



Project Document Cover Sheet

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Project Information			
Project Acronym	eCrystals		
Project Title	eCrystals Federation		
Start Date	01/01/2008	End Date	31/03/2009
Lead Institution	University of Southampton		
Project Director	Simon Coles		
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Partner Institutions	UKOLN, University of Cambridge		
Project Web URL	http://wiki.ecrystals.chem.soton.ac.uk		
Programme Name (and number)	Repositories and Preservation		
Programme Manager	Andrew McGregor		

Document Name			
Document Title	<i>Project Plan</i>		
Reporting Period	<i>n/a</i>		
Author(s) & project role	Simon Coles, Project Director		
Date	07/02/2008	Filename	eCrystals projectplan.doc
URL	<i>if document is posted on project web site: when agreed by partners</i>		
Access	X Project and JISC internal	General dissemination	

Document History		
Version	Date	Comments
1.0	07/02/2008	Draft for comment



JISC Project Plan

Overview of Project

1. Background

Whilst institutional repository networks which provide managed storage and open access to the textual interpretations of research, are emerging e.g. SHERPA (<http://www.sherpa.ac.uk/>) and DRIVER (<http://www.driver-repository.eu/>), the data repository landscape within institutions is considerably less mature. Well-established community archives such as the UK Data Archive and the EBI sequence databanks for bio-informatics data, provide curated resources in certain disciplines. However, the technical infrastructure and associated support for research data remains fragmented and there are gaps in provision as exemplified by Open DOAR where out of the 76 recorded UK institutional repositories a mere 4 contain datasets. This is against a backdrop of an increasing “deluge” of data generated by both large-scale facilities and institution-based small-science. In addition, the highly social, participative, (and chaotic) constructs of the current Web environment are changing scholarly communications, and we are starting to see scientific data as well as textual information, being shared, discussed and evaluated in blogs and wikis e.g. within the associated R4L Project <http://www.jisc.ac.uk/conference2007/>. This is in contrast to the more formal standards-driven service-oriented architectural approach of the eFramework.

The pioneering JISC funded eBank-UK project (three phases since Sept 2003), has constructed an institutional repository that makes available the raw, derived and results data from a crystallographic experiment (<http://ecrystals.chem.soton.ac.uk>), developed the the eBank aggregator service for metadata harvesting by 3rd parties and promoted the linking from primary data to other research outputs within the scholarly knowledge cycle (Lyon, Ariadne July 2003). Phase 3 also investigated preservation and curation aspects of the data repository and evaluated approaches to audit and certification. Phase 3 was positioned as a transitional scoping study for the proposed eCrystals Federation, and this bid describes the first stages of full implementation. The results from Phase 3 are currently being assimilated and collated into a series of reports, however there are a number of outcomes which are already evident:

- Crystallographic laboratory practices are very varied, ranging from a more automated workflow with outputs handled and manipulated digitally, to a very “hands-on” process where an individual crystallographer oversees the process and maintains paper copies of results in a filing cabinet.
- This variation in laboratory practice has implications for the ease of adoption of a standard metadata schema such as the eBank Application Profile.
- Crystal structure data and associated information is complex, should be considered as compound objects and will require the use of a metadata packaging format such as METS or MPEG DIDL.
- There are likely to be a range of persistent identifiers in use within any discipline. The allocation of identifiers by the issuing agency must be efficient, reliable and scaleable.
- When considering preservation and curation, these aspects need to be addressed: audit and certification processes and procedures, representation information for crystallography data, preservation metadata for crystallography data, conformance to the OAIS Reference Model of repository software in use within the Federation.
- It is clear that preservation and curation issues will have to be addressed politically by both institutions and the community.
- Advocacy programmes will be essential to assist with populating the data repositories, since there is no established culture of sharing data within the chemistry domain.
- The implementation of a data embargo procedure/policy will be an important factor in encouraging searchers to deposit data destined for eventual open access.

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- The pro-active support of professional societies, publishers, data centres and other key domain stakeholders is essential to achieve buy-in from the scholarly community.
- It is unclear as to the exact nature of the relationship between subject-based and institutional repositories and mechanisms for machine to machine interoperability will be necessary.

