. The final R-factors are .122 and .157 respectively.

Laueite,



$a=5.28$, $b=10.66$, $c=7.14$ Å, $\alpha=107^\circ55'$, $\beta=110^\circ59'$, $\gamma=71^\circ07'$, has Mn at 000, Fe at $0\frac{1}{2}0$ and $0\frac{1}{2}\frac{1}{2}$; 1 P and 9 O in general positions in an asymmetric unit of structure. The structure consists of infinite vertex-linked chains of Fe-centered oxygen octahedra and isolated Mn-centered oxygen octahedra. With O_p representing oxygen associated with the PO_4^{3-} tetrahedral tetradentate group, and O_h as either watermolecule or hydroxyl oxygen, the chains can be specified as



The isolated octahedron is trans-Mn(O_h) $_4$ (O_p) $_2$. Possible structures for the stewartite and strunzite polymorphs are suggested.

Metastrengite, $\text{Fe}^{3+}(\text{H}_2\text{O})_2(\text{PO}_4)$, $P2/n$, $a=5.30$, $b=9.77$, $c=8.73$ Å, $\beta=90^\circ36'$, has 1 Fe, 1 P, and 6 O, all in general positions, in an asymmetric unit of structure. The octahedral asymmetric unit is cis-Fe(O_p) $_4$ (O_h) $_2$.

Structure classification is based on the general formula (here, for metals of +2 charge):



where X is metal, OH^- , PO_4^{3-} , (H_2O) $_x$ are ligands. The formula $n\text{P}$, where $\text{P}=r+2n+z$ relates cell stoichiometry to type of octahedral linkage.

PROOF OF THE FORMULA OF SHATTUCKITE, $\text{Cu}_5(\text{SiO}_3)_4(\text{OH})_2$

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A chemical analysis of a shattuckite concentrate from Ajo, Arizona, established its formula as $\text{Cu}_5(\text{SiO}_3)_4(\text{OH})_2$. The concentrate contained several per cent of quartz as tiny inclusions, which appeared as an insoluble residue in the analytical procedure. Electron-probe analyses of 4 single crystals used for x-ray studies gave an atomic ratio of Cu/Si = 5:4, thus confirming the analytical procedures used. An infra-red absorption band at 3.15μ revealed the presence of (OH) groups, and absence of the 6μ band showed that water molecules were not present.

Shattuckite crystals are prismatic, elongated [001]; nine prism forms and seven general forms were identified by goniometry; cleavages (010) and (100), perfect and easy. Color dark blue, streak pale blue; hardness $\sim 3\frac{1}{2}$. Indices of refraction, close to previously re-

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ported values, are: $\alpha=1.752$, $\beta=1.782$, $\gamma=1.815$ (all ± 0.002), $2V$ large. Pleochroism: $X=b$, very pale blue; $Y=a$, pale blue; $Z=c$, deep blue. Space group $Pcab$: $a=9.876 \pm 0.001$ Å, $b=19.812 \pm 0.003$ Å; $c=5.381 \pm 0.001$ Å; $Z=4$; cell volume 1052.86 Å³; $D_c=4.138$ g cm⁻³, $D_m=4.11$ g cm⁻³.

The formula $4 [Cu_5(SiO_3)_4(OH)_2]$, which differs from those formerly proposed, fulfills the requirement of the space group symmetry that atoms in the structure be present in multiples of 4, contains only hydroxyl groups, and gives close agreement between measured and calculated specific gravity. Application of the Gladstone-Dale relation to this formula, using the specific refractive energy value of $k_{CuO}=0.173$ (Am. Mineral. **50**, 288, 1963) and the calculated specific gravity 4.138, gives a mean calculated n of 1.786, in excellent agreement with the mean measured n of 1.783.

THE STRUCTURE OF TSUMEBITE¹

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Three dimensional single crystal data has been used to determine the crystal structure of tsumebite. The crystal used was from the Morenci, Arizona locality. Due to the extreme tendency of tsumebite to occur as intimately intergrown crystals, considerable difficulty was encountered in obtaining a suitable, single crystal.

The unit cell is monoclinic with $a=8.70$, $b=5.80$, $c=7.85$ Å, $\beta=111.5^\circ$ and two formula units per unit cell. The space group is $P2_1/m$. Lead and copper coordinates were determined from a Patterson synthesis. The remaining atoms were found using least-square and Fourier methods. The structure determination has indicated that the previous formula $(Pb_2Cu)(PO_4)(OH)_3 \cdot 3H_2O$ is incorrect. Subsequent fluorescence analysis has shown that the formula is most likely $Pb_2Cu(PO_4)(SO_4)OH$.

THE CRYSTAL STRUCTURE OF MIZZONITE, A CALCIUM AND CARBONATE RICH SCAPOLITE

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The crystal structure of a 70.1% meionite scapolite from Grenville, Quebec, with $a=12.169 \pm .004$, $c=7.569 \pm .003$ Å, and space group $I4/m$ has been refined using three-dimensional x-ray intensities collected by integrated Weissenberg film techniques. Starting with positional parameters from a refined marialite scapolite structure (Papike and Zoltai, 1965, *Am. Mineral.* **50**, 290) the model was completed by Fourier methods and refined by least squares. The refined structure is basically the same as that of marialite with the interesting differences concerning the aluminum distribution in the tetrahedral framework and the crystal chemical role of carbonate.

	<i>x</i>	<i>y</i>	<i>z</i>
(Ca,Na,K)	.1428 $\pm$.0003	.2170 $\pm$.0003	0
(Si,Al)-1	.3391 $\pm$.0003	.4084 $\pm$.0003	0
(Si,Al)-2	.3393 $\pm$.0002	.0866 $\pm$.0002	.2069 $\pm$.0004
O-1	.4581 $\pm$.0007	.3480 $\pm$.0007	0
O-2	.3120 $\pm$.0008	.1280 $\pm$.0008	0
O-3	.0510 $\pm$.0005	.3489 $\pm$.0005	.2081 $\pm$.0010
O-4	.2332 $\pm$.0005	.1354 $\pm$.0005	.3263 $\pm$.0011
(C,S)	0	0	0

¹ Work performed under the auspices of the U. S. Atomic Energy Commission.