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The crystal structure of calaverite

Author(s): G. Tunell and C. J. Ksanda

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empirically by the use of ferrous ammonium sulfate as a standard substance.

CRYSTALLOGRAPHY.—*The crystal structure of calaverite.*<sup>1</sup> G. TUNELL and C. J. KSANDA, Geophysical Laboratory, Carnegie Institution of Washington.

The morphology of calaverite has been thoroughly investigated by a number of crystallographers.<sup>2</sup> Goldschmidt, Palache, and Peacock<sup>3</sup> concluded that calaverite crystallizes in the monoclinic system although they pointed out that an orthorhombic interpretation was not excluded with certainty by the evidence then available. They determined accurately the following values of the crystallographic elements of calaverite:<sup>4</sup>  $a:b:c = 1.6298:1:1.1492$ ,  $\beta = 90^{\circ}08'$ . Concerning the value of  $\beta$  they<sup>5</sup> wrote: "Aus diesen Messungen erhalten wir  $89^{\circ}52'$  als besten Mittelwert des Winkels zwischen den zwei Achsen in der Projectionsebene. Dieser Winkel ist so nahe an  $90^{\circ}$ , dass die Frage, ob der Neigungswinkel von  $90^{\circ}$  verschieden ist, nicht aus den Messungen entschieden werden kann." In their comprehensive joint study of the form system of calaverite they report that it has a two-fold axis of symmetry.<sup>6</sup> From the statements of Penfield and Ford,<sup>7</sup> together with his own observations, Peacock<sup>8</sup> concludes that it has also a plane of symmetry. From its crystal habit, then, calaverite appears to belong to the holohedral symmetry class,  $2/m (C_{2h})$ , of the monoclinic system.

Crystals of calaverite from Cripple Creek, Colorado, have been studied by the present authors by means of the Weissenberg X-ray goniometer and the two-circle reflection goniometer. The reciprocal lattice of calaverite was established by means of Weissenberg photographs taken with Cr-, Cu-, and Mo-radiation, although the crystals of calaverite were not single individuals. The structural lattice has elements strictly analogous to the fundamental morphological elements of Goldschmidt, Palache, and Peacock (their *S*-elements).

<sup>1</sup> Received December 8, 1934.

<sup>2</sup> See V. GOLDSCHMIDT, C. PALACHE, and M. PEACOCK, *Neues Jahrbuch für Mineralogie, Geologie und Paläontologie, Beilage-Band 63*: Abt. A, S. 50-52. 1931, and M. A. PEACOCK, *American Mineralogist* 17: 318. 1932, for references to previous work.

<sup>3</sup> *Op. cit.*, pp. 6, 7, see also M. A. PEACOCK, *op. cit.*, pp. 324, 325.

<sup>4</sup> M. A. PEACOCK, *op. cit.*, p. 325.

<sup>5</sup> V. GOLDSCHMIDT, C. PALACHE, and M. PEACOCK, *op. cit.*, p. 5.

<sup>6</sup> V. GOLDSCHMIDT, C. PALACHE, and M. PEACOCK, *op. cit.*, pp. 6 and 21.

<sup>7</sup> *Am. Jour. Sci.* (4) 12: 236. 1901.

<sup>8</sup> Personal communication to G. TUNELL, dated April 25, 1934.

The dimensions of the unit cell, determined by purely röntgenographic measurements, are:  $a_0 = 7.18 \text{ \AA}$ ,  $b_0 = 4.40 \text{ \AA}$ ,  $c_0 = 5.07 \text{ \AA}$ , all  $\pm 0.03 \text{ \AA}$ ,  $\beta = 90^\circ \pm 30'$ . Our Weissenberg films also yield decisive evidence on the question of the crystal system of calaverite. On the Weissenberg films the planes,  $hkl$  and  $h\bar{k}l$ , in general yield diffraction spots of very different intensity. This would not be possible if calaverite belonged to the orthorhombic system, irrespective of the space group in the orthorhombic system with which it might be isomorphous. It is therefore certain that calaverite does not belong to the orthorhombic system. The systematic extinctions of the X-ray diffraction effects on our films limit the monoclinic space groups possible for calaverite to three:  $C2/m$  ( $C_{2h}^3$ ),  $C2$  ( $C_2^3$ ), or  $Cm$  ( $C_s^3$ ), the extinctions of these three space groups being identical. The density of calaverite calculated from the X-ray data is 9.31. This agrees well with the measured<sup>9</sup> densities and fixes the number of molecules of  $\text{AuTe}_2$  in the unit cell as 2. The two gold atoms can only occupy the positions, 0, 0, 0, and  $\frac{1}{2}$ ,  $\frac{1}{2}$ , 0, no matter which of the three monoclinic space groups listed above is that of calaverite. By means of the intensities alone all arrangements of the tellurium atoms possible in the space group,  $Cm$ , have been excluded. From the intensities it is also certain that the tellurium atoms do not occupy fixed positions or positions with one variable parameter in the space group,  $C2/m$ . Hence the tellurium atoms must occupy the positions,  $m$ , 0,  $p$ ;  $\bar{m}$ , 0,  $\bar{p}$ ;  $m + \frac{1}{2}$ ,  $\frac{1}{2}$ ,  $p$ ;  $\frac{1}{2} - m$ ,  $\frac{1}{2}$ ,  $\bar{p}$ , in the space group,  $C2/m$ , or the positions,  $\bar{m}$ ,  $n$ ,  $p$ ;  $\bar{m}$ ,  $n$ ,  $\bar{p}$ ;  $m + \frac{1}{2}$ ,  $n + \frac{1}{2}$ ,  $p$ ;  $\frac{1}{2} - m$ ,  $n + \frac{1}{2}$ ,  $\bar{p}$ , in the space group,  $C2$ . From the intensities of the successive orders of reflection of (100) and (001) the  $m$ - and  $p$ -parameters of the tellurium atoms have been determined to be  $m = 0.69$  ( $2\pi m = 247^\circ$ ) and  $p = 0.29$  ( $2\pi p = 105^\circ$ ) no matter which of the two remaining space groups,  $C2/m$  and  $C2$ , is that of calaverite. From the intensities of the other reflections the parameter along the  $b$ -axis must be close to 0. Thus the tellurium atoms occupy the positions,  $m$ ,  $n$ ,  $p$ ;  $\bar{m}$ ,  $n$ ,  $\bar{p}$ ;  $m + \frac{1}{2}$ ,  $n + \frac{1}{2}$ ,  $p$ ;  $\frac{1}{2} - m$ ,  $n + \frac{1}{2}$ ,  $\bar{p}$ , where  $m = 0.69$ ,  $n = 0.00$ , and  $p = 0.29$ , all  $\pm 0.05$ .<sup>10</sup> The results of the intensity calculations will be given in greater detail in a subsequent communication.

<sup>9</sup> Cf. S. L. PENFIELD and W. E. FORD, *Am. Jour. Sci.* (4) 12: 246. 1901, *Zeit. f. Kryst. und Min.* 35: 450. 1901; G. F. H. SMITH, *Min. Mag.* 13: 149. 1902, *Zeit. f. Kryst. und Min.* 37: 234. 1902; E. S. SIMPSON, *Geological Survey of Western Australia, Bulletin* 42: 107. 1912.

<sup>10</sup> The correspondence between the positive and negative senses of our axes and those of Goldschmidt, Palache, and Peacock has not been established as yet but only the correspondence between the directions of our axes and those of Goldschmidt, Palache, and Peacock.