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KOTTENHEIMITE, $\text{Ca}_3\text{Si}(\text{OH})_6(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$, A NEW MEMBER OF THE ETTRINGITE GROUP FROM THE EIFEL AREA, GERMANY

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ABSTRACT

The new ettringite-group mineral kottenheimite was found at Bellerberg, near Kottenheim, Eastern Eifel area, Rhineland-Palatinate (Rheinland-Pfalz), Germany, and named for the type locality. Associated minerals are wollastonite, clinocllore, ellestadite, melilite, cuspidine, and earlier formed sanidine, clinopyroxene, and magnetite. Kottenheimite forms white radiated and random aggregates of hair-like subparallel clusters of minute crystals. The Mohs' hardness is 2-2.5; $D_{\text{meas}} = 1.92(2)$ g/cm³, $D_{\text{calc}} = 1.926$ g/cm³. The new mineral is uniaxial (-), $\omega = 1.490(2)$, $\epsilon = 1.477(2)$. The IR spectrum of kottenheimite is in accordance with the chemical composition and contains absorption bands in the range 3300-3700 cm⁻¹ (O-H-stretching vibrations), at 1650 and 1683 cm⁻¹ (bending vibrations of H₂O molecules), 1158, 1086, and 987 cm⁻¹ (showing the presence of distorted SO₄²⁻ groups), 752 and 725 cm⁻¹ (corresponding to Si-O stretching vibrations of Si(OH)₆ octahedra). The chemical composition is (electron microprobe, mean of 6 analyses, wt.%; H₂O and CO₂ determined by gas chromatography): CaO 26.04, MgO 0.20, FeO 0.19, Al₂O₃ 0.25, SiO₂ 8.95, SO₃ 24.26, CO₂ 0.58, H₂O 41.30; total 101.77. The empirical formula calculated on the basis of 26 anions is Ca_{3.015}Mg_{0.03}Fe_{0.02}Al_{0.03}Si_{0.97}(OH)_{5.94}(SO₄)_{1.97}(CO₃)_{0.09}·11.91H₂O. The simplified formula is Ca₃Si(OH)₆(SO₄)₂·12H₂O. The crystal structure was refined by the Rietveld method ($R_p = 0.0487$, $R_{\text{vp}} = 0.0623$, $R_B = 0.087$) based on the structural model of carraraite, Ca₃Ge(SO₄CO₃)₂(OH)₆·12H₂O. The new mineral is hexagonal, space group $P6_3/m$, $a = 11.1548(3)$, $c = 10.5702(3)$ Å, $V = 1139.04(5)$ Å³, and $Z = 2$. The strongest lines of the powder diffraction pattern [d in Å (I) (hkl)] are: 9.72 (100) (100), 5.590 (60) (110), 4.645 (26) (102), 3.840 (54) (112), 2.751 (34) (302), 2.536 (27) (213), 2.185 (30) (223). The channels in the crystal structure of kottenheimite are only filled by sulfate anions and water molecules. Type material is deposited in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 4102/1.

Keywords: kottenheimite, ettringite group, thaumasite, new mineral, crystal structure, cement, Eifel area, Germany.

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INTRODUCTION

Minerals belonging to the ettringite group represent a wide family of compounds in which the crystal structures are composed of columnar units $\text{Ca}_6[M_2(\text{OH},\text{O})_{12}\cdot 24\text{H}_2\text{O}]$ ($M = \text{Si}, \text{Ge}, \text{Mn}^{4+}, \text{Al}, \text{Fe}^{3+},$ or Cr) oriented along the c axis of the hexagonal (trigonal) lattice; intercolumn channels are occupied by charge-balancing anions such as SO_4^{2-} , CO_3^{2-} , $\text{PO}_3\text{OH}^{2-}$, $\text{B}(\text{OH})_4^-$, and H_2O molecules (Moore & Taylor 1970, Effenberger *et al.* 1983, Grier *et al.* 2002, Martucci & Cruciani 2006). The archetype members of this group, ettringite $\text{Ca}_6\text{Al}_2(\text{OH})_{12}(\text{SO}_4)_3\cdot 24\text{H}_2\text{O}$ (Moore & Taylor 1970) and thaumasite $\text{Ca}_3\text{Si}(\text{OH})_6(\text{SO}_4)(\text{CO}_3)\cdot 12\text{H}_2\text{O}$ (Edge & Zobetz 1971), play an important role in cement and concrete compositions (Batic *et al.* 2000, Brown & Hooton 2002, Brown *et al.* 2003). Structural studies of these minerals, first carried out on natural crystals, led to an explanation of the chemical behavior of their artificial counterparts in cement. The possible existence of a hypothetical high-sulfate analogue of thaumasite, $\text{Ca}_3\text{Si}(\text{OH})_6(\text{SO}_4)_2\cdot 12\text{H}_2\text{O}$, with intercolumnar channels completely occupied by sulfate ions, has been questioned for a long time. In the present paper, we describe this enigmatic member of the ettringite group. It was discovered near Kottenheim, in the Eifel area, Germany, and named kottenheimite after the type locality. The mineral and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (IMA no. 2011-038). The type material is deposited in the collection of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 4102/1.

