

Annual Operational Report for 2007

Frank H. Allen, Executive Director

Robin Taylor *Development Director*

John Liebeschuetz *Applications & Marketing Manager*

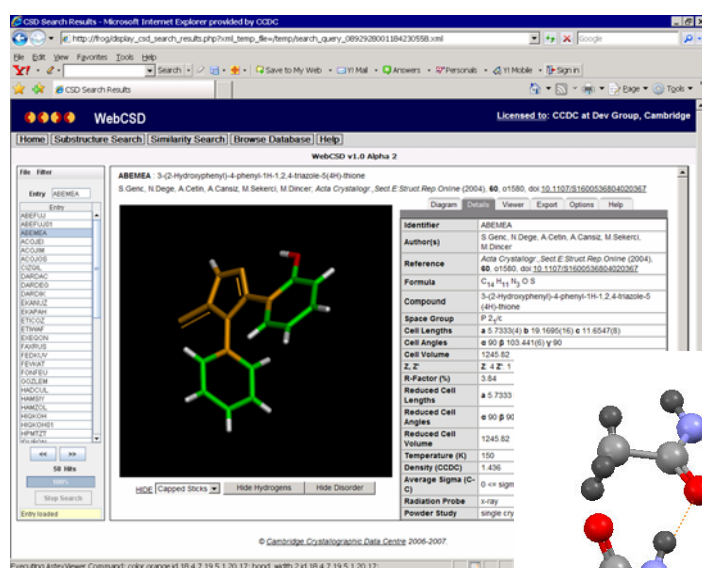
Jason Cole, *Principal Scientific Software Engineer*

Jenny Field *Principal Scientific Editor*

Stephen Salisbury *Business Director*

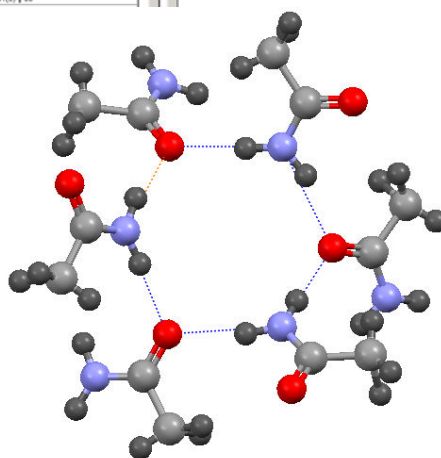
Owen Johnson *Technical Support Manager*

Ian Bruno, *Principal Scientific Software Engineer*

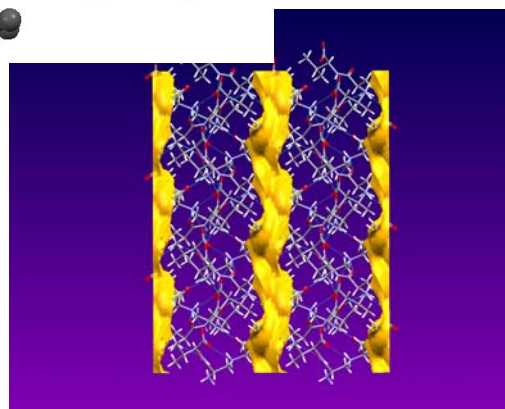


← WebCSD: the Results pane

Intermolecular interaction motif located by Materials Mercury →



Display of crystal structure voids in Mercury →



New developments at the CCDC in 2007

The Cambridge Crystallographic Data Centre (CCDC)

Registered in England No. 2155347 Registered Charity No. 800579

Registered Office

12 Union Road, Cambridge CB2 1EZ, United Kingdom

ANNUAL OPERATIONAL REPORT FOR THE YEAR ENDED 31 DECEMBER 2007

Objectives of the CCDC

The Cambridge Crystallographic Data Centre (CCDC) was originally established in the University of Cambridge Chemical Laboratory in 1965. Its principal remit is to compile and distribute a computerised database (the Cambridge Structural Database, or CSD) containing data for organic and metal-organic compounds studied by X-ray and neutron diffraction. The CSD is comprehensive for all results published in the open literature since the inception of the technique in the early 1900s. Additional unpublished data deposited by individual scientists are also included in the CSD after full validation by CCDC staff. The continuous development of software is also fundamental to the CCDC's objectives in order to: (a) create and maintain the CSD, (b) provide facilities for searching and analysing CSD data, and (c) generate products that make use of CSD data in academic and industrial applications.

Today, the CCDC is a charitable company limited by guarantee having been established on 18 August 1987. It is governed by a Memorandum and Articles of Association, which were last amended on 14 May 2003. Its objects are the general advancement and promotion of the science of chemistry and crystallography in all its branches for the public benefit.

The CCDC serves the scientific community through the acquisition, evaluation, dissemination and use of the world's output of small molecule crystal structures by:

- Compiling the Cambridge Structural Database (CSD)
- Developing scientific products and services
- Maximising world-wide accessibility to the CSD
- Performing and supporting fundamental research using chemical structural data
- Promoting and supporting applications of structural data in academia and industry

Governance, Organisation and Management

Governors' Meetings

The Board of Governors met twice during 2007: on 22 May, incorporating the Annual General Meeting of the CCDC, and on 13 November. A meeting of the Governors' Finance Committee was held on the preceding day in each case. Each Board Meeting was preceded by a briefing session, to acquaint Governors with important recent developments. At the May meeting, senior managers and staff presented a survey on CSD and Relibase integration and in November, the current status of two new CCDC products, Materials Mercury and WebCSD, were demonstrated.

At the May meeting also, Governors received the annual report and audited financial statements for 2006. At the November meeting they received a summary of the CCDC's achievements against objectives for 2007, together with the operational objectives set for the company during 2008. These two documents form the basis for this operational report. The

financial performance of the CCDC during 2007 was discussed at both meetings, and the outline budget for 2008 was presented and discussed at the November meeting. The Board also received regular Quarterly Reports during the year, together with other related documents.

Organisation, Management and Staffing

The Senior Management Team is responsible for the operational and strategic briefings that normally precede Board Meetings and which inform papers presented to the Board for discussion. They also report to Governors on operational progress against objectives, and present operational plans for the coming year.

