General Electric XRD-5 are essentially identical with X-ray data for bindheimite compiled by Mason and Vitaliano (1953).

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MEASUREMENT OF THE DISTORTION INDEX (DELTA) OF CORDIERITE

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### Abstract

Identification and use of  $K_{\alpha_1}$  reflections in the X-ray diffraction pattern permit more reliable determination of the distortion.

Miyashiro and his affiliates first discovered that cordierite, (Mg, Fe, Mn)<sub>2</sub>Al<sub>4</sub>Si<sub>5</sub>O<sub>18</sub>, occurs in different structural states (Miyashiro & Iiyama, 1954; Miyashiro, Iiyama, Yamasaki & Miyashiro, 1955; Miyashiro, 1957). This phenomenon probably reflects long-range order-disorder relations of Al-Si and Mg-Al (Miyashiro, 1957, p. 45; Schreyer & Yoder, Yoder, 1964, p. 311; Gibbs, 1966, p. 1072). The disorder arrangement would be realized in hexagonal high cordierite (called indialite by the earlier Japanese authors), whereas an increase in ordering would result in an orthorhombic crystal structure. The ordering is thought to be a continuous process, its degree, and thus the degree of distortion from the hexagonal structure being tied to a certain maximum. The degree of ordering in a certain cordierite would be mainly dependent on P-T conditions during and subsequent to its growth (Schreyer, 1966). The variation in structure can be demonstrated in X-ray diffraction diagrams, preferably between  $2\theta = 29^{\circ}$  and  $2\theta = 30^{\circ}$ , Cu K<sub> $\alpha$ </sub>. The hexagonal high cordierite shows one peak in this region, 1231 (Iivama, 1956); whereas in orthorhombic forms it is split up into as many as 3 peaks, 511 (A), 421 (B) and 131 (D) (Iiyama, 1956). Empirically, Miyashiro (1957) found that an appropriate measure for ordering in cordierite is given

by the distortion index:  $\Delta = 2\theta_{131} - \frac{2\theta_{511} + 2\theta_{421}}{2}$ , CuK<sub>al</sub>-radiation.

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This parameter has been universally accepted to describe the structural state of cordierite, see for instance, Schreyer (1966).  $\Delta = 0^{\circ}$  for high-cordierite, and  $\Delta$  increases continuously with increasing ordering to a maximum value of  $0.29^{\circ}-0.31^{\circ}$  for any Fe/Mg ratio of the mineral. Meagher & Gibbs (1965) and Gibbs (written communication, 1969) called attention to the point that  $\Delta$  is not only a function of the structural state of cordierite, but that it is also influenced by its chemical composition.<sup>1</sup>

Since  $\Delta$  was introduced, no further specification has been given for its exact measurement. There is even disagreement among the various authors about the interpretation of the peak topography in the pertinent region (Schreyer, 1966, pp. 228-229, versus Iiyama, 1956, and Miyashiro, 1957, 44). To solve this problem, a number of diffractometer charts and step-scan recordings were made of an approximately 90% pure cordierite concentrate (see Fig. 1a,b,c,d). In particular, the step-scan recordings (one of which is shown in Fig. 1a) strongly suggest that Iiyama's interpretation is correct: the peak configuration dominated by three strong  $CuK_{\alpha 1}$  peaks is complicated by the occurrence of their  $K_{\alpha 2}$  components. The measured angular separation between the supposed  $K_{\alpha 1}$ - $K_{\alpha 2}$  pairs is  $0.075^{\circ} 2\theta$ , which is exactly the figure expected from the difference in wavelength between  $CuK_{\alpha 1}$  and  $CuK_{\alpha 2}$ . No indication was found in support of the explicit conclusion of Schreyer (1966, pp. 228-229) that the appearance of peak C is a grain size effect, bound to disappear with intensive grinding.

In computing the values of  $\Delta$ , the  $K_{\alpha_1}$  reflections were used. The location of the mean of a  $K_{\alpha_1}$  peak was established rather high in the peak body, roughly half way between the top and the place where the  $K_{\alpha_2}$  reflection visibly distorts the peak (cf. Fig. 1). Peaks A and B were not evaluated separately, but the  $2\theta$  value corresponding to their combined peak was used. The author is aware of the fact that, due to overlapping of the peaks, the true positions of the  $K_{\alpha_1}$  reflections cannot be obtained in this way. The exact locations may be found by Fourier analysis, cleaning away the instrumental peak broadening. Alternatively, diffraction diagrams should be made with monochromatic X-rays. As facilities for these more precise measurements are not available for many mineral-

<sup>1</sup> Note added in proof: Recently, D. S. Harwood & R. R. Larson (1969, Amer. Mineral., 54, 896-908) described cordierites with varying values of  $\Delta$  from a contact aureole in Maine (U. S.) and they concluded that the variations in  $\Delta$  can be related to variations in T within the contact aureole, and that  $\Delta$  is a measure of the Al-Si distribution in cordierite. They found  $\Delta$  to be independent of the MgO/(MgO+FeO) and Al<sub>2</sub>O<sub>3</sub>/(Al<sub>2</sub>O<sub>3</sub>+SiO<sub>2</sub>) ratios of the cordierites, but it varies inversely with the beryllium content (ranging from 7 to 15 ppm). The minor variations in Be are thought to indicate that the ability of cordierite to accommodate Be varies with its structural state [cf. also R. C. Newton (1966) Mineral. Mag., 35, 920-927].



ogists-petrologists, the method explained above will still be used for the time being. The author believes that, when using this method for fairly rich concentrates of cordierite with a fairly high  $\Delta$  value, a series of strip-chart diagrams will suffice to determine  $\Delta$  within 0.01°-0.02°. For rather poor cordierite concentrates and presumably for cordierite with

a small  $\Delta$  value, a step-scan recording becomes necessary (cf. Fig. 1e). In that case automatic step-scan devices, including a print out, come in handy. During the step-scan procedure it is recommended to run the strip-chart recorder simultaneously in order to check the stability of the apparatus.

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FIG. 1. X-ray diffraction diagrams of cordierite concentrates, which served to measure the distortion index,  $\Delta$ . a and e are step-scan recordings; b, c and d are diagrams produced by continuous chart registration. Except for e, which represents sample Z 73 Ho (a cordierite-bearing volcanite described in Zeck, 1968, pp. 35–61), the diagrams are made from the same concentrate of cordierite derived from sample Z 15 Ho, (cordierite-bearing) almandine-biotite-sillimanite gneiss (Zeck, 1968, pp. 65–72). Grain size of the concentrates was below 10  $\mu$ m. Apparatus used: Philips wide-angle powder diffractometer (PW 1050) and electronic circuit panel (PW 1051), copper tube, normal line focus, take-off angle 3°, Ni-filter attached to the receiving slit, 1 kW generator (PW 1010) used on 40 kV, 20 mA, proportional counter, 1675 V. Further specific conditions for each diagram: (a) step-scan recording, steps 0.01° 2 $\theta$ , 120 sec. counting time each step, slits: 1/6°, 0.05 mm, 1/6°; (e) ditto, but 240 sec. counting time each step; b-continuous chart registration, slits 1/2°, 0.1 mm, 1/2°, goniometer speed 1/4° per min., paper speed 80 cm/h, scale factor 1/4, time constant 4 sec.; c, d-ditto, but scale factor 1/8.