OCCURRENCE, GENERAL APPEARANCE
AND PHYSICAL PROPERTIES

Kottenheimite occurs at Bellerberg, near Kottenheim, 2 km north of Mayen, Laacher See region, eastern Eifel area, Rhineland-Palatinate (Rheinland-Pfalz), Germany. The new mineral was found in a late hydrothermal assemblage related to alkali olivine basalt. Associated minerals are wollastonite, clinocllore, ellestadite, melilite, cuspidine and earlier plagioclase, sanidine, clinopyroxene, and magnetite.

Kottenheimite forms snow-white radiating and random aggregates of hair-like subparallel clusters in mirolitic cavities, encrusting cuspidine and melilite, in alkali basalt (Figs. 1, 2). Clusters reach 0.2 mm in length and consist of minute crystals that are curved and split. Crystal forms could not be indexed with certainty, but apparently the main form is the prism $\{10\bar{1}0\}$. Individual crystals are colorless under the microscope. The luster is vitreous in separate crystals and silky in aggregates. The mineral is brittle, with a Mohs' hardness of 2-2½. The fracture is uneven and there is no obvious cleavage. The density, measured by flotation in

heavy liquids, is 1.92(2) g/cm³. The calculated density is 1.93 g/cm³.

The new mineral is optically uniaxial (-), $\omega = 1.490(2)$, $\epsilon = 1.477(2)$.

CHEMICAL DATA

Six electron-microprobe analyses for Ca, Mg, Fe, Al, Si, and S were carried out using a VEGA TS 5130MM SEM equipped with an EDX analyzer [INCA Si(Li) detector], at an operating voltage of 15.7 kV and a beam current of 0.5 nA. The electron beam was rastered over an area $8 \times 8 \mu\text{m}^2$. Attempts to use the WDS mode, with higher beam currents, were unsuccessful because of the instability of the mineral resulting from its volatile component. Both H₂O and CO₂ contents were determined by gas chromatography (CHN analysis) of the products by annealing at 1200 °C. Contents of other elements with atomic numbers higher than oxygen, as well as nitrogen (by CHN analysis), are below detection limits (*i.e.*, below 0.05-0.2 wt.%). Analytical data are given in Table 1.

In spite of the precautions taken, the contents of components as measured by the electron-microprobe analyses seem to be somewhat overestimated due to partial dehydration of the mineral under electron beam. As a result, the total sum in Table 1 is 101.77%.

The empirical formula of kottenheimite (based on 26 O atoms) is $\text{Ca}_{3.015}\text{Mg}_{0.03}\text{Fe}_{0.02}\text{Al}_{0.03}\text{Si}_{0.97}(\text{OH})_{5.94}(\text{SO}_4)_{1.97}(\text{CO}_3)_{0.09}\cdot 11.91\text{H}_2\text{O}$.

The simplified formula is $\text{Ca}_3\text{Si}(\text{OH})_6(\text{SO}_4)_2\cdot 12\text{H}_2\text{O}$.

The Gladstone-Dale compatibility index (Mandarin 1981) calculated from the empirical formula is $1 - (K_P/K_C) = 0.010$ (*Superior*).



FIG. 1. Aggregates of acicular crystals of kottenheimite (white), with earlier melilite crystals, on cuspidine. Field of view: 1.2 mm.

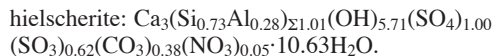
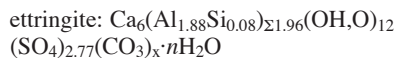
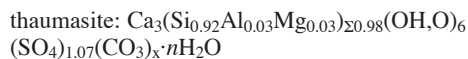
INFRARED SPECTROSCOPY

The kottenheimite sample was mixed with anhydrous KBr, pressed into a pellet, and analysed using a Specord 75 IR spectrophotometer. The IR spectrum of the pure KBr disk was subtracted from the overall spectrum. Polystyrene and gaseous NH₃ were used as frequency standards; the precision of frequency measurement is ± 1 cm⁻¹; the mean resolution for the region 400–1600 cm⁻¹ is 0.8 cm⁻¹.

