The phase transition from P4/mnc to P21/n in the antifluorite K₃TeBr₆ is shown, by X-ray and heat capacity measurement, to undergo two independent strain-coupled processes. The angle \( \beta \) between the \( a \)- and \( c \)-axes in the tetragonal phase increases sharply from 90° at about 400K, on cooling, the temperature at which the thermal expansivity of the \( c \)-axis changes sign, see figure below [Abrahams, Irfinger, Marsh & Nassau (1984)]. To be published. Further cooling to 359K breaks the identity of the \( a \)- and \( b \)-axial lengths. Mode analysis of the antifluorite structure in P4/mnc at the zone center shows that each \( E' \) basis vector reduces the symmetry to \( P21/n \). Two order parameters \( Q_1 \) and \( Q_2 \) of identical symmetry, defined respectively as the displacement of the K⁺ ion in the [010] direction from the tetragonal \( [010] \) of the TeBr₂⁻ octahedra at the phase transition, are shown to follow an identical critical power law but with different critical temperatures. Decomposition of the strain tensor and the corresponding order parameters makes the monoclinic angle \( \beta \) (400 - T)° and the corresponding axial length difference \( a-b \) (359 - T)°. The two relationships are seen in the figure to hold well, close to the critical temperatures. The incompatible symmetry of the \( E_g \) mode, leading to the monoclinic distortion, with the \( A_{1g} \) mode that orignates in the phase transition from cubic to tetragonal and leads to an increasing octahedral TeBr₂⁻ rotation about \([001]\), results in further rotation becoming blocked by the displacement of the K⁺ ion from their special positions and the consequent abrupt change in \( c-a \) at 400K. Comparable relationships are expected in all antifluorite structures at the tetragonal-to-monoclinic phase transition, although it is not possible to predict the relative order of the two critical temperatures or their difference by mode analysis. Related structures that are expected to undergo similar soft modes include the elpasolites (e.g. Rb₂NaDyF₆), the cryolites (e.g. (NH₄)₃FeF₆) and the K₃Co(CN)₆ family: others may include the K₃Co(NO₃)₆ family. In each case, careful heat capacity and differential high resolution X-ray diffraction measurement would indicate not only the transition temperatures but would also identify broadened transitions such as that in the accompanying figure at which critical temperature differences become appreciable.

II. Below 119K the Bragg reflexions are surrounded in \( c \)-direction by up to ten orders of satellites due to a mutual periodic deformation of host and guest. The appearance of the satellites is preceded by a weak diffuse scattering in \( c \)-direction. No clear indication of an inelastic \( n \)-component could be found. There is a hysteresis of about 15K around the transition temperature.

III. Continuous layer-lines perpendicular \( c \) are found in all antifluorite phases with a period slightly longer than 2c of urea. They are sharp along \( c \) in the whole range and do not change with temperature until 119K, where Bragg-reflexions arise on the layers with \( h \) and \( k \) of urea. This is explained by screw disorder of the whole chains. No pure translational or rotational disorder is possible as shown by structure analysis. The diffraction pattern at \( T_c \) has been reproduced by calculating Fourier-Bessel-transforms for the chains in their extended planar zig-zag configuration. While X-ray data reveal no difference between a cylinder-symmetrical and a sixfold azimuthal orientation of the chains about their axes, neutron data make allowance also for the \( H \)-atoms clearly pointing towards the latter possibility. This is confirmed by the analysis of the contributions of the chains to the k3O reflexions.

IV. Three observable orders of broad (static) diffuse layers (also perpendicular \( c \) show the typical intensity distribution of a longitudinal disordered \( \beta \)-helix built by the zig-zag fragments of the alkene chains. The temperature dependence is the same as in section III. The \( h \)- and \( k \)-reflexions do not increase with \( Q \)-From these longitudinal displacements of the atoms in the fragments are derived. It is concluded, that the interaction between guest and host takes place by intramolecular distortion of the chains in accordance with the fine structure of the host. (Supported by funds of the BMBF under 03-I02A04).