Members of the CCDC's Senior Management Team on 31 December 2007 were:

<i>Frank H. Allen PhD FRSC</i>	<i>Executive Director & Database Group Manager</i>
<i>Robin Taylor PhD</i>	<i>Development Director</i>
<i>Stephen A. Salisbury PhD</i>	<i>Business Director</i>
<i>Owen Johnson PhD</i>	<i>Technical Support Manager</i>
<i>John W. Liebeschuetz PhD</i>	<i>Applications and Marketing Manager</i>
<i>Jenny C. Field BSc</i>	<i>Principal Scientific Editor (Database Group)</i>
<i>Ian J. Bruno PhD</i>	<i>Principal Scientific Software Engineer</i>
<i>Jason C. Cole PhD</i>	<i>Principal Scientific Software Engineer</i>

Mrs Kathleen Foreman retired from her position as Principal Scientific Editor on 31 May 2007 after 23 years service to the company. Following internal interviews, her role is now fulfilled by two experienced Senior Scientific Editors, Dr Gwenda Kyd and Dr Matthew Lightfoot. At the end of 2007, and including advertised vacancies, the CCDC had 51 Staff assigned to operational groups as follows: Database (16), Development (15), Applications & Marketing (6), Pfizer Institute (2), Technical Support (6), and Business & Administration (6).

CCDC staff are encouraged to become members of relevant professional organisations, to serve on scientific committees and advisory panels, and becoming involved as referees and editors of scientific journals. These activities broaden professional experience and enhance the CCDC's reputation within the scientific community.

The third implementation of the new CCDC salary structure, using objectives reviews and performance assessments for all staff, was carried out successfully early in 2007, within a salary budget ratified by the Board of Governors in November 2006. Also during 2007, a major revision of the CCDC Staff Handbook, and a major revision of information provision to staff via the CCDC's Intranet were finalised following periods of staff consultation.

General CCDC Activities

Scientific Collaborations

The CCDC has always had close and effective collaborations with scientists from academia, government laboratories and industry. A number of the academic collaborations involve partial funding of PhD students by the CCDC at the host institution. A list of major collaborators during the past few years is provided in Annex 1.

The CCDC is one of the three partners in the Pfizer Institute for Pharmaceutical Materials Science (PIPMS). This major research venture, established in 2002, also involves two Departments of Cambridge University (Chemistry and Materials Science & Metallurgy) and the leading pharmaceutical company Pfizer Inc, who provide direct funding. The CCDC's Executive Director is a member of the PIPMS Board of Governance. During 2007, the scientific work of the Centre continued to develop impressively, and involvement with the Institute is also valuable in the development of our new product, Materials Mercury. During 2006 the CCDC had received Pfizer funding to employ two postdoctoral researchers during the calendar years 2006-2008 inclusive, and in December 2007 this funding was extended to cover 2009.

A feature of 2007 was the fourth CCDC Crystal Structure Prediction Workshop held in September. At this meeting, a step-jump in performance of CSP software was demonstrated by participants, which led to several positive reports in the scientific media. A full publication on the outcomes is in preparation.

Awards and Prizes

The CCDC has established agreements with a number of professional organisations to sponsor CCDC Awards for Younger Scientists at meetings of these organisations. Awards are made to scientists up to the age of 35 for excellence in scientific research in the broad field of "*chemical crystallography or the scientific applications of small-molecule structural data*". The CCDC also sponsors a triennial award to a senior scientist selected by the Royal Society of Chemistry for excellence in structural chemistry. Recipients of CCDC awards in 2007 are given in Annex 1.

Risk Analysis

The CCDC's SMT had conducted a two-day Strategy Review Meeting in September 2006. A full risk analysis, taking account of perceived threats and company opportunities, was conducted, including full discussion of the possible threats posed by open-access scientific publishing initiatives. These risks were closely monitored during 2007, including the growing threat to the CSD itself from 'open data' proponents and their activities. During 2007 also, the CCDC has begun to implement the strategic directions determined in the Review, including continued development of Materials Mercury and WebCSD and furthering the use of the CSD as an educational resource. Work to improve the throughput of data to the CSD has also been a major feature of software development work. Plans put in place during 2007 provide resources for a thorough investigation, during the early months of 2008, of potential new products for the CCDC's portfolio.

Contents of this Operational Report

The Annual Operational Report summarises the principal activities and achievements of the six organisational Groups of the CCDC. The following information is provided for each group: (a) Group remit, (b) operational achievements in 2007, and (c) operational objectives for 2008. The report concludes with Annexes of statistical and other data on CCDC activities during 2007.

Database Group

The Cambridge Structural Database (CSD)

Remit

The CSD is the largest of five numerical crystal structure databases maintained worldwide, and contains about 66% of all compounds for which a structure has been published. The CSD has a high reputation for completeness and accuracy and it is the Group's aim to maintain this position by working with the crystallographic community, professional organisations and scientific journals to maximise the number of crystal structures available to science via the CSD. To achieve this aim, the Group undertakes:

- Acquisition of relevant published crystal structure data through formal arrangements with scientific journals, and by scanning the appropriate literature.
- Working with journals to involve them in the CCDC's pre-publication data deposition scheme.
- Working with individual scientists to attract and process unpublished data to the CSD.
- Creation of a pre-publication data archive, and making its contents available to journal referees and to individual scientists once the data are published.
- Adding value to the raw experimental data by including bibliographic and chemical information.
- Validation of all information, referring back to journals and authors to resolve inconsistencies.
- Archiving completed structure data to the distributed CSD.
- Maintain the WebCite database of literature references to published applications of CCDC products.
- Maintaining accurate statistical information to inform future resourcing of Group activities.

Group achievements in 2007

Summary statistical data for CSD growth over the past 5 years are tabulated below.

	2003	2004	2005	2006	2007
<i>No. of entries at year end</i>	306,364	335,280	367,496	401,529	436,436
<i>No. of entries archived to the CSD</i>	25,001	28,916	32,216	34,033	34,907
<i>Entries in progress at year end</i>	8,723	8,701	8,094	6,636	7,727
<i>No. of entries passed for processing</i>	28,311	28,827	31,341	37,890	35,796
<i>No. of electronic data sets received</i>	26,230	27,794	30,545	37,539	35,177
<i>No. of hard-copy data sets received</i>	2,081	1,033	796	351	619
<i>% electronic data sets received</i>	92.6%	96.4%	97.4%	99.1%	98.3%
<i>Data requests (Web, e-mail, referees)</i>	5,364	7,448	9,518	12,507	13,947

- Succession planning has continued with 2 senior-grade staff taking further line-management responsibilities, following the retirement of Kathleen Foreman in May 2007.
- The appointment of a Scientific Editor to replace Kathleen Foreman maintained the staff resource at 10 full-time Scientific Editors.
- Gill Heale retired at the end of 2007. Here duties will now be undertaken by Tracy Allgood.
- Two full-time Editorial Assistants were appointed to replace part-time departees
- 98% of new data have arrived electronically during 2007, and prior-to-publication deposition arrangements are in place for around 100 journals; authors in many other journals also use this facility.

