

05.2-4 X-RAY MORPHOLOGY AND PREFERRED ORIENTATION OF CRYSTALLINE PHARMACEUTICAL PRODUCTS

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A quantitative description of crystal habit as it affects tableting behaviour can be based upon measurement of preferred orientation. An X-ray powder diffraction pattern is then measured for crystals of each habit extreme on specially prepared samples. The samples are prepared in such a manner that preferred orientation effects are maximized. A ratio of the relative peak intensities of critical lines in this diffraction pattern serves to indicate the average habit crystals. The ratio is useful in predicting tableting behaviour as well as serving, when desired, as a manufacturing specification.

Using the lattice parameters of crystal and atomic coordinates of the molecule obtaining from single crystal X-ray data we have calculated the intensities of a "theoretical" powder pattern. From the theoretical and the measured patterns obtained from crystals with various habit we can calculate the following factors:

$$P_{hkl} = \frac{I_{hkl}}{\sum I} \quad f_{hkl} = \frac{P_{hkl \text{ obs}}}{P_{hkl \text{ theor}}}$$

The orientation of crystals within tablets we calculated by the equation

$$T_{or} = \frac{f_{hkl \text{ tabl}}}{f_{hkl \text{ cryst}}}$$

The tableting ability is measurable by the hardness of tablets /e.g. can be measured by its crushing strength/. The  $\alpha$ -Lactose monohydrate,  $\beta$ -D-Mannitol, L-Ascorbic Acid and L- $\alpha$ -methyl-DOPA were examined. We have found the following correlation between the tableting ability and crystal habit: in case of the ratio of faces being parallel with the cleavage /perpendicular on the cohesion minimum/ is increasing in the crystalline powder the tableting ability is getting worse.

05.2-5 X-RAY INVESTIGATIONS OF THE DOPING OF SILLENITES CRYSTALS. By E.N. Khabarov, E.I. Leonov, V.A. Lopo, Krasnodar university, Leningrad physics-technical institute, Brest pedagogical institute, USSR..

The displacement of the doping neutral atoms in the structural holes of sillenites crystals (i.e.  $\text{Bi}_{12}\text{GeO}_{20}$ ) was investigated. These holes are the results of bismuth-oxygen heptahedra coordination and their filling can be corroborated by poly- and monocrystals X-ray methods. The sillenites' diffractive reflexes  $h+k+l=2n$  exist, but  $\langle \Delta F \rangle = \langle F_{\text{obs}} - F_{\text{cal}} \rangle > 0$  for all even hkl and  $\langle \Delta F \rangle < 0$  for mixed even hkl. These theoretical deductions conform with the experimental data. The method of calculation of sillenites stereochemical formula based on their chemical composition is developed. The stability of sillenite oxygen sublattice is postulated. The atoms' size and their placement in structural polyhedra and in the holes influence physical properties of sillenite crystals.

05.2-6 A METHOD TO CALCULATE ELASTIC CONSTANTS FROM CRYSTAL STRUCTURE DATA. By M. Catti, Dipartimento di Chimica Fisica ed Elettrochimica, Università, Milano, Italy

Calculations of anisotropic elastic properties of crystals are usually based on lattice dynamics. A different approach involves the stress-strain response of the static crystal structure, provided that a suitable interatomic potential is available. The derivatives of the total crystal energy with respect to strain components (at constant temperature) are approximated by derivatives of the static (lattice) energy only. These can be related to components of the fourth-rank elasticity tensor by thermodynamic equations (Catti, Acta Cryst. (1981) A37, 72), and then they are transformed into derivatives with respect to cell edges and angles. This corresponds to a process of mechanical deformation of the crystal unit-cell to a general triclinic geometry, independently of the original symmetry. If a correct model is assumed for the lattice energy of the crystal structure, its first and second derivatives and then the elastic constants, too, can be calculated. Electrostatic ( $\propto r^{-1}$ ), dispersive ( $\propto r^{-6}$ ,  $\propto r^{-8}$ ) and repulsive ( $\propto \exp(-r)$ ) interactions were considered; by combining them appropriately, both ionic and molecular crystals can be taken into account. Analytical formulas were obtained for the energy derivatives, and a computer program was written to perform calculations. If molecules or molecular ions are present in the structure, the program is able to carry out energy differentiation by keeping their internal geometry unchanged while the lattice is deformed. The method was checked on some simple crystal structures, for which the elastic constants were calculated and compared to experimental values.