The search for new materials which have new or greatly improved properties is an intrinsic part of materials science. One aspect of such a search is to identify relations, regularities, rules, models and laws within experimentally determined data. In the field of inorganic and intermetallic materials there are over 4,000 distinct types of ordering of atoms, called structure types. Since the crystal structures are a first indicator for the existence of specific intrinsic properties, they should be the first element to be analysed. One approach to such studies is the use of structure maps and Quantum Structural Diagrams (QSD). Structure maps order the vast amount of structural information within 2- and 3-dimensional plots, using a Mendeleeyerian philosophy, such that materials with a given structure type cluster together. Quantum Structural Diagrams (QSD) systematize the relationship between composition and structure type and employ atomic size difference, electronegativity difference and sum valence electrons as coordinates. We will show, with examples, how such maps are used in the search for superconducting materials, quasicrystals and permanent magnets. The use of other maps showing relationships between mechanical properties and structure will be reviewed. An attempt will be made to explain if violations of structure types lead us to the discovery of new, yet unknown, exotic materials.

MS-18.01.07 NEW TOOLS FOR SCIENTIFIC DATA EXCHANGE. N. Spadaccini, Department of Computer Science, University of Western Australia.

The proliferation of scientific data and related information has necessitated the development of automated procedures to speed archiving and retrieval. Many databases have invested years of effort to develop fast access algorithms designed specifically for their own format. Attempts to pool information across database systems is hampered by incompatible formats and access software. Agreement on a single database format is not practical, however the adoption of a standardised exchange format (e.g. Protein Seq Data Avul 1, 27-39, 1987) with more straightforward conversion routines to most other database formats has been widely suggested. Many of these exchange formats are specific to particular applications or disciplines. They are generally fixed or pre-defined free forms, both of which require significant prior knowledge to facilitate access data and are inflexible to evolving data requirements.

Hall (ICCS 32, 325-335, 1991) has reported a flexible, self-defining file format known as STAR. The file can be easily extended to incorporate new data storage requirements as they evolve without violating the original file structure. The data can be automatically validated against either universal or defined data dictionaries (e.g. the CIF dictionary) or can be extended to user defined dictionaries. The crystallographic community has adopted the CIF format, a restricted implementation of STAR, as its basis for data exchange and retrieval. This paper reviews the underlying advantages of the STAR approach and elaborates on its structure.

Spadaccini, Hall & Hall (Star Base Users Manual, 1993) have developed a query language known as Star Base to facilitate data access from STAR files. Star Base provides a number of options including the extraction of data, both on nodal statements over a variety of user defined scopes. The language makes it possible to access data as required by the user with less prior knowledge of the file structure. Possible future extensions of Star Base to a full application level language will be presented.

PS-18.01.08 PCDFWIN - SEARCH/RETRIEVE PROGRAM FOR THE ICDD POWDER DIFFRACTION DATABASE ON CD-ROM. R. Jenkins, F. Nishihara*, International Centre for Diffraction Data, Swarthmore, PA, USA, R. Garvey, North Dakota State University, USA; S. Lin, Nankai University, China.

The PCDFWIN program uses Brue and bitmap algorithms to search and retrieve the ICDD PDF2 (Powder Diffraction File) database on CD-ROM, which contains 150 MB of information. This information includes interplanar spacings, relative intensities, Miller indices, crystal system, space group symbol, unit cell lengths, interaxial angles and several chemical and physical properties. Among its many search parameters, the PCDFWIN program includes: Three Strongest Intertplanar Spacings, Three Longest Interplanar Spacings, Cell Parameters, Cell Volume, and Density. In addition, it provides over 250 organic functional groups as search criteria for the organic substances in the database. A two-