- 39,959 incoming data sets were archived to Catdep during 2007.
- In collaboration with Wiley, CCDC are hoping to be able to make cifs for 'Early View' Angewandte Chemie papers available via the CCDC data request form for published cifs.
- Further discussions have been had with the ACS with regard to direct deposition from their journals. We expect significant progress in 2008.
- The final number of Private Communications processed by the year end will again be in excess of 500 due to major contributions from both UK and German Universities.
- With permission 33 unpublished cifs from the eCrystals (Electronic Data Repository) in Southampton were included in the 2007 release of the CSD, with a link back to the e-Repository.
- Around 92% of depositions are matched after three years; at the time of the report.
- Following legal advice, no unpublished structures will be processed into the CSD without specific permission from the author(s).
- 34,907 new CSD entries were processed in 2007 against a target of 31,800 for the year.
- Data processing targets have been monitored regularly during the year.
- 3,948 existing CSD entries were edited
- 12,826 requests for CIFs associated with any one publication were supplied, 96% being provided via the Web-based request form, including requests via ConQuest
- 948 requests for datasets for refereeing purposes were fulfilled; 77% via the Web-based request form.
- Work with the Development Group to maintain PDB information in Relibase+ has continued in 2007.
- The MySQL journal codens database has been maintained with a further 123 new codens added in the year.
- All existing software for CSD creation and maintenance has been monitored and bugs or suggested improvements logged.
- The Development Group has made significant progress with the new software for the creation and maintenance of a new cif archive and work has continued on CSD building software, specifically involving ACD Batch name, bond type analysis and the 2D sketcher.
- The WebCite database, now has 1883 entries, and carries classification and search functionalities, together with DOI access to the original paper. WebCite has received an average of around 460 Web-visitors per month in 2007.
- The Group has interacted with the IUCr, RSC, ACS and other professional bodies and journal publishers; two Scientific Editors represented the Database Group at meetings, one at the BCA meeting in Canterbury and another at the 24th European Crystallographic Meeting in Morocco.

Group objectives for 2008

Cambridge Structural Database

- Continue to develop Database Group staff as part of succession planning.
- Maintain current CSD input taking account of progress on working practices and new software implementations, and with a minimum processing target of 32,125 new entries.
- Improve currency of the CSD available to the WebCSD product during 2008
- Ensure that edits to existing CSD entries are managed and completed in a timely manner.
- Fulfil requests for individual data sets in a timely manner, further promoting the web-based services to individuals and journal referees. Aim to create accessible logs of all queries and data requests, liaising with other CCDC Groups as required.
- Maintain information provision to depositors, journals, referees and requestors of data through the CCDC Web pages and elsewhere, collaborating with other groups as necessary, and monitor the use of the 'Request-a-Structure' service and other Web pages relevant to the Group.
- Continue regular monthly monitoring of data processing and other statistics to identify problem areas and contribute to discussions of current working practices.

Electronic Data Archive, data deposition and external liaison

- Ensure that all incoming electronic data depositions and hard-copy material are managed together, and processed in a timely manner to create the CCDC Electronic Data Archive.
- Continue to interact with journal publishers and editors to improve the quantity, quality and integrity of deposited electronic data, particularly by extending the CCDC's scheme for the direct deposition of crystal structure data to the Electronic Data Archive prior to publication.
- Continue to work with publishers to improve the quality and integrity of CIF data, and in particular continue to develop the CCDC's interaction with the American Chemical Society.
- When appropriate, establish Memoranda of Understanding with journal publishers regarding the use of published data for input to the CSD
- Continue to publicise the availability of direct electronic deposition of Private Communications to the CSD, working with Universities and others to assist in data deposition where appropriate.
- Collaborate with the Development Group to ensure the timely processing of relevant PDB information into Relibase+.

Working practices and implementation of new software

- Carry out a thorough examination of current working practices so as to align resource needs within guidelines which take full account of the business needs of the CCDC, by
 - Examining and prioritising all processing and checking activities for new CSD entries
 - Implementing and maximising the use of new software for automating current procedures
 - Identifying additional procedures suitable for automation by software development
- Liaise and consult with the Database Software Team of the Development Group concerning testing and implementation of the next generation of data processing and acquisition software.
- Contribute to discussions leading to the creation of a 'Stop Press' section of the CSD.
- Contribute to discussions concerning the development of a possible CCDC e-journal.

WebCite

- Continue to maintain currency of the WebCite database, using modified procedures for creating entries to reduce resource needs.

Development Group

Software Product Development

Remit

Software development is of central importance to the CCDC. The Development Group comprises 13 Scientific Software Engineers who are responsible for the following areas:

- The CCDC software infrastructure: the OO/C++ toolkit.
- CSD System software for information access, structure display, and data analysis.
- Software for applications of the CSD and other structural data in the life sciences.
- Software for the creation and maintenance of the CSD and related knowledge-bases.
- Contributions to the CCDC's marketing efforts, and provision of expert back-up to the CCDC's support groups in answering scientific queries from customers.
- Engineering interfaces to the software products of other organisations and companies that will bring CCDC data and techniques to the desktops of scientists worldwide.

Within this general remit, the Group are responsible for development of the following software products:

- CSD System software: *ConQuest* for searching the CSD, *Mercury* for visualising structures and *Vista* for analysis of retrieved information, together with knowledge bases of intermolecular interactions (*IsoStar*) and intramolecular geometry (*Mogul*), both derived from the CSD.
- *SuperStar*, which uses *IsoStar* information to predict preferred interactions of ligands with protein active sites.
- *GOLD*, for protein ligand docking using a genetic algorithm, together with some information derived from the CSD.
- *Relibase* and *Relibase+*, a database system which provides advanced search and analysis capabilities for protein ligand complexes derived from the Protein Data Bank (PDB).
- *enCIFer*, a program for checking the format and syntax of crystallographic information files; the program is used as part of in-house validation and is made freely available to scientists.
- *CatDep*, *PreQuest*, *Register* and other novel software for CSD creation and maintenance
- The *Materials Module of Mercury* designed to aid pharmaceutical materials development
- *WebCSD*, the CCDC's initial work to bring the CSD to an Internet audience.

This is a major portfolio of software products, and not all programs receive equal development time in any year. For the more mature products, especially those which require updating of their underlying data from the CSD, agreed work is delegated to the Technical Support Group.

