CRYSTALLOGRAPHY OF DOLEROPHANITE

W. E. RICHMOND AND C. W. WOLFE, Harvard University, Cambridge, Mass.

Crystals of dolerophanite, Cu₂SO₅, formed during the eruption of Mt. Vesuvius in October 1868, were described by Scacchi (1873). V. Goldschmidt (1886) chose a different orientation from that of Scacchi and calculated new elements. Dana (1892) adopted Scacchi's elements, but interchanged the a- and c-axes. Strandmark (1902), working with artificial crystals found in copper slag, selected a still different orientation; and Zambonini (1935), in an exhaustive study of the morphology, adopted Strandmark's orientation but calculated new elements based on more reliable measurements.

Table 1. Dolerophanite: Correlation of Settings

Forms	Scacchi	Goldschmidt	Dana (1892)	Strandmark- Zambonini		
a 100	g	g	g	g		
b 010	C	$\overset{\circ}{C}$	$\overset{\circ}{b}$	$\overset{\circ}{\mathcal{C}}$		
c 001	A	A	a	\overline{A}		
m 110	t	1	1	t		
o 410	-	-	-	0		
ω 011	-	-	-	ω		
l 201	-	_		l		
$\mu = 304$	-	-	-	u		
j 405	~	-		j		
d 101	d	d	d	J		
B = 403	B	B	C	В		
$e \overline{201}$	e	e	e	3		
f 401	f	f	f	f		
v 111	-		-	v		
r I12	r	r	r	r		
p 314	Þ	Þ	Þ	Þ		
n = 133	n	n	n	n		
s 111	S	s	s	S		
q 312	q	q	a	a		
$h \overline{803}$	-	h	4	$egin{array}{c} q \ h \end{array}$		
y 601	_	-		n y		

An x-ray crystallographic study shows that the orientation and unit of Goldschmidt correspond with the face-centered lattice generally chosen by x-ray crystallographers, and the orientation of Strandmark is the corresponding body-centered lattice of the same network. The transformations of other orientations to the Goldschmidt orientation and unit are:

Scacchi to Goldschmidt -400/040/303Dana to Goldschmidt -004/040/303Strandmark to Goldschmidt -101/010/001

The correlation of forms is given in Table 1. The letters used here are those of Scacchi except that the pinacoids and unit prism have been given letters conforming to standard usage.

The accepted forms of dolerophanite are shown on the gnomonic projection (Fig. 1). A typical crystal is illustrated in Fig. 2.

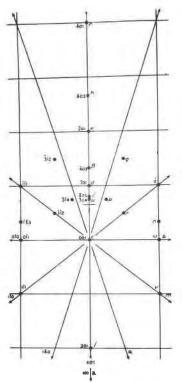


Fig. 1. Gnomonic projection of the accepted forms of dolerophanite.

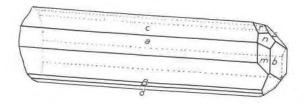


Fig. 2. Typical crystal of dolerophanite.

Since Zambonini's measurements are probably the best, his elements, transformed to Goldschmidt's orientation are adopted in the angle table (Table 2).

Table 2. Angle Table of Dolerophanite, $\mathrm{Cu_2SO_5}$ Monoclinic; prismatic—2/m

 $\begin{array}{l} a:b:c=1.4842:1:1.2089;\ \beta=122^{\circ}18\frac{1}{2}';\ p_{0}:q_{0}:r_{0}=0.8145:1.0217:1\\ r_{2}:p_{2}:q_{2}=0.9787:0.8127:1;\ \mu=57^{\circ}41\frac{1}{2}';\ p_{0}'=0.9637,\ q_{0}'=1.2089,\ x_{0}'=0.6324 \end{array}$

