08.X-1 REPORT PREPARED FOR THE MICROSYMPOSIUM ON THE NOMENCLATURE OF INORGANIC STRUCTURE TYPES. By a Subcommittee of the Nomenclature Commission of the IUCr: J. Lima-de-Faria (Chairman), E. Hellner, E. Makovicky, F. Liebau and E. Parthé, Crystallographic and Mineralogical Center of I.I.C.T., Alameda A.Afonso Henriques 41 - 4º E, 1000 Lisbon, Portugal.

The aim of the microsymposium is to discuss in an open session the report of the Subcommittee on the Nomenclature of Inorganic Structure Types in order to incorporate the comments and suggestions into the final version of the report.

The report presented by the Subcommittee attempts to give concise definitions for different degrees of similarity between inorganic structure types (the isopointal structures, the configurational and crystal chemical isotypes, homeotypes, parent and derivative structures of different categories). Each definition is accompanied by a comment on the problems involved in its practical applications.

Furthermore, it recommends some basic rules for crystal chemical notation for inorganic structure types, attempts to elaborate the coordination notation and presents the principal categories which have to be considered in the realm of topology, conformation, packing, and in the Bauverband approach.

The proposed notational scheme attempts to be open for additions, improvements and omissions according to the individual needs of different specialists.

A copy of the report will be available at the Congress prior to the microsymposium.

08.1-1 SCHLEGEL PROJECTIONS AND DIAGRAMS AS A NEW TOOL TO DESCRIBE AND UNDERSTAND SOLIDS. By R. Hoppe, Institute for Inorganic Chemistry, University of Gießem, W.-Germany.

By adding interatomic distances and bond angles to SCHLEGEL projections of coordination polyhedra (CP), very easily information of deviations from regular or semiregular polyhedra is obtained. Structural peculiarities are indicated.

By adding next-but-one neighbours one obtains SCHLEGEL diagrams. Including the symmetry of the unit cell, from such drawings even complicated structures of solids can simply be described topologically.

Examples are given. For instance the number of topologically principally different modifications of $TiO_2 - TiO_{6/3}$ can be counted for the first time, including metastable ones. Other intergrowths between α-PbO_2 and anatase-type except for brookite are described.

So-called Partial SCHLEGEL DIAGRAMS show very easily relationships between parts of structures of chemical quite different compounds like salts and intermetallics.

08.1-2 OBTAINING NEW STRUCTURES FROM OLD. By I.D. Brown, Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada.

Inorganic crystal structures can be modelled using empirical rules that describe the properties of observed crystal structures. Such rules are obtained from data stored in the Inorganic Crystal Structure Database (ICSD) with the aid of the program STRUMO which is also used to develop the modelling techniques that make use of these rules. It is an interactive program with a sophisticated infrastructure of symmetry handling and bond manipulation routines (D. Altermatt and I.D. Brown, Acta Cryst A, in press). Initially the various modelling steps are performed by the operator but, as experience is acquired, the modelling rules are gradually built into the program. Current work is directed toward the initial generation of trial coordinates by developing routines that construct groups of strongly bonded atoms (complexes) from the chemical formula. In order to do this we are developing algorithms which will decide which anions and which cations will bond together and which will predict the appropriate coordination numbers based on an analysis of coordination numbers found in the ICSD. The operator must decide on the placing of the complexes in the unit cell but the coordinates are then refined using a Distance Least Squares routine which generates its own target distances and can place atoms within 0.05 Å of their observed positions. In addition to modelling new crystal structures, STRUMO can be used to model structural features that are not easily measured such as defects, disorder and surfaces.