This project will begin to establish a global and sustainable federation of data repositories for crystallography: the **eCrystals Federation**, and builds on and is informed by three previous phases of work from the **eBank Project** (<http://www.ukoln.ac.uk/projects/ebank-uk/>). In particular eBank Phase 3 was a preliminary scoping study for the deployment, interoperation, harvesting and preservation of such a Federation. eCrystals addresses the stated need to “*create[ing] the technical conditions required for interoperability for resource discovery and access to resources held within digital repositories*”. The proposal is submitted to the Repositories and Preservation Programme strand D, section b) Repository enhancement projects. The 15-month project will be led by the University of Southampton, with the core partners at UKOLN (Bath), DCC (Edinburgh) and Cambridge.

The eCrystals Federation will make a major contribution to the development of a repository-based e-infrastructure for research data, and represents an instantiation of the “Federation Data Deposit Model” described in the *Dealing with Data Report* from a recent study completed by UKOLN. The project will establish a solid foundation of crystallography data repositories across an international group of partner sites, with metadata harvested by a number of aggregator services. Building on the eBank Phase 3 results, partners will work together to harmonise the metadata application profiles from repositories operating on different platforms (EPrints, DSpace, Fedora & ReciprocalNet), investigate aggregation issues arising from harvesting metadata from repositories within the networked information environments in other countries (EU, USA & Australia) and enable the Federation of institutional archives to interoperate with international subject archives (IUCr and CCDC) and other third party harvesters. eCrystals will provide a testbed for the StORe middleware and the CLADDIER “Ping” mechanism to enable the linking of data to derived resources such as primary publications. The project will build on eBank-UK achievements already made in the areas of data curation, preservation and provenance by application to an operational Federation and through the provision of a testbed for the DRAMBORA Toolkit. Co-ordinated advocacy and training approaches, will be promoted through the Federation Framework, and these will directly inform the “data aspects” of the Repository Support Project, in which UKOLN and Southampton are partners.

Federation partners can broadly be broken down into the following groups:

- 1) Institutions: Repository providers are the federation partners and have expressed their support (see Appendix). They comprise the Universities of Southampton, Cambridge, Glasgow, Newcastle, Indiana (USA, ReciprocalNet), Sydney and ARCHER (Australia) and STFC and represent institution-based repositories. The partners have been selected on the basis of their significance in crystallography, but also because they represent a truly global multi-platform data network.
- 2) Scientists: the individual crystallographers in the laboratory and practising chemists who create the crystal structures as part of their routine workflow.
- 3) Data centres: CCDC is a professional body with a subject repository for crystal data and CDS is a national service that provides federated searching across chemistry databases. They may be considered as the primary data harvesters of eCrystals.
- 4) Publishers: IUCr is the learned society representing crystallography, is a publisher of 8 journal titles and maintains standards for communicating and representing crystal structures. The RSC is a key publisher in the field and Chemistry Central is an emerging Open Access publisher who will operate a repository to store and link data relating to publications in their journals.
- 5) Users: scientists in related disciplines, students and other third parties who have a requirement to use crystallographic data as part of their research.

There are also two additional groups who are associated with the Federation:

- 6) Advisory services: the DCC will provide guidance on preservation and curation practice including the creation of preservation metadata and audit and certification tools. Institutional library and information services will play an important role in the sustainability and preservation of repositories and will be engaged in policy matters from the outset (Cambridge

and Southampton University Libraries leading). In addition IUCr has an interest in the preservation of federation data and scoping the operation of a subject repository.

- 7) Third party services: it is expected that third party services will develop across repository federation infrastructure and the model is being developed with this in mind. Whilst such service development will be the subject of future proposals, integration with the StORe project middleware and the CLADDIER Ping mechanism, which provide services to link data and publications, will be implemented as part of this proposal and the eCrystals Federation will act as a testbed.

2. Aims and Objectives

The key broad aims of this project are:

1. To create an operational Federation of data repositories in the crystallography domain thereby testing the effectiveness of the Federation Data Deposit Model, both within the crystallography community, and as a potential framework for other disciplines.
2. To make recommendations on preservation good practice for institutional data repositories.
3. To assess the socio-political and technical interactions between subject and institutional repositories and sustainable models for partnership.

