American Mineralogist, Volume 66, pages 376–384, 1981

The crystal structure of bartonite, a potassium iron sulfide, and its relationship to pentlandite and djerfisherite

HOWARD T. EVANS, JR.

U.S. Geological Survey,
Reston, Virginia 22092

AND JOAN R. CLARK

U.S. Geological Survey,
Menlo Park, California 94025

Abstract

The structure of a bartonite crystal from Coyote Peak, Humboldt County, California, has been solved and refined in anisotropic mode to a conventional $R = 0.068$ for 504 observed reflections. The tetragonal unit cell [space group $I4/mmm$, $a = 10.424(1)$, $c = 20.626(1)$Å] contains 2 formula units, which were found by site–occupancy refinement to be $(K,Na)_{5.68}(Fe,Cu,Ni)_{20.27}S_{26}(S,Cl)_{0.93}$. The structure is closely related to those of the cubic minerals pentlandite and djerfisherite. All three minerals have cubic close-packed sulfur layers, which with eight Fe atoms in edge-shared FeS_4 tetrahedra form Fe_8S_{14} cube clusters. Substitutions of K for S in the close-packed layers, the stacking sequence of the cube clusters, and variations in the kinds of atoms and vacancies occupying octahedral and tetrahedral sites explain the structural differences among the three minerals. Average bond distances in bartonite are: Fe–S, 2.289Å; Fe–Fe, 2.724Å; and K–S, 3.369Å.

Introduction

Bartonite was discovered at Coyote Peak, Humboldt County, California, and a complete mineralogical description is given in the accompanying paper by Czamanaske *et al.* (1981). From their study and the present one, bartonite is assigned the idealized chemical formula $K_{6-x}Fe_{24-y}S_{26}(S,Cl)_{1-z}$ with 2 formula units in the tetragonal cell of $I4/mmm$: $a = 10.424(1)$, $c = 20.626(1)$Å. A preliminary description of the crystal structure was given by Clark *et al.* (1979).

Bartonite has a close relationship to pentlandite ($Fm3m$, $a = 10.04$Å) and djerfisherite ($Pm3m$, $a = 10.36$Å), with a shift to tetragonal symmetry and doubled c axis. This property was recognized to be the result of a change in stacking sequence of the Fe_8S_{14} clusters, which are a prominent feature of these structures. The structure analysis showed that other factors, including cation substitutions and vacancies, also are significant in the crystal chemistry of bartonite.

Experimental and computational details

The crystal selected for intensity measurements was cut from a larger crystal to obtain an irregular fragment about 0.1 mm in longest dimension, slightly elongated in an oblique direction. The unit cell parameters determined by Czamanske *et al.* (1981) are given in Table 1. The c axis was oriented parallel to the ϕ axis of a Picker single-crystal diffractometer and 1742 reflections in the angular range 5° to 60° 2θ were measured in Nb–filtered Mo$K\alpha$ radiation. A standard reflection was monitored after each 30 measurements; no significant variation was noted during the data collection. Following correction of intensities for Lorentz and polarization effects and conversion to $|F_0|$, the symmetry-equivalent reflections ($hkl = khl$) were averaged and a set of 817 data was obtained, of which 504 with $|F_0| > 3\sigma(F)$ (where σ was based on counting statistics) were used for the structure analysis. No absorption corrections were made because the crystal shape was irregular al-

0003–004X/81/0304–0376$02.00

Table 1. Crystallographic and other data for bartonite, djerfisherite, and pentlandite

	Bartonite	Djerfisherite		Pentlandite	
Source, ref. (see below)	(1)	(2)	(3)	(4)	(5)
Space group	I4/mmm	Pm3m	Pm3m	Fm3m	Fm3m
a (Å)	10.424(1)	10.358(5)	10.465(1)	10.038(1)	10.521(3)
c	20.626(2)				
V ($Å^3$)	2241.2	1111.3	1146.1	1011.4	1164.6
Formula unit	$K_6Fe_{21}S_{26}(S,Cl)$	$K_6LiFe_{24}S_{26}Cl$	$K_6NaFe_{24}S_{26}Cl$	$(Fe,Ni)_9S_8$	$Ag(Fe,Ni)_9S_8$
Z	2	1	1	4	4
Vol. of S(K,Cl) ($Å^3$)	34.0	33.7	43.7	31.6	36.4

Sources, references:

