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Mössbauer analysis of synthetic djerfisherite

DJERFISHERITE, $K_6(Fe,Ni)_{26}S_{26}Cl$, is one of three naturally occurring potassium transition element sulphides that have been discovered in recent years. Only limited data are as yet available concerning the structure and composition range of this material; published results have been reviewed by Clarke (1977). In this note we discuss the results of a ^{57}Fe Mössbauer analysis of a synthetic djerfisherite of composition $K_{5.85}(Fe_{0.53}Ni_{0.47})_{26.30}S_{25.94}Cl_{1.06}$. The preparation technique and the analysis of the composition of this sample (24F̄) were discussed by Clarke (1977); in addition to djerfisherite, it contained minor (< 10%) amounts of other phases.

A room-temperature ^{57}Fe Mössbauer spectrum was obtained using a conventional constant-acceleration Mössbauer spectrometer. The spectrum is shown in fig. 1. It was computer-analysed in terms of two symmetrical doublets of Lorentzian lines. In the figure the positions of the lines and their relative intensities are indicated. The low-intensity doublet has Mössbauer parameters similar to those obtained for $KFeS_2$ (Raj and Puri, 1969; Kerler *et al.*, 1963) and may indicate small amounts of unreacted potassium thioferrite in the sample.

The major doublet in our spectrum is that due to djerfisherite. The Mössbauer parameters for this doublet are given in Table I. We discuss this doublet in relation to results obtained in the mineral pentlandite $(Fe,Ni)_9S_8$, which has a structure very similar to the one proposed for djerfisherite. In pentlandite, of the thirty-six cations (four formula units) per unit cell, thirty-two are contained in tetrahedral sites, arranged in clusters of eight cations forming a simple cube (Rahamani and Prewitt, 1973). The four remaining cations are in octahedral sites. In the structure proposed for djerfisherite (Dmitrieva and Ilyukhin, 1976), the same arrangement of cations in tetrahedral sites is found but the octahedral sites remain empty. Distances from a tetrahedrally coordinated cation to the near-neighbouring sulphur and metal atoms are given for samples of each material in Table II.

Although interatomic distances in djerfisherite are somewhat larger than the corresponding distances in pentlandite, the overall near-neighbouring coordination is sufficiently similar that one may expect comparable Mössbauer parameters. In Table I we have also listed Mössbauer parameters measured for pentlandites. It is obvious from an inspection of these results that the

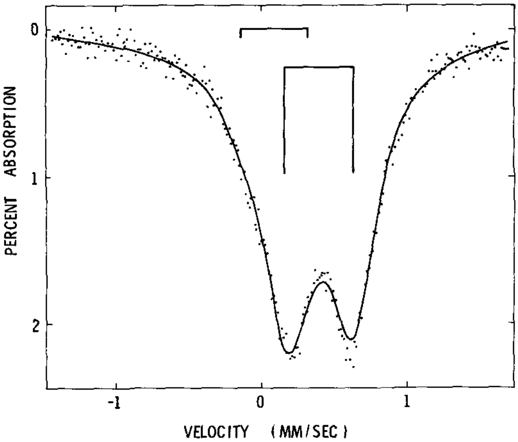

FIG. 1. Mössbauer spectrum of djerfisherite.

TABLE I. *Mössbauer parameters of ^{57}Fe in pentlandite and djerfisherite; room temperature*

Samples	Fe coordination	IS* (mm/s)	ΔE_Q (mm/s)	References
Pentlandite	Tetrahedral	0.36	0.37	Vaughan and Ridout (1971)
	Octahedral	0.57	0	
Pentlandite	Tetrahedral	0.36-0.38	0.29-0.31	Knop *et al.* (1970)
	Octahedral	0.65-0.68	0	
Djerfisherite	Tetrahedral	0.39	0.46	This work

* Relative to metallic iron.

TABLE II. *Distances from a tetrahedrally coordinated transition metal ion to near-neighbouring atoms in pentlandite and djerfisherite*

Sample	M-S_1	M-S_2($\times$ 3)	M-M($\times$ 3)	References
Pentlandite	2.15	2.25	2.52	Raj and Puri (1969)
Djerfisherite	2.29	2.31	2.76	Kerler *et al.* (1963)

Mössbauer parameters of tetrahedrally coordinated Fe are similar in djerfisherite and pentlandite, and no evidence is found that the octahedral sites are occupied by Fe in djerfisherite, as opposed to the additional singlet found in pentlandite Mössbauer spectra, which was attributed to Fe in those sites.

Thus our Mössbauer results support the structure proposed by Dmitrieva and Ilyukhin (1976) for djerfisherite.

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Mossite discredited

MOSSITE was originally described by Brøgger (1897) from Berg, Råde, near Moss, Norway. The precise locality remains unknown but Brøgger (1906) assumed Berg or Elvestad in Råde. Lake Vannsjø, situated just east of Moss, is surrounded by a number of classic feldspar quarries which date back to 1870-80. The quarries were in dikes; the accessory minerals in the dikes were columbite, monazite, uraninite, and beryl (Bjørlykke, 1939). The dikes are presently inaccessible due to overgrowth and the use of some of them for the storage of refuse.

Mossite has been considered until now to be an iron niobate referred to the tetragonal tapiolite group and having the ideal formula, $Fe(Nb,Ta)_2O_6$. It has been considered the niobium analogue of tapiolite, $FeTa_2O_6$, and, together, mossite and tapiolite have been considered the tetragonal analogues of orthorhombic ferrocolumbite and ferrotantalite, respectively. Recently, it has been postulated that mossite does not exist as a valid species (Clark and Fejer, 1978). In addition, Moreau and Tramasure (1965) indicated that mossite is unlikely to occur in nature.

The existence of mossite as a legitimate species has long been doubted by various investigators. The original analysis had a Ta_2O_5:Nb_2O_5 ratio of 118:116 and Schaller (1912) correctly noted that