Specific objectives within these broad aims include:

1. Deploying the eCrystals software, an output of the eBank-UK project, in a number of active crystallography laboratories and exploring the advocacy and working practice issues that arise.
2. Using the Federation of repositories as a testbed for emergent technologies for describing and enabling reuse of data repository content, specifically the Open Archives Initiative – Object Reuse and Exchange (OAI-ORE) protocol.
3. Provision of an advocacy and support role for the emergent federation members and beginning to highlight issues that will arise as the federation grows.
4. Initial development of alternative software platforms to be employed within the federation.
5. Publishing a description of the resources i.e the eCrystals data collections, and a list of providers in the Information Environment Service Registry (IESR).
6. Using the first phase federation members to achieve agreement and adherence to a “core” Federation Application Profile.
7. Working towards a formalisation of the relationship between data in the federation, data centres, subject repositories and scholarly articles.
8. Development of third party services based on the Federation.
9. Establishing an effective mechanism for data centres to discover repositories with appropriate content and subsequently harvest that data.
10. Finding and addressing the federation issues surrounding data preservation and curation.
11. Developing recommendations for institutional policies surrounding data preservation.
12. Enlightening the wider, global crystallographic community as to the benefits of joining the federation.

3. Overall Approach

The overall approach that this project is adopting to achieve its goals is one of total engagement of the communities involved with every aspect of the crystallography research data lifecycle. The work will be structured into work packages as outlined in Appendix 2, with specific approaches and important matters that require addressing and elaboration outlined below.

As such the project will undertake extensive advocacy, roadshow and dissemination programs. To achieve this the project team will go out in the field to engage the crystallographic community by installing software and advising on its use, as well as conducting open data roadshows to demonstrate the benefits of the Open Data approach to practitioners **and** their ‘customers’. This will be performed by Dr Simon Coles, the project manager, an experienced crystallographer well known to the UK community and with an international reputation. Simon Coles will be assisted by Dr Richard

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Stephenson (50%), who is a member of staff on the EPSRC National Crystallography Service (NCS) and will work on the eCrystals project as the funded contribution from NCS. The project will be concerned only with crystallographic data from the chemical community and will not address any of the wider data types and issues in the chemistry domain.

The project will work in close collaboration with OAI-ORE team at Cornell and Los Alamos to address the issues of interoperability and complex object packaging for the chemistry domain. There is agreement from all parties to develop OAI-ORE in this direction and this 'eChemistry consortium' is awaiting a proposal to gain funding to undertake (in part) this work, which will begin to deliver in the timescale of this project.

The project seeks to initiate developments in the provision of different software platforms, based on both the institutional repository model and a more 'lightweight' approach, which will be collaborative work between core project members. Further collaborative work between experts at UKOLN and practitioners and developers in Southampton will focus on the population of service registries and development of the core federation application profile.

The dissemination and engagement program will be pitched at all stakeholder communities involved in the research data lifecycle, this includes crystallographers, data managers, librarians, data centres, publishers, funders, third party service providers and chemical information provision. The core partners will work with supporting partners representing each of these stakeholders and evaluate approaches to engaging with these communities. In doing this work the project will seek to bring together the appropriate parties to formalise the relationship between data in the federation, data centres, subject repositories and scholarly articles.

The project will work in very close collaboration with supporting partners, CCDC & IUCr, to evaluate the requirements, business and sustainability models surrounding a subject repository. Additionally these partners will assist in the evaluation of possible solutions for discovering and harvesting repositories and their content, including considering new protocols such as OAI-ORE.

The development of some demonstrator third party services, based on a Federation of data repositories, will be conducted in collaboration with the JISC data cluster projects CLADDIER and StORe. We will investigate their project outputs, namely the 'ping' mechanism and data - article linking middleware, for applicability and suitability as services that link repository material with other digital objects available on the web.

The eBank-UK project has performed a considerable amount of work on preservation and curation of the data contained within the eCrystals repository, producing a highly cited report (<http://www.ukoln.ac.uk/projects/ebank-uk/curation/>) that speculates on issues that an Open Data Federation may face in this respect. The project, led by the DCC and in conjunction with UKOLN and NCS, will address these matters when an initial federation has been constructed. We will provide a testbed for the DCC DRAMBORA toolkit, feeding back and tailoring as appropriate for a data federation, in addition to developing representation information that will enable the long term preservation of the federation data.

Simon Coles serves on an institutional working group convened to scope the issues, problems and scale of preserving the digital research output of an entire institution. Working in this role, he is now involved in a bid to JISC to attempt to assess the financial implications of enacting such a policy and the university will also be assessing the emergent HEFCE shared services infrastructure.