(1) This study; Czamanske et al (1981).
(2) Synthetic; Tani (1977).
(3) Khibina, Kola Peninsula, USSR; Dmitrieva and Ilyukhin (1976); Czamanske et al (1979).
(4) Frood Mine, Sudbury, Ontario; Rajamani and Prewitt (1973).
(5) Bird River Mines, Ore Fault Claims, Manitoba; Hall and Stewart (1973). These authors also report a refinement of the structure of pentlandite from the Frood Mine, closely similar to that given by Rajamani and Prewitt.

though approximately spherical, and the values of the symmetry-equivalent reflections were in good agreement ($\mu = 83.0$ cm^{-1} for Mo*Kα*). The diffraction profiles were all sharp, and there was no evidence for any diffuse scattering, twinning, or other abnormalities.

The computer program XRAY76 of Stewart (1976) was used during the structural study. The scattering factors for neutral atoms in analytical form and anomalous dispersion factors were taken from Doyle and Turner (1968). The initial atomic coordinates were based on those reported for djerfisherite by Tani (1977), but with Fe_8S_{14} clusters centered at 1/2, 1/2, 0; 1/2, 0, 1/4; and 0, 0, 1/2. The atomic sites in *I4/mmm* are given in Table 2.

Preliminary refinement in anisotropic mode brought the conventional reliability index to $R = 0.078$. The density of bartonite has been measured by R.C. Erd as 3.305(10) g/cm^3, and this value, together with the analytical data (Czamanske *et al.*, 1981) clearly indicated the presence of considerably less than 48 Fe atoms in the unit cell. Therefore, population parameters (P) were introduced for the Fe atoms, and subsequently also for K and S(6). Refinement was repeated in graduated stages, with parameters x, y, z, and U varied first, then those for Fe only with P varying, then the same for K and S(6); following this the P values were held constant and x, y, z, and U_{ij} varied for all atoms. In the last cycles all parameters (53) were varied together, and also weighting factors $\sqrt{w} = 1/\sigma(F)$ were introduced. In this way the refinement proceeded smoothly and with sharp convergence to $R = 0.068$. The correlation coefficients in the last cycle for scale factor with P for Fe was -0.7, and with other P values, -0.5 or less. The correlation of P with the diagonal elements U_{ii} for any atom ranged from 0.2 to 0.5. Although the main sulfur framework [S(1) to S(5) atoms] was assumed to be fully occupied, significant deficiencies were found in the cation site populations. When weights were introduced, no structure shifts resulted that were more than 2σ for the structure parameters, but larger changes occurred for the population and thermal parameters. The most notable change occurred with K(1); it had previously appeared strongly anisotropic in thermal motion, but became essentially isotropic and identical with K(2). In the final stages, composite scattering factors for K and Fe, based on the tables of Doyle and Turner (1968) and the microprobe analysis (see next section), were also introduced. Changes resulting from this procedure were not greater than 1σ for any parameter.

The results of the final, weighted calculations are given in Table 2. The conventional reliability index is $R = 0.068$ and the weighted factor $R_w = 0.076$; the standard deviation of an observation of unit weight is

Table 2. Structure and thermal parameters for bartonite

Structure parameters:

Atom	Site	Occupancy	x	y	z	$\bar{u}$, Å
K(1)	8i	0.920(17)	0.2996(6)	0.0	0.0	0.188(11)
K(2)	4e	1.0	0.0	0.0	0.1539(4)	0.172(10)
Fe(1)	32o	0.841(4)	0.1299(2)	0.3687(2)	0.1841(1)	0.131(4)
Fe(2)	16m	0.864(6)	0.3688(2)	=x	0.0659(1)	0.131(6)
S(1)	16m	1.0	0.2307(3)	=x	0.1159(2)	0.139(6)
S(2)	16n	1.0	0.0	0.2495(3)	0.2510(2)	0.137(8)
S(3)	8j	1.0	0.2506(6)	0.5	0.0	0.135(14)
S(4)	8g	1.0	0.0	0.5	0.1237(2)	0.137(14)
S(5)	4e	1.0	0.0	0.0	0.3726(4)	0.146(15)
S(6)	2a	0.925(34)	0.0	0.0	0.0	0.183(20)

