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Empressite, AgTe, from the Empress-Josephine mine, Colorado, U.S.A.: Composition, physical properties, and determination of the crystal structure

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ABSTRACT

The chemistry and composition of empressite, AgTe, a rare silver telluride mineral, has been mistaken in the mineralogical literature for the silver telluride stützite ($Ag_{5-x}Te_3$). Empressite from the type locality, the Empress-Josephine deposit (Colorado), occurs as euhedral prismatic grains up to 400 μm in length and contains no inclusions or intergrowths with other minerals. It is pale bronze in color and shows a grey-black to black streak. No cleavage is observed in empressite but it shows an uneven to subconchoidal fracture and Vickers hardness (VHN_{25}) of 142 kg/mm². Empressite is greyish white in color, with strong bireflectance and pleochroism. Reflectance percentages for R_{min} and R_{max} are 40.1, 45.8 (471.1 nm), 39.6, 44.1 (548.3 nm), 39.4, 43.2 (586.6 nm), and 38.9, 41.8 (652.3 nm), respectively.

Empressite is orthorhombic and belongs to space group *Pmnb* (*Pnma* as standard), with the following unit-cell parameters: $a = 8.882(1)$, $b = 20.100(5)$, $c = 4.614(1)$ Å, $V = 823.7(3)$ Å³, and $Z = 16$. Electron microprobe analyses gave the chemical formula $Ag_{1.01}Te_{0.99}$. The calculated density (from the ideal formula) is 7.59 g/cm³. The crystal structure has been solved and refined to $R = 4.45\%$. It consists of edge-sharing $AgTe_4$ tetrahedra forming sheets parallel to (010). The connectivity between the sheets is provided by Te-Te contacts (<2.9 Å) to complete the framework. The structural study presented here shows that empressite and stützite have different crystal structures.

INTRODUCTION

Empressite, AgTe, is a rare orthorhombic mineral that forms in gold-silver veins (e.g., Bradley 1914, 1915; Honea 1964; Berbeleac 1980; Kovalenker et al. 1997; Pals and Spry 2003), magmatic nickel (e.g., Abel et al. 1979; MacTavish 1992), and base metal sulfide deposits (e.g., Weibel and Koeppel 1963; Cook 1996; Zhong et al. 1997). It usually occurs in trace amounts with other tellurium-bearing minerals, particularly those in the Ag-Te system. For example, empressite coexists with hessite (Ag_2Te) and stützite ($Ag_{5-x}Te_3$) (e.g., Huangshaping Pb-Zn deposit, P.R. China; Zhong et al. 1997); hessite (e.g., Sulitjelma Cu-Zn deposit, Norway; Cook 1996), native tellurium (e.g., Empress-Josephine Au-Ag deposit; Bradley 1914), and stützite (e.g., Empress-Josephine Au deposit; Stumpfl and Rucklidge 1968). As a result of similar compositions and X-ray diffraction patterns and due to the inability, to date, to synthesize empressite in the laboratory there has been some confusion concerning the physical and chemical differences between empressite and stützite.

A mineral with the formula AgTe was first identified by Bradley (1914) from the Empress-Josephine deposit, Kerber Creek district, Colorado. This composition was reconfirmed by him the following year (Bradley 1915) using new data from a different analyst. Thompson et al. (1951) subsequently conducted microscopic and experimental studies in the system Ag-Te and suggested that the formula for empressite should be $Ag_{2-x}Te_{1+x}$. However, Donnay et al. (1956), on the basis of density and X-ray diffraction data, suggested that the formula for empressite should be $Ag_{5-x}Te_3$. Further compositional and structural studies by Honea (1964) suggested the original formula proposed by Bradley (1914) was correct and that the mineral with the formula Ag_5Te_3 should be termed stützite. Honea (1964), Cabri (1965b), and Kracek et al. (1966) did experimental studies in the system Ag-Te but were unable to synthesize AgTe. However, the results of a differential thermal study of a natural crystal of AgTe suggested to Honea (1964) that empressite was stable up to 210 °C whereupon it broke down to stützite and native tellurium. Cabri (1965a) challenged the results of Honea's (1964) study and suggested that due to similarities between the X-ray patterns of synthetic $Ag_{5-x}Te_3$ and Honea's AgTe there was no need to redefine empressite. Responding to Cabri's concerns, Honea (1964) argued that the rules of synonomy had been followed and that differences in optical data, chemical compositions, and X-ray data between AgTe and $Ag_{5-x}Te_3$ had been identified. Moreover, measured and calculated specific gravities of AgTe undertaken by him matched and reaffirmed the identity of AgTe. Subsequent electron microprobe studies by Stumpfl and Rucklidge (1968) of the sample used by Thompson et al. (1951) showed that it contained both AgTe and $Ag_{5-x}Te_3$. Although the names empressite and stützite have been retained in the literature since Stumpfl and Rucklidge's (1968) study, questions still remain concerning the correct structural characterization of empressite and why most of the lines of the powder X-ray patterns for empressite and stützite in Honea's (1964) study are the same. These issues were discussed by Cabri (1965a) and Honea (1965) but have never been adequately explained.