There are a number of factors critical to the success of the project, which include:

- Development of the eCrystals software to a 'distribution' level
- Adaptation of the software to cope with different laboratory working practices
- Adoption of the eCrystals software by partner sites
- Population of eCrystals data repositories by partner sites
- The acceptance and possible modification of the Federation application profile

- Construction or modification of crystallography data repositories on different software platforms

4. Project Outputs

The project will deliver in a number different ways as outlined below:

- Construction of a community Wiki to coordinate project partners
- Production of a new version of the eCrystals software, which will be an EPrints2 to EPrints3 migration with numerous enhancements, such as - enhanced access features for private records, data toolbox and other file manipulation software integrated into the ingest workflow, versioning and enhanced embargo control
- Construction of mass upload tool for legacy data (generally CIF only) held by federation partners/adopters
- Formal establishment of DOI registration
- Capability of software to be configured for different workflows and lab practices and development of installer procedure
- Collaboration with JISC funded PRESERV2 project to assess preservation services in the archival of raw data
- Use of the Federation as an example in developing an advocacy program for the crystallographic community – enable promotion and wider uptake, - particularly a data publication workshop at the IUCr international Congress (Osaka, Aug. 2008) to engage the community
- Investigation of the emergent OAI-ORE protocol for chemical / crystallographic information
- Development of preservation metadata
- Incorporation into the Information Environment Services Registry
- Interactions with other projects as a testbed – StOReLink, DRIVER, Data Audit Framework, eChemistry, myExperiment and a number of consultancy activities

5. Project Outcomes

The project expects to deliver against a number of broad outcomes:

1. Raised awareness and understanding amongst the research community of the benefits of openly sharing data, and of data deposit within a managed Institutional Repository: eCrystals will contribute through the Federation Advocacy Programme and Dissemination activities.
2. More informed repository managers and developers who are/wish to implement data repositories within their institution: the eCrystals experience will be shared with the Repository Support Project and promoted more widely through this activity.
3. Enhanced understanding of the critical relationships and interactions between IRs, subject repositories, learned societies and data centres: eCrystals will work with IUCr, CDS and CCDC to provide mutually beneficial services and support, in addition to scoping the requirements for a subject based repository.

6. Stakeholder Analysis

Stakeholder	Interest / stake	Importance
Crystallographer	Facilitation of publishing process and thorough archival of results data	High
Data Manager	Ability to manage and preserve data in a structured manner	Medium
Librarian	Exemplar for the inclusion of data repositories in a community Federation framework	High

Data Centre	Simple approach to obtaining a larger amount of data	High
Publisher	Structured community approach to publishing data in a way that doesn't impinge on the scholarly publication process	High
Crystallographic information reuser	Comprehensive data sets made available in an structured fashion so that provenance can be established by the reuser	Medium
Funder	Getting value for money as more results data is made available to the public domain	High
Third party service provider	Data made available in a structured (machine to machine) fashion	Medium

7. Risk Analysis

Risk	Probability (1-5)	Severity (1-5)	Score (P x S)	Action to Prevent/Manage Risk
Staffing (failure to recruit or loss of staff)	5	5	25	Subcontract work to existing EPrints / Chemistry staff
Organisational (Management & coordination of partners)	3	3	9	Make more use of National Crystallography Service and UKOLN infrastructure
Technical	3	3	9	Consult EPrints team
External suppliers	1	1	1	Source different suppliers
Legal	2	2	4	Consult JISC Legal & University of Southampton legal experts

8. Standards

Name of standard or specification	Version	Notes
OAI-ORE		
OAI-PMH		
Dublin Core		
Perl		
XML		

9. Technical Development

The project will follow best practice for software development and will deploy a development system so that live software is not modified. If development occurs between partner sites then critical versioning software will be used.

10. Intellectual Property Rights

The host institution of the researchers performing the work will own the IPR.

Project Resources

11. Project Partners

Consortium agreement to be signed mid February 2008.

This project is led by the University of Southampton, [Simon Coles] with core partners at UKOLN (University of Bath) [Liz Lyon], the Digital Curation Centre [Chris Rusbridge] and the Unilever Centre (University of Cambridge) [Peter Murray-Rust].