Thermal parameters: U×1000 in $\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{23}k\ell b^*c^*)]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K(1)	34(4)	37(4)	35(4)	0	0	0
K(2)	30(3)	$=U_{11}$	29(4)	0	0	0
Fe(1)	16(1)	18(1)	18(1)	-1(1)	1(1)	-2(1)
Fe(2)	18(1)	$=U_{11}$	15(1)	1(2)	1(1)	$=U_{13}$
S(1)	22(2)	$=U_{11}$	15(2)	3(2)	3(1)	$=U_{13}$
S(2)	26(3)	10(2)	21(2)	0	0	0
S(3)	18(4)	23(4)	14(3)	0	0	0
S(4)	19(4)	23(4)	15(3)	0	0	0
S(5)	22(4)	$=U_{11}$	21(6)	0	0	0
S(6)	31(6)	$=U_{11}$	38(9)	0	0	0

Standard deviations given in terms of last significant digit; zero when not shown.

1.15. The list of structure factors is available on request.[1]

Description of the structure

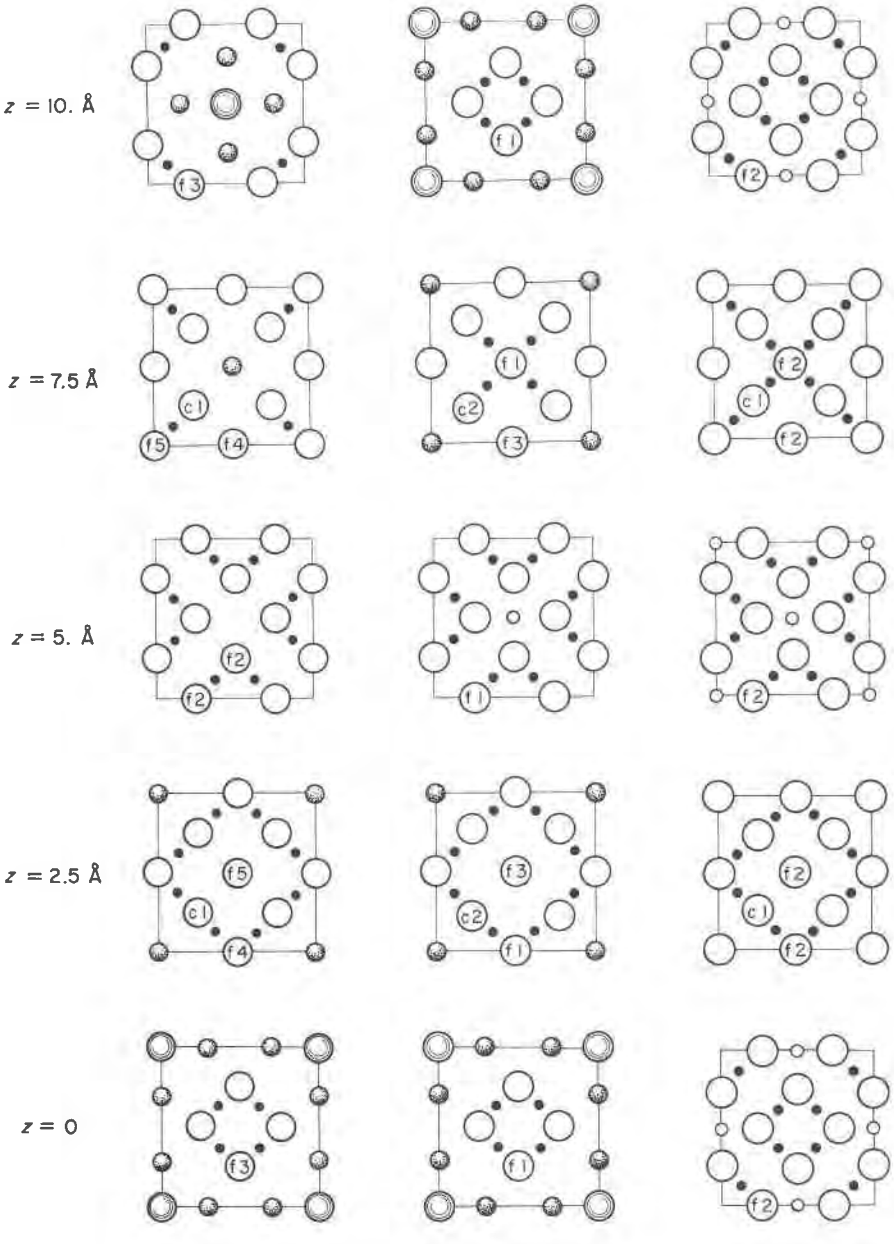
The structure of bartonite is so closely related to the structures reported for pentlandite and djerfisherite that all three are readily considered together. Table 1 summarizes the relevant data and references for the three structures used in the comparison. The idealized, cubic-close-packed layers for each structure are illustrated in Figure 1, which shows the similarities and differences. A summary of the names and coordinates assigned to the sulfur atoms in all three minerals is given in Table 3. Individual bond lengths and angles for bartonite are listed in Table 4. Principal averaged bond lengths in all three minerals are listed for comparison in Table 5.