Group achievements in 2007

- Finish replacing *Catdep* and *Lassie*. Release *Decifer 1.0* (providing reasonable level of automated disorder analysis, bond detection, bond-type assignment, compound naming and diagram generation) and enable it to be used with existing database-building software [3.2 person years]: *Partly done. A working Classie prototype should be delivered by end of year, containing most but not all of the functionality required for replacing Catdep, but working only on test data and with an interface that requires improvement. Decifer 1.0 is not achieved at the time of writing (late September) but all of the components are in place and the program should be delivered by end of year.*
- Release a version of *GOLD* with a new user interface, especially to allow easy set up of ensemble dockings and dockings into proteins with flexible side-chains. Release *GoldMine 1.0* and continue its development with the addition of charting functionality and substructure-based ligand classification. Produce some improvement to one of the *GOLD* scoring functions, e.g. by use of receptor density scaling. [2.55 person years]: *Mostly done. At time of writing, the new GOLD interface is partly done and expected to be complete by end of year. A release of GOLD was made mid-year*

containing a new scoring function, an option to generate diverse solutions and improved handling of flexible side chains. GoldMine 1.0 was released on time and included charting functionality. Substructure-based classification is not yet done. Receptor density scaling is done and is effective.

- Release a new version of Relibase+ by mid 2007 with at least the following: CSD similarity searching, links from Reliview to Mogul and IsoStar, improved editing, better export options. Implement option to protonate protein structures. Further improve Relibase+ with priorities determined via a user questionnaire, but possibly including improved interworking with Oracle. [2.15 person years]: *Done. New version released with all scheduled features. Protein protonation implemented but not yet released. User questionnaire highlighted Oracle implementation and display of electron density surfaces as top priorities and substantial progress has been made on both.*
- Produce an interface to SuperStar in Reliview and GoldMine so that surfaces can be generated for protein binding sites. [0.4 person years]: *Done, but initial interface highlighted the need for a general-purpose Reliview/Mercury widget for listing and manipulating graphics objects and release of the SuperStar interface was delayed while work progressed on this "object explorer".*
- Make essential improvements in response to feedback on the test release of intranet-only WebCSD; make a full release of intranet-only WebCSD 1.0. Produce an initial prototype of an Internet version of WebCSD, including suitable licence enforcement assuming a subscription-based licensing policy. [0.8 person years]: *Done, with slight variations. Intranet WebCSD 1.0 could be released before end of year but effort will be directed instead to enable an earlier than planned release of the Internet version, which should be achievable in early 2008.*
- Produce a Mogul ring library; if time, implement Mogul conformational checking of GOLD docking solutions. [1.0 person years]: *Only partially done. An experimental program was almost complete to enable the underlying scientific methodology to be explored but a releasable ring library is still a long way off. Progress slowed by resignation of Lucia Rodriguez-Monge. Some improvements in Mogul library building implemented.*
- Respond to feedback on the Materials Mercury test release; add functionality to aid crystal-structure comparison, as prototyped in COMPACK; make another Materials Mercury release. [0.9 person years]: *Done, with slight variations. Some resource devoted to interfacing Materials Mercury with Accelrys's Materials Studio, at the cost of not quite completing some of the crystal-structure comparison items (although some comparison features were included in the release).*
- Release a new version of Mercury with a small number of improvements, including. void detection and an interface to IsoStar. Enable hit fragments from ConQuest searches to be highlighted in Mercury [0.25 person years]: *Done.*
- Produce a maintenance release of ConQuest, possibly including upgrade to a later version of Python, at least for Mac version. [0.25 person year]: *Done, but Python upgrade judged unnecessary.*
- Work with Tripos to improve interfaces between Tripos and CCDC products, e.g. Sybyl-ConQuest, Sybyl-GOLD. [0.3 person years]: *Not done. Meeting held with Tripos but no substantive work done (legal agreement not yet in place).*
- Perform maintenance on the Toolkit C++ class libraries, including any performance improvements necessary for WebCSD and some of the items prioritised by the Toolkit Maintenance Group. [0.6 person years]: *Partly done. Improvements necessary for WebCSD done. Work on TMG priorities has been left until late in the year, so it is unknown at the time of writing how much will be achieved, but it may well be relatively little.*
- Improve the development infrastructure, particularly with respect to build speeds and use of Qt4 [0.3 person years; part may be outsourced]: *Anticipated that work on improving build speeds, and some other build-related issues, will be done by end of year. Qt4 port was outsourced to Bugless Ltd.*
- Perform essential maintenance and bug fixing on DASH [0.1 person years].

Exceeded. Temporary Scientific Software Engineer hired from May onwards to finalise next version of DASH and add further enhancements. At time of writing, it is probable that the new version will be complete but possibly not released by end of year.

- Assist support groups as necessary, particularly while they have unfilled vacancies. [0.3 person years]: *Done*.
- Contribute to CCDC's marketing effort. [0.25 person years]: *Done*.
- Collaborate with AMG to identify opportunities for new products. [0.25 person years]: *Not done*.

Group Objectives for 2008

Complete Classie and move Database Building project to the next phase

- Finish Classie so that catdep and Lassie can be decommissioned
- Integrate Classie and Decifer; improve Decifer reporting/algorithms in the light of feedback
- Complete main requirements for the Editorial Sketcher
- Start work on an application that will ultimately replace PreQuest

Exploit immediate potential of WebCSD

- Release WebCSD 1.0; add any functionality deemed important as a result of user feedback
- Offer early access to published structures within WebCSD; develop alerting services
- Develop a Web-based service that uses Mogul to provide a quality report for a given structure
- Exploit WebCSD to enhance existing services or offer new ones if opportunities arise
- Possibly investigate use of MACCS keys to improve similarity searching

Maintain and capitalise on Materials Mercury momentum

- Develop and release new functionality associated with H-bond propensities
- Support promotion of Materials Mercury and activities of the Crystal Form Club
- Make functionality improvements arising from feedback, the Crystal Form Club or otherwise

Extend and maintain CSD System software

- Implement and release a subset of Vista functionality within Mercury
- Continue work towards provision of functionality for assessing ring conformations
- Make minor improvements to Mercury and Mogul as needs dictate or time allows
- With PSEng, investigate an upgrade to ConQuest's Python version
- Support release of the 2008 CSD System

Maintain and improve development infrastructure

- Make improvements to C++ code base including licencing code
- Make improvements to infrastructure dictated by Release and Build reviews
- Investigate implementation of a scripting interface to selected C++ libraries
- Investigate usage of wiki software in conjunction with web-based products