The positions of absorption bands in the IR spectrum of kottenheimite (Fig. 3a,b) and their assignments (cm⁻¹; s: strong band, w: weak band, sh: shoulder) are: 3620 sh, 3512, 3400 sh, 3350 s (O–H stretching vibrations of H₂O molecules and OH groups), 1683, 1650 (bending vibrations of H₂O molecules), 1393 w (stretching vibrations of CO₃²⁻ anions), 1158 s, 1086 s (asymmetric stretching vibrations of SO₄²⁻ anions), 987 w (symmetric stretching vibrations of SO₄²⁻ anions), 870 sh, w, 752 s, 725 sh [Si–O stretching vibrations of Si(OH)₆ octahedra], 670, 621 s, 600 sh (bending vibrations of SO₄²⁻ anions), 497 s, 460 sh [O–Si–O bending vibrations of Si(OH)₆ octahedra].

The IR spectrum confirms the very low content of CO₃ groups in kottenheimite, unlike thaumasite. Bands of B-bearing groups [a doublet of relatively broad bands in the range 950–1000 cm⁻¹ corresponding to B(OH)₄⁻, as well as bands of BO₃³⁻ in the range 1185–1240 cm⁻¹; see Pöllmann *et al.* 1989, Malinko *et al.* 2001] are absent in the IR spectrum of kottenheimite. Bands in the range 930–970 cm⁻¹, corresponding to S–O stretching vibrations of sulfite groups in the SO₃-dominant ettringite-group mineral hielscherite (IMA 2011-037), are also not observed in the IR spectrum of the SO₃²⁻-dominant ettringite-group mineral kottenheimite. Thus SO₃²⁻ groups are absent in kottenheimite.

For comparison, IR spectra of some other ettringite-group minerals are given in Figures 3a and b. Their empirical formulae, calculated from electron microprobe analyses on the basis 3 or 6 Ca atoms pfu, are given below:



The IR spectrum of kottenheimite differs from those spectra obtained for all other ettringite-group minerals. The most important distinctive feature of the kottenheimite IR spectrum is the splitting of the band corresponding to the triply degenerate asymmetric SO₄ mode ν_3 into two components with absorption maxima at 1086 and 1158 cm⁻¹. Another distinction from most

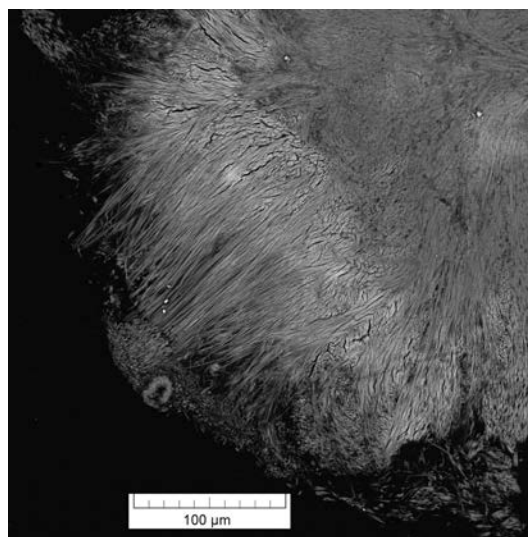


FIG. 2. Fibrous aggregate of kottenheimite. Polished section. BSE image.

TABLE 1. CHEMICAL COMPOSITION OF KOTTENHEIMITE

Constituent	Experimental data for the holotype			Theoretical composition of Ca ₃ Si(OH) ₆ (SO ₄) ₂ ·12H ₂ O, wt. %
	wt. %	Ranges	Probe standard	
CaO	26.04	25.25–26.81	Diopside	25.54
MgO	0.20	0–0.34	Diopside	
FeO	0.19	0.10–0.32	Fe	
Al ₂ O ₃	0.25	0–0.41	Albite	
SiO ₂	8.95	8.77–9.24	Diopside	9.12
SO ₃	24.26	23.81–24.72	BaSO ₄	24.31
CO ₂	0.58			
H ₂ O	41.30			41.03
Total	101.77			100.00

