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Buchwaldite, a new meteoritic phosphate mineral

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Abstract

A new mineral, buchwaldite, $NaCaPO_4$, has been found within troilite nodules in the Cape York iron meteorite. It is orthorhombic, $Pmn2_1$, $a = 5.167$, $b = 9.259$, $c = 6.737$ Å, $Z = 4$. It is associated with chromite and other, apparently new, phosphate phases.

Occurrence

Buchwaldite occurs as minute inclusions within troilite nodules in the Cape York iron meteorite (specifically, the Agpalilik specimen). The inclusions are fairly sparse and small. The dimensions in our sample are mostly < 10 μm across. One inclusion was 40 μm across, and most of our data were obtained from it. Optical examination showed that the inclusion was polycrystalline, made up mostly of compact, interlocking masses of fine needles. It was impossible to obtain single-crystal X-ray data. A few grains were large enough to obtain optical data.

The mineral was discovered early in 1974, and the composition determined. It was not until the end of 1974 that X-ray data could be obtained free of impurity lines. Two other phosphate phases were discovered at the same time, but we were unable to obtain adequate compositional and X-ray data for them. In August of 1975 we learned from Drs. A. Kracher and G. Kurat of the Naturhistorisches Museum, Wien, that they had discovered four phosphate phases in Cape York (Kracher and Kurat, 1975), for which they had compositional data but no X-ray data. One of these phases was similar to buchwaldite, but had 7 percent FeO, 2.5 percent MnO, and 1.86 percent MgO. Because it appeared that the two discoveries were simultaneous, it was amicably agreed we should publish the buchwaldite description on our specimen, which is compositionally purer and for which we had X-ray data, and they would publish descriptions of the other phosphates when X-ray data could be obtained.

Optical

Buchwaldite is biaxial negative, $2V$ is approximately 65° (estimated), or 70°45′ (calculated). Indices are $\alpha = 1.607$, $\beta = 1.610$, $\gamma = 1.616$; extinction is parallel, and the sign of elongation is positive. One platy cleavage or parting is present. The mineral is colorless in transmitted light.

Composition

The composition was obtained by electron microprobe on several of the inclusions. The fully corrected analysis is: P_2O_5 44.9, CaO 35.6, MnO 0.06, Na_2O 19.5, Sum 100.06. Nondispersive X-ray analysis for other elements showed no peaks above background (generally, the 0.01% level).

The oxide formula is almost exactly Na_2O:$2CaO$:P_2O_5, or $NaCaPO_4$. The calculated analysis for this composition is: P_2O_5 44.91, CaO 35.48, Na_2O 19.61.

X-ray

Table 1 gives the powder diffraction pattern. The 40 μm inclusion was quite soft, and a small portion was X-rayed in a 57.3 mm Gandolfi camera, using Ni-filtered Cu-radiation. Attempts to obtain a useable pattern with a larger camera were unsuccessful. Because of the impossibility of obtaining a single crystal, the unit-cell parameters were obtained by simulation. We attempted to synthesize this composition and to have syntheses made by colleagues at other institutions. In each case the synthetic material was unsuitable for single-crystal work, usually because several polymorphs were present or because compositions that were off stoichiometry resulted. Thus, it was necessary to resort to computer simulation.

$NaCaPO_4$ is considered by us to be isostructural with Na_2SO_4-III and with β-K_2SO_4 on the basis of similarity of powder patterns. Adjustments in the cell parameters of each were made for the substitution of NaCa for NaNa and KK, and of P for S, and the powder patterns calculated. The adjusted Na_2SO_4-III pattern gave the better overall fit with the observed $NaCaPO_4$ pattern, although there are discrepancies. Lines are present in the observed pattern that have calculated intensities of zero, and other lines show significant intensity differences between calculated and observed values. Discrepancies may be due to the presence of more than one polymorph in the natural occurrence. Based on the indexing of the Na_2SO_4-III pattern, least-squares refinement yields the cell parameters of buchwaldite: $a = 5.167 \pm 0.025$, $b = 9.259 \pm 0.045$, $c = 6.737 \pm 0.032$; orthorhombic, $Pmn2_1$, $Z = 4$.

Physical properties

It was impossible to measure specific gravity or hardness due to the minute amount of material available. The calculated density is 3.21 grams/cm^3. The color is white. In collecting from the inclusion with a very sharp tungsten needle it was estimated that the hardness of the polycrystalline aggregate was fairly low, probably < 3 (Mohs).

