

Paulkellerite, a new bismuth iron phosphate mineral from Schneeberg, Germany

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ABSTRACT

Paulkellerite, $\text{Bi}_2\text{Fe}^{3+}(\text{PO}_4)_2(\text{OH})_2$, is monoclinic, $C2/c$, with $a = 11.382(6)$, $b = 6.690(4)$, $c = 9.666(6)$ Å, $\beta = 114.73(5)^\circ$, and $Z = 4$. Microprobe analysis yielded Bi_2O_3 71.6, Fe_2O_3 14.5, P_2O_5 11.3, H_2O 2.9, sum = 100.3 wt%. Optically, it is biaxial, positive, $2V = 37(2)^\circ$, with $\alpha = 1.762(2)$, $\beta = 1.767(2)$, and $\gamma = 1.825(5)$. Paulkellerite is light greenish-yellow, without cleavage, and occurs in wedge-shaped lustrous crystals associated with native bismuth, a skutterudite-group mineral, pyrite, erythrite, and bismutoferrite at the Neuhilfe mine, Schneeberg, East Germany. The name honors Professor Dr. Paul Keller of the University of Stuttgart.

INTRODUCTION

The mineral described herein was originally labeled atelestite, from Schneeberg, and physically resembles that species. The specimen was acquired from the Bergakademie Freiberg through the courtesy of Drs. F. Hofmann and H.-J. Roesler. Preliminary investigation indicated that it was a mineral new to scientific knowledge, and our subsequent investigation has confirmed this. We have named this new mineral *paulkellerite* in honor of Professor Dr. Paul Keller of the University of Stuttgart, in recognition of his extensive contributions to mineralogy, especially the mineralogy of the secondary minerals from ore deposits. The new mineral and the name were approved by the Commission on New Minerals and Mineral Names, IMA. The holotype specimen, designated by the criteria of Dunn and Mandarino (1987), is preserved at the Smithsonian Institution (NMNH no. 163777). Part of the holotype is in the National Museum of Natural Sciences in Ottawa (NMNS no. 53450), and the remainder is at the Bergakademie Freiberg, D.D.R.

PHYSICAL AND OPTICAL PROPERTIES

Paulkellerite occurs in wedge-shaped, euhedral crystals, with slightly curved faces, which vary from 0.2 to 0.8 mm in size (Fig. 1). The observed morphology is simple, displaying two dominant prisms, $\{110\}$ and $\{011\}$, and a poorly developed pinacoid $\{\bar{1}01\}$. A representative crystal drawing is shown in Figure 2. It is greenish-yellow, with a very light yellow streak. The luster is vitreous, inclining to adamantine, and the mineral is transparent with no discernible fluorescence in ultraviolet radiation.

The hardness (Mohs) is approximately 4; cleavage was not observed. The density is greater than 4.2 g/cm^3 , but could not be precisely determined owing to small grain size and paucity of material. The calculated density is 6.17 g/cm^3 .

Optically, paulkellerite is biaxial, positive, with $2V_{\text{meas}} = 37(2)^\circ$, $2V_{\text{calc}} = 34^\circ$. The indices of refraction, measured in Na light, are $\alpha = 1.762(2)$, $\beta = 1.767(2)$, and $\gamma = 1.825(5)$. The orientation is $X \wedge \mathbf{a} = 25^\circ$ in the obtuse angle β , $Y = \mathbf{b}$, $Z = \mathbf{c}$; pleochroism and dispersion are absent or indiscernible.

CHEMICAL COMPOSITION

Paulkellerite was analyzed using an ARL-SEM-Q electron microprobe, utilizing an operating voltage of 15 kV and a sample current, measured on brass, of $0.025 \mu\text{A}$. A wavelength-dispersive microprobe scan confirmed the absence of elements with atomic number greater than 8, except those reported herein. The standards used were maricite (Fe, P) and BiVO_4 (Bi), and the data were corrected using a modified version of the MAGIC-4 program. Water was determined by TGA-EGA using a Mettler TA1 thermoanalyzer for thermogravimetric analysis and an Inficon IQ 200 mass spectrometer for evolved-gas analysis (F. J. Wicks and R. A. Ramik, in prep.). The operating conditions were sample weight 2.899(2) mg at 23°C and 40% relative humidity, Pt crucible with a loose Pt lid, TG support stick, quartz-glass furnace, initial vacuum 4×10^{-8} torr stabilized over 2 h, heating rate $10^\circ\text{C}/\text{min}$, and heating range 20–900 $^\circ\text{C}$. The lightly crushed sample had been hand picked to at least 98% purity at optical