To help resolve these issues, we present new crystal structure data for empressite from its type locality together with physical and chemical data.

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PHYSICAL AND OPTICAL PROPERTIES

Empressite is pale bronze in color and shows a grey-black to black streak. The mineral is opaque in transmitted light and exhibits a metallic luster. No cleavage is observed and the fracture is uneven to subconchoidal. The calculated density ($Z = 16$) for ideal AgTe is 7.59 g/cm^3. Unfortunately, the density could not be measured because of the small grain size. Micro-indentation measurements carried out with a VHN load of 25 g give a mean value of 142 kg/mm^2 (range: 135–151) corresponding to a Mohs hardness of about 3-1/2.

In plane-polarized incident light empressite is greyish white in color, with moderate to strong bireflectance (from white to brownish grey) and pleochroism. Under crossed polars, empressite shows strong anisotropism, with a distinct change from light to dark. Internal reflections are absent and there is no optical evidence of growth zonation.

Reflectance measurements were performed in air by means of an MPM-200 Zeiss microphotometer equipped with a MSP-20 system processor on a Zeiss Axioplan ore microscope. The filament temperature was approximately 3350 K. An interference filter was adjusted, in turn, to select four wavelengths for measurement (471.1, 548.3, 586.6, and 652.3 nm). Readings were taken for specimen and standard (SiC) maintained under the same focus conditions. The diameter of the circular measuring area was 0.1 mm. Reflectance percentages for R_{min} and R_{max} are 40.1, 45.8 (471.1 nm), 39.6, 44.1 (548.3 nm), 39.4, 43.2 (586.6 nm), and 38.9, 41.8 (652.3 nm), respectively.

X-RAY CRYSTALLOGRAPHY AND CRYSTAL-STRUCTURE DETERMINATION

A small crystal fragment (15 × 20 × 20 μm) was selected for the X-ray single-crystal diffraction study. Unit-cell parameters, determined by centering 25 high-θ (20–25°) reflections with an automated diffractometer (Enraf Nonius CAD4), are shown in Table 1. Intensity data were collected using Mo$K\alpha$ radiation monochromatized by a flat graphite crystal in ω scan mode. Intensities were corrected for Lorentz-polarization effects and subsequently for absorption following the semi-empirical method of North et al. (1968). The values of the equivalent pairs *hkl* and $\overline{h}kl$ were averaged. The merging *R* for the ψ-scan data set decreased from 15.29% before absorption correction to 5.42% after correction. Systematic absences ($h0l$: $h + l = 2n$; $hk0$: $k = 2n$; $h00$: $h = 2n$; $0k0$: $k = 2n$; $00l$: $l = 2n$) were consistent with the space groups $P2_1nb$ ($Pna2_1$ as standard) and *Pmnb* (*Pnma* as standard). Statistical tests on the distribution of |*E*| values strongly indicated the presence of an inversion centre, suggesting space group *Pmnb*. We decided to solve the structure in the non-standard space group *Pmnb* in order to maintain the original orientation (Honea 1964).