Aside from the close-packed layers, the important feature these sulfides have in common is the presence of distinctive "cube clusters" in the structure. These Fe_8S_{14} clusters have been illustrated in pentlandite by Rajamani and Prewitt (1973) and by Hall and Stewart (1973). General views of these clusters and their environment are shown for bartonite, djerfisherite, and pentlandite in Figure 2. As far as we know, these three minerals are the only ones in which such clusters have been found.

The atomic thermal motions are shown as 50 percent probability ellipsoids in a partial stereoscopic view of the structure (Figure 3). The atoms in the K_6S group are practically isotropic, whereas the remaining atoms appear to be librating generally about the centers of the Fe_8S_{14} clusters. Figure 3 also shows

---

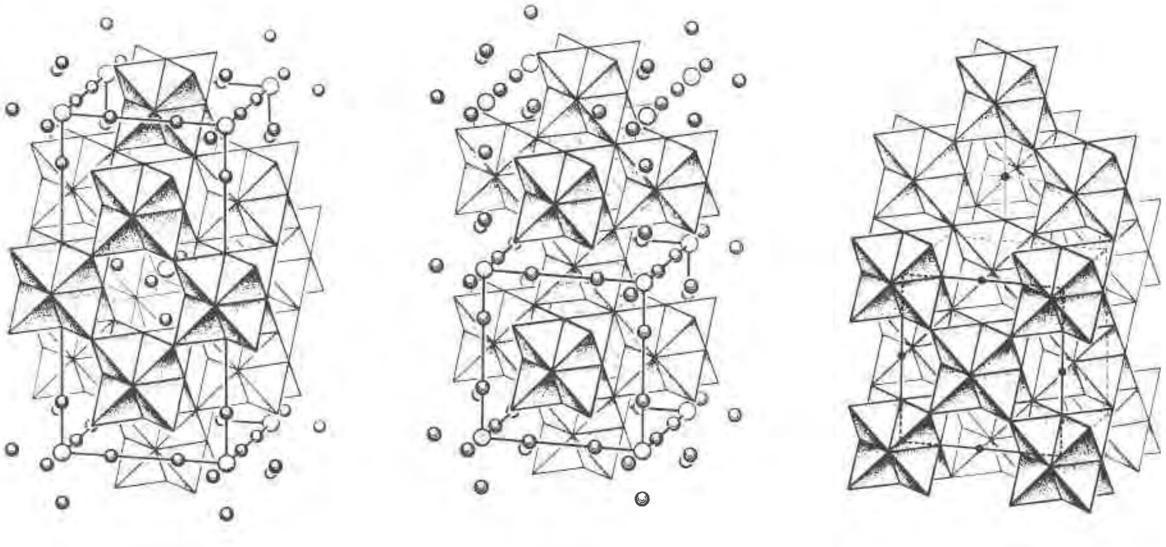
[1] A copy of this table may be obtained by ordering Document AM-81-152 from the Mineralogical Society of America, 2000 Florida Ave. NW, Washington, D.C. 20006. Please remit $1.00 in advance for the microfiche.



Atom key		BARTONITE	DJERFISHERITE	PENTLANDITE
S	○			
X	◎	S, Cl	Cl	—
A	●	K	K	—
M(*tet*)	• (*at* z + 1.25 Å)	Fe,Ni,Cu	Fe,Cu	Fe,Ni
B(*oct*)	○	—	Na,Li	Fe,Ni,Ag

(c = *cube corner*, f = *cube face*)

Fig. 1. Atomic layer sequences in bartonite, djerfisherite and pentlandite projected along the *c* axis. Type numbers for typical S atoms in each layer correspond to original structure descriptions (see Table 3).