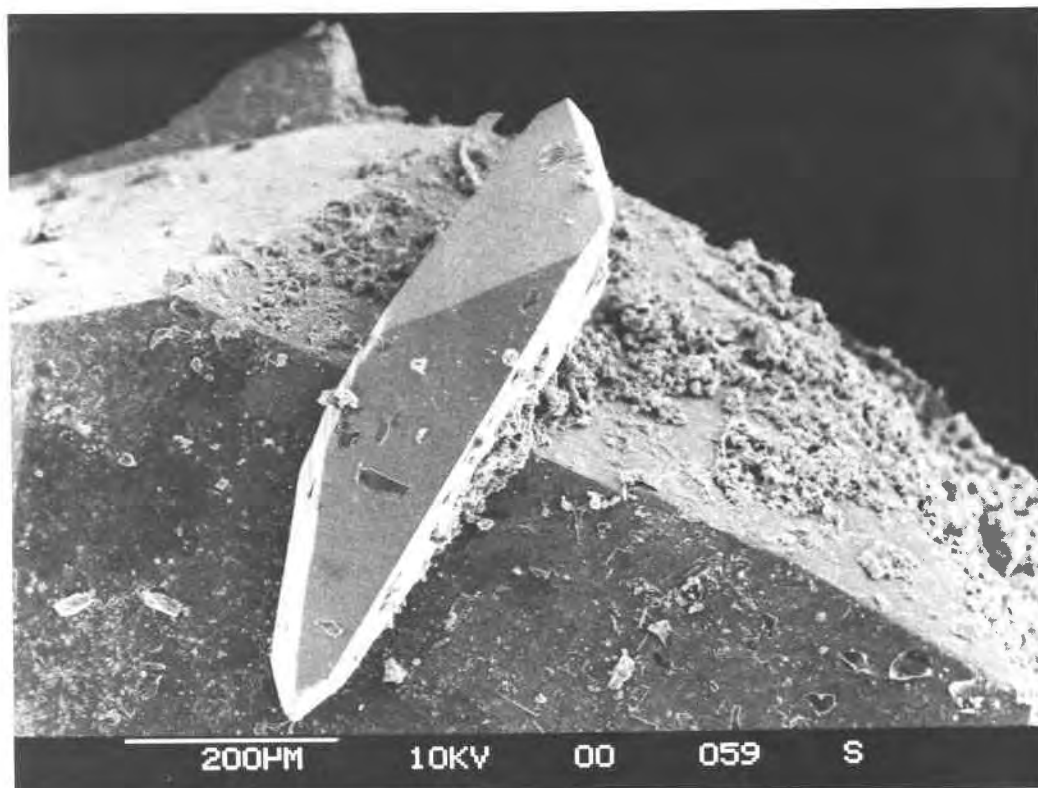


Fig. 1. SEM photomicrograph of euhedral crystals of paulkellerite from Schneeberg.

resolution. No volatiles were lost while the sample was at vacuum prior to analysis. A 2.9(3) wt% water loss was recorded in a simple, single-step loss beginning at 270 °C, peaking at 480 °C, and ending at 520 °C. Minute traces of CO₂ were also detected. A minor, sharp, water-loss peak was detected with the mass spectrometer at 600 °C, but the quantity lost was too small to be recorded on the analytical balance. Fusion and recrystallization of the sample followed this event. The temperature and form of the water loss suggests that it is present as (OH) and is thus an integral part of the structure. The oxidation state of Fe was determined using microchemical tests and confirmed by crystal-structure analysis (Grice and Groat, 1988).

The resultant composition is Bi₂O₃ 71.6, Fe₂O₃ 14.5, P₂O₅ 11.3, H₂O 2.9, total = 100.3 wt%. The empirical formula, calculated on the basis of 16 oxygen atoms, is Bi_{3.80}Fe_{2.25}P_{1.97}H_{3.98}O₁₆. The chemical formula for paulkellerite is therefore Bi₂Fe³⁺(PO₄)₂(OH)₂ with Z = 4, and this formula has been confirmed by solution of the crystal structure by Grice and Groat (1988).

