IUCr IPC Meeting

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On behalf of COMCIFS
Vilnius University, LSC, IBT

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Main objectives

- Main topic – coordination of efforts!
- Re-use of data presentation standards
- (Formal) relations between standards in different application areas (chemistry, material science, medicine, etc.)
- Formalization of data meaning

Connections with other topics/MS

- Mathematical crystallography (e.g. via formal reasoning on crystallographic ontologies)
- COM Data – standardization and representation
- Applications of machine learning
- Teaching – tools for representing crystals/structures
- ...

CIF 2.x developments

- Importance of standardization in data exchange
- CIF 2 new features – their use
- CIF 2 DDLm dictionaries
- Image data: cbf, Nexus, HDF5

Ontologies

- EMMO ontology and crystallography
- Ontologies for computational material sciences
- Provenance of computational and experimental data
- Comparison of experimental measurements and theoretical calculations

Database interfaces

- OPTIMADE standard – REST API for computational and experimental databases
- OPTIMADE extensions for biological macromolecule data and molecular dynamics

Provenance and Ontologies of derived information

- representation of derived chemical information (with IUPAC?)
- representation of computed material properties
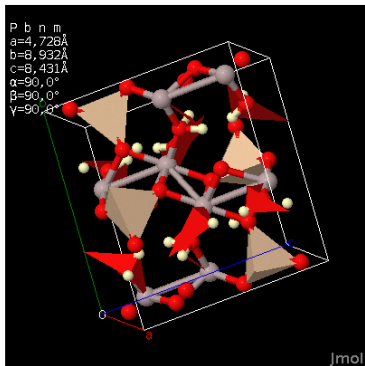- provisions for multi-scale modeling (what is "material"?)

Microsymposia?

- A CIF(2)/standardization/representation MS?
- Merging with COMData MS?

Thank you!

Coordinates	[2207377.cif](2207377.cif)
Original IUCr paper	HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html