BARTONITE DJERFISHERITE PENTLANDITE

Fig. 2. Pictorial representation of the structures of bartonite, djerfisherite, and pentlandite, showing Fe_8S_{14} clusters as condensed tetrahedra. Circle-shaded atoms are K, large circles are S or Cl, small filled circles (in pentlandite) are Fe, Ni, or Ag.

the relative locations of the different kinds of atoms in the structure.

The cube clusters

These clusters contain eight highly-condensed FeS_4 tetrahedra sharing edges. Two crystallographically distinct Fe_8S_{14} clusters are present in the unit cell, four of one type that contains 8Fe(1) atoms and two of the second type with 8Fe(2) atoms, but their dimensions are quite similar. The eight Fe atoms in each cluster are located nearly at corner positions of a cube with an average edge of 2.726[±0.011]Å (maximum deviation 0.018Å). This dimension is close to that found by Tani (1977) in a synthetic lithium djerfisherite (2.72Å), but considerably larger than that in pentlandite (2.53Å). The smaller size of the cluster in pentlandite is probably mainly a result of the extensive replacement of Fe by Ni. There are two main kinds of sulfur atom in the cluster: six [types S(2), S(3), S(4), S(5)] located opposite the faces of the Fe cube, each sharing 4Fe atoms, and which we denote S(f); and eight [type S(1)] located at the corners of the cube, each sharing 3Fe atoms (in different cubes; sharing 4Fe atoms in tetrahedra in pentlandite), which we denote S(c). The identities of the various sulfur atoms in the three structures in terms of these two types are shown in Table 3 and Figure 1.

The environment of the clusters in the three struc-

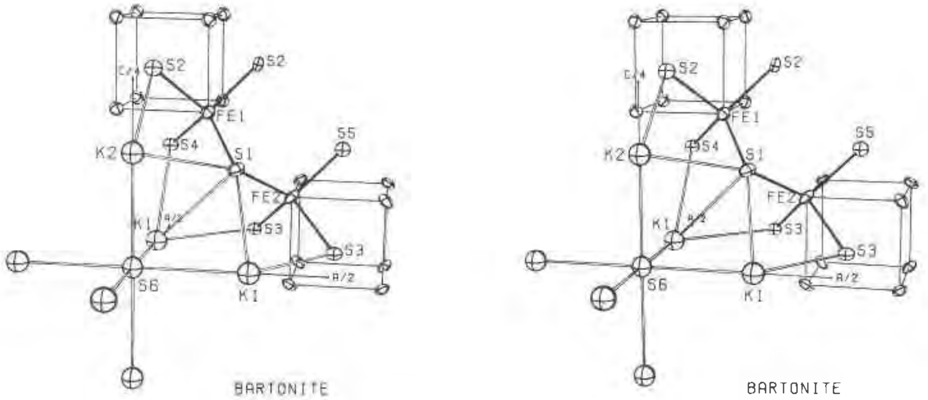


Fig. 3. Detail of the structure of bartonite in stereo view, showing 50 percent probability thermal ellipsoids. Two typical Fe_8 cubes are shown, but only two FeS_4 tetrahedra.

Table 3. Nomenclature and atomic coordinates compared for bartonite, djerfisherite, and pentlandite

Mineral	S(c)	S(f)				Origin site
Bartonite[1] I4/mmm	S(1),16m	S(2),16n	S(3),8j	S(4),8g	S(5),4e	S(6),2a
x	0.2307	0.0	0.2506	0.0	0.5	0.0
y	0.2307	0.2495	0.5	0.5	0.5	0.0
2×z	0.2318	0.5020	0.0	0.2474	0.2548	0.0
Djerfisherite[2] Pm3m	S(2),8g	S(1),12h			S(3),6f	Cl,1a
x	0.226	0.0	0.247	0.0	0.5	0.0
y	0.226	0.247	0.5	0.5	0.5	0.0
z	0.226	0.5	0.0	0.247	0.251	0.0
Pentlandite[3] Fm3m	S(1),8c	S(2),24e				(Vacant)
x	0.25	0.0	0.2368	0.0	0.5	
y	0.25	0.2368	0.5	0.5	0.5	
z	0.25	0.5	0.0	0.2368	0.2632	