The International Union of Crystallography (<http://www.iucr.org/>) [Peter Strickland], a body serving the world community of crystallographers, promoting international standardisation and cooperation in crystallography and enabling international publication of crystallographic research; **The Cambridge Crystallographic Data Centre** (<http://www.ccdc.cam.ac.uk/>) [Frank Allen / Owen Johnson], operator of the world repository for all small-molecule organic and metal-organic crystallographic data published in journal articles; **The Royal Society of Chemistry** (<http://www.rsc.org/>) [Richard Kidd], the largest organisation in Europe for advancing the chemical sciences supported by a worldwide network of members and an international publishing business; **The Chemical Database Service** (<http://www.cds.dl.ac.uk/>) [Bob McMeeking], provider of a single interface to search all available crystallographic databases (CSD, ICSD, CrystMet); **Chemistry Central** (<http://www.chemistrycentral.com/>) [Bryan Vickery], an emergent Open Access series of journals, covering all aspects of the chemistry domain; **StORe** (<http://jiscstore.jot.com/WikiHome>) [Ken Miller], a JISC Digital Repositories Programme project, involved in linking 'source' and 'output' repositories; **CLADDIER** (<http://claddier.badc.ac.uk/trac>) [Brian Matthews], a JISC Digital Repositories Programme project, concerned with linking data to publications; **The Research Information Network** (<http://www.rin.ac.uk/>) [Michael Jubb], an organisation funded to assess and coordinate the provision of research information in the UK; **ReciprocalNet** (<http://www.reciprocalnet.org/>) [John Huffman], a well established consortium of partners (US based but also including USyd and NCS) sharing and publishing crystallographic data; **ARCHER** (<http://archer.edu.au/>) [Andrew Treloar], a DEST project based on data repositories supporting the research process; **The University of Sydney** (<http://mmsn.net.au/>) [Peter Turner], a lead partner in the Molecular and Materials Structure Network, (an Australian Research Council funded project); **The Science and Technology Facilities Council** (<http://www.scitech.ac.uk>) [Brian Matthews], a multidisciplinary research organisation supporting scientists and engineers world-wide through operation of large-scale research facilities and provision of strategic advice to the government on their development; **University of Glasgow** (<http://www.chem.gla.ac.uk/xtal/>) [Andy Parkin], a UK Chemistry department with a strong crystallographic section that supports a wide range of research; **Newcastle University** (<http://www.ncl.ac.uk/xraycry/>) [Bill Clegg], a well established crystallography laboratory with world leading experience in operating a synchrotron based national service and a strong background in data-based publishing.

12. Project Management

The project will establish a steering group, which will meet twice a year. The composition of the steering group will be minimal, so as to maximise the opportunity for the whole group to meet face to face and will have representation from parties outside the project in the fields of digital libraries, crystallography, publishing and data management. Senior staff on the project from each core partner site will also be members of this group. Internally the core partners on the project and interested supporting partners will meet face to face on a quarterly basis, otherwise internal communication will be via email and the project Wiki. The project will deploy and continue to develop a Wiki throughout its duration (<http://wiki.ecrystals.chem.soton.ac.uk>). The Wiki will be used as a project management

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and dissemination tool and will enable partners to openly contribute to content and discussion. All reporting will be coordinated and collated by the University of Southampton partners.

The project will make use of any pertinent JISC training events that are organised during its lifetime and the technical development members of staff will regularly attend EPrints training events to continue to be aware of new developments concerning this core software.

The core team comprises:

University of Southampton

Simon Coles (Project Director)
TBA (Project Developer and General Manager)
Andrew Milsted (eCrystals software consultant)
Richard Stephenson (0.5 FTE; dual role with NCS and responsible for systems administration and crystallography laboratories outreach)
Mike Hursthouse and Jeremy Frey (Crystallographic and eScience advisors)

UKOLN

Liz Lyon (UKOLN leader)
Manjula Patel (DCC 0.5 FTE Preservation researcher)
Pete Cliff (Research Assistant)

University of Cambridge

Peter Murray-Rust (Cambridge Leader)
Jim Downing (Advisor)

The Steering Group will comprise a member of the digital libraries community, a member of the publishing community, a member of the crystallographic information community and the JISC programme manager, in addition to at least one representative from each of the core partners.

13. Programme Support

Potentially the programme could assist with staff recruitment and training of project team members in key aspects of Digital Repositories research and development.