TABLE 1. Data and experimental details for the selected empressite crystal

Space group	*Pmnb* (*Pnma* as standard)
Cell parameters	$a = 8.882(1)$ Å $b = 20.100(5)$ Å $c = 4.614(1)$ Å $V = 823.7(3)$ Å^3
Crystal size (μm)	15 × 20 × 20
Wavelength (26 mA × 50 kV)	Mo$K\alpha$
Theta-range (°)	1–32
Scan mode	ω
Scan width (°)	2.60
Scan speed (°/min)	2.06
μ (mm^{-1})	23.15
Independent refl.	1504
Refl. With $F_o > 4\sigma(F_o)$	1052
R_{obs} (%)	4.45
R_{all} (%)	6.49

The position of most of the atoms (Ag1, Ag2, Te1, Te2, Te3) was determined from the three-dimensional Patterson synthesis (Sheldrick 1997a). A least-squares refinement using these heavy-atom positions and isotropic temperature factors yielded an *R* factor of 12.88%. Three-dimensional difference Fourier synthesis yielded the position of the remaining silver atom (i.e., Ag3). The full-matrix least-squares program SHELXL-97 (Sheldrick 1997b) was used to refine the structure. Anisotropic temperature factors for all the atoms led to $R = 4.45\%$ for 1052 observed reflections [$F_o > 4\sigma(F_o)$] and $R = 6.49\%$ for all 1504 independent reflections. Neutral scattering curves for Ag and Te were taken from the *International Tables for X-ray Crystallography* (Ibers and Hamilton 1974). Inspection of the difference Fourier map revealed that the maximum positive and negative peaks were 4.09 and 3.94 e$^-$/Å^3, respectively. Experimental details and *R* indices are given in Table 1. Fractional atomic coordinates and anisotropic-displacement parameters are shown in Table 2. Table 3[1] lists the observed and calculated structure factors.

CHEMICAL COMPOSITION

A preliminary chemical analysis using energy dispersive spectrometry, performed on the same crystal fragment used for the structural study, did not indicate the presence of elements ($Z > 9$) other than Ag and Te and only very minor amounts of Cu and Fe. The chemical composition was determined using wavelength-dispersive analysis (WDS) by means of a Jeol JXA-8600 electron microprobe. Major and minor elements were determined at 20 kV accelerating voltage and 40 nA beam current, with variable counting times: 30 s for Ag and Te and 60 s for the minor elements Cu and Fe. For the WDS analyses the following lines were used: Ag$L\alpha$, Te$L\alpha$, Cu$K\alpha$, and Fe$K\alpha$. The estimated analytical precision is: ±0.20 for Ag and Te and

TABLE 2. Fractional coordinates and anisotropic displacement parameters for empressite

	x	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	U_{eq}
Ag1	3/4	0.05130(7)	0.1669(3)	0.0434(8)	0.0330(6)	0.0293(7)	0	0	0.0069(6)	0.0352(3)
Ag2	1/4	0.15582(7)	0.7433(3)	0.0317(7)	0.0321(7)	0.0337(7)	0	0	0.0073(6)	0.0325(3)
Ag3	0.5201(1)	0.06565(6)	0.6499(3)	0.0427(6)	0.0517(6)	0.0599(7)	0.0224(5)	–0.0233(6)	–0.0336(6)	0.0514(4)
Te1	0.5228(1)	0.15783(3)	0.0999(1)	0.0140(3)	0.0168(3)	0.0187(3)	0.0004(2)	0.0019(9)	0.0003(3)	0.0165(2)
Te2	1/4	0.26324(4)	0.3510(2)	0.0164(4)	0.0152(4)	0.0172(4)	0	0	–0.0012(4)	0.0163(2)
Te3	1/4	0.03365(5)	0.3417(2)	0.0149(4)	0.0158(4)	0.0214(4)	0	0	0.0005(4)	0.0174(2)

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[1] For a copy of Table 3, document item AM-04-065, contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. Deposit items may also be available on the American Mineralogist web site at http://www.minsocam.org.

±0.02 for Fe and Cu. The standards employed were: Ag metal (Ag), synthetic Sb_2Te_3 (Te), marcasite (Fe), and Cu metal (Cu). The empressite fragment was found to be homogeneous within analytical error. The average chemical composition (15 analyses from different spots), together with ranges of wt% of elements, is reported in Table 4. On the basis of 2 atoms, the formula of empressite is $Ag_{1.01}Te_{0.99}$, ideally AgTe.

DESCRIPTION OF THE STRUCTURE AND DISCUSSION

The structure of empressite consists of edge-sharing $AgTe_4$ tetrahedra forming sheets parallel to (010). The connectivity between the sheets is provided by Te–Te contacts (<2.9 Å) (Fig. 1). In particular, Ag3 atoms form corner-sharing chains parallel to the **a** axis which are linked by edge-sharing with Ag1 and Ag2 atoms. Each Ag1 atom shares two edges with Ag3 atoms and a vertex with Ag2. In the same way, each Ag2 atom shares two edges with Ag3 atoms and a vertex with Ag1.