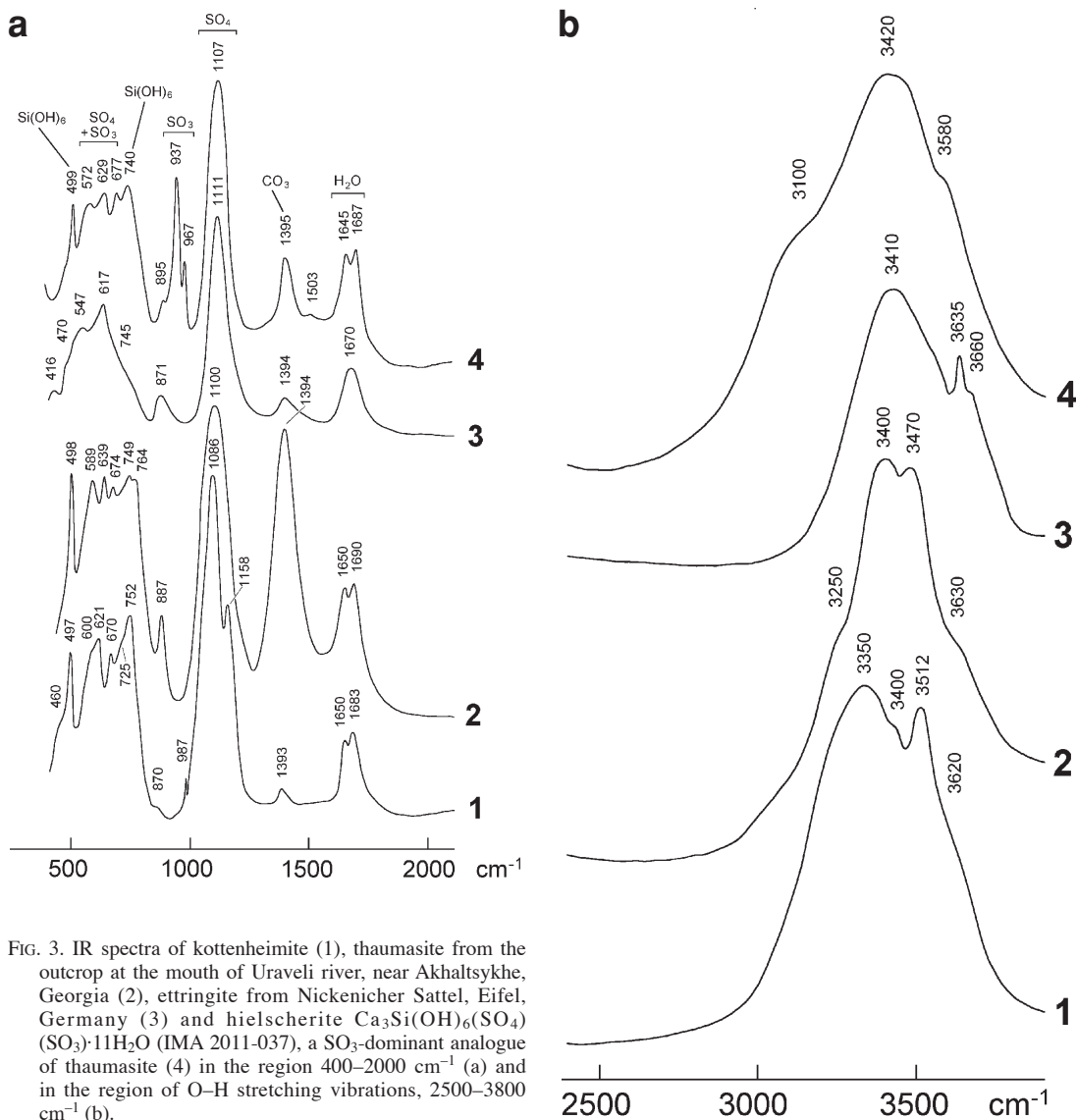


FIG. 3. IR spectra of kottenheimite (1), thaumasite from the outcrop at the mouth of Uraveli river, near Akhaltsykhe, Georgia (2), ettringite from Nickenicher Sattel, Eifel, Germany (3) and hielscherite $\text{Ca}_3\text{Si}(\text{OH})_6(\text{SO}_4)(\text{SO}_3)\cdot 11\text{H}_2\text{O}$ (IMA 2011-037), a SO_3 -dominant analogue of thaumasite (4) in the region 400–2000 cm^{-1} (a) and in the region of O–H stretching vibrations, 2500–3800 cm^{-1} (b).

other ettringite group minerals is the presence of a weak but distinct narrow band at 987 cm^{-1} corresponding to the non-degenerate symmetric stretching SO_4 mode ν_1 . Both these features indicate strong distortion of SO_4 tetrahedra. Strong bands at 752 and 497 cm^{-1} indicate the presence of $\text{Si}(\text{OH})_6$ octahedra in kottenheimite. Similar bands are observed in the IR spectrum of thaumasite, but they are absent in the IR spectra of Si-free ettringite-group minerals (in particular, in the spectrum of ettringite; Fig. 3a). The splitting of the H–O–H bending band into two components, with maxima at 1687 and 1645 cm^{-1} , in the IR spectrum of kottenheimite reflects the presence

of locally non-equivalent H_2O molecules. Characteristic bands of SO_3^{2-} anions at 937 and 967 cm^{-1} are present in the IR spectrum of hielscherite, but are not observed in the spectrum of kottenheimite.

