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The PDB archive is an international repository managed by the Worldwide Protein Data Bank (wwPDB). wwPDB members curate, annotate, and distribute PDB data, while focusing on maintaining consistency and accuracy across the archive. As the PDB grows, new structures and new technologies challenge how all structures are represented. To address this, the wwPDB is developing a new working format to replace the current PDB format.

The working format does not replace current archival PDB formats such as mmCIF/PDBx and PDBML. Rather, the role of this working format is to provide a simple and efficient—yet powerful—means for programs to exchange the most widely used items of PDB data, free from the restrictions imposed by the record-oriented PDB format. The wwPDB Working Format (PWF) is designed to preserve the popular simple organization of the current PDB format while providing a framework that can support larger molecular systems and can capture ever-evolving methodological details. The PWF combines format features from the PDB format and macromolecular crystallographic information file (mmCIF). In this presentation, we present the features of the new PWF and how this format fully exploits the both the content and software tools that have been developed to support mmCIF and the PDB Exchange Data Dictionary.

The wwPDB members are: RCSB PDB (supported by NSF, NIGMS, DOE, NLM, NCI, NINDS and NIDDK), PDBe (EMBL-EBI, Wellcome Trust, BBSRC, NIGMS, and EU), PDBj (NBDC-JST) and BMRB (NLM).

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## MS.89.5

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### Active Data Dictionaries: A Future Role for DDLm

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A 2009 editorial *Data's Shameful Neglect* in *Nature* (461, pp 145) and several accompanying articles drew attention to the scandalous shortfall in data sharing between researchers. It highlighted the lack of technical, institutional and cultural frameworks for supporting open data access and archiving.

The crystallographic community recognised these issues 20 years ago and developed a *Crystallographic Information Framework (CIF)* which is now the mainstay of all open data access, exchange and archiving, at least within structural chemistry. The submission of experimental and model data is mandated for all publications of the IUCr, for data deposition to the PDB and several chemical databases.

The *CIF* is a subset of the *STAR* format, the latest version of which was presented at the 2008 IUCr Osaka Congress as the basis for a new *CIF* formalism. Extensions to *STAR* facilitate the active dictionary definition language *DDLm* that can extend dictionary definitions via *dREL*-based methods.

This paper will review the underpinning syntactic and structural simplicity of *STAR*. We will show that semantically rich definitions are possible through an active dictionary definition language that supports an expandable range of data types and functions, and invokes the full scope of *dREL*-methods capabilities.

**Keywords:** STAR, CIF, DDL

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### Quantum nature of the hydrogen bond

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Hydrogen bonds are weak, generally intermolecular bonds, which hold much of soft matter together as well as the condensed phases of water, network liquids, and many ferroelectric crystals. The small mass of hydrogen means that they are inherently quantum mechanical in nature, and effects such as zero-point motion and tunneling must be considered, though all too often these effects are not considered. As a prominent example, a clear picture for the impact of quantum nuclear effects on the strength of hydrogen bonds and consequently the structure of hydrogen bonded systems is still absent. Here, we report ab initio path integral molecular dynamics studies on the quantum nature of the hydrogen bond. Through a systematic examination of a wide range of hydrogen bonded systems we show that quantum nuclear effects weaken weak hydrogen bonds but strengthen relatively strong ones. This simple correlation arises from a competition between anharmonic intermolecular bond bending and intramolecular bond stretching. A simple rule of thumb is provided that enables predictions to be made for hydrogen bonded materials in general with merely classical knowledge (such as hydrogen bond strength or hydrogen bond length). Our work rationalizes the influence of quantum nuclear effects, which can result in either weakening or strengthening of the hydrogen bonds, and the corresponding structures, across a broad range of hydrogen bonded materials [1-3]. Furthermore, it highlights the need to allow flexible molecules when anharmonic potentials are used in force field-based studies of quantum nuclear effects.

[1] X.-Z. Li, B. Walker, A. Michaelides *P.N.A.S* **2011**, (in press). [2] X.-Z. Li et al, *Phys. Rev. Lett.* **2010**, *104*, 066102. [3] B. Walker, A. Michaelides, *J. Chem. Phys.* **2010** *133*, 174306.

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### Quantum protons in hydrogen bonds

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The momentum distribution of the protons participating in hydrogen bonds in water and ice deviates considerably from the classical equilibrium distribution. As a consequence the molecular structure of water and ice is directly affected by quantum mechanics [1]. Yet the effect is essentially quasi-harmonic and quasi-classical in nature [2]. New physics arises in presence of proton tunneling, which is collective and dominated by strong local correlations.

[1] J. A. Morrone and R. Car, *Physical Review Letters* **2008**, *101*, 017801. [2] L. Lin, J. A. Morrone, R. Car, and M. Parrinello, *Physical Review B* **2011**, *83*, 220302(R)

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