Selected bond distances and angles are given in Table 5. As observed by Van der Lee and de Boer (1993) for the crystal structure of hessite, the Ag-tetrahedra in empressite are also strongly distorted. The bond distances are in the range 2.783(1)–3.142(2) Å (Table 5), which compares favorably with those observed for the hessite structure [2.8415(7)–3.034(1) Å; Van der Lee and de Boer 1993]. The bond angles for empressite show less variation, 74.79(4)–121.84(5)°, than those reported for hessite [94.85(2)–155.79(3)°; Van der Lee and de Boer 1993] and vulcanite, CuTe [69.7–120.5°; Pertlik 2001]. However, the averages of the Te-Ag-Te bond angles for the Ag1 and Ag2 tetrahedra in empressite [109.24(4) and 109.42(5)°, respectively] are close to the ideal value, whereas the Ag3 tetrahedron is slightly more distorted [107.80(5)°]. The Ag–Ag distances [3.001(2) to 3.463(2) Å] are in the range observed for several silver-bearing minerals [2.841(1)–3.133(1) Å for the structure of hessite, Van der Lee and de Boer (1993); 3.04–3.71 Å for the low-temperature modification of Ag_2S, Frueh (1958); and 2.93–3.68 Å for the low-temperature modification of Ag_2Se, Wiegers (1971)].

The most interesting crystal-chemical feature observed in the structure of empressite concerns the environment of the tellurium atoms. The Te2 atom has two neighboring Te1 atoms with Te1-Te2 = 2.812(1) Å, thus forming a Te_3 group with a Te1-Te2-Te1 angle of 91.71(4)° (Fig. 2). After krennerite, $(Au,Ag_x)Te_2$ (Pertlik 1984a), this is the second occurrence of a Te_3 group in a mineral crystal structure. As suggested by Pertlik (1984a), this structural feature is strictly comparable to a section of the chain in native tellurium (Te-Te = 2.835 Å, Te-Te-Te = 103.2°; Cherin and Unger 1967). Te-Te contacts <2.9 Å are also observed in the crystal structures of sylvanite ($AgAuTe_4$; Pertlik 1984b) and stützite (Peters et al. 1996). However, in these structures the Te–Te contacts only form Te_2 dumbbells.

Table 6 compares the X-ray powder pattern reported by Ho-

TABLE 4. Electron microprobe analyses for empressite (means and ranges in wt % of elements; *n* = 15)

Element	Wt%	Range
Ag	46.06	45.88–46.25
Te	53.77	53.10–54.21
Cu	0.04	0.01–0.06
Fe	0.04	0.01–0.05
Total	99.91	

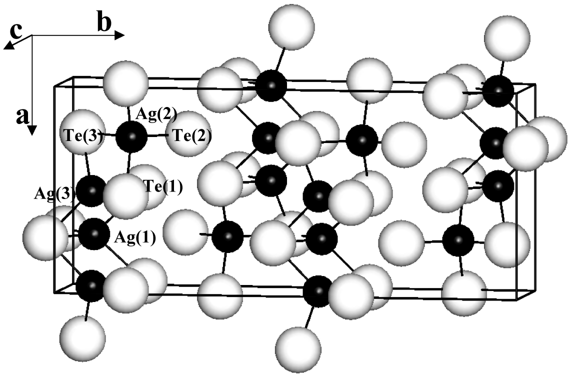

FIGURE 1. The crystal structure of empressite projected down [001]. The black and white circles refer to Ag and Te atoms, respectively. The unit cell is outlined.