THE CRYSTAL STRUCTURE AND X-RAY POWDER DIFFRACTION DATA

X-ray powder-diffraction data for kottenheimite (Table 2) were collected with a STOE IPDS II single-crystal diffractometer equipped with an image-plate detector ($\text{MoK}\alpha$ radiation; the distance between sample

TABLE 2. X-RAY POWDER DIFFRACTION DATA FOR KOTTENHEIMITE

l_{obs}	d_{obs}	l_{calc}	d_{calc}	h	k	l	l_{obs}	d_{obs}	l_{calc}	d_{calc}	h	k	l
100	9.72	100	9.66	1	0	0	7	1.931	10	1.933	5	0	0
69	5.590	60	5.579	1	1	0			3	1.918	2	2	4
		2	5.285	0	0	2			1	1.882	3	1	4
15	4.907	13	4.934	1	1	1	1	1.874	1	1.876	3	2	3
		6	4.832	2	0	0			1	1.860	3	3	0
26	4.645	34	4.637	1	0	2			9	1.832	3	3	1
1	4.399	2	4.394	2	0	1	9	1.827	7	1.830	2	1	5
54	3.840	67	3.837	1	1	2			4	1.815	5	0	2
5	3.645	6	3.652	2	1	0			4	1.800	4	2	1
12	3.568	13	3.566	2	0	2			1	1.783	4	0	4
21	3.455	24	3.452	2	1	1			1	1.767	3	0	5
		2	3.310	1	0	3			3	1.762	0	0	6
16	3.222	18	3.221	3	0	0	6	1.755	10	1.754	3	3	2
1	3.075	1	3.081	3	0	1			2	1.736	5	1	0
4	2.983	4	2.979	1	1	3			5	1.733	1	0	6
34	2.751	39	2.750	3	0	2			1	1.713	5	1	1
		2	2.680	3	1	0	2	1.676	6	1.680	1	1	6
8	2.639	11	2.643	0	0	4			5	1.660	3	1	5
10	2.600	11	2.598	3	1	1			5	1.649	5	1	2
27	2.536	36	2.536	2	1	3	11	1.649	14	1.648	4	1	4
		2	2.467	2	2	2	4	1.610	7	1.611	6	0	0
		1	2.416	4	0	0			2	1.589	4	3	0
4	2.391	3	2.390	3	1	2			3	1.571	4	3	1
		1	2.388	1	1	4	4	1.561	7	1.560	5	0	4
3	2.318	5	2.318	2	0	4			1	1.546	3	0	6
		8	2.217	3	2	0			1	1.541	6	0	2
		5	2.197	4	0	2			1	1.502	4	2	4
30	2.185	35	2.187	2	2	3			3	1.493	4	1	5
8	2.166	11	2.170	3	2	1	4	1.488	5	1.490	2	2	6
15	2.133	20	2.133	3	1	3			3	1.485	5	2	2
		4	2.109	4	1	0			1	1.472	3	1	6
		2	2.068	4	1	1	1	1.450	1	1.451	5	1	4
		2	2.065	1	0	5			1	1.448	4	3	3
3	2.046	4	2.044	3	2	2			1	1.419	6	1	2
		1	1.992	4	0	3	1	1.416	3	1.417	5	2	3
		3	1.977	1	1	5	1	1.396	2	1.396	3	3	5
3	1.961	3	1.959	4	1	2							

and detector was 200 mm) using the Gandolfi method. They indexed well in the hexagonal system, space group $P6_3/m$.

Individual crystals of kottenheimite consist of differently oriented blocks and are curved. Owing to the lack of crystals suitable for a single-crystal data collection, the crystal structure of kottenheimite was refined by the Rietveld method using the FullProf (v. 2005) program suite (Rodríguez-Carvajal 1993) (Tables 3–5, Figs. 4, 5) on the basis of cell parameters taken from the powder data and a structural model adopted from carraraite $\text{Ca}_3\text{Ge}(\text{OH})_6(\text{SO}_4, \text{CO}_3) \cdot 12\text{H}_2\text{O}$ (Merlino & Orlandi 2001). Site positions for all atoms were refined unconstrained. Atom sites related to the framework (*i.e.*, Ca and Si polyhedra) were assumed to be fully occupied, whereas site occupancies of atoms in the sulfate anion were freely refined. Because attempts to attain positive