			_										
F	orms	φ	9	ρ	9	0	ψ2	ρ_2	=B		C		A
с	001	90°	00′	32°	18½′	57	°41½′	90°	°00′	0,	00′	57	°41\f
b	010	0 (00	90 (00	-		0	00	90	00	90	00
a	100	90 (00	90 (00	0	00	90	00	57	$41\frac{1}{2}$	0	00
m	110	38 3	$33\frac{1}{2}$	90 (00	0	00	38	$33\frac{1}{2}$	70	$32\frac{1}{2}$	51	$26\frac{1}{2}$
0	410	72 3	$35\frac{1}{2}$	90 (00	0	00	72	$35\frac{1}{2}$	59	20	17	$24\frac{1}{2}$
ω	011	27 3	37	53	$45\frac{1}{2}$	57	$41\frac{1}{2}$	44	23	45	37		03
μ	304	-90 (00	5	$13\frac{1}{2}$	95	$13\frac{1}{2}$	90	00	37	32	95	$13\frac{1}{2}$
j	405	-90 (00	7 .	$53\frac{1}{2}$	97	$53\frac{1}{2}$	90	00	40	12	97	$53\frac{1}{2}$
d	T01	-90 (00	18 :	20	108	20	90	00	50	$38\frac{1}{2}$	108	20
В	403	-90 (00	33 ($07\frac{1}{2}$	123	$07\frac{1}{2}$	90	00	65	26	123	07½
l	201	90 (00	68 3	$39\frac{1}{2}$	21	$20\frac{1}{2}$	90	00	36	$21\frac{1}{2}$		$20\frac{1}{2}$
e	201	-90 (00	52	$19\frac{1}{2}$	142	$19\frac{1}{2}$	90	00	84	38	142	_
h	803	-90 (00	62 4	42	152	42	90	00	95	$00\frac{1}{2}$	152	42
f	401	-90(00	72	$45\frac{1}{2}$	162	$45\frac{1}{2}$	90	00	105	04	162	$45\frac{1}{2}$
у	601	90 (00	81 ($)8\frac{1}{2}$	8	$51\frac{1}{2}$	90	00	48	50	8	$51\frac{1}{2}$
r	Ī12	13 5	59	31 3	35	81	$26\frac{1}{2}$	59	08	38	13	82	39½
v	111	52 5	$51\frac{1}{2}$	63	$27\frac{1}{2}$	32	04	57	$18\frac{1}{2}$	40	$38\frac{1}{2}$	44	$30\frac{1}{2}$
S	Ī11	-151	$19\frac{1}{2}$	51 2	25	108	20	41	04	65	$22\frac{1}{2}$	101	$55\frac{1}{2}$
r	Ī33	14 2	26	51	18	72	43	40	54	50	$46\frac{1}{2}$	78	47
þ	$\overline{3}14$	-16 4	$19\frac{1}{2}$	17 3	$31\frac{1}{2}$	95	$13\frac{1}{2}$	73	15	40	$35\frac{1}{2}$	95	00
q	$\overline{3}12$	-532	$22\frac{1}{2}$	45 2	$22\frac{1}{2}$	129	07	64	$52\frac{1}{2}$	73	14	124	50

3.

Uncertain forms: 10.0.1, 13.0.1, 14.0.1, 883, 269.

X-RAY STUDY

Richmond (1939) determined the lattice constants of dolerophanite. The crystal used for this work was approximately 0.5 millimeter in length and 0.25 millimeter in section. Rotation and Weissenberg photographs were taken about the b[010] and c[001] axes, using copper radiation.

Reciprocal lattice projections were made of the zero and first layer-line photographs taken about the b[010] axis.

The reciprocal lattice chosen to conform to morphological conventions resulted in a body-centered lattice. The alternate face-centered lattice was therefore adopted. The reflections on the Weissenberg photographs, referred to this lattice, are:

$$(hkl)$$
 = with h and k even
 $(h0l)$ = with h even
 $(0k0)$ = with k even

These criteria, together with the fact that previous morphological investigations indicated holohedral symmetry, give the space group $C_{2h}^3 - C_2/m$.

The lattice constants, calculated from the Weissenberg photographs are:

$$a_0 = 9.39 \text{ Å}$$

 $b_0 = 6.30 \text{ Å}$
 $a_0: b_0: c_0 = 1.490: 1: 1.209; \beta = 122°41\frac{1}{2}'$
 $c_0 = 7.62 \text{ Å}$

Contents of the unit cell. The analysis by Zambonini and a new specific gravity (4.17) determined by Richmond, together with the lattice constants, give the content of the unit cell as shown in Table 3.

TABLE 3. DOLEROPHANITE: CONTENTS OF THE UNIT CELL

1	2	3		4	5	6
65.20	66.06	0.830	Cu	0.830	7.98	8
33.49	33.94	0.424	S	0.424	4.07	4
1.31	_	-	О	2.120	20.20	20
100.00	100.00					
	33.49	33.49 33.94 1.31 —	33.49 33.94 0.424 1.31 — —	33.49 33.94 0.424 S 1.31 — O	33.49 33.94 0.424 S 0.424 1.31 — O 2.120	33.49 33.94 0.424 S 0.424 4.07 1.31 — O 2.120 20.20

- 1. Analysis of dolerophanite; analyst, Zambonini.
- 2. Analysis recalculated to 100%.
- 3. Molecular proportions.
- 4. Atomic proportions.
- 5. Number of atoms in the unit cell.
- 6. Theoretical number of atoms in the unit cell.

From column 6 the unit cell contains 4[Cu₂SO₅].

OPTICAL PROPERTIES

Zambonini gave incomplete optical data. Therefore, Dr. Harry Berman determined the indices of refraction and optical orientation of dolerophanite which, in Goldschmidt's orientation, are:

		Indices (Na	a)
X	deep brown	1.715	positive
Y = b	brownish yellow	1.820	$2V = 85^{\circ}$
$Z \wedge c = -10^{\circ}$	lemon yellow	1.880	r > v, very strong, crossed dispersion

References

Dana, E. S.: System of Mineralogy, New York, 924 (1892). Goldschmidt, V.: Index d. Kryst. Min., Berlin, 511 (1886). Richmond, W. E.: Thesis, Harvard University (1939). Scacchi, A.: Atti. Accad. Napoli, 5 (1873).

Strandmark, J. E.: Zeits. Kryst., **36**, 457 (1902). Zambonini, F.: Min. Ves., 2d ed., 161 (1935).