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CARLHINTZEITE, A NEW CALCIUM ALUMINUM FLUORIDE HYDRATE FROM THE HAGENDORF PEGMATITES, BAVARIA, GERMANY

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ABSTRACT

Carlhintzeite $Ca_2AlF_7 \cdot H_2O$ is a new mineral associated with rockbridgeite, pyrite, strengite and apatite in the Hagendorf pegmatites, Bavaria, Germany. The mineral is triclinic (pseudomonoclinic, $C\bar{1}$ or $C1$, with a 9.48(5), b 6.98(3) c 9.30(5)Å, α 91.14(10), β 104.85(10), γ 90.0(10)°. The strongest lines in the X-ray diffraction pattern are 3.48 (100), 4.56 (70), 3.69 (60), 1.46 (40), and 2.852 (40). Carlhintzeite crystals are prismatic along [010], always twinned about [010], with forms {100}, {001} and the face (110). Two closely agreeing analyses average: Al_2O_3 10.27 CaO 29.86, F 52.1, H_2O 7.0, sum 99.23 wt. %, in agreement with $Ca_2AlF_7 \cdot H_2O$. Carlhintzeite is white to colorless. D(meas.) = 2.86 g/cm^3, D(calc.) = 2.89 g/cm^3 with Z=4. Carlhintzeite is biaxial (+), $2V$ = 77(2)° (meas.), $2V$ = 78° (calc.); α 1.411, β 1.416, γ 1.422. The name honors the late Professor Carl Hintze, author and compiler of *Handbuch der Mineralogie.*

SOMMAIRE

On trouve la nouvelle espèce carlhintzeite $Ca_2AlF_7 \cdot H_2O$, accompagnée de rockbridgeite, pyrite, strengite et apatite, dans une pegmatite de Hagendorf (Bavière). Triclinique, elle est pseudo-monoclinique de groupe spatial $C\bar{1}$ ou $C1$, avec la maille a 9.48(5), b 6.98(3), c 9.30(5)Å α 91.14(10), β 104.85(10), γ 90.0(10)°. Les cinq raies les plus intenses du cliché de poudre sont: 3.48(100), 4.56(70), 3.69(60), 1.46(40) et 2.852(40). Les cristaux sont prismatiques [010] et invariablement maclés suivant l'axe [010]; ils possèdent les formes {100} et {001} et la face (110). Deux analyses concordantes donnent la moyenne: Al_2O_3 10.27, CaO 29.86, F 52.1 et H_2O 7.0 (Σ 99.23% en poids), qui justifie bien la formule idéale. La carlhintzeite varie de blanche à incolore. D(mes.) = 2.86, D(calc.) = 2.89 avec Z = 4. Biaxe positive, $2V$ = 77(2)° (mes.), 78° (calc), α 1.411. β 1.416, γ 1.422. Elle est dédiée à feu le D^r Carl Hintze, rédacteur du *Handbuch der Mineralogie.*

(Traduit par la Rédaction)

INTRODUCTION

Carlhintzeite, ideally $Ca_2AlF_7 \cdot H_2O$, was initially noted by one of the authors (PJD) during an examination of some phosphophyllite specimens from a pegmatite near Hagendorf, Bavaria, Germany. The new mineral is named for Dr. Carl Hintze (1851–1916) who was Professor of mineralogy at the University of Breslau. We take pleasure in honoring Dr. Hintze in this manner because of his significant contributions to mineralogy, most notably in the compilation of his monumental *Handbuch der Mineralogie*. It is indeed a pleasant coincidence that the new mineral comes from Germany and was found in the mineral collection of the late Dr. Carl Bosch, a German mineral collector. Both the new mineral and the name have been approved by the I. M. A. Commission on New Minerals and Mineral Names. Type material is preserved in the mineral collection of the Royal Ontario Museum (# M35498) and in the National Museum of Natural History, Smithsonian Institution, Washington, D. C. (# B20119).

X-RAY CRYSTALLOGRAPHY

Single crystals were investigated using standard Weissenberg and precession X-ray diffraction techniques. Initial results indicated that carlhintzeite is monoclinic. However, the presence of doubled reflections resolvable on *b*-axis upper-level photographs indicated that the mineral is triclinic, pseudomonoclinic, and twinned. Lattice parameters are *a* 9.48(5), *b* 6.98(3), *c* 9.30(5)Å, α 91.14(10), β 104.85(10), γ 90.0(10)°. The space group is $C\bar{1}$ or $C1$. This unconventional *C*-centred unit cell has been chosen to emphasize the pseudomonoclinic lattice geometry and to obtain the simplest indexing of the morphological elements. Twinning occurs by rotation about [010]. Several single crystals, each less than 0.1 mm in greatest dimension, all show the presence of twinning, with approximately equal intensities for equivalent reflections from each of the two domains. Individual twin domains therefore must be extremely small; it is unlikely that an untwinned crystal suitable for structural analysis will be obtained from the single hand-specimen currently available.

