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The orientation of the Miller–Bravais axes of α-quartz.

By A. R. LANG, *H. H. Wills Physics Laboratory, University of Bristol, England*

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The major rhombohedron of α-quartz, *r*, which has indices {100} referred to rhombohedral Miller axes, will have indices $\{10\bar{1}1\}$ or $\{01\bar{1}1\}$ in the Miller–Bravais system according to whether the rhombohedral axes are set in the obverse or reverse orientation with respect to the hexagonal axes. The former, obverse orientation is established practice in morphological descriptions of α-quartz: it is used by Tschermak (1884), by Michel Lévy (Lévy & Lacroix, 1888), by *Dana's System of Mineralogy* (Dana 1920, Frondel 1962) and by Tutton (1911). It is also the orientation adopted in *International Tables for X-ray Crystallography* (Henry & Lonsdale, 1952) as standard for rhombohedral to hexagonal unit-cell transformations. Miller–Bravais indices came into use rather slowly in English mineralogies; some texts use the alternative setting and could cause confusion. Story-Maskelyne (1895) and Miers (1902, 1929), while using none other than rhombohedral axes in their descriptions of trigonal crystals, both give the Miller to Miller–Bravais transformation with the rhombohedron in the reverse orientation.

In the classic structure determination of Bragg & Gibbs (Bragg & Gibbs, 1925; Gibbs, 1926) the conventional obverse orientation is used. This is clear from Gibbs's report, for example, that the $10\bar{1}1$ reflexion was stronger than the $10\bar{1}\bar{1}$, and the $30\bar{3}1$ very much stronger than the $30\bar{3}\bar{1}$. In the later structure analysis of Wei (1935), on the other hand, the reverse orientation is used. The effect of this change is simply described (when Friedel's Law is obeyed) as a reversal of the sign of all Wei's *l* indices with respect to those of the morphological descriptions and of Gibbs. Wei's indexing has been followed by Brill, Hermann & Peters (1942), Bond & Armstrong (1946), and quite recently by Young & Post (1962) and Smith & Alexander (1963). However, the conventional indexing was used in the X-ray intensity measurements of Wooster & Macdonald (1948) and de Vries (1958).

Wei used coordinates of equivalent positions in space group $P3_121$ derived by Wyckoff (1922). The four parameters to be determined in the α-quartz structure are, in Wyckoff's notation, *u* for silicon and *x*, *y* and *z* for oxygen. In *Strukturbericht* (Ewald & Hermann, 1931) Wyckoff's coordinates of equivalent positions were quoted but the possible values of *x* and *y* derived from Gibbs's (1926) data were apparently miscalculated, as pointed out by Wei. Wyckoff's own estimates of these parameters (Wyckoff, 1931) came close to the values found by Wei. Now Wyckoff (1922) used a *left*-handed hexagonal coordinate system for his expressions for equivalent positions in trigonal and hexagonal space groups. (In *Internationale Tabellen* (Hermann, 1935) transformation of Wyckoff's left-handed system to a right-handed system is made without comment). Wei has drawn the α-quartz structure, analytically described by Wyckoff's left-handed coordinates, in right-handed axes. Besides altering the hand of the structure, this has the effect of changing from obverse to reverse orientation. Thus, in Wei's axes the plane which is structurally the major rhombohedron, *r*, will be given the indices $\{01\bar{1}1\}$. From this accident, so it appears, arose the unconventional orientation of Wei and those who have followed him. Curiously, Wyckoff (1948) repeats his original left-handed coordinates for the right-handed structure $P3_121$ but depicts the structure in right-handed coordinates like Wei. Hence the structure appears left-handed and in reverse orientation. Wyckoff's (1948) coordinates and figure are copied by Frondel (1962).

Calling Wyckoff's left-handed hexagonal axes a_1', a_2' and *c*, his coordinates show that his $P3_121$ and $P3_221$ cells have a twofold axis at height zero parallel to a_1'. The corresponding cells in *International Tables for X-ray Crystallography*, with axes here referred to as a_1, a_2 and *c*, have a twofold axis at height zero parallel to $\mathbf{a}_1+\mathbf{a}_2$. [The disposition of symmetry elements in Wyckoff's $P3_121$ cell when drawn in right-handed axes, as by Wei, is the same as in the $P3_221$ cell drawn by Buerger (1956)]. Thus the relations between the axes a_1 and a_2 of *International Tables* and Wyckoff's a_1' and a_2' are $\mathbf{a}_1=-\mathbf{a}_1'-\mathbf{a}_2'$, $\mathbf{a}_2=\mathbf{a}_2'$. When using the coordinates of equivalent positions of space groups $P3_121$ and $P3_221$ as given in *International Tables* instead of as by Wyckoff no change need be made in Wyckoff's parameters *u*, *x* and *y*, but Wyckoff's *z* must be replaced by $\frac{1}{3}-z$.

Many studies of α-quartz are performed on polished plates whose orientation with respect to the morphological axes must be unambiguously determined. This information can be obtained conveniently by comparing intensities of non-equivalent pairs of reflexions such as *hkil* and *hkil̄* provided that there is no ambiguity of indexing in the published intensity data. It is clearly desirable to use the same axes in X-ray intensity measurements on α-quartz as are accepted in the morphological description. Thus one should follow Gibbs, or Wyckoff (1931) (remembering the hand of his axes!), and not Wei.

In view of the confusion in the literature it is useful to have a mnemonic for the correct, obverse orientation of the Miller–Bravais axes with respect to the α-quartz structure. Place the origin on one of the threefold screw axes that intersect the twofold axes [as is done in *International Tables* (1952)]. Look along this threefold screw axis towards the origin. The six silicon atoms surrounding the threefold screw axis project on the basal plane as a distorted hexagon, with included angles alternately more acute and more obtuse than 120°. In $P3_121$ the axes a_1, a_2 and a_3 run outwards from the more obtuse corners of the distorted hexagon, whereas in $P3_221$ they run outwards from the more acute corners.

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