Relibase

- Complete the refactoring of the existing system to use a relational database back end.
- Replace cavity viewer with visualisation inside ReliView
- Incorporate Difference Electron Density Surfaces and incorporate external links to other sites.
- Generate a quality report from Mogul in the web page.
- Incorporate SecBase into the ReliBase+ system
- Complete implementation of cavity clustering in ReliBase
- Add void calculation and least squares superposition of ligands into ReliView

Gold & GOLDMine

- Complete improved GOLD interface; use SMARTS codes to facilitate specification of flexible bonds in GOLD; implement better ring searching, perhaps via pre-specified ring templates.
- Develop GOLDMine as a resource for storing docking results directly from GOLD and as a resource for storing input data sets & configurations for docking runs.
- Implement support for other RDBMS systems if users request it.
- Work towards implementing protein flexibility with ChemScore.
- Research new scoring function improvements via, for example, clash terms/ Gold-Score RDS/Bad contact penalisation/finer tuned H-Bonding terms.
- Add in substructure filtering to GOLDMine and to ReliView descriptors. Work towards including tools for pose analysis and/or significance testing.

- Work towards making GOLDMine operate without a protein.
- Add in grid-driven descriptor which could be used with any field to evaluate sums of interpolated field values for atoms of given type.

IsoStar & SuperStar

- Complete interface to superstar into ReliView/GOLDMine
- Create descriptors based on the Superstar surface
- Improve methodology to specify the IsoStar server in ReliView-IsoStar/Mercury-IsoStar links.

DASH

- Release DASH 3.1.
- Improve the CIF output to make it more publication compliant.
- Implement further improvements to DASH such as ring flexibility in the SA, use of alternative Search Methodologies (e.g. Hybrid Monte-Carlo), better handling of special positions for use with inorganic structures, further improvements to rigid body Rietveld refinement.

General

- Contribute to CCDC's marketing effort, and assist the Support groups as necessary
- Collaborate with AMG to identify opportunities for new products

Applications & Marketing Group

Scientific Support, Product Applications, Promotion and Marketing

Remit

The Applications and Marketing Group is responsible for: (a) promoting the use of the CCDC's products and services to existing and potential customers, (b) carrying out basic research in the life sciences, crystal chemistry and crystalline materials, so as to generate papers in the scientific literature, contributions to scientific conferences, applications notes for CCDC products, and workshop examples, (c) ensuring responsive customer support for all scientific queries, (d) providing scientific product testing and support as part of software releases, (e) coordinating the involvement of the CCDC at external and internal events, and (f) undertaking market research and analysis to support the development of both products and markets.

Promotional activities and marketing

- Promote and market existing and future products and services to both academia and industry
- Plan, organise and coordinate the CCDC's marketing activities at meetings, conferences and workshops, involving managers and staff of other Groups as required.
- Play a leading role in the scientific promotion of the CCDC by generating research publications in the open literature, contributions to scientific conferences, applications notes for CCDC products, and examples for use in workshops on CCDC products.
- Co-ordinate the production and publication of product information and promotional material, ensuring that marketing information is kept up to date in the CCDC Web pages.

Research

- Identify and conduct original research in crystal chemistry, crystalline materials and the life sciences. These applications will normally use existing CCDC products or the crystallographic and chemical information that underpins those products.
- Enter into collaborative research projects with external academic and industrial organisations, and supervise the activities of external collaborators and students assigned to the Group.
- Identify research software and other research output that is suitable for public release or which will enhance the information content of the CCDC's databases or knowledge bases, and liaise with the Development and Technical Support Groups in furthering these activities as required.
- Maintain awareness of scientific research in fields that are relevant to the CCDC, and invite appropriate external speakers to the CCDC to present seminars and software demonstrations.

Product releases and support

- Undertake the scientific testing of all CCDC product releases, new features and bug fixes, reporting back to CCDC Project Managers on the outcomes
- Be responsible for the timely maintenance and updating of scientific product and release documentation in collaboration with other Groups in the CCDC.
- Provide expert scientific guidance to customers, working with the Development and Technical Support Groups as necessary

Market research and development

- Obtain, analyse and circulate regular feedback from customers and potential customers on CCDC products, working with other Groups in the CCDC as necessary.
- Undertake strategic research to assess potential new markets for existing products and requirements for new products in existing markets.
- Assist recognised educators to generate teaching examples and aids using CCDC products for use in undergraduate programmes in chemistry and crystallography
- Advise on pricing and licensing strategies for all products, including strategies for handling smaller companies.
- Advise on product enhancements and development strategies.

Group achievements in 2007

General

- Two new staff members have been inducted and trained in all areas of the AMG remit.
- All members of AMG now have the opportunity to engage in research activities, that promote the CCDC and its products.
- A review of marketing strategy and tactics has been carried out and a number of recommendations have been developed. Some have been implemented (e.g. pull-up individual product posters, web seminars for customers). Others (e.g. an external CCDC newsletter) cannot be implemented without further resource.
- The Student Day was this year organised by AMG. It proved to be a successful and stimulating event.

Customer Support

- Collaborated with Technical Support Group to manage the overall support function.
- Scientific support queries continue to be answered effectively, either directly, or in consultation with or transfer to scientific software developers. Response within 48 hrs has been achieved in almost all cases.
- Increased resource means that the individual scientific support load has effectively been reduced. The total support load remains steady at between 0.5 – 1.0 full time employee at any given time, depending on normal fluctuations in demand.
- Scientific queries on GOLD predominate, with the CSD System and Relibase+ being the other major contributors. GOLD queries are the most time consuming. Thus, the support load is heaviest on those trained to answer issues with the life science software.
- There was again little resource available to update FAQ pages on the web site.

Product Releases

- Testing, documentation, tutorial updates, release notes and html conversions have been carried out as appropriate for releases of Relibase+, GOLD, and the CSD System. Minor releases of SuperStar and Encifer have also been handled. The release of GOLD also involved the release of GoldMine, and the release of the CSDS incorporated the release of Materials Mercury, both requiring significant testing and documentation. A third new product, WebCSD was delayed for release till 2008.
- Problems with release scheduling in 2006 have been avoided by better planning in 2007.

