

Estimation Cation Site-Occupancy in Amphibole by Means of Powder XRD

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The method that estimation cation site-occupancy in amphibole with intensity of peaks in powder diffraction pattern is discussed in this paper. Two linear statistic models, which is function about cation site-occupancy to intensities of diffraction peak, are built by step by step regression with 18 peaks in pattern of calc-amphibole and 15 peaks in that of alkali-amphibole.

Experimental data proved that this method is reliable not only in fact of theory but also in experiment. For calc-amphibole or alkali-amphibole, precision of estimation are both up to 90% or so. So the result can meet needs of studying crystal-chemistry on amphibole.

Comparison with names from composition by chemical analysis and estimated cation site-occupancy according to table of international classification for amphibole, they are very similar and about 80~85% are equal. Therefore, the statement of elder scholar, which is that amphibole group can't be studied by powder XRD, is negated.