08.4–28 THE MYTH OF LOEWENSTEIN'S RULE. By Wulf Depmeier, Chimie appliquée, University of Geneva, Geneva, Switzerland.

Loewenstein's rule (W.Loewenstein, Amer. Miner.39, 92; 1954) essentially states that AlO_4 tetrahedra should not share corners in tetrahedral framework structures, if this can be avoided. This rule is sometimes misunderstood as an absolute prohibition. This is valid especially in zeolite chemistry where it is frequently argued that a lower limit of the ratio Si:Al must be 1, "because of Loewenstein's rule". Furthermore, using the same argument, any excess of Al in the total composition, if present, is explained by the postulation of Al-rich occlusions within the cages. However, there are several examples known where Loewenstein's rule is not obeyed. The sodalite family seems to exhibit a variable framework composition with a Si:Al ratio between almost ∞ and 0 (Depmeier, Acta Cryst.40B, in press,1984) and stuffed tridymite-like structures are known with pure AlO_4 frameworks (e.g., Hörkner & Müller-Buschbaum, J.inorg.nucl.Chem. 38,983,1976). Another example is found in the series gehlenite - pentacalcium trialuminate (Louisnathan, Can. Miner.10,822,1970; Vincent & Jeffery,Acta Cryst.B34, 1422,1978) where one AlO_4 tetrahedron having framework character is connected with other AlO_4 tetrahedra. These examples suggest that a Si:Al ratio < 1.0 in the framework should not be excluded a priori. Similarly, the answer to the question whether Al-rich zeolites exist must not necessarily be in the negative. It seems that the violations of Loewenstein's rule are often connected with severe distortions of the tetrahedra (Depmeier,Acta Cryst.B40, in press, 1984).

08.4–29 WHOLE PATTERN REFINEMENT OF RANDOMLY INTERSTRATIFIED CLAY MINERALS
By I.G. Wood and G. Brown, Soils and Plant Nutrition Department, Rothamsted Experimental Station, Harpenden, Herts. AL5 2JQ, U.K.

The information necessary to characterise interstratified clay minerals is the number, type and distribution of interlayer species and the average number of alumino-silicate layers in each coherently diffracting unit. In principle, all of these parameters may be determined from the intensity distribution along the line in reciprocal space normal to the plane of the alumino-silicate layers. Provided that suitably oriented samples can be prepared, the use of these basal reflections simplifies the problem considerably as then only the calculation of a one-dimensional diffraction pattern is required. If the different interlayer species are also assumed to occur in a random sequence further simplification results. The auto-correlation function may then be determined simply from the concentrations and spacings of the different interlayers and the thicknesses of the coherently diffracting domains, leading to an analytical solution of the problem (Wright, A.C. (1975). Clays and Clay Minerals 23, 278-88).

Previous analyses of interstratified minerals have usually involved manual adjustment of the parameters to obtain a calculated intensity distribution that resembles the one observed. This is unsatisfactory as it gives no indication of the probable error of the values obtained or of correlations between variables. A program has, therefore been developed which allows least-squares refinement of the structural parameters to obtain the best fit over the entire pattern. The procedure is similar to that used in Rietveld refinement (Rietveld, H.M. (1969). J. Appl. Cryst. 2, 65-71). It requires, however, a much more exact calculation of the diffraction pattern to include the structural disorder and small particle size. Terms describing the background intensity (which appears to be of the form expected from amorphous material) and the effects of the preferred orientation of the clay particles on the Lorentz factor must also be included. Applications of the program to complex interstratifications in a calcium-montmorillonite at different relative humidities (Ormerod, E.C. and Newman, A.C.D. (1983). Clay Minerals 18, 289-99) and to illite-smectite interstratifications in weathered Oxford Clay (Weir, A.H. and Rayner, J.H. (1974). Clay Minerals 10, 173-187) will be presented. Atomic coordinates are determined to within approximately ±0.02Å, site occupancies to ±0.2 atoms and interlayer separations to ±0.01Å.

Although designed primarily for use in the study of soil clays, the method is applicable to any material randomly disordered in one dimension.

08.4–30 CRYSTAL STRUCTURE AND LOCAL DEFORMATION IN $K_2M_2^{++}(SO_4)_3$ - COMPOUNDS OF THE LANGBEINITE - TYPE. By D. Speer and E. Salje, Institut für Kristallographie und Petrographie, Universität Hannover, Welfengarten 1, 3000 Hannover 1, Federal Republic of Germany.

The high temperature modifications of potassium -langbeinites $K_2M_2^{++}(SO_4)_3$ (M^{++} = Zn, Ni, Co and Mg) show cubic symmetry with S.G. = $P2_13$ (Z=4). The structure is described as a network of SO_4 - tetrahedra which share common corners with distorted oxygen octahedra around the divalent metal positions.
The potassium atoms fill the larger holes of the structure. The local deformation of the $(M^{++}O_6)$ - octahedra changes significantly with chemical composition and is closely related to the structural polymorphism $P2_13$ - $P2_12_12_1$.
Two types of deformations were found:

a) a tilt around the trigonal axis of two triangular faces of the octahedra and
b) an offcentering of M^{++} along the trigonal axis.

The two symmetry - inequivalent octahedra show dominantly either the deformation of type a) or b). The tilt angle and the magnitude of the offcentering increase with increasing ion - radius of M^{++}. Only $K_2Zn_2(SO_4)_3$ shows a slightly different behaviour. The known struc-