Mineral	M(tet)		B(oct)	A	
Bartonite	Fe(1),32o	Fe(2),16m	(Absent)	K(1),8i	K(2),4e
x	0.1299	0.3688		0.2996	0.0
y	0.3687	0.3688		0.0	0.0
2×z	0.3682	0.1318		0.0	0.3078
Djerfisherite	Fe,24m		Li,1b	K,6e	
x	0.1310	0.3683	0.5	0.296	0.0
y	0.3683	0.3683	0.5	0.0	0.0
z	0.3683	0.1310	0.5	0.0	0.296
Pentlandite	M(T),32f		M(O),4b	(Absent)	
x	0.1261	0.3739	0.5		
y	0.3739	0.3739	0.5		
z	0.3739	0.1261	0.5		

[1] This study (from Table 2).
[2] Tani (1977); synthetic.
[3] Rajamani and Prewitt (1973); Frood Mine.

tures is distinctly different, leading to small adjustments of bond lengths and angles within the clusters. In pentlandite the site symmetry of the cluster is the highest, *m*3*m* and all six S(f) atoms are coordinated additionally to an octahedral (Fe,Ni) or Ag atom. In djerfisherite the site symmetry is 4/*mmm* and only two S(f) atoms are coordinated to an octahedral cation (Na or Li). In bartonite two types of cluster are found in the unit cell, two containing Fe(2) with site symmetry 4/*mmm* and four containing Fe(1) with site symmetry $\bar{4}m2$ no octahedral cation sites are present. There does not seem to be any rational way to account for the variations in detailed dimensions in the cluster that are observed within the bartonite structure or among the three structures. For example, it is not clear why in bartonite all the S–Fe–S angles are 107±1° except for one type in each cluster at 119° (Table 4); or why the S(c)–Fe–S(f) angles are 107.50 and the S(f)–Fe–S(f) angles are 111.50 in Frood Mine pentlandite, whereas the reverse is true in silver pentlandite (Table 5).

K_6S groups.

These groups consist of a central S(6) atom at the origin surrounded octahedrally by 4K(1) and 2K(2) atoms (see Figs. 2 and 3). Table 4 shows moderate departures from ideal cubic symmetry in this group. The average K–S(6) distance is 3.15Å, considerably shorter than the other K–S bonds in the ninefold coordination. This bond is comparable with that in K_2S, which has the antifluorite structure and K in fourfold coordination, with a K–S distance of 3.19Å. The other eight bonds for the two K atoms range from 3.283 to 3.490Å, averaging 3.39Å. These may be compared with 3.36Å in lithium djerfisherite, 3.39Å (3.306 to 3.476Å) in $KFeS_2$ (Stevens, 1979; personal communication), and 3.52Å (3.41 to 3.70Å) in rasvumite, KFe_2S_3 (Clark and Brown, 1980). It is

Table 4. Bond lengths and angles in bartonite

Bond lengths (Å):				
Fe-S(c):	Fe(1)-S(1)	2.269(3)	Fe(2)-S(1)	2.282(3)
Fe-S(f):	Fe(1)-S(2)	2.298(4)	Fe(2)-S(3)	2.289(4)(×2)
	-S(2)'	2.290(4)	-S(5)	2.313(5)
	-S(4)	2.293(3)		
S(c)-S(f):	S(1)-S(2)	3.686(5)	S(1)-S(2)'	3.931(5)
	-S(3)	3.693(7)	-S(5)	3.977(4)
	-S(4)	3.700(3)		
S(f)-S(f):	S(2)-S(2)'	3.701(6)	S(3)-S(3)'	3.677(8)
	-S(4)	3.703(5)	-S(5)	3.697(6)
Fe-Fe:	Fe(1)-Fe(1)'	2.708(3)	Fe(2)-Fe(2)'	2.735(3)
	-Fe(1)"	2.739(3)	-Fe(2)"	2.720(3)(‖c)
	-Fe(1)	2.718(3)(‖c)		
	Fe(1)-Fe(1)	3.520(3)	Fe(2)-Fe(1)	3.485(2)
Bond angles (deg.):				
S(c)-Fe-S(f):	S(1)-Fe(1)-S(2)	107.6(1)	S(1)-Fe(2)-S(3)	107.8(2)
	-S(2)'	119.1(1)	-S(5)	119.9(2)
	-S(4)	108.4(1)		
S(f)-Fe-S(f):	S(2)-Fe(1)-S(2)'	107.2(2)	S(3)-Fe(2)-S(3)'	106.9(1)
	-S(4)	107.5(1)	-S(5)	106.9(1)
	-S(4)'	106.5(1)		
K_6S group:	K(1)-S(1)	3.466(3)(×4)	K(2)-S(1)	3.490(3)(×4)
	-S(3)	3.346(6)(×2)	-S(2)	3.283(6)(×4)
	-S(4)	3.300(5)(×2)	-S(6)	3.174(4)
	-S(6)	3.120(6)		
	K(1)-K(1)'	4.413(9)	K(2)-K(1)	4.451(7)

