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 research 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 exchange for teaching programs which includes some referee system. Only in this way programs already functioning in a few laboratories will become available to the crystallographic teachers at large.

Table 1

Pearson symbol	Structure type	Space group	Space group number
t I18	Al3Zr1	I4/mmm	139

Author: G.Brauer
1939 242 Pl Monatsheft für Chemie
Remarks: also called Bi2Sr1Zn1, Bi1 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]	γ	Atoms	point set	X	Y	Z	occ.
Hg2Na3	P42/mmm	Pearson symbol	0.852	0.852	90	90	Hg	8(j)	.125	.125	.190	1.0
		Hg2Na3	0.780		90		Na1	4(c)	.0	.5	.0	1.0
		tP20					Na2	4(f)	.368	.368	.0	1.0
							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 inorganic chemistry is far behind because of the lack of a simple ball and stick model to describe chemical structure 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 * (anion oxidation number) and 0.038 * (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