B_{iso} for oxygen O4 were unsuccessful, we fixed its B_{iso} at the reasonable value of 1.00 (Table 4). The refinement of other parameters was stable and converged into the values given in Table 4. The basic structural features of thaumasite and kottenheimite are essentially the same: they are dominated by a hexagonal arrangement of positively charged columnar units $\text{Ca}_3[\text{Si}(\text{OH})_6 \cdot 12\text{H}_2\text{O}]^{4+}$ composed of sequences of $\text{Ca}(\text{OH})_4(\text{H}_2\text{O})_4$ polyhedra and $\text{Si}(\text{OH})_6$ octahedra alternating along the c axis, as is characteristic for the topology of ettringite group minerals. Differences in symmetry (space groups $P6_3$ for thaumasite and $P6_3/m$ for kottenheimite) are related to order-disorder features in the distribution of charge-balancing intercolumnar anions SO_4^{2-} and CO_3^{2-} (Fig. 5). The crystal structure of kottenheimite, with the channels fully occupied by symmetrically identical sulfate groups, is consistent with the ideal symmetry of an

undistorted thaumasite "skeleton". The lower symmetry of thaumasite is due to the ordered distribution of SO_4^{2-} and CO_3^{2-} in the interchannel space.

Selected interatomic bond distances in the crystal structure of kottenheimite are given in Table 5. The S–O distances in the sulfate group of kottenheimite are substantially shorter than the corresponding bond lengths in thaumasite (Fig. 5). The same phenomenon [S–O(1) = 1.448(49), S–O(2) = 1.439(17) Å] has been reported for carraraite (Merlino & Orlandi 2001). The nonequivalence of S–O bond-lengths in kottenheimite [S1–O5 = 1.451(10), S1–O6 = 1.431(5) Å] is in a good

agreement with specific features of the IR spectrum (*i.e.*, the splitting of the ν_3 band and the presence of the ν_1 band).

The chemical analyses gave 24.26 wt.% SO_3^{2-} , which corresponds to the site occupation parameter for the S position of 0.985. However, the corresponding value determined from the analysis of the crystal structure is 0.94 (Table 4). This discrepancy could be due to a possible overvaluation of the S content in the electron microprobe analyses (see Chemical Data).

DISCUSSION

Comparative data for kottenheimite and some related ettringite-group minerals are given in Table 6. Taking into account the simplicity of the chemical composition of kottenheimite, one would expect its widespread occurrence both in natural associations and cements. Looking through numerous available data on ettringite-group minerals, however, one can say that kottenheimite is extremely rare in nature. The same can be said of the synthetic analogue of kottenheimite; its existence is still not well proven (Lukas 1970a, 1970b). The reasons for the rarity of kottenheimite can be clarified by further studies of its complex chemical and thermal behavior, as well as conditions of its formation. Hypothetically, kottenheimite should be formed via the oxidation of hielscherite $\text{Ca}_3\text{Si}(\text{SO}_4)(\text{SO}_3)(\text{OH})_6 \cdot 11\text{H}_2\text{O}$ (IMA 2011-037, Pekov *et al.* 2011), a recently described sulfite-dominant analogue of thaumasite. Hielscherite and intermediate members of the solid solution series hielscherite-thaumasite are common minerals in the Eifel area. The possibility of the oxidation of SO_3^{2-} to SO_4^{2-} in a synthetic sulfite analogue of ettringite was demonstrated by Motzet & Pöllmann (1999). On the other hand, the new (in particular, well-established IR spectroscopy) data provided in the present paper will facilitate possible recognition of kottenheimite

TABLE 3. RIETVELD REFINEMENT DETAILS FOR KOTTENHEIMITE

Diffractometer	Stoe Stadi P
Geometry	Transmission
Wavelength (Å)	1.540598
2 θ min, max (°)	12.00, 90.00
Scan step, 2 θ (°)	0.01
no. of data points	7799
no. of observed reflections	446
Peak profile	Pseudo-Voigt
Background function	6-coefficients polynomial
Peak intensity cut-off	none applied
no. of refined parameters	44
no. of restraints	0
Space group	$P6_3/m$
a (Å)	11.1548(3)
c (Å)	10.5702(3)
V (Å ³)	1139.04(5)
Z	2
R_p (%)	4.87
R_{wp} (%)	6.23
R_{exp} (%)	4.13
χ^2	2.28
R_B (%)	8.70
R_F (%)	7.41