CRYSTALLOGRAPHY

X-ray precession photographs show paulkellerite to be monoclinic with possible space groups *C2/c* or *Cc*. The crystal-structure analysis (Grice and Groat, 1988) showed *C2/c* to be the correct space group. Unit-cell dimensions

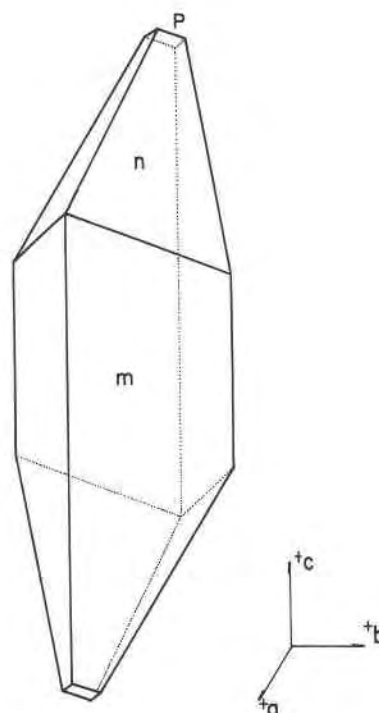


Fig. 2. Crystal drawing of paulkellerite showing prisms *n*{011} and *m*{110} and pinacoid *p*{101}.

TABLE 1. X-ray powder diffraction data for paulkellerite

<i>hkl</i>	<i>d</i> _{calc}	<i>d</i> _{obs}	<i>I</i> _{est}	<i>hkl</i>	<i>d</i> _{calc}	<i>d</i> _{obs}	<i>I</i> _{est}
110	5.617	5.651	1	132	1.887	1.888	2*
200	5.169	5.125	2	330	1.872	1.874	<1
202	4.367	4.368	1	024	1.835	1.838	<1
112	3.918	3.913	2*	133	1.827	1.823	1
020	3.345	3.338	2	204	1.771	1.774	1
311	3.299	3.306	<1	604	1.759	1.762	<1
112	3.131			331	1.752	1.752	<1
021	3.126	3.123	10	600	1.723	1.723	1*
310	3.064	3.060	<1	515	1.690	1.686	<1
202	2.815	2.836	<1	133	1.679	1.675	<1
220	2.808	2.804	3*	622	1.649	1.651	1
313	2.669	2.681	<1	041	1.643	1.638	<1
022	2.661	2.660	<1	425	1.624	1.624	1*
400	2.585	2.580	1*	241	1.620	1.605	<1
204	2.416	2.424	1	332	1.596	1.596	2*
113	2.383	2.380	1*	512	1.580	1.580	2*
223	2.305	2.310	<1	316	1.566	1.566	1
114	2.223	2.224	2*	241	1.531	1.531	2*
004	2.195	2.199	1	116	1.502	1.504	1
312	2.163			134	1.483	1.483	2*
131	2.160	2.162	4	006	1.463	1.462	<1
511	2.117	2.122	<1	625	1.452	1.452	<1
131	2.073	2.074	1	710	1.442	1.442	3*
420	2.045	2.044	2*	442	1.438		
132	2.025	2.028	1	135	1.430	1.432	<1
423	2.019	2.008	<1	531	1.423		
224	1.959	1.964	1	621	1.422	1.423	<1
331	1.922	1.925	<1	802	1.410		
602	1.896	1.897	2*	404	1.408	1.408	<1

Note: FeK α radiation, visually estimated intensities, and Si as an internal standard.

* Used in cell refinement.

refined from X-ray powder-diffraction data (Table 1), collected with a 114.6-mm-diameter Debye-Scherrer camera using FeK α radiation and NBS Si as an internal standard, yield $a = 11.382(6)$, $b = 6.690(4)$, $c = 9.666(6)$ Å, $\beta = 114.73(5)^\circ$, $V = 668.6(5)$ Å³. The X-ray powder-diffraction

data and unit-cell dimensions are not similar to any mineral known to us.

OCCURRENCE AND PARAGENESIS

Paulkellerite occurs in the Neuhilf mine, Schneeberg, near Zwickau in the Erzgebirge area of East Germany. The mineral was found in a NW-SE vein in the Bi-Ni-Co ores in 1881. The holotype specimen consists of a small specimen of native bismuth mixed with an unanalyzed skutterudite-group mineral and quartz. Secondary minerals have formed by alteration of this ore. These are greenish-yellow bismutoferrite as a thin coating, light pink erythrite in freely growing 1.0-mm rosettes, some massive secondary pyrite, and greenish-yellow crystals of paulkellerite. Upon casual observation, paulkellerite closely resembles some atelestite, and additional paulkellerite samples may reside mislabeled in systematic collections.

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