not possible to rationalize all these variations by means of an empirical bond length–strength function such as is commonly used in oxide structures, and the causes for them are unknown. This difficulty is also found in the Fe–S bond system, especially where Fe–Fe interactions may be involved.

Chemical composition

The generalized formula for bartonite found from this structure determination is $K_{6-x}Fe_{24-y}S_{26}(S,Cl)_{1-z}$, where (S,Cl) represents the unique atom at the origin. In the crystal used for this study, the crystal structure analysis indicates a composition with $x = 0.32(10)$, $y = 3.73(8)$, and $z = 0.07(4)$:

$$(K,Na)_{5.68}(Fe,Cu,Ni)_{20.27}S_{26}(S,Cl)_{0.93}$$

After the structure analysis, the crystal was mounted and polished for microprobe analysis by G. Czamanske, who determined the following results:

	wt.%	atoms	
Na	0.14	.14	5.70
K	9.46	5.56	
Fe	50.9	20.92	21.23
Co	0.08	.03	
Ni	0.19	.07	
Cu	0.58	.21	
S	37.6	26.93	(standard)
	98.95		

Chlorine was not detected. Although the microprobe gave a marginally higher Fe/S ratio than the structure analysis, the agreement is remarkably good. Further confirmation of the determined nonstoichiometric composition is provided by the density calculated from the X-ray result, 3.286(11) g/cm^3, which is in excellent agreement with the measured value (from a different specimen) of 3.305(10) g/cm^3 (Czamanske *et al.*, 1981). The value predicted by the microprobe analysis is 3.366 g/cm^3.

For comparison with pentlandite and djerfisherite,

Table 5. Average bond lengths and angles in bartonite, djerfisherite, and pentlandite

Atoms	Bartonite	Djerfisherite		Pentlandite	
B=	--	Li	Na	2(Fe,Ni)	2Ag
Average bond lengths (Å):					
B-S	--	2.58(2)	2.63	2.380(2)	2.676(2)
K-S	3.391	3.36(2)	3.40	--	--
K-(S,Cl)	3.147	3.07(2)	3.13	--	--
M-S(c)	2.276(6)	2.31(1)	2.32	2.154(1)	2.243(2)
M-S(f)	2.295(5)	2.30(2)	2.30	2.258(1)	2.264(2)
M-S(all)	2.289	2.30	2.31	2.232	2.259
M-M	2.726(11)	2.72(2)	2.76	2.531(1)	2.670(2)
Average bond angles (deg.):					
S(c)-M-S(f)	107.9 119.5	107.2	107.	107.18(4)	111.26(3)
S(f)-M-S(f)	107.0	106.4 121.9	107. 122.	111.66(4)	107.63(3)
M-S(c)-M	100.5	97.9	99.	109.47	109.47
M-S(f)-M	72.8 114.2	72.8 113.7	73. 115.	68.19(4)	72.29(5)
References (see Table 1)	(1)	(2)	(3)	(4)	(5)

the composition of bartonite may be expressed more generally as follows:

bartonite	$A_{6-x}M_{24-y}S_{26}X_{1-x}$
djerfisherite	$A_{6-x}BM_{24-y}S_{26}X_{1-x}$
pentlandite	$B_2M_{24-y}S_{26}X_{1-x}$

In these formulas, the tetrahedral M site (M(T) of Rajamani and Prewitt, 1973) may contain Fe, Co, Ni, and Cu. In pentlandite the octahedral B site (M(O) of Rajamani and Prewitt) may contain Co, Fe, Ni, or Ag; in djerfisherite B may be occupied by Cu, Na, or Li. A in bartonite or djerfisherite is K with a little Na; X is S or Cl, mainly S in bartonite, Cl in djerfisherite. The B site is absent in bartonite, and may also have vacancies in the other structures.