Associated minerals

Numerous single crystals of chromite, often euhedral with rounded faces, are present in the troilite nodules. The chromite is virtually pure $FeCr_2O_4$. Buchwaldite occurs embedded in troilite and in contact with chromite. The troilite is polycrystalline due to a moderate-level shock history (Lipschutz, 1968). We have also found two other new phosphate phases. One of these is a Cr-rich phase with an analysis: P_2O_5 46.0, CaO 11.3, Na_2O 19.3, K_2O 5.3, Cr_2O_3 16.1, MnO 1.5, sum 99.5. The other is a Mn-rich phase with an analysis: P_2O_5 41.1, Al_2O_3 0.2, K_2O 0.3, Na_2O 28.8, MnO 20.1, Cr_2O_3 3.2, FeO 3.0, sum 96.7. The *latter* phase occurred as a single inclusion of approximately 5 μm. Both of these analyses are unsatisfactory; no reasonable stoichiometric proportions could be obtained from either. No X-ray data could be obtained from these minerals. The Cr-rich phosphate was dark green and occurred in several larger (10–20 μm) inclusions; however, optical examination showed the green coloration was not uniformly distributed but consisted of specks and streaks intimately mixed with the white buchwaldite. The microprobe analysis was of two phases. The X-ray patterns obtained were principally that of buchwaldite with some additional peaks of low intensity.

Table 1. X-ray powder pattern of buchwaldite

hkl	I/Io	d(Å)(Obs)	d(Å)(calc)
120	90	3.79	3.81
130	20	2.80	2.80
220	100	2.72	2.72
031	60	2.63	2.65
002	50	2.58	2.58
012	40	2.51	2.49
140	40	2.19	2.19
231	20	2.08	2.08
202	20	2.04	2.05
141,311	10	2.01	2.01
240	80	1.91	1.91
232	10	1.70	1.70
341	30	1.54	1.54
332,061,430	10B	1.48	1.48
431	20B	1.42	1.42
043,351	10B	1.38	1.38
521,352,333	30	1.25	1.25
281,244,443	10	1.07	1.07
182,372,462	10	1.04	1.04
731,652,633	10	0.90	0.90
750,464,165	10B	0.85	0.85
393,226,505	30B	0.82	0.82

At this time neither of these phases can be characterized well enough for consideration as new minerals. As noted earlier, Kracher and Kurat (1975) reported four phosphates in their sample of Cape York (Agpalilik): (1) a $NaFePO_4$ phase, (2) a $Na_4Mn(PO_4)_2$ phase, (3) a Na–Ca–Cr phosphate with (Na + K):Ca:Cr ≈ 4:1:1, and (4) $NaCaPO_4$ with significant amounts of FeO (7%), MnO (2.5%), and MgO (1.86%). Phase 4 is very probably the same as buchwaldite with substitutions of Fe, Mn, and Mg in the formula, but this is subject to confirmation by X-ray examination. With the substitutions it is possible this phase could be a different polymorph of buchwaldite. Also, it appears that their phases 2 and 3 are the same ones we found in our sample. Their samples, however, contain larger inclusions of these other phosphates, and work is in progress to fully characterize them (Kracher, personal communication).

Discussion

Buchwaldite is named after Dr. Vagn Buchwald, of the Department of Metallurgy at Danmarks Tekniske Høјskole, Lyngby, Denmark. Dr. Buchwald has made major contributions to the understanding of iron meteorites over the past decade. He has recently made an intensive study of the Cape York iron meteorite, in which this phase is found. It is appropriate his name be given to this new mineral. The name has been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association prior to publication.

In the literature dealing with industrial phosphates, the name *rhenanite* has been applied to the composition $NaCaPO_4$ (Ando, 1958). This name has never entered the mineralogical literature (Fleischer, 1975). Spencer (1940) noted that rhenanite is a name applied to an artificially-prepared fertilizer made by the industrial process called the Rhenania Process. He noted that rhenanite is a mixture of 4:1 $NaCaPO_4:Na_2CO_3$. Bredig (1942) and Ando (1958), nevertheless, applied the name of this industrial mixture to the several polymorphs of pure, synthetic $NaCaPO_4$.

Because the industrial product is a mixture and because the industrial name has never entered the mineralogical literature, no confusion will arise by giving the name, buchwaldite, to the only natural occurrence of $NaCaPO_4$. This is, for example, analogous to the phase Fe_3C, which is called cohenite in the mineralogical literature and is known as cementite in industrial literature.

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