TABLE 4. ATOMIC COORDINATES AND ISOTROPIC DISPLACEMENT PARAMETERS (Å²) FOR KOTTENHEIMITE*

Atom	Site	x/a	y/b	z/c	B_{iso}	SOF**
Ca1	6h	0.193(3)	−0.0124(4)	1/4	0.14(7)	1
Si1	2b	0	0	0	1.1(2)	1
S1	4f	1/3	2/3	0	0.8(1)	0.91(1)
O1	6h	0.390(1)	0.2325(11)	1/4	1.1(3)	1
O2	6h	0.137(1)	−0.254(1)	1/4	1.5(3)	1
O3	12i	1/3	−0.0155(5)	0.4257(4)	0.6(1)	1
O4	12i	0.1353(6)	0.1278(6)	0.1030(2)	1.00***	1
O5	4f	1/3	2/3	−0.137(1)	7.9(5)	0.86(2)
O6	12i	0.1912(5)	0.6133(7)	0.0334(6)	5.3(2)	0.99(1)

* Site designations are given according to Merlino and Orlandi (2001).

** Atom sites of the coordinating framework cations (Ca and Si) were assumed to be fully occupied.

*** Refinement of O4 resulted in negative value of B_{iso} . Therefore B_{iso} was fixed at a reasonable value.

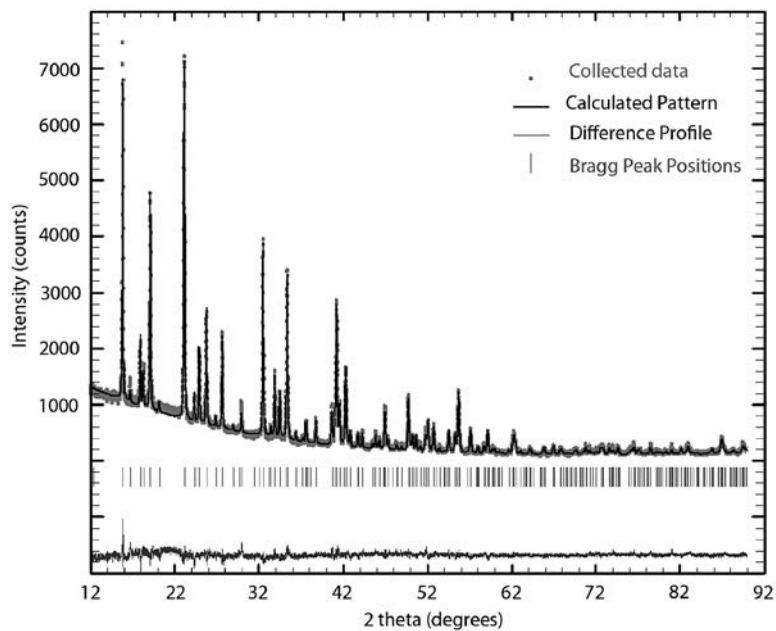


FIG. 4. Observed, calculated, and difference patterns from the Rietveld refinement of kottenheimite.

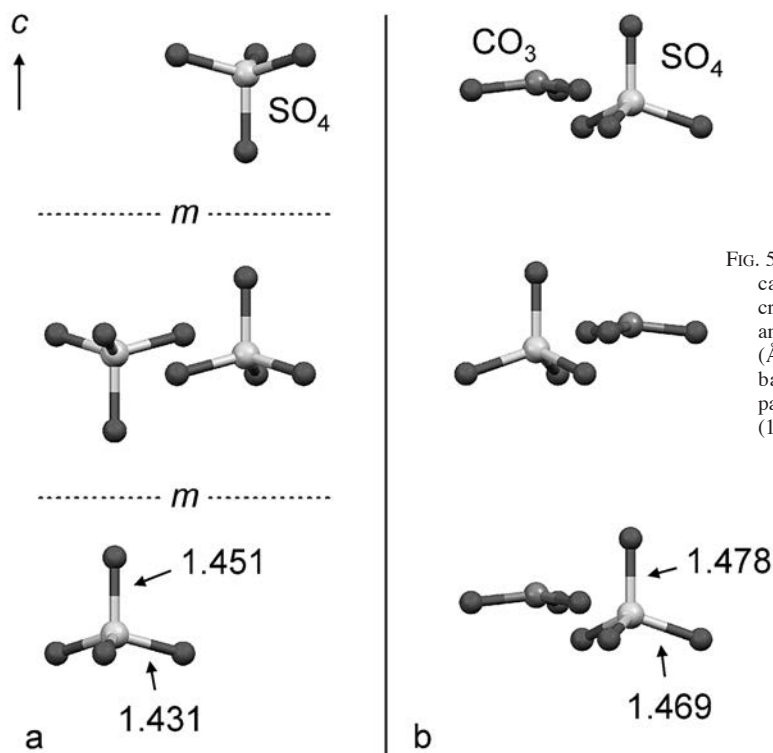


FIG. 5. Relative arrangement of sulfate and carbonate groups in the channels of crystal structures of kottenheimite (a) and thaumasite (b). S-O bond distances (Å) in sulfate groups are calculated basing on data taken from present paper (a) and after Effenberger *et al.* (1983) (b).

