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THE CRYSTAL STRUCTURE OF YAVAPAIITE:
A DISCUSSION

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ABSTRACT

The crystal structure of yavapaiite, recently determined by Graeber and Rosenzweig (1972), is shown to be similar to those of FeSO_4 and Na_2SO_4 (III). Crystal data and atomic parameters determined in this study are presented.

The crystal structure of the mineral yavapaiite, $KFe(SO_4)_2$, was recently determined by Graeber and Rosenzweig (1972). We had finished preparation of a manuscript dealing with that structure when we discovered that their work was in press. We feel that some of the conclusions we had reached regarding the yavapaiite structure are worthy of note as additions to their work.

Graeber and Rosenzweig suggest that the structure of yavapaiite is closely related to that of krausite (Graeber, Morosin, and Rosenzweig, 1965). We had noted instead the relationship of yavapaiite to several of the simpler nesotetrahedral compounds. We would compare the structure of yavapaiite to those of $FeSO_4$ and Na_2SO_4 (III). The crystal data of these compounds are compared to those of yavapaiite in Table 1.

$FeSO_4$ is one of a group of isostructural compounds which includes $CrVO_4$, $CaCrO_4$, $CoCrO_4$, $CuCrO_4$, $NiCrO_4$, $ZnCrO_4$, $NiSO_4$, $MgSO_4$, $MnSO_4$, $CoSO_4$, $InPO_4$, and $TiPO_4$ for which $CrVO_4$ is considered to be the type structure (Brandt, 1943; and Wyckoff, 1965). A projection of the structure of $FeSO_4$ (Coing-Boyat, 1959) on the b - c plane is shown in Figure 1 for comparison with yavapaiite. The similarities between the two arrangements are seen in the locations and orientations of the SO_4 tetrahedral units and in the analogous special positions occupied by the potassium and ferric iron ions of yavapaiite and by the ferrous iron ions of $FeSO_4$. The distortion of the $FeSO_4$ structure to make room for the large potassium ions in half of the special positions and the smaller ferric iron in the other half, brings about a rotation of the SO_4 units around axes normal to the plane of the projection and leads to the development of monoclinicity, general lowering of symmetry, and the notable lengthening of the c unit cell edge of yavapaiite relative to $FeSO_4$. The six-fold coordination by oxygen of the ferrous iron atoms in $FeSO_4$ is increased to ten for

Table 1. Crystal data for yavapaiite and compounds of similar structure

	Yavapaiite		$FeSO_4$	Na_2SO_4 (III)
	(Graeber and Rosenzweig, 1972)	(Present study)	(Coing-Boyat, 1959)	(Das Gupta, 1954)
a	8.152(5) Å	8.150(4) Å	b 7.97 Å	8.726 Å
b	5.153(4)	5.162(3)	a 5.25	5.592
c	7.877(5)	7.855(5)	c 6.59	6.953
β	$94^{\circ}54'$ (1)	$94^{\circ}52'$ (2)	90°	90°
Space Group	$C2/m$	$C2/m$	$Cmcm$	$Cmcm$
V^0 calc.	2.891	2.895		
Z	2	2	4	4

the potassium atom in the equivalent sites in yavapaiite, while the coordination of the smaller ferric iron atoms remains six fold.

Comparison of the yavapaiite structure to that of orthorhombic Na_2SO_4 (III) (Das Gupta, 1954) follows a very similar course. The

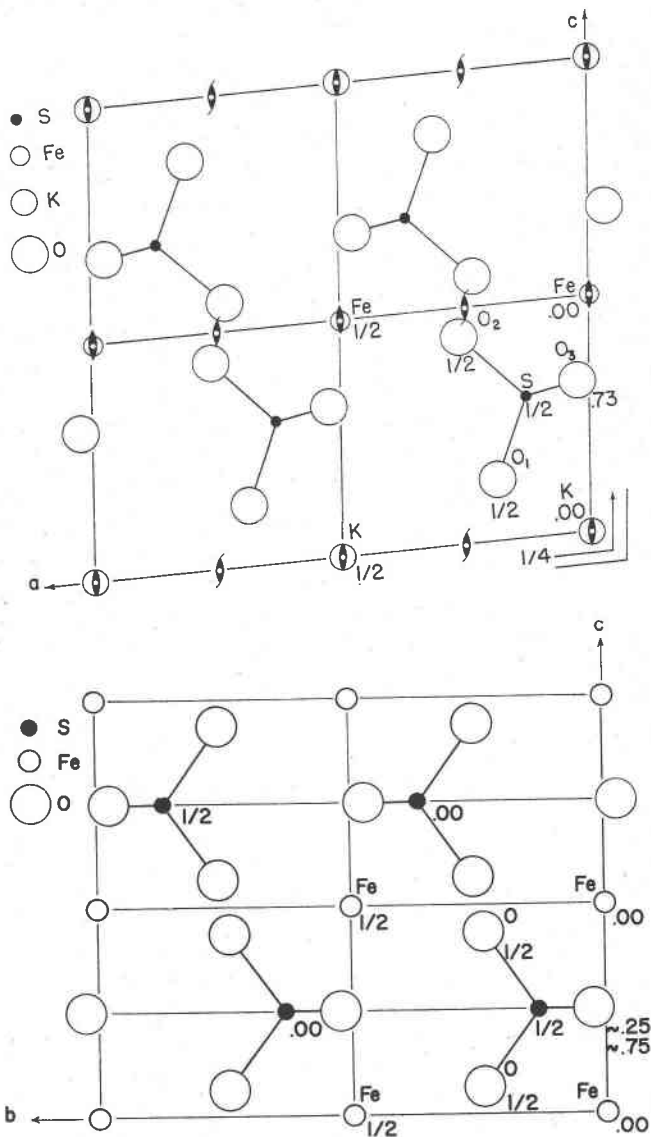


FIG. 1. A. The structure of yavapaiite viewed in projection along b .
B. The structure of FeSO_4 , (after Coing-Boyat) viewed in projection along a .

Table 2. Positional and temperature parameters for yavapaiite. Parameters listed on top are those of Graeber and Rosenzweig and those below are from the present work with origin converted to that of Graeber and Rosenzweig.

	x	y	z	B
Fe	.0000	.0000	.0000	0.67 0.45(2)
K	.0000	.0000	.5000	1.69 1.50(1)
S	.3701(1) .3700(1)	.0000 .0000	.2020(1) .2020(1)	0.56 0.47(1)
O(1)	.2371(3) .2369(4)	.0000 .0000	.0626(4) .0628(4)	1.08 0.89(4)
O(2)	.3128(4) .3124(5)	.0000 .0000	.3702(4) .3700(5)	1.76 1.49(5)
O(3)	.4741(3) .4741(3)	.2325(4) .2330(6)	.1807(3) .1810(3)	1.22 1.08(3)

structure of Na_2SO_4 (III) requires an additional cation site for sodium. Replacement of one-fourth of the sodium atoms in Na_2SO_4 (III) by the larger potassium accounts for the increased c cell parameter in yavapaiite (Table 1), while the substantially larger a and b cell dimensions of Na_2SO_4 (III) result from the additional sodium site.

It is perhaps also worthwhile to compare the positional and temperature parameters for the yavapaiite structure as determined by Graeber and Rosenzweig with those determined in the present study (Table 2). In the present work an automated diffractometer was used to measure 1168 reflections from a sphere ground from Jerome material. After correction for normal effects and for absorption the structure was solved routinely from a three dimensional Patterson synthesis and refined to an R factor of 0.071 with isotropic temperature factors.

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