

08.X-1 REPORT PREPARED FOR THE MICROSYP-
SIUM ON THE NOMENCLATURE OF INORGANIC STRUCTURE
TYPES. By a Subcommittee of the Nomenclature
Commission of the IUCr: J. Lima-de-Faria (Chair-
man), E. Hellner, E. Makovicky, F. Liebau and
E. Parthé, Crystallographic and Mineralogical
Center of I.I.C.T., Alameda A.Afonso Henriques
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The aim of the microsymposium is to dis-
cuss in an open session the report of the Sub-
committee on the Nomenclature of Inorganic St-
ructure Types in order to incorporate the com-
ments and suggestions into the final version of
the report.

The report presented by the Subcommittee
attempts to give concise definitions for differ-
ent 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 accom-
panied by a comment on the problems involved in
its practical applications.

Furthermore, it recommends some basic ru-
les for crystal chemical notation for inorganic
structure types, attempts to elaborate the coordi-
nation 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 omis-
sions according to the individual needs of dif-
ferent 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 Gießen,
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 peculiar-
ities 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 - $TiO_{6/7}$, can be counted for the first time, includ-
ing 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 ob-
served 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 coordi-
nates by developing routines that construct groups of
strongly bonded atoms (complexes) from the chemical
formula. In order to do this we are developing algo-
rithms which will decide which anions and which cations
will bond together and which will predict the ap-
propriate 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 struc-
tural features that are not easily measured such as
defects, disorder and surfaces.