TABLE 5. SELECTED BOND DISTANCES (Å)
IN THE STRUCTURE OF KOTTENHEIMITE

Atom1	Atom2	Length
Ca1	O1	2.507(9)
Ca1	O2	2.440(10)
Ca1	O3 (x2)	2.438(5)
Ca1	O4 (x2)	2.498(6)
Ca1	O4'(x2)	2.508(8)
Si1	O4 (x6)	1.829(4)
S1	O5	1.451(10)
S1	O6 (x3)	1.431(5)

*Atom labels are given according to Merlino and Orlandi (2001).

in natural assemblages and cements. Such recognition might help in a better understanding of some chemical processes such as the “thaumasite form of sulfate attack” which results in rapid and serious deterioration of cement and concrete (Crammond 1985, Sims & Huntley 2004).

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TABLE 6. COMPARATIVE DATA FOR KOTTENHEIMITE
AND SOME RELATED ETTRINGITE GROUP MINERALS

Mineral	Kottenheimite	Hielscherite IMA 2011-037	Thaumasite	Carraraite
Idealized formula	Ca ₃ Si(OH) ₆ (SO ₄) ₂ ·12H ₂ O	Ca ₃ Si(OH) ₆ (SO ₄) (SO ₃)·11H ₂ O	Ca ₃ Si(OH) ₆ (SO ₄) (CO ₃)·12H ₂ O	Ca ₃ Ge(OH) ₆ (SO ₄ ,CO ₃) ₂ ·12H ₂ O
Crystal system	Hexagonal	Hexagonal	Hexagonal	Hexagonal
Space group	<i>P</i> 6 ₃ / <i>m</i>	<i>P</i> 6 ₃	<i>P</i> 6 ₃	<i>P</i> 6 ₃ / <i>m</i>
<i>Unit cell data</i>				
<i>a</i> , Å	11.1548(3)	11.1178(2)	11.02–11.08	11.056(3)
<i>c</i> , Å	10.5702(3)	10.5381(2)	10.37–10.44	10.629(6)
<i>V</i> , Å ³	1139.04(5)	1128.06(3)	1091–1111	1125 2
<i>Z</i>	2	2	2	2
Strongest reflections of the X-ray powder pattern: <i>d</i> , Å ³ – <i>I</i>	9.72 – 100 5.590 – 69 4.645 – 26 3.840 – 54 3.455 – 21 2.751 – 34 2.536 – 27 2.185 – 30	9.62 – 100 5.551 – 50 4.616 – 37 3.823 – 64 3.436 – 25 2.742 – 38 2.528 – 37 2.180 – 35	9.56 – 100 5.51 – 40 3.78 – 16 3.41 – 20 3.18 – 16 2.713 – 14 2.155 – 13	9.67 – vs 5.53 – s 3.83 – s 3.56 – ms 3.44 – m 2.74 – ms 2.53 – m
Density, g cm ⁻³	1.93 (calc.) 1.92(2) (meas.)	1.791 (calc.)	1.84–1.89	1.979 (calc.)
<i>Optical data</i>				
<i>ω</i>	1.490(2)	1.494(2)	1.498–1.507	1.509(1)
<i>ε</i>	1.477(2)	1.476(2)	1.458–1.490	1.479(1)
Optical sign	(–)	(–)	(–)	(–)
IR bands in the characteristic region 900–3800 cm ⁻¹ ; strongest bands are marked in bold; stretching vibrations of sulfite groups SO ₃ are marked with asterisks	3620 3512 3400 3350 1683 1650 1393 1158 1086 987	3580 3420 3100 1687 1647 1395 1107 967* 937*	3630 3470 3400 3250 1690 1650 1394 1100	No data
Reference	This work	Pekov <i>et al.</i> (2011); our data on the IR spectrum	Anthony <i>et al.</i> (1995); Jacobsen <i>et al.</i> (2003); Martucci & Cruciani (2006); our data on the IR spectrum	Merlino & Orlandi (2001)

Note: m = medium, s = strong, ms = medium strong, vs = very strong.

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