Internal Research

- Lack of available personnel until mid-year has restricted the small molecule research effort this year.
- It was decided that some effort would be expended in examining why the DASH/Mogul link was unsuccessful. A defect in the sampling algorithm was identified that may well be responsible for this flaw.
- Several research projects suggested by the Theses of past students have been commenced.
- A study that showed GOLD in a poor light has been refuted and best practise protocols for use of GOLD have been drawn up and published on the CCDC website, presented orally and a paper is in press. The impact on hit quality of post-processing using GoldMine, is being investigated.
- Validation of protein flexibility functionality within GOLD has been pursued. Some promising results will be presented shortly. Nevertheless this is a difficult area and much remains to be done. Employing protein flexibility effectively in docking is a very difficult problem that many are struggling with.
- Some examples that exemplify the use of the CSDS in pharmaceutical drug discovery were created.
- Work has been initiated in developing worked examples and tutorials for Materials Mercury
- Jana Hennemann, a 6-month diploma student from Marburg University, worked on two projects:
 - Investigations, using Mogul, of the quality of ligand/protein structures in the PDB. Clear proof was found that at least 15% of submitted structures contain poorly refined ligand geometries and that Mogul is a useful tool in identifying them. A paper is in preparation.
 - Use of pharmacophore models to tailor a GOLD fitting point file.

Research Collaborations

- Two studentships (P. Wood, Edinburgh; G. Minguez, Sheffield) have reached successful conclusions and generated a number of high quality papers. Work on symmetry and phase changes under pressure is now being continued by Russell Johnstone (Edinburgh).
- Three new CCDC funded studentships are being set up for initiation in late 2007/early 2008. These will include a project on artificial enzymes, a project on identifying positive and negative motifs for inhibitor

binding in classes of proteins to aid in ligand design; and continuation of work on the crystal engineering of metal-organics and structure determinations using DASH.

- *A collaboration on the intersection of chirality with hydrogen bonding motifs, is showing promising results.*

Product Promotion

- *The initiative to promote the CSDS through undergraduate teaching is progressing. High quality teaching examples are now in hand. Our US collaborator, Prof. Greg Ferrence now has an NSF funded fellowship to promote this initiative in Mid-West colleges, a significant boost to this effort.*
- *Worked examples have been prepared for new software products GoldMine and Materials Mercury. Resource has not allowed much additional work to be done although some of the research may be worked up.*
- *Contributions have been made to the maintenance and development of the CCDC Website.*
- *Product information flyers have been continually updated to take account of new developments.*
- *Resource was not available to organise a CCDC users meeting in 2007.*

External Events (full details are in Annex 3)

- *Calendars of conferences and other external events, and of Scientific Support and Marketing Group activities, have been generated and maintained on the CCDC Intranet*
- *The Group have participated in, or coordinated, CCDC attendance at:*
 - *Conferences in the UK(3), USA (5), Morocco (1) and Japan (2).*
 - *Customer visits in UK, USA and Japan, plus 3 web presentations.*
- *The proposed fact finding trip to China did not take place, due to pressure of other commitments.*
- *A visit to Japan was undertaken in November. DASH, including new functionality, was presented at a special symposium. The CSDS was promoted for use in pharmaceutical discovery at another meeting and several customer visits were made.*

The Group gave scientific presentations at the BCA meeting (Canterbury), the Fall ACS meeting (Boston, MA, USA), the e-Cheminfo Interaction meeting (Bryn Mawr PA, USA), a QSAR meeting, (Kyoto, Japan) and a DASH symposium (Tokyo, Japan).

Group objectives for 2008

Management and Training

- *Develop the research aspect of the AMG remit and ensure that release and promotional activities are distributed evenly such that staff have significant periods applied to other activities.*
- *Organise the annual CCDC Student Day.*

Customer Support

- *Interact with the TSG to ensure smooth management of the CCDC's customer support function*
- *Ensure that scientific queries are dealt with in a timely manner*
- *Ensure that sufficient quality of response is maintained*
- *Contribute to the development of customer support FAQ pages on the CCDC Website*

Product releases

- *Work with the TSG and individual project managers to develop timed schedules for the beta-testing and release of CCDC products during 2008, allowing adequate spacing between releases.*
- *Contribute to releases through scientific testing, documentation, tutorials etc. as timetabled.*
- *Contribute as required to releases of the new product: WebCSD.*

Internal Research

*Continue and develop a programme of internal and collaborative research, including, *inter alia*:*

- *Relationships between molecular shape, chirality, crystal packing patterns and space group*
- *Energy calculations of intermolecular interactions using CADPAC and PIXEL.*
- *Studies of intramolecular geometry and conformation that exemplify the value of the CSD.*
- *Research applications that exemplify Materials Mercury.*
- *Complete validation of GOLD's protein flexibility functionality and investigate tailoring GOLD fitting point files according to SuperStar interaction maps, for more efficient docking.*
- *Complete GOLD/GoldMine work on optimising virtual screening through post-processing.*
- *Coordinate relationships with CCDC-supported PhD students and supervisors, providing supervision as appropriate.*

Product Promotion

- Develop application and tutorial examples for all CCDC products for use in workshops, training sessions, customer visits, etc., collaborating with staff in other Groups as required
- Take a leading role (with Dev) in publicising Materials Mercury and the Crystal Form consortium through a program of conference attendance/talks/papers and company visits.
- Continue to develop worked examples that can be employed to teach principles of organic and metal-organic chemistry, working in collaboration with the academic community.
- Support the work of Greg Ferrence in setting up a community of Mid-Western colleges who will be guided in the use of the CSDS for education.
- Publish papers on the teaching initiative
- Contribute to the maintenance of accurate information on the CCDC Website

External Events

- Develop a rolling calendar of external events and deadlines, and coordinate CCDC attendance at major conferences for 2008, including, *inter alia*: ACS Spring & Fall Meetings (New Orleans & Philadelphia, PA), BCCE Meeting (Indiana, IN, USA) and IUCr Triennial Congress (Japan)
- Organise a 2-day CCDC User Group Meeting to take place in Cambridge
- Participate in commercial exhibitions at major conferences, and coordinate and contribute to product demonstrations and workshops, as required by the meetings calendar
- Attend and contribute with oral and poster presentations at scientific meetings.
- Coordinate and contribute to customer visits by CCDC staff as required

Pfizer Institute

CCDC-Based Research in Pharmaceutical Materials Science

Remit

The scientific aims of the Institute as they pertain to the CCDC largely centre around the use of the Cambridge Structural Database to further the development of novel formulations for use in drug delivery. This involves the study of, *inter alia*, intermolecular interactions and motif formation in crystal structures, crystal structure systematics of salts, hydrates and other solvates, polymorphism, crystal structure prediction, and structure determination, especially using powder diffraction. An important part of the work carried out at the CCDC involves the development of novel software for CSD analysis in support of the types of projects outlined above. There is a significant collaboration with Pfizer Institute Staff in the Department of Chemistry, and the CCDC provides software and scientific support for their applications of CSD information. Two Research Associates were responsible for this work during 2007.

