ECRYSTALS(.CHEM.SOTON.AC.UK): Open Archive Publication of Crystal Structure Data

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The eCrystals Repository has been developed as part of the eBank-UK project, to serve as an examplar and testbed for open archive publication, linking and aggregation of digital scientific data.

This poster outlines a "pre-print"[1] procedure for the rapid and effective dissemination of structural information "@source", based on the "e-print" concept. An eCrystals record makes available, for assessment and/or re-use, all raw, derived, results and validation data generated during the course of a crystallographic experiment. During the deposition process metadata, comprising bibliographic and chemical identifiers, are associated with a dataset, and key items of data are automatically extracted and displayed on a HTML jumpoff page, which is then offered over the internet by standard Open Archive Initiative (OAI) protocols. The bibliographic, crystallographic and chemical metadata relating to an eCrystals record may be 'harvested' by information providers through the OAI Protocol for Metadata Harvesting (OAI-PMH)[2]. Developing metadata standards allow this information to be linked and aggregated with existing literature and electronic resources to provide 'added value' to the chemical and crystallographic literature.

[1] Garson L.R., Acc. Chem. Res., 2004, ASAP Article, DOI: 10.1021/ar0300017. [2] Heery R., Duke M., Day M., Lyon L., Hursthouse M., Frey J., Coles S., Gutteridge C., Carr L. ESA/ESRIN, 2004, Frascati, Italy, European Space Agency, 8pp. (http://eprints.soton.ac.uk/9705/).

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