TABLE 5. Selected bond distances (Å) and interatomic angles (°) for empressite

Ag1^{i}–Te1^{i,ii}	2.958(1)	Te1^{i}–Ag1^{i}–Te1^{ii}	86.01(5)
–Te3^{iv}	2.838(2)	Te1^{i,ii}–Ag1^{i}–Te3^{iii}	109.96(4)
–Te3^{iii}	2.902(2)	Te1^{i,ii}–Ag1^{i}–Te3^{iv}	121.26(4)
Ag1^{i}–Ag3^{i,ii}	3.036(2)	Te3^{iii}–Ag1^{i}–Te3^{iv}	106.98(6)
–Ag3^{vii,viii}	3.153(2)	Ag3^{i}–Ag1^{i}–Ag3^{ii}	84.52(6)
–Ag3^{iv,ix}	3.463(2)	Ag3^{i}–Ag1^{i}–Ag3^{vii}	96.38(4)
		Ag3^{ii}–Ag1^{i}–Ag3^{viii}	96.38(4)
		Ag3^{i}–Ag1^{i}–Ag3^{viii}	169.13(7)
		Ag3^{ii}–Ag1^{i}–Ag3^{vii}	169.13(7)
		Ag3^{i}–Ag1^{i}–Ag3^{iv}	110.56(5)
		Ag3^{ii}–Ag1^{i}–Ag3^{ix}	110.56(5)
		Ag3^{iv}–Ag1^{i}–Ag3^{vii}	134.05(4)
		Ag3^{viii}–Ag1^{i}–Ag3^{ix}	134.05(4)
		Ag3^{vii}–Ag1^{i}–Ag3^{ix}	78.36(5)
		Ag3^{iv}–Ag1^{i}–Ag3^{viii}	78.36(5)
Ag2^{i}–Te1^{v,vi}	2.929(1)	Te1^{v}–Ag2^{i}–Te1^{vi}	111.63(6)
–Te2^{i}	2.817(2)	Te1^{v,vi}–Ag2^{i}–Te2^{i}	110.50(4)
–Te3^{i}	3.076(3)	Te1^{v,vi}–Ag2^{i}–Te3^{i}	110.45(4)
Ag2^{i}–Ag3^{i,x}	3.037(2)	Te2^{i}–Ag2^{i}–Te3^{i}	102.99(6)
		Ag3^{i}–Ag2^{i}–Ag3^{x}	104.34(7)
Ag3^{i}–Te1^{v}	2.783(1)	Te1^{i}–Ag3^{i}–Te2^{v}	102.12(4)
–Te1^{i}	3.142(2)	Te1^{i}–Ag3^{i}–Te3^{i}	74.79(4)
–Te3^{iv}	2.856(1)	Te1^{i}–Ag3^{i}–Te3^{iv}	114.68(5)
–Te3^{i}	2.862(1)	Te1^{v}–Ag3^{i}–Te3^{iv}	116.68(4)
Ag3^{i}–Ag1^{i}	3.036(2)	Te1^{v}–Ag3^{i}–Te3^{i}	121.84(5)
–Ag1^{v}	3.153(2)	Te3^{i}–Ag3^{i}–Te3^{iv}	116.68(4)
–Ag1^{xi}	3.436(2)	Ag1^{i}–Ag3^{i}–Ag1^{v}	96.38(4)
–Ag2^{i}	3.037(2)	Ag1^{i}–Ag3^{i}–Ag1^{xi}	125.48(5)
–Ag3^{ix}	3.001(2)	Ag1^{i}–Ag3^{i}–Ag2^{i}	133.79(6)
		Ag1^{v}–Ag3^{i}–Ag2^{i}	117.30(5)
		Ag1^{i}–Ag3^{i}–Ag3^{ix}	70.01(5)
		Ag1^{v}–Ag3^{i}–Ag3^{ix}	110.20(6)
		Ag2^{ii}–Ag3^{i}–Ag3^{ix}	119.75(7)
Te1^{i}–Te1^{ii}	4.036(2)	Te1^{ii}–Te1^{i}–Te2^{i}	135.10(5)
–Te2^{xii}	2.812(1)	Te1^{ii}–Te1^{i}–Te3^{i}	131.55(5)
–Te2^{i}	3.421(2)	Te2^{i}–Te1^{i}–Te2^{xii}	107.29(5)
–Te3^{i}	3.653(2)	Te2^{i}–Te1^{i}–Te3^{i}	81.37(4)
Te2^{i}–Te1^{xiii,xiv}	2.812(2)	Te2^{xii}–Te1^{i}–Te3^{i}	170.45(5)
–Te1^{i,x}	3.421(2)	Te1^{i}–Te2^{i}–Te1^{xiii}	88.82(4)
Te3^{i}–Te1^{i,x}	3.653(2)	Te1^{x}–Te2^{i}–Te1^{xiv}	88.82(4)
		Te1^{i}–Te2^{i}–Te1^{x}	90.20(4)
		Te1^{xiii}–Te2^{i}–Te1^{xiv}	91.71(4)
		Te1^{i}–Te2^{i}–Te1^{xiv}	174.88(5)
		Te1^{x}–Te2^{i}–Te1^{xiii}	174.88(5)
		Te1^{i}–Te3^{i}–Te1^{x}	83.10(4)