14. Budget

See Appendix A

Detailed Project Planning

15. Workpackages

See Appendix B

16. Evaluation Plan

Timing	Factor to Evaluate	Questions to Address	Method(s)	Measure of Success
Project end	Uptake of software by crystallographic community	Has the project managed to establish a federation of data	Audit	Number of repositories; Quantity of deposits

		repositories in the crystallography community		
Project end	Population of Federation repositories	Are there barriers to deposit?	Audit	Significant numbers of records in all repositories across the Federation
Project end	Introduction of (or requests for) new repositories / partners in the Federation	Is there interest from the community outside the core partners	Audit	Unplanned repositories included in the federation by the end of the project
Project end	Preservation workpackage outputs	Is there a solution to long term preservation of data in repositories	Report evaluation	Reports accepted and cited
Project end	Interoperability and protocols	Can we implement the protocols into our software?	Assessment	Successful implementation across a number of services / resources

17. Quality Plan

Output	Quality criteria	QA method(s)	Evidence of compliance	Quality responsibilities	Quality tools (if applicable)
Project end	Are all partners integrated into the Federation	Audit	Revised application profile accommodating all partners		
Project end	Can repositories and services interoperate	Testing	Full integration		
Project end	Are third parties making use of repository content	Audit	Records being harvested by CCDC & CDS		

18. Dissemination Plan

As a component of the advocacy workpackage the team will regularly make presentations and demonstrations about the eCrystals software to practising crystallographers as part of the roll out plan for the software / federation. Additionally presentations at a number of conferences and workshops will be performed in order to inform the digital repositories, computer science, crystallographic and chemical information communities; a selection of these opportunities are outlined below.

Timing	Dissemination Activity	Audience	Purpose	Key Message
Dec 2007	CNI Taskforce	Information		Importance of

	conference presentation	specialists		data repositories
Dec 2007	DCC conference presentation	Digital Libraries Preservation community		Importance of data repositories and preservation
Dec 2007	JISC/Mellon closed workshop presentation	Senior developers and researchers	Inform funders of areas to invest in	Advocacy, lab practices, funding models.
Jan 2008	DRIVER II summit meeting presentation	DRIVER project partners and interested parties	Inform the network of the issues involved with data federations	Federation considerations for data repositories
Mar 2008	Presentation at NaCTeM chemical information workshop	Chemical informaticians	Promote eCrystals as best practice	How to manage chemical information
Apr 2008	Paper presentation at OR08 conference	Repositories community	Promote eCrystals as exemplar of data repository federation	Federation considerations for data repositories
Apr 2008	Demonstration and presentation at British Crystallographic Association Spring meeting	UK crystallography community	Promote eCrystals	Best practice in crystallographic data capture, management and dissemination
May 2008	Presentation at Royal Society of Chemistry SIG on chemical information	Chemical Informaticians	Promote eCrystals	Exemplar of chemical information management
Aug 2008	Host workshop on data publication at IUCr international congress (Osaka)	Global crystallographic community	Raise awareness and promote new routes to crystallographic data publication	Vital to adopt new routes to data publication to cope with data deluge.

19. Exit and Sustainability Plans

Project Outputs	Action for Take-up & Embedding	Action for Exit
Deployed repositories	Advocacy and training for adopters	Advice on management and assistance with entering negotiations with host institutions for inclusion and support in their IR portfolio
Interoperability, data audit and data linking testbeds	Deployment across federation and demonstration of worth	Work with project leads to ensure outputs are embedded and there is a sustainable future

Project Outputs	Why Sustainable	Scenarios for Taking Forward	Issues to Address
Data repository federation	Adopted by practising crystallographers	Investigation of business models to be built on top of	Acceptance and adoption by

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		federation; endorsement by International Union of Crystallography; incorporated into 'whole community' model and current practice	crystallographic community
eCrystals software	Built on EPrints; large scale adoption; endorse by International Union of Crystallography	Public release of software in an easily installable and manageable form	Reluctance by practitioner to deploy and maintain heavyweight (institutional) software
Project Wiki	Partner and Community ability to contribute content regarding Federation project matters	Hosted by NCS	In the event that NCS ceases to exist will be taken on by IUCr

Appendixes

Appendix A. Project Budget

Appendix B. Workpackages