Rajamani and Prewitt made a careful study of the crystal chemistry of pentlandite, from which they concluded that the stability of the structure is related to the maintenance of 7 *d* electrons per metal atom in the M_8 cubic unit. This accounts for the confinement of pentlandite to compositions having more or less equal Fe and Ni occupancy (Fe/Ni = 0.65 to 1.5) and a complete solid solution with cobalt pentlandite, Co_9S_8. In djerfisherite and bartonite the situation is more complicated, and the role of *d* electrons is unknown.

Rajamani and Prewitt pointed out that in pentlandite there is clearly a strong M–M interaction in the M_8 cube, and therefore the true oxidation state of M does not correspond to the formal valence ratio ($14/8 = +1.75$, assuming B and S are divalent). In terms of the available electrons and the oxidation potential of the phase with respect to the environment, the formal valence of M may be qualitatively significant. In both pentlandite and djerfisherite the formal valence is low (1.78 and 1.92, respectively) but in bartonite it is 2.38. In other iron sulfide minerals from the Coyote Peak diatreme, higher formal valences are found (e.g., 2.50 for rasvumite KFe_2S_3, 3.0 for erdite $NaFeS_2 \cdot 2H_2O$). The paragenesis of these minerals and their possible relationship to the oxidation potential of the environment are topics discussed by Czamanske *et al.* (1981).

Conclusion

When these three cluster structures and their various occupancies, substitutions, and vacancies are considered, further variations are easily envisioned in the sites that could produce different but related structures. The limits within which any one structure will persist are less easily defined. Clearly, much synthetic and crystallographic work lies ahead if all the characteristics of these fascinating and versatile sulfides are to be revealed and understood.

Acknowledgments

We thank our colleagues at the U.S. Geological Survey, Menlo Park, G. K. Czamanske and R. C. Erd, who provided the bartonite crystal and much helpful discussion of the problems. Judith A. Konnert, U. S. Geological Survey, Reston, gave valuable assistance with computer programs. Some stimulating discussions about the structure were held with G. E. Brown, Jr., Department of Geology, Stanford University, and Emil Makovicky, Institute of Mineralogy, University of Copenhagen, Denmark. We also thank Dr. R. E. Stevens of State University of New York at Buffalo for providing us with information about $KFeS_2$ previous to publication.

References

Clark, J. R., Brown, G. E. Jr., Konnert, J. A., and Evans, H. T. Jr. (1979) Atomic arrangements of three alkali iron sulfide minerals. American Crystallographic Association, Program and Abstracts, Series 2, 6(2), 88.

Czamanske, G. K., Erd, R. C., Leonard, B. F., and Clark, J. R. (1981) Bartonite, a new potassium iron sulfide mineral. American Mineralogist 66, 369–375.

Czamanske, G. K., Erd, R. C., Sokolova, N. M., Dobrovol'skaya, M. G., and Dmitrieva, M. T. (1979) New data on rasvumite and djerfisherite. American Mineralogist 64, 776–778.

Dmitrieva, M. T. and Ilyukhin, V. V. (1975) Crystal structure of djerfisherite. Doklady Akademiia Nauk USSR 223, 343–346 (transl. Soviet Physics Doklady 20, 469–470, 1976).

Doyle, P. A. and Turner, P. S. (1968) Relativistic Hartree-Fock X-ray and electron scattering factors. Acta Crystallographica A24, 390–397.

Hall, S. R. and Stewart, J. M. (1973) The crystal structure of argentian pentlandite $(Fe,Ni)_8AgS_8$ compared with the refined structure of pentlandite $(Fe,Ni)_9S_8$. Canadian Mineralogist 12, 169–177.

Rajamani, V. and Prewitt, C. T. (1973) Crystal chemistry of natural pentlandites. Canadian Mineralogist 12, 178–187.

Stevens, E. D. (1979) Experimental electron density distribution of potassium iron disulfide. American Crystallographic Association, Program and Abstracts, Series 2, 7(1), 49.

Stewart, J. M., Editor (1976) The X-ray system-version of 1976. Tech. Report TR-446, Computer Science Center, University of Maryland, College Park, Maryland.

Tani, B. S. (1977) X-ray study of $K_6LiFe_{24}S_{26}Cl$, a djerfisherite-like compound. American Mineralogist 62, 819–823.

Manuscript received, July 7, 1980;
accepted for publication, October 22, 1980.