s8b.m4.p1 **Improvement of the Inorganic Crystal Structure Database ICSD.** R. Allmann, *Institut für Mineralogie, Hans Meerwein Str. D35043, Marburg. E-mail: napieral@mailer.uni-marburg.de*
Keywords: database, inorganic structures, authors.

The ICSD, published by Fachinformationszentrum Karlsruhe, now contains more than 50,000 structures, including about 10,000 mineral structures. A new retrieval program written by NIST under Windows should be ready at the time of this meeting.

My first work for ICSD after my retirement in 1996 was updating the mineral names. About 4,000 were missing, even if the structures themselves were in ICSD. Then about 700 structures with misprints in their publications could be corrected, the most often errors being missing signs, missing leading zeros, interchanged digits, and wrongly doubled digits (for instance: .133 instead of .113), an error very difficultly to be detected in proof-reading. Further errors were wrong origins of unit cells (most often in $P2_12_12_1$), wrong space groups, transformed co-ordinates with non-transformed unit cells, and missing angles ß for monoclinic cells. Another problem are the correct constraints for anisotropic displacement factors, especially in trigonal and hexagonal space groups. If possible, cross references to the Powder Diffraction File PDF for new and revised entries are given.

During the last two years I added about 5,000 overlooked or forgotten structures published in 1960-1990 (entries 40,000 to 45,000). To my experience about 10 % of the structures were missing. The best way for finding forgotten structures would be by assistance of the authors themselves. **Authors**, please, check your publication lists against ICSD and send me reprints of the missing papers!!! If your list contains more than 50 inorganic structures, I am willing to do this for you: just send me your publication list.

Another reason for missing structures is their non-publication. Nearly half of all structures presented at meetings like this will never be published in full. If the poster itself can be cited, you may send me the full data set for inclusion in ICSD (there with the remark: "Atomic parameters from author").

The coming Windows program will provide a new field "Structure type". Part of my further work will be the filling of this field. Another new field will be "Mineral group". In the recent version of ICSD the second mineral name mostly stands for the mineral group (group as in PDF).

s8b.m4.p2 **An Environment for Searching and Mining Multiple Structural Databases**. P.S. White, *Department of Chemistry, University of North Carolina at Chapel Hill, NC 27599-3290, USA,* Y. Le Page, *ICPET, National Research Council of Canada, Ontario K1A 0R6, Ottawa, Canada* and J.R. Rodgers, *Toth Information Systems, Inc. 2045 Quincy Ave., Gloucester, Ontario K1J 6B2, Canada.*
Keywords: methods crystallography, data mining, data bases.

For the past couple of years, CRYSTMET® the database of intermetallic structures has been available in the form of a relational database with a search program that runs on PCs and the Windows operating system. A quite similar Web based search routine has also been available. This paper will describe a new version of the search program that has been generalized to permit the inclusion and concurrent searching of multiple databases.

The software uses a relational database structure that is consistent with archiving data for all types of small molecule structures. This structure is extensible and can also contain other information such as computed powder diffraction patterns and observed or computed physical properties. At present the available databases are the CRYSTMET® database of metals and intermetallic compounds, and the ICSD[1] database of inorganic compounds. Searches may be performed on individual databases or across multiple databases.

The search software has been designed with a GUI based user interface so that complex queries can be made in an intuitive manner. Individual sets of results can then be combined logically and/or edited manually to provide a final result set.

A second part of the software provides a set of tools for looking at entries. Individual entries can be looked at in detail; Geometries can be computed; Structures can be displayed with a wide variety of options so that interesting features can be emphasized and atomic environments can be studied; Powder patterns can be computed and visualized; and there is a routine based on MISSYM[2] to check the validity of an entry.

It is also possible to export data in standard formats either for input into more detailed analysis routines or other software that may be available locally.

[1] © FIZ Karlsruhe and National Institute of Standards and Technology
[2] Y. Le Page, J. Appl. Crystallog. **21**, 983-4, 1988.