Group achievements during 2007

Management

- Contribute to the overall management and development of the Pfizer Institute through membership of its Board of Management: *All management board and scientific implementation panel meetings have been attended.*
- Contribute to the scientific activities of the Institute by working with its staff, and liaising with principal investigators, particularly in relation to Chemistry Department projects under the direction of Prof. Bill Jones, ensuring timely reporting and presentation of results: *Quarterly reports meetings have been organised and attended, and reports prepared. Collaborations with chemistry staff have been ongoing throughout 2007.*
- Collaborate as required with other CCDC staff on scientific and software development issues: *Support was given towards Mercury and DASH development, and to the Database Group as needed.*

Scientific activities

- Provide specific scientific and software support to Pfizer Institute projects in relation to applications of the Cambridge Structural Database and the COSET and DASH programs, and contribute appropriate software to the CCDC's OO/C++ toolkit: *Updates to the Coset software following discussions with Pfizer Institute staff and Pfizer scientists have been carried out. All updates form part of the CCDC C++ toolkit.*
- Specifically, use DASH to determine structures of co-crystals (Pfizer project NP4) and of new polymorphs and hydrates (Project P13): *Collaboration with members of the cocrystal project continued and results published. An efficient cocrystal screening methodology is described that is based on liquid-assisted grinding and structure determination using DASH.*
- Continue to develop the logit methodology to predict the most likely hydrogen-bond group-pairings for a given molecule using hydrogen bond propensities: *A new GUI application has been developed named MIDAS, forming part of the C++ toolkit. Eight separate 'blind tests' have been performed on Pfizer drug candidates using MIDAS with a view to implementing the methodology within the Pfizer company.*
- Study co-crystal formation in the CSD using molecular properties and hydrogen bond propensity to predict most likely co-crystal formation agents for a given molecule: *Molecular property correlations have been investigated and complementary properties identified. An initial investigation of cocrystals with the hydrogen bond propensity model has been performed and work continues.*

- Investigate relationships of molecular shape and packing patterns for organic co-crystals and salts: *Important shape relationships between molecules of cocrystals have been revealed using the "box model"*.

Scientific publications and conference attendance

- Originate and/or contribute to scientific journal publications arising from Pfizer Institute, research, aiming to publish at least 10 papers in 2007 including papers on, inter alia: (a) the COSET program, (b) the hydrogen bond propensity model, (c) hydrogen bond motifs of amino acids, and (d) hydrogen bond motifs of secondary amides: *11 articles have been published in academic journals. These included publication of the logit methodology, results of cocrystal studies, investigation of crystal hydrate and solvate formation and crystal structure prediction. Other papers are in preparation.*
- Attend and contribute to internal meetings of the Pfizer Institute and to quarterly reporting to staff of Pfizer Research Laboratories: *Done. Visits have also been made to the Pfizer R&D site in Sandwich, Kent to work with Pfizer scientists. A presentation of recent developments was made to staff in Pfizer Global R&D materials sciences, and at a 1-day symposium at Sandwich in November 2007. Four Pfizer scientists have visited the CCDC during the past 12 months in addition to quarterly meetings.*
- Attend scientific conferences, meetings and workshops as appropriate and as required: *Pfizer institute staff attended 3 conferences, 1 crystallography school, presented 2 scientific talks and 4 scientific posters, and gave 2 CSD system demonstrations.*

Group objectives for 2008

Management

- Contribute to the overall management and development of the Pfizer Institute through membership of its Board of Management.
- Contribute to the scientific activities of the Institute by working with its staff, and liaising with principal investigators, particularly in relation to Chemistry Department projects under the direction of Professor Bill Jones, ensuring timely reporting and presentation of results.

Scientific activities

- Provide specific scientific and software support to Pfizer Institute projects in relation to applications of the Cambridge Structural Database and the COSET, MIDAS and DASH programs.
- Collaborate as required with other CCDC staff on scientific and software development issues and contribute appropriate software to the CCDC's OO/C++ toolkit.
- Cooperate with Pfizer scientists over potential implementation and application of results, using feedback to give a practical focus on research directions.
- Conduct further research into co-crystals within Pfizer project NP4, using DASH to determine crystal structures from powder patterns.
- Apply the logit hydrogen bonding propensity model to more challenging cases. Attempt to develop the methodology to obtain better confidence for difficult compounds. Continue with scientific implementation within Pfizer.
- Investigate predictive applications of the molecular property relationships and hydrogen bond propensity models to find the most likely co-crystal formation agents for a given molecule.

Scientific publications and conference attendance

- Originate and/or contribute to scientific journal publications arising from Pfizer Institute, research, aiming to publish at least 5 papers in 2008.
- Organise, attend and contribute to internal meetings of the Pfizer Institute and to quarterly reporting to staff of Pfizer Research Laboratories.
- Attend scientific conferences, meetings and workshops as appropriate and as required.

Technical Support Group

Systems Administration, Product Release and Technical Support

Remit

The Technical Support Group comprises two systems engineers/administrators and three Product Support Engineers (PSEs). Together they are responsible for:

- Internal hardware and systems support throughout the company, including purchase and support of PC, Unix and Mac-based systems, and any other systems used for product testing, and the maintenance of all IT and Internet-based communications systems
- Maintenance and development of the CCDC's Intranet and external Web pages, and assistance with editing existing material as required.
- Monitoring the use of IT and communications facilities by CCDC staff, and of the Web pages by external users.
- Preparation and technical testing of all CCDC product releases, including the generation of new data releases of e.g. IsoStar, Mogul, etc. that do not involve the generation of new development code, and close liaison with the Development Group.
- Management of the help desk and the provision of technical product support for CCDC's customer base, involving close liaison with the Applications and Marketing Group.
- Other technical matters that may be referred to the Group by others in the CCDC, e.g. the development, implementation and maintenance of administrative systems etc.

