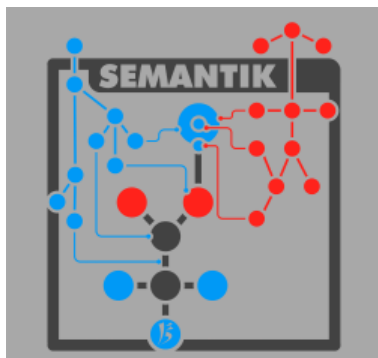


Articles

Semantic physical science

Edited by: Dr Peter Murray-Rust, Henry Rzepa
 Collection published: 3 August 2012
 Last updated: 24 May 2013



In January 2012 we held an invited workshop (hackathon) and symposium to investigate and formalise the use of semantics in physical sciences ("Semantic Physical Science" or "SPS"). Although the primary concentration is on physical, instrumental and computational chemistry, many of the principles and tools relate to other sciences rich in numeric data. The primary technologies are based on chemical markup language (CML) and, very recently, MathML, and we show that it is possible to create fully semantic declarative scientific objects. The papers in this series represent the outputs of a number of leading groups e.g. CSIRO, PNNL, STFC, Kitware, IUCr, the Blue Obelisk and the Unilever Centre for Molecular Science Informatics (who hosted the meeting.) The papers will be published by the journal asynchronously involving the normal process of peer-review.

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We thank the EPSRC for a "Pathways to Impact" award which funded the workshop and also the Cambridge-related article processing charges.

Readers should also consult our earlier thematic series, "Visions of a Semantic Molecular Future", which laid the groundwork last year for much of the basis of the workshop.

 Research article **Open Access** **Highly accessed**
From data to analysis: linking NW Chem and Avogadro with the syntax and semantics of Chemical Markup Language

Wibe A de Jong, Andrew M Walker, Marcus D Hanwell

Journal of Cheminformatics 2013, **5**:25 (24 May 2013)

Abstract | Full text | PDF | ePUB | PubMed | Graphical abstract

 Commentary **Open Access** **Highly accessed**
Chemical datuments as scientific enablers

Henry S Rzepa

Journal of Cheminformatics 2013, **5**:6 (23 January 2013)

Abstract | Full text | PDF | PubMed | Editor's summary | Graphical abstract

Research article [Open Access](#)**Applied and implied semantics in crystallographic publishing**

Brian McMahon

Journal of Cheminformatics 2012, **4**:19 (30 August 2012)[Abstract](#) | [Full text](#) | [PDF](#) | [PubMed](#)**Software** [Open Access](#) **Highly accessed****Avogadro: an advanced semantic chemical editor, visualization, and analysis platform**

Marcus D Hanwell, Donald E Curtis, David C Lonie, Tim Vandermeersch, Eva Zurek, Geoffrey R Hutchison

Journal of Cheminformatics 2012, **4**:17 (13 August 2012)[Abstract](#) | [Full text](#) | [PDF](#) | [PubMed](#) | [Editor's summary](#) | [Graphical abstract](#)

Potential Applications
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Database [Open Access](#) **Highly accessed****The semantics of Chemical Markup Language (CML) for computational chemistry : CompChem**

Weerapong Phadungsukanan, Markus Kraft, Joe A Townsend, Peter Murray-Rust

Journal of Cheminformatics 2012, **4**:15 (7 August 2012)[Abstract](#) | [Full text](#) | [PDF](#) | [PubMed](#) | [Cited on BioMed Central](#)**Editorial** [Open Access](#)**Semantic physical science**

Peter Murray-Rust, Henry S Rzepa

Journal of Cheminformatics 2012, **4**:14 (3 August 2012)[Abstract](#) | [Full text](#) | [PDF](#) | [PubMed](#)