Determination of Chlorite Compositions by X-Ray Spacings and Intensities

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Abstract: The cell dimensions and compositions of four chlorites whose crystal structures have been determined in detail are used to test existing graphs and regression equations designed to give tetrahedral and octahedral compositions. It is found that the thicknesses of the tetrahedral sheet, the 2:1 octahedral sheet, the interlayer sheet, and the space between the 2:1 layer and the interlayer can vary appreciably from specimen to specimen quite independently of tetrahedral composition. Total octahedral composition, the number of octahedral vacancies, cation ordering, and the distribution of trivalent cations and of charge between the two octahedral sheets must have effects on *d*(001) that are additional to the effect of tetrahedral composition. Nevertheless, Brindley's *d*(001) graph and a regression equation by Kepezhinskas both should give tetrahedral compositions with an average error of 10%, or about $0 \cdot 1$ Al^{IV}, for most trioctahedral chlorites. They are not valid for dioctahedral or di, trioctahedral species. Equations derived from the data of von Engelhardt and of Shirozu relating the *b* parameter to octahedral Fe, Mn content give results with an average error of 10%, or $0 \cdot 1$ Fe, Mn, for the four test chlorites provided Cr is included with the Fe, Mn, as does a regression equation by Kepezhinskas that contains terms for both the *b* parameter and *d*(001). Methods using the (00*l*) intensities or structure amplitudes give less consistent results for heavy atom contents than the spacing methods, but can be used to give approximate values for the asymmetry in distribution of heavy atoms between the 2:1 octahedral sheet and the interlayer.

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