Note: Symmetry codes are: (i): *x*, *y*, *z*; (ii): 3/2 – *x*, *y*, *z*; (iii): 1/2 + *x*, –*y*, –*z*; (iv): 1/2 + *x*, –*y*, 1–*z*; (v): *x*, *y*,1 + *z*; (vi): 1/2 – *x*, *y*, 1 + *z*; (vii): *x*, *y*, –1 + *z*; (viii): 3/2 – *x*, *y*, –1 + *z*; (ix): 1 – *x*, –*y*, 1 – *z*; (x): 1/2 – *x*, *y*, *z* ; (xi): –1/2 + *x*, –*y*, 1 – *z*; (xii): 1 – *x*, 1/2 – *y*, –1/2 + *z*; (xiii): 1 – *x*, 1/2 – *y*, 1/2 + *z* ; (xiv): –1/2 + *x*, 1/2 – *y*, 1/2 + *z* .

nea (1964) with that calculated using the structural parameters obtained in this study. Calculated and observed data are in good agreement, although one diffraction line with very low intensity (d = 2.97 Å, *hkl*: 250; Honea 1964) is forbidden by the space group used in this study.

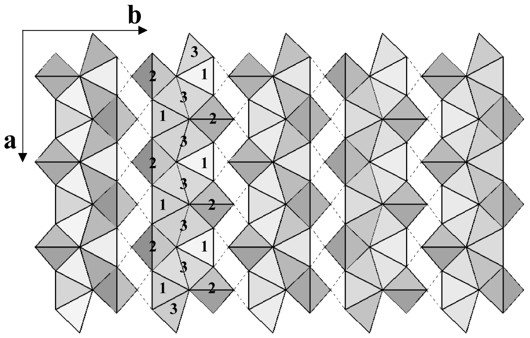

FIGURE 2. The structure of empressite projected down [001]. The numbers (1,2,3) on tetrahedra refer to Ag1, Ag2, and Ag3, respectively. The dashed lines represent the short Te-Te contacts.

The structural study presented here shows that empressite and stützite have different crystal structures. In stützite, highly mobile silver cations are distributed in a tellurium framework forming Frank-Kasper polyhedra (Peters et al. 1996; Kälin and Günter 1996). In addition, tellurium exists as Te^{2-} as well as Te_2 dumbbells and forms three types of tetrahedral sites. By means of a high-resolution electron diffraction study, Kälin and Günter (1996) showed that the crystal structure of stützite can be described as a superstructure of elemental tellurium. The lattice constants a and b of the basic tellurium structure are modulated with a period of 3. Each third spiral chain of the tellurium crystal structure is retained in the tellurium sublattice of $Ag_{4.53}Te_3$. On the other hand, in the crystal structure of empressite (this study), the silver atoms are located at specific positions, without a suggestion of possible diffusion paths. In addition, a careful examination of precession photographs of empressite did not reveal the presence of any extra reflections due to a possible modulated structure.

