19. X—11 MICROCOMPUTERS IN CRYSTALLOGRAPHIC TEACHING.
By H. Schenk, Laboratory of Crystallography, University
of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam,
The Netherlands.

Present-day microcomputers offer a wealth of computing
power at very limited costs. In fact, it is now well
possible, as we showed some years ago, to have a simple
least-squares structure refinement program running on
a $ 1000.- computer.

Another, and possibly more important, field in which
microcomputers can be applied is teaching. As a rule,
crystallographic methods depend heavily on computing,
and the associated programs are nearly always black
boxes which do not elucidate anything of what is going
on. To explain these methods to students, simulations
can be used. As an example, a direct method teaching
simulation on a microcomputer should leave all the
essential decisions to the students, and should itself
do only checking and administrative tasks, so that in
the end a student may grasp what's going on in the re-
search program. Other possibilities for computers in
teaching are of course computer-assisted instruction
and computer-managed instruction.

Along these lines, in the author's laboratory several
teaching programs have been developed, illustrating
Fourier Synthesis, Direct Methods, Model Building, etc.
and some results will be shown.

In the view of the author there should be set up an ex-
change for teaching programs which includes some referee
system. Only in this way programs already functioning in
a few laboratories will become available to the crystal-
lographic teachers at large.

Table 1

Pearson symbol	Structure type	Space group	Space group number
t I18	Al3Zrl	I4/mmm	139

Author
G.Brauer
1939 242 Pl Monatsheft für Chemie
Remarks: also called Bi2SrlZnl,
Bil 4(c), Bi2 4(e), Sr 4(e), Zn 4(d)

a = 0.4014   b = 0.4014   c = 1.732   [nm]
α = 90   β = 90   γ = 90   [degrees]
Origin at 4/mmm

Atoms	Site	Symmetry	X	Y	Z	occupancy
Al 1	4(c)	mmm	0.0	0.5	0.0	1.00
Al 2	4(d)	-4m2	0.0	0.5	0.25	1.00
Al 3	4(e)	4mm	0.0	0.0	0.361	1.00
Zr	4(e)	4mm	0.0	0.0	0.122	1.00

Followed by a table of compounds crystallizing in this structure type

Table 2

Phase	Space group	Structure type	a_b [nm] $_c$	α_β [D] $_\gamma$	Atoms	point set	X	Y	Z	occ.
Hg2Na3	P42/mmm	Pearson	0.852	90	Hg	8(j)	.125	.125	.190	1.0
		symbol	0.852	90	Na1	4(c)	.0	.5	.0	1.0
		Hg2Na3	0.780	90	Na2	4(f)	.368	.368	.0	1.0
		tP20			Na3	4(g)	.210	.790	.0	1.0

Space lattice (c)	(T)	(p)	Remarks		Name Year	Coden Vol page
			Structure like Al2Zr3 except Na1 in 4c not 4d; s.l. varies from 32 to 45 at% Hg, fig. given in ref. 2		Niels 1954	ACCRA9 7 277

**19. 1—1   HANDBOOK OF CRYSTALLOGRAPHIC DATA FOR
INTERMETALLIC PHASES, P. VILLARS, L.D. Calvert and
W.B. Pearson, Eidgenössische Technische Hochschule,
Zürich, National Research Council of Canada and
University of Waterloo.**

This handbook covers the world literature for this
area from 1913 to 1983. It includes all metallic
phases (elements, binary, ternary etc.) for which data
were found. Also included are simple oxides and
sulphides, but complex minerals and halogen containing
phases have been excluded.
This book is a critical evaluation of the best data
available and not a historical collection of structure
data. All type structures are given in standard
setting. The old data from the classical structure
compilations have been reevaluated and replaced where
necessary. For 1963-1983 the original literature
directly scanned covers over 20,000 publications, of
which around 15,000 contained useful citations. Part
1 is a handbook of all structure types (~1000)
ordered according to the Pearson symbol. A typical
entry is shown in Table 1.
Part 2 contains critically evaluated data for each of
the ~20,000 individual phases found. These are
alphabetically ordered and follow the pattern given in
Table 2.
This book is planned to be published in 1985.

**19. 1—2   ATOMS, BONDS AND COMPUTERS. By I. D. Brown
and D. Altermatt, Institute for Materials Research,
McMaster University, Hamilton, Ontario, Canada L8S 4M1.**

Computers are now widely used in organic and biological
chemistry for model building and **data retrieval**, but in-
organic chemistry is far behind because of the lack of a
simple ball and stick model to describe chemical struc-
ture and chemical connectivity.

The present project addresses two questions:

1. Can a computer, using only coordinates obtained
   from, for example, the Inorganic Crystal Structure
   Database, calculate a recognisable chemical
   description of the structure, i.e. can it identify
   the chemical bonds?

and

2. Can one use the resulting description of bonds for
   computer modelling of inorganic solids?

Considerable success has been achieved in answering the
first question with the program SINDBAD. This uses the
bond valence model that works well for compounds that
are formally ionic, i.e. contain bonds only between
anions and cations.

The program has 3 parts. In the first ranges are set
for interatomic distances that correspond to bonds. For
cation-anion bonds these are distances with bond valences
lying between 1.2 $\times$ (anion oxidation number) and 0.038 Å
(cation oxidation number). Anion-anion and cation-
cation bonds are only expected when both ions have less
than their maximum oxidation number. In the second part,
bond distances and bond valences are calculated and
checked to see if the bond valence sum around each atom
corresponds to its oxidation number. If it does not,
the third part of the program attempts to locate