Committee on Data for Science and Technology
of the International Council of Scientific Unions

CODATA '96

15th International CODATA Conference
SCIENTIFIC DATA IN THE AGE OF NETWORKING
Their Use for Global Prosperity and Better Human Life

SCIENTIFIC PROGRAM
EXTENDED ABSTRACTS
AND PROCEEDINGS

compiled and edited by
Phyllis S. Glaeser, Christina Prado, and Akira Tsugita

The Auditorium of
the Agency of Industrial Science & Technology
Tsukuba, Japan
29 September - 3 October 1996

THE FACTUAL DATABASE IN MACROCYCLIC CHEMISTRY

Mikhail V. Alfimov[1], Ninel N. Kochanova[1], Vitally P. Solov'ev[2], Maria S. Stuklova[1], Olga A. Eremeeva[1] and Elena V. Koltunova[1]
[1]The Russian Federation Institute of Scientific and Technical Information
125219, Usievich Str. 20, Moscow, Russia
[2]Institute of Physiologically Active Compounds of the Russian Academy of Sciences
142432, Chernogolovka, Moscow region, Russia

Work on the factual database Macrocyclic Compounds and their Complexes is in progress with the aid of computer technology. It has been implemented on a personal computer and is being created by professional chemists who are experts in coordination chemistry.

The factual database contains information from the new Russian periodic literature (more than fifty journals from Russia and other states of the CIS are included). This database includes three main information sections:
- bibliographic data: title of work, authors, source;
- identification of chemical data: registration number, chemical name, molecular formula, molecular weight, molecular 2D-structure, substructure fragments;
- physical, chemical and biological data: synthesis, melting point, boiling point, density, refractive index and other physical data (stability constants, enthalpy, entropy, etc.) about reactions of the complexation; also application in chemical technology and others.

The factual database Macrocyclic Compounds and their Complexes is programmed to use the original graphic user interface under both DOS and WINDOWS. The fields in each information section of the database are searchable and displayable.