TABLE 6. X-ray powder diffraction patterns for empressite

	1		2		
hkl	d_{calc} (Å)	I/I_o	*hkl*	d_{obs} (Å)	I/I_o
020	10.05	15	020	10.04	4
140	4.374	< 3	140	4.37	1
111	4.012	15	111, 050	4.02	4
031	3.800	31	031, 121	3.81	6
240	3.3277	30	060, 240	3.33	6
141	3.1742	26	141	3.18	5
221	3.0489	< 3	221, 051	3.04	1
–	–	–	250	2.97	½
231	2.8873	15	151, 231	2.89	4
151	2.8685	7	–	–	–
320	2.8400	9	320	2.85	3
241	2.6990	100	061, 330, 241	2.70	10
161	2.5928	7	161	2.60	2
080	2.5125	4	340, 080, 301, 251	2.51	2
251	2.5035	3	–	–	–
071	2.4379	5	071, 321	2.43	2b
180	2.4176	6	–	–	–
261	2.3138	23	261	2.32	4
002	2.3070	3	–	–	–
012	2.2920	3	012	2.29	1
341	2.2324	6	–	–	–
400	2.2205	34	400, 090, 341, 360, 112	2.23	8
112	2.2193	9	–	–	–
081	2.2066	7	–	–	–
280	2.1868	4	280, 032, 122, 420	2.18	3
032	2.1813	11	–	–	–
271	2.1371	20	181, 271	2.14	5
132	2.1184	4	–	–	–
351	2.1179	14	132, 351, 430	2.12	4
202	2.0472	5	–	–	–
212	2.0367	18	202, 142, 212, 440	2.04	5
0.10.0	2.0100	16	0.10.0, 091, 222, 052, 361	2.01	4
421	1.9623	< 3	421, 232, 1.10.0	1.962	1
431	1.9172	6	431, 062, 380	1.920	3
380	1.9157	6	–	–	–
441	1.8589	< 3	441, 162	1.864	½
291	1.8313	< 3	2.10.0, 291, 252	1.833	½
072	1.7984	< 3	072, 3.12.1, 322, 451	1.796	1
381	1.7692	3	510, 381	1.771	1
332	1.7561	5	332, 470, 520	1.757	2b
182	1.6690	< 3	0.12.0, 182, 272, 1.11.1, 480	1.669	2
511	1.6522	< 3	511, 1.12.0, 471	1.650	1b
092	1.6046	< 3	092, 402, 362	1.604	1b
192	1.5791	3	422, 192, 541, 490, 0.12.1	1.578	2b
541	1.5743	4	–	–	–
481	1.5652	3	481, 2.12.0, 3.10.1, 432	1.562	1b
432	1.5561	6	–	–	–
0.10.2	1.5155	< 3	1.13.0, 103, 0.12.2, 113, 570	1.516	1b
4.10.0	1.4902	9	1.10.2, 491, 4.10.0, 452, 561	1.490	4
561	1.4858	4	–	–	–
043	1.4707	< 3	382, 3.11.1, 043, 620	1.471	1b
0.11.2	1.4324	5	223, 053, 571, 0.14.0, 2.12.2, 0.11.2	1.436	2
640	1.4200	< 3	640, 233, 153, 4.10.1	1.421	1
512	1.4041	5	512, 472, 621, 243	1.403	1b
2.11.2	1.3632	4	0.14.1, 253, 303, 073	1.363	3b
641	1.3572	7	–	–	–
263	1.3333	< 3	–	1.333	1
2.14.1	1.3099	6	–	1.312	2
273	1.2967	4	–	1.296	2b
353	1.2924	4	–	–	–
283	1.2580	< 3	–	1.257	1b
3.14.1	1.2440	< 3	–	1.245	1
443	1.2261	< 3	–	1.224	1vb
4.11.2	1.2037	4	–	1.205	1
592	1.1907	4	–	1.191	½b
3.13.2	1.1783	< 3	–	1.180	½
751	1.1704	3	–	1.172	½
780	1.1326	< 3	–	1.134	1vb
4.15.1	1.1134	< 3	–	1.112	1
781	1.1000	< 3	–	1.099	½b
244	1.0899	< 3	–	1.089	1b
274	1.0757	< 3	–	1.074	1vb
264	1.0592	< 3	–	1.059	½
593	1.0313	< 3	–	1.032	1b
6.14.1	1.0058	< 3	–	1.007	1vb
723	0.9742	< 3	–	0.974	1vb
733	0.9685	< 3	–	0.970	½
3.20.0	0.9517	< 3	–	0.952	1
2.12.4	0.9290	< 3	–	0.929	½b
2.17.3	0.9172	< 3	–	0.918	½b
912	0.9064	< 3	–	0.905	1
644	0.8953	< 3	–	0.896	½b
992	0.8406	3	–	–	–

Notes: 1 = calculated powder pattern and indexing for empressite of this study. d values calculated on the basis of a = 8.882(1), b = 20.100(5), c = 4.614(1) Å, and with the atomic coordinates reported in Table 2. Intensities calculated using XPOW software version 2.0 (Downs et al. 1993). 2 = observed powder pattern and indexing originally reported by Honea (1964).

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