19. X–4 IN-HOUSE IMPLEMENTATION OF DATABASES. By John. R. Rodgers, National Research Council of Canada, Ottawa, CANADA K1A 0R6.

The National Research Council of Canada has acquired several databases dealing with chemistry and physics. These cover the spectral, chemical thermodynamics and the x-ray crystallography areas. This paper will describe the in-house implementation of the crystallographic databases. These crystallographic databases contain bibliographic and structural data for organic (Cambridge Crystallographic Database), inorganic (Inorganic Crystal Structure Database) and metallic substances. The metallic section of these crystallographic databases, called the Metal Data File, is being developed in the Chemistry Division of the NRC. In addition to the structural databases there is the NBS Crystal Data File which contains bibliographic and crystallographic data on ~60000 substances. The methods involved in searching, retrieving and displaying these data will be described. The research underway in the developement of new methods of accessing these data will also be described.

19. X–5 USE OF THE CRYSTAL DATA AND POWDER DIFFRACTION FILE COMPUTER DATABASES IN CRYSTAL CHEMISTRY. G. J. McCarthy, North Dakota State University, Fargo, ND, A. D. Mighell and C. R. Hubbard, National Bureau of Standards, Washington, DC and M. C. Nichols, Sandia National Laboratory, Livermore, CA, USA.

We have been exploring the utility in crystal chemical research of two computer databases distributed by the JCPDS-International Centre for Diffraction Data. The Crystal Data database prepared at the US National Bureau of Standards (NBS) contains entries for dimensions of the reduced cell, crystal system, space group, density, name, formula and references for 70,000 phases. Software has just been released that will calculate a reduced cell from a direct cell and will do crystalline phase identification based on this reduced cell and derivative cells. Computer routines for retrieving any combination of the entries in the database have been developed in a joint effort of the National Research Council (Canada) and the NBS. The latter system proved to be more applicable to crystal chemical research.

Portions of the JCPDS Powder Diffraction File (PDF) have been available in computer-readable form since 1965 and numerous crystalline phase identification routines have been developed that search the d-I and chemical data in the database. However, the PDF is of limited value in crystal chemistry research due to the absence of the crystallographic data (cell parameters, space group, Z, density) available on the familar printed card. These data along with other information (e.g. Pearson symbol) have just been added to the computer database and a rigorous editorial and error correction effort is nearing completion. The research presented here is part of the process of deciding which portions of this very large database would be of sufficient value to be made available for lease or for time-sharing networks at the completion of the project in early 1985.

Examples to be discussed include using space group, Z and cell parameters to retrieve all entries for a particular structure type and combining the above specifications to retrieve such listings as "spinels containing Co and Zn", "fluoride perovskites" and "cubic and tetragonal alloys containing Pt, Pd or Ru."

19. X–6 ADVANCES IN PUBLISHING SCIENTIFIC JOURNALS. By S. C. Abrahams, AT&T Bell Laboratories, Murray Hill, NJ 07974, USA.

Scientific journal publishing is in a state of unusually rapid change. Traditional monotype setting, which had experienced only incremental improvement over many decades, has been totally displaced in the last half-dozen years by computer-controlled photocomposition with its attendant economies. Simultaneously, multiple subscriptions to the more important journals traditionally held by major institutions have been drastically reduced with resulting financial pressures on publishers. Numerous future changes are now apparent. Authors using word processors are able, in principle, to submit compuscripts of their papers after editorial typescript acceptance which could lead to substantial reductions in publisher's composition costs. Alternatively, optical scanning devices can currently "read" all clean typescripts except for multilevel mathematics, tables and figures: the combination of representing digitally the full information content on a page with the expected decrease in mass storage cost will remove this limitation. Beyond the printed page in the subscriber's library lies the document delivery service and the electronic journal. In the former, central libraries with single subscriptions to most journals will offer to mail photocopies of requested articles, identified most likely by a computer search of the secondary literature, to readers for a modest fee. In the latter, articles will be electronically transmitted to a video display terminal at the reader's location: a logical extension of the electronic journal will use existing network services to link authors, editors and referees with the publisher and hence with the reader. Each of the outlined changes will eventually affect most crystallographers, whose views on their potential impact and value will be sought at the Open Meeting of the Commission on Journals in Hamburg.