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Possible unit cell for danielsite

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Abstract

The X-ray powder-diffraction pattern of danielsite, $(Cu,Ag)_{14}HgS_8$, can be indexed on an orthorhombic unit cell with $a = 9.644$, $b = 9.180$, and $c = 18.156$ Å. This unit cell contains four formula units and gives a calculated density of 6.541 g/cm³.

Introduction

Danielsite was described as a new mineral by Nickel (1987). Microprobe analyses gave a composition corresponding to $(Cu,Ag)_{14}HgS_8$, with Cu:Ag approximately 1.6. This formula is similar to that of balkanite, $Cu_9Ag_5HgS_8$, which has Cu:Ag = 1.8 (Atanassov and Kirov, 1973), but the X-ray powder-diffraction patterns of the two minerals are quite different. According to Nickel (1987), it was not possible to obtain single-crystal diffraction patterns of danielsite, and attempts to calculate a unit-cell consistent with the powder-diffraction pattern were unsuccessful. Consequently, the published X-ray diffraction pattern of danielsite was not indexed, and the description lacked unit-cell parameters. This brief contribution is intended to overcome that shortcoming.

Proposed unit-cell parameters

The X-ray powder-diffraction pattern of danielsite is given in Table 1. The attempt to find a unit cell was started by assuming an orthogonal cell, with the first three diffraction peaks (highest d values) corresponding to ($0kl$), ($0k2$), and ($0k3$). This gave a trial value for c and for the b^*-c^* interrelationship, which enabled the value of 2 to be assigned to k. An estimation of the value of a was based on the value of the density of balkanite, which appears to be isochemical with danielsite.

The preliminary values of the unit-cell parameters were then used to index the d values of the danielsite powder-diffraction pattern by means of a least-squares computer program. The final values are $a = 9.644(6)$, $b = 9.180(5)$, and $c = 18.156(9)$ Å. The d values calculated from the cell parameters are given in Table 1. As can be seen, all the lines can be indexed, and there is satisfactory agreement between the calculated and measured values.

The calculated density of danielsite—using the unit-cell given above and the chemical composition reported by Nickel (1987) and assuming Z to be 4—is 6.541 g/cm³, which is reasonably close to the measured value of synthetic $Cu_9Ag_5HgS_8$ (balkanite), namely 6.32 g/cm³.

The unit cell of balkanite has been reported as being orthorhombic, with $a = 10.62$, $b = 9.42$, and $c = 3.92$ Å

TABLE 1. Indexed X-ray powder-diffraction pattern of danielsite

I_{est}*	d_{obs}*	d_{calc}†	*hkl*
2	4.44	4.450	021
1	4.11	4.107	104
		4.096	022
2	3.648	3.657	023
		3.631	005
½	3.493	3.488	213
½	3.401	3.398	105
1	3.314	3.325	220
		3.305	204
½	3.198	3.187	115
2B	3.018	3.026	006
		3.017	031
½	2.885	2.887	106
		2.880	131
3	2.831	2.839	303
10	2.622	2.627	133
		2.623	304
1	2.564	2.563	206
		2.558	231
1	2.475	2.469	216
5	2.392	2.407	305
		2.390	401
½	2.222	2.225	042
		2.217	217
1	2.080	2.081	333
		2.078	422
1	2.034	2.034	028
1	1.991	1.992	334
		1.991	128
		1.986	326
6	1.959	1.960	243
6	1.875	1.877	511
		1.874	228
2	1.692	1.692	147
1	1.642	1.638	055
½	1.588	1.590	239
		1.589	346
		1.588	351
½	1.512	1.513	0.0.12
		1.512	621
		1.511	445
½	1.425	1.427	058
		1.426	2.1.12
		1.424	0.4.10
1B	1.279	1.280	1.5.10
		1.279	462
1	1.259	1.258	168
		1.257	609

* From Nickel (1987).
† Calculated from an orthorhombic cell with $a = 9.644$, $b = 9.180$, and $c = 18.156$ Å.

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(Atanassov and Kirov, 1973). These unit-cell parameters are different from those of danielsite, and there does not seem to be a simple relationship between the unit cells of the two minerals. From a compositional standpoint, the two minerals appear to be dimorphs, apart from the difference in their Cu:Ag ratios, which may or may not be a significant factor. From the reported occurrences of the two minerals, it is apparent that balkanite is the high-temperature, and danielsite the low-temperature, form.

Although the unit cell for danielsite proposed here provides a satisfactory indexing of the X-ray powder-diffraction pattern and gives reasonable cell contents and calculated density, a definitive characterization of its crystallographic parameters must await a single-crystal X-ray diffraction study. The type specimen, from Coppin Pool in Western Australia, does not provide suitable material for such a study, and, until more suitable material is found, the proposed unit cell will have to suffice.

References cited

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