By the "breathing mode" a sequence of large and small Te-squares is formed in such a way that a big Te-square is located between two Nb atoms of short bond distance and a smaller Te square is formed when the Nb-atoms are further apart. By the oscillatory motion of the libration mode Te-Te pair bonds occur between Te atoms of different antiprisms about $(0,0,z)$ and about $(1/2,1/2,z)$. The bond lengths vary between 2.90(1) Å and 2.95(1) Å . In the Nb-chain along c the bond lengths vary between 3.08(1) Å for a Nb-Nb pair and 3.96 Å between Nb_3-groups.

By the refinement calculations in the space-group P4 the following R-values have been obtained : R=0.062 for the modulated structure (1024 unique reflections), R=0.062 for the average structure (290 unique main reflections) and R=0.046 for the complement structure (734 unique satellite reflections).

The scale factor has been refined by the main reflections (average structure), whereas, the atomic shifts have been determined by the satellite reflections alone (complement structure).

The evaluation of the Patterson-function as well as a Fourier-synthesis confirm the obtained results.

TABLE

Space groups	Type of modulation	main reflections R_M	satellites R_S	common R
$P^I\,{}^{mmm}_{\bar{1}s1}$	occupational	0.0611	0.1617	0.0894
$P^I\,{}^{2mm}_{ss1}$	occupational	0.0619	0.1380	0.0833
$P^I\,{}^{mmm}_{\bar{1}s1}$	mixed	0.0553	0.0908	0.0653
$P^I\,{}^{2mm}_{ss1}$	mixed	0.0555	0.0822	0.0630

The improvement due to the superposed displacive wave (displacement of ions along y, only) is evident. The difference between the two space groups, solves the p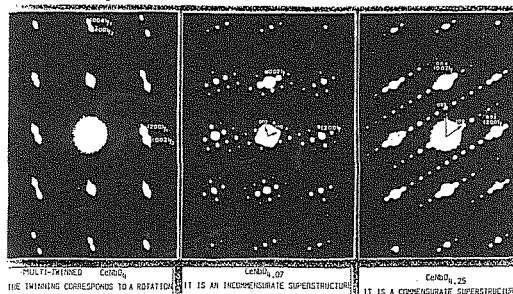roblem of phase shifts between the modulating waves. Contrary to $P^I\,{}^{2mm}_{ss1}$, the $P^I\,{}^{mmm}_{\bar{1}s1}$ group excludes all relative phase shifts between the individual waves. The phase shifts, however, do exist as indicated by the significant lowering of R_S index (see Table). The occupational wave of NO_2 group is shifted in respect to Na^+ ion wave by about $22°$. There are practically no phase shifts between the individual displacive and occupational waves. The amplitude of the displacive wave of Na^+ was found almost two times as big as that of NO_2, with the occupational amplitudes being approximately the same.

20.4–6   RE-EXAMINATION OF THE MODULATED STRUCTURE OF THE $NaNO_2$ IN ANTIFERROELECTRIC PHASE.

By W.A. Paciorek and D. Kucharczyk, Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland.

The structure of the antiferroelectric phase of $NaNO_2$ has been refined (Kucharczyk et al., Ferroelectric (1978) 21, 445) for a mixed occupational and displacive modulation model. This was later supported by theorethical studies (Michel, Phys. Rev. B (1981) 24, 3998; Mc Connell & Heine, Phys. Rev. Lett. (1981) 46, 1091). However, due to a number of simplifications concerning the symmetry treatment, the refinement procedure and some arbitraryness in phase relationships of the modulating waves, the obtained structure is no longer the good base for more detailed studies. We decided, therefore, to reinvestigate this structure by applying the recently developed approach to modulated structure determination. The special least squares program for modulated structures refinement by use of $(3+1)$-dimensional symmetry (de Wolff et al., Acta Cryst. (1981) A37, 625) has been written by one of us (W.A.P.). The refinement was carried out in two superspace groups (see Table) with a data set of 214 reflections (seven of them removed due to extinction reasons). At the begining, in addition to positional and anisotropic thermal parameters, only the individual occupational waves were taken into account. Next, all the possible displacive waves were added. However, the components of the displacive waves along x and z were proved negligibly small and consequently set to zero. Furthermore, the rigid body like behaviour of NO_2 group was detected and for the final refinement all modulation parameters of the N and O atoms, were constrained. The final discrepancy indices obtained for different space groups for pure occupational and mixed modulation are as follows:

20.4–7   ANION INSERTION IN THE COMMENSURATE-INCOMMENSURATE FERGUSONITE-LIKE PHASES $CeNbO_{4+x}$.

By J.L. Hodeau and M. Marezio, Laboratoire de Cristallographie. C.N.R.S., associé à l'U.S.M.G., 38042 Grenoble-Cedex, France, and R.S. Roth, National Measurements Laboratory, N.B.S. Washington, D.C. 20234, U.S.A.

The compound $CeNbO_4$ can be oxidized at relatively low temperatures (∼ 600°C), the reaction products are discrete compounds $CeNbO_{4+x}$, x = 0.07, 0.25, 0.33. X-ray, electron diffraction and electron microscopy results on the two first compounds are reported :

MULTI-TWINNED $CeNbO_4$
THE TWINNING CORRESPONDS TO A ROTATION
$CeNbO_{4.07}$ IT IS AN INCOMMENSURATE SUPERSTRUCTURE
$CeNbO_{4.25}$ IT IS A COMMENSURATE SUPERSTRUCTURE

Commensurate phase $CeNbO_{4.25}$

The supercell is 12 times that of the fergusonite. Its structure was determined by X-ray diffraction. The anion insertion mechanism corresponds to a rotation of one edge of the oxygen tetrahedra around some of the niobium atoms. The compression of the anion framework resembles that of Vernier structures. Oxygen clusters containing 3 extra anions are formed. The cation displacement are rather small. however, the anion clusters are located close to those zones of the crystal where the cation displacements are larger. The final values of the R fac-