Group achievements in 2007

Systems and Services

- Maintenance of systems, networks, and services.
Computer systems have been maintained and enhanced as appropriate. Time has been spent to understand virtualisation of machines and to exploit this to provide backup servers running on virtual hosts. Hardware used for software testing has been replaced. The Linux cluster head node was replaced and five new nodes added replacing old, slow nodes. New nodes have local disk space which is mirror-ed for safety. A new home directory server for UNIX was purchased at the start of the year in the hope of moving from the home-grown solution to a more robust, purpose-designed product. While this offers a higher degree of safe, duplicated storage, it has had more than its fair share of problems and some issues await resolution.
- Resilience & security of IT systems.
New, smaller uninterruptable power supply (UPS) units were purchased for the basement server room. The old UPS was retired to give more room to accommodate a growing number of servers. Firewall and email spam firewalls have been maintained with one failure on the latter leading to a slight loss of incoming mail. Mailhost and web proxy logging systems, backup & recovery measures have been maintained.
- Tools and services for internet and intranet.
Re-designed intranet pages populated with required company information were published. Servers for WebCSD development and testing were provided and investigations made into suitable entry-level hardware, load balancing and redundancy for in-house hosting. Investigations were made into enhancing the videoconference equipment to provide live video streams for demonstrations. This was not pursued and the Applications & Marketing group make use of a service, WebEx, to give demonstrations.
- Contribute technical expertise to project developments.
A licensing system and database for GoldMine was developed using PHP & MySQL to track FLEXIm user-based licences, & administration tools were written for the Office. A PHP-enabled Apache web server was prepared for Relibase+ 2.2 which could be used in other products requiring a bundled web server. The version of Relibase available freely on the web was upgraded to 2.2.1 and a registration system based on email address implemented. DOI's continue to be obtained for the references of CSD entries.

Product Release and Support

- **Resourcing**
A third Product Support Engineer was recruited in January.
- **Product Release**
Major software releases prepared and tested included Relibase+ 2.2, GOLD 3.2 & GoldMine 1.0 and the CSD System (CSD v529, ConQuest 1.10, Mercury CSD 2.0, Mogul 1.1.2 and IsoStar 2.0.1). An upgrade to the freely-available Mercury (1.4.2), an alpha test release of GoldMine and a maintenance release of SuperStar were prepared & tested in the first quarter. Three interim CSD data update releases were prepared and packaged for third-party applications. Upgrade releases for Reliview and GoldMine were generated such that they would access Mogul within the 2008 CSD System release. A Windows installer was prepared for a new release of DASH which includes a copy of Mercury. The 2008 CSD v529 has been converted to SDfile and Unity database formats
- **User Support**
Front line user support has been maintained and technical queries resolved. Liaison with other groups providing support to users has continued. A Request Tracker upgrade has been obtained & is being tested
- **Product Support**
Linux build platforms have been discussed & it was decided to build the CSD System on RedHat and move development builds to Debian. A 64-bit build of GOLD was released with GOLD 3.2 and support for Sun Solaris was withdrawn. Support for Debian 4.0, RedHat 5.0 and Microsoft Vista has been added where possible with product releases made this year. Regression tests were run during Relibase+ release preparations but no progress has been made in the use of testing tools for our Qt interfaces. Investigations have commenced on arranging the CSD System software for quick launching on the Mac OSX platform.

Group objectives for 2008

Systems and Services

- **Maintenance of systems, networks, and services.**
*Maintain desktop & server hardware.
Monitor usage of the Linux cluster and work to resolve outstanding issues.
Monitor growth of machines on the network and the allocation of machine addresses.
Maintain systems for tape backup, onsite & offsite storage, internet and email firewalls & backup systems for key services.*
- **System provision.**
*Provide dedicated hardware for WebCSD roll-out and other web services as required.
Liaise with developers for provision of systems for development, build, testing & production to agreed policies.
Provide necessary build machines for product developments and porting.
Provide server machines required for client-server developments.*
- **Systems support.**
*Provide responsive systems support for all staff and visitors.
Extend records of systems setup & in-house procedures and make centrally available.*

Product Release and Support

- **Product Release**
*Undertake pre-release generation of software and technical testing.
Major releases include GOLD & GoldMine, Relibase+, the CSD System and WebCSD.
Other releases include DASH, Mercury, SuperStar and enCIFer.
Prepare maintenance and update releases of software as required and periodic data updates.*
- **User Support**
*Undertake front line user support and resolve technical queries.
Liaise with other groups providing support to users.*

- **Product Support**

Undertake technical product support (porting, testing, installation, packaging, distribution).

Add support for new computer platforms and operating systems as appropriate.

Contribute resource to work arising from the Release and Build Reviews.

Make some investigation into upgrading the python version used by ConQuest.

Business & Administration Group

Product Distribution, Contracting, Financial Affairs & Facilities

Remit

The Business & Administration Group is responsible for:

- All financial and legal affairs of the CCDC, including the drawing up of customer contracts, invoicing of customers, and the maintenance of proper income and expenditure accounts.
- Close liaison with the CCDC's National Affiliated Centres (NACs) for academic distribution of the CSD System, acting as the distribution centre for a number of smaller countries where an NAC would not be viable
- Sales, contracts, licensing and distribution of all products to industrial customers and of all non-CSD System products to academia worldwide.
- Liaison with the CCDC's professional legal, financial and investment advisers when required.
- The personnel function, including the maintenance of employment contracts, personnel records, providing (or obtaining) proper advice for staff, and the maintenance of absence and other records.
- Provision of secretarial services and general administrative support to all CCDC Managers and Groups and to the Governing Body, including arrangements for UK and foreign travel.
- Maintaining the infrastructure of the CCDC Building.

The permanent full-time staff of the Group are augmented by a small number of part-time employees and occasional (agency) staff who assist in maintaining the infrastructure of the CCDC Building, or help with the despatch of major product releases.

Group achievements in 2007

General Administration and Services

- Continue to maintain high levels of services in all areas of the group's responsibilities, these principally include:
 - Secretarial services
 - Assistance and support services for the Board of Governors
 - The personnel function
 - Accounting and payroll
 - Facilities management
 - Business development, contracting and invoicing
 - Conference registration and all travel arrangements for staff
 - Exhibition booking arrangements and shipping
 - Liaison with legal, financial and human resources consultants

All this ongoing work was carried out successfully.

- Make progress with ventilation and heating improvements
E-stack Limited commissioned to produce feasibility study on natural ventilation solutions to climate improvement
- Upgrade the emergency lighting system
Pendant lights upgraded to include emergency power supplies; illuminated signs fitted along emergency exit routes; original, fibre optic system retired
- Upgrade riser duct covers to current fire safety standards
Deferred pending completion of higher priority tasks

- Roof repairs
These were finally completed during 2007
- New central heating boilers
New boilers were installed, following failure of original, now obsolete equipment
- Drainage pumps
New waste water drainage pumps and pipe work installed after failure
- Guestroom
This room has been refurbished to convert to a Staff office
- CCDC Intranet
The contents of the CCDC Intranet has been completely reviewed, upgraded and reorganised. In particular, the CCDC Staff Handbook and the CCDC Health & Safety Handbook have both been