Powder diffraction data (Table 1) were obtained using a powdered sample in a 114.6 mm diameter Gandolfi camera, Cu*K*α radiation and NBS silicon as an internal standard. Indices and calculated *d* values are not listed because the lattice pseudosymmetry leads to ambiguous indexing for virtually all reflections. For the same reason, we were unable to refine the lattice parameters using the powder diffraction data.

TABLE 1. X-RAY POWDER DIFFRACTION DATA FOR CARLHINTZEITE

d(obs)	I/Io	d(obs)	I/Io
9.0	10	1.813	20
5.51	10	1.799	10
4.56	70	1.760	10
4.41	10	1.739	10
3.69	60	1.639	10
3.48	100	1.624	20
3.24	5	1.547	2
2.852	40	1.537	1
2.791	20	1.523	5
2.665	20	1.492	1
2.480	2	1.476	2
2.277	30	1.460	40
2.242	30	1.437	2
2.214	20	1.425	2
2.190	20	1.414	2
2.081	30	1.368	2
2.047	20	1.273	10
1.976	30	1.260	2
1.900	20	1.242	1
1.869	20	1.160	5

Cu Kα nickel-filtered X-radiation.
Gandolfi camera 114.6 mm diameter; polycrystalline sample
Intensities visually estimated.
Values of *d* corrected using a silicon standard.

MORPHOLOGY, OPTICAL AND PHYSICAL PROPERTIES

Individual crystals of carlhintzeite up to 2.0 mm long are flattened on (001) and elongate parallel to [010]. The forms present are {100} and {001}; on some crystals, the face (110) is also present. The crystals occur as tufts and bundles of crystals that have (001) in common and are twinned about [010]. In its radiating habit and colorless nature, the species resembles pectolite.

The density, determined by flotation in heavy liquids, is 2.86 gm/cm^3, in excellent agreement with the calculated value of 2.89 g/cm^3 for $Z=4$. The streak is white, the lustre is vitreous; the mineral does not respond to ultraviolet radiation.

Carlhintzeite is biaxial (+), 2*V* (meas.) = 77(2)°, (calc.) = 78°; α 1.411(2), β 1.416(2), γ 1.422(2). Dispersion of the optic axes is indiscernible. The orientation of the indicatrix and determination of 2*V* were made using the universal stage. The orientation could not be detetrmined with an accuracy of greater than ±5° because of twinning and very small crystal size. Angles α and γ are very close to 90° and the orientation is given as for a monoclinic mineral: *X* very nearly parallel to *b*, and $c \wedge Z = 10(5)°$ in the acute angle between *a* and *c*. The specific refractive energy *K* of carlhintzeite, calculated from the chemical composition and Gladstone–Dale constants (Mandarino 1976), is 0.136. The value obtained from the density and refractive indices is 0.145.

CHEMISTRY

Carlhintzeite was chemically analyzed using an ARL–SEMQ electron microprobe utilizing an operating voltage of 15 kV and a beam current of 0.15 μA. The intensities were corrected using the MAGIC-4 computer program. The standards used were CaF_2 for Ca, MgF_2 for F, and hornblende for Al. Water was determined by DTA/TGA; a weight loss of 7% occurs between 315 and 370°C. Although the relatively high temperature of the weight loss might seem consistent with the loss of hydroxyl, other calcium aluminum fluorides, *e.g.*, gearksutite, dehydrate at temperatures as high as 398°C (Solov'ev & Levando 1958, Mel'nik & Razumeeva 1969, Korzhinskii *et al.* 1960). An emission spectrographic analysis proved the absence of any elements with atomic number below nine, and a wavelength-dispersive microprobe scan indicated that only Ca, F and Al were present in measurable quantities; Mn is present only as a trace.

An average of two analyses in close agreement yields: Al_2O_3 10.27 CaO 29.86, F 52.1, H_2O 7.0, sum 99.23 wt.%, in agreement with the theoretical composition of $Ca_2AlF_7 \cdot H_2O$: Al_2O_3 10.45, CaO 31.05, F 51.52, H_2O 6.98, sum 100.00 wt.%. This yields the empirical formula $Ca_{1.90}Al_{0.97}F_{7.00} \cdot 0.96H_2O$ on the basis of F=7 atoms.

OCCURRENCE AND PARAGENESIS

Carlhintzeite is known only from one museum specimen, the label of which states only "Hagendorf". The matrix and associated species are similar to those from the Hagendorf pegmatites, but we cannot identify the pegmatite in the Hagendorf area of Bavaria from which the specimen came. The mineralogy of these pegmatites has been described by many investigators: Laubmann & Steinmetz (1920), Mücke (1977), Müllbauer (1925), Strunz (1952), Strunz & Forster (1975), Strunz & Wilk (1960), Strunz *et al.* (1975, 1976).

On the type and only specimen, carlhintzeite is associated with rockbridgeite, pyrite, strengite and apatite; it is younger than the first three listed. Carlhintzeite was thus formed during the hydrothermal alteration of the primary triphylite, the precursor of the secondary phosphate minerals. Interestingly, the chemically related mineral pachnolite $NaCaAlF_6 \cdot H_2O$ has been reported from the Hagendorf pegmatites (Mücke 1977).

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