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STAR↔XML TOOLS: LINKS TO W3C EXCHANGE STANDARDS

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The eXtensible Markup Language (XML) is a language developed for the exchange of information over the Internet independent of particular application domains. XML has been adopted by most software vendors as a preferred exchange medium and is well supported with parsers and editing tools. However, XML and its schema have significant limitations compared to Star File dictionaries [1] in the precise specification of data and particularly in the retention of semantic information, such as the relationships between data items [2]. There are also concerns that the syntax of XML, which is driven largely by commercial pressures, will evolve significantly, and is therefore unsuitable as a long-term archival medium.

The Star File offers established archives (including those in the taxanomic sciences) advantages in interoperability because its syntax is simple, extensible and stable, and its dictionaries are capable of a much higher level of semantic definition. Even so, exchange activities over disparate data collections are likely to need access to, or generation of, XML files at some stage, even if its only for communication purposes. This paper will describe generic processes for converting Star Files into XML instance documents, and the reverse, and the automatic translation of Star dictionaries into an XML schema (XSD). Such approaches are also useful for gaining access to commercial browser/editors such as XmlSPY.

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INVERSE MELTING IN POLYMERS

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We report some unusual phase behavior, of general implication for condensed matter, on the polymer poly-4-methyl pentene-1 (P4MP1) induced by changes in pressure (P) and temperature (T), as observed by in-situ X-ray diffraction and high pressure DSC. Upon increasing pressure beyond a threshold value, the polymer, crystalline at ambient conditions, looses its crystalline order isothermally. The process is reversible. This behavior is observed in two widely separated temperature regions, one below the glass transition temperature (< 50°C) and one close to the melting temperature (250°C), thus showing solid state amorphization and inversion in the melting temperature with increasing pressure. This further suggests inverse melting, i.e. re-entrant of the two widely separated liquid and amorphous phases along the T-axis at fixed P. This is confirmed experimentally as disordering in the crystalline structure on cooling. The inverse melting in P4MP1 raises the possibility of exothermic melting and endothermic crystallization as anticipated by Tammann (1903), see reference 1. The anticipated exothermic melting and endothermic crystallization is confirmed experimentally in the one component system P4MP1. We are observing similar features in a range of polymers like syndiotactic polystyrene, syndiotactic poly-p-methyl styrene, poly-diethyl siloxanes etc.

Keywords: PRESSURE, AMORPHIZATION, POLYMERS

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HOW THE PDB USES mmCIF

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The Protein Data Bank (PDB; **http://www.pdb.org/**) is the international repository for the processing and distribution of three-dimensional structural data. These data are deposited and processed using the dictionary technology of the Macromolecular Crystallographic Information Format (mmCIF). The mmCIF dictionary contains 2000 terms that define the macromolecular structure and the crystallographic experiment[1,2]. The PDB now uses an extended data dictionary which includes the content of the mmCIF dictionary as well as terms describing further details of crystallographic structure determination, electron microscopy, NMR, protein production, and other information for data tracking and management purposes (**http://deposit.pdb.org/mmcif/**).

In the US (**http://deposit.pdb.org/adit/**) and Japan (**http://pdbdep.protein.osaka-u.ac.jp/adit/**), ADIT (AutoDep Input Tool) is used for the deposition and annotation of PDB structures. This software tool is built on top of the PDB exchange data dictionary, which helps to ensure that the data submitted are consistent with dictionary definitions. In addition to precise definitions and examples, these dictionary definitions specify allowed data types, enumerations, boundary values, and relationships between data values.

The PDB is managed by three members of the RCSB: Rutgers, NIST, and SDSC. The PDB project is funded by the NSF, DOE, and two units of the NIH: NIGMS and NLM.

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YAXDF AND THE INTERACTION BETWEEN CIF AND XML

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Yet Another Extended Data Framework (yaxdf) is a meta-data framework within which to discuss various data frameworks and the interactions among them. We present a proposal for managing the interaction between two important data frameworks, the Crystallographic Information File (CIF) and the Extensible Markup Language (XML), which is a simplified markup language that integrates well with HTML for web applications. Both XML and CIF have a similar 'flavor', providing information associated with tags, but they differ in significant details. XML allows a highly nested, order-dependent presentation of information. XML also allows various attributes of tags to be assigned values. There are many alternate ways in which documents with such features could be embedded as data within a CIF document. Even though there is no fully agreed presentation of tables within the tree-structure of XML, translation from CIF to XML is relatively simple. Faithful translation from XML to CIF is not simple. In yaxdf we propose an extension of the CIF format to be used in parsing certain data values within a CIF which, while similar in style to CIF, also permits recursive nesting, optional order-dependence, optional use of associated parameters, optional preservation of white space, and other extensions. These facilitate a faithful representation of XML documents within yaxdf documents, with much less syntactic noise than is seen in XML documents, while allowing use of both CIF-based and XML-based tools.

Keywords: XML CIF YAXDF