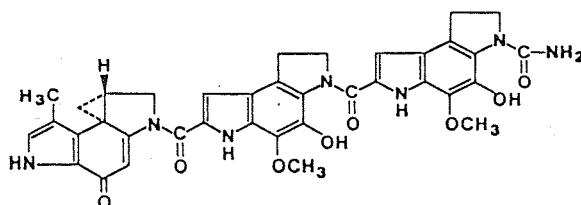


## 21. STRUCTURAL RESULTS FROM METHODS OTHER THAN DIFFRACTION-315

After extension by some extra rules, the same procedure of subgroup relations are applicable to complex polytypes (clay minerals etc.) and also to commensurable and incommensurable superstructures. Examples of polytypes and modulated structures with different complexity will be presented.

21.1-1 STRUCTURAL STUDIES ON CC-1065/DNA INTERACTIONS. By D.C. Rohrer, T.A. Scahill and W.C. Krueger, The Upjohn Co., Kalamazoo, MI 49001, USA.

CC-1065 is a novel antitumor antibiotic isolated from *Streptomyces zelensis* which binds covalently to DNA. CC-1065 is made up of three fused-ring subunits (see structural formula below), one of which contains a reactive cyclopropane. A covalent bond is formed to N3 of adenine from the antibiotic by opening the cyclopropane while the antibiotic is positioned in the minor groove of the B form of DNA. The shape of the molecule lends itself to fitting along the minor groove of the "natural" enantiomer extending from the bonded adenine in the 5' to 3' direction. Only minor perturbation of the B conformation of the DNA structure is observed with the CC-1065 bound. While no actual crystal structure of the antibiotic/DNA complex has been determined, NMR and CD spectral results give data which has been used in conjunction with molecular mechanics and dynamics calculations to determine model structures for this complex.



21.1-2 CHROMIUM INCORPORATION INTO MULLITE. By H. Rager, Department of Geosciences, University of Marburg, FRG, and H. Schneider, Research Institute of the Feuerfest-Industrie, Bonn, FRG.

Mullites containing chromium in solid solution were synthesized from homogenized SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, and Cr<sub>2</sub>O<sub>3</sub> powders in a laboratory furnace at 1650 C. The experiments yielded mullites with Cr<sub>2</sub>O<sub>3</sub> contents up to 12wt%. The Cr enriched mullites exhibit a strong substitution induced deformation of the crystal structure, i.e. the relative cell expansion is strong along c and smaller along a and b. Because only little information is available on the mode of Cr incorporation into the mullite structure EPR measurements were carried out. The EPR spectra were taken at 9.5GHz and 100kHz modulation. The EPR signals were labelled by their effective g-values, g<sub>eff</sub>. The EPR spectra of all investigated mullites show qualitatively the same pattern, i.e. narrow EPR signals -denoted as A- around g<sub>eff</sub> = 5 and a broad structured EPR band -denoted as B- around g<sub>eff</sub> = 2.5. If the Cr<sub>2</sub>O<sub>3</sub> content exceeds 9wt% an EPR signal appears at g<sub>eff</sub> = 1.98 which is due to antiferromagnetically coupled Cr<sup>3+</sup> ions. The intensity ratio, I(B)/I(A), of the signals B and A seems to increase with the Cr content in an exponential manner. Signal A is due to Cr<sup>3+</sup> ions in a strong crystal field and corresponds very likely with the octahedrally coordinated Al position. Signal B is due to Cr<sup>3+</sup> ions in a rather weak crystal field and corresponds to Cr<sup>3+</sup> sites where fluctuations in the local crystal fields are responsible for the signal broadening. It may, thus, result from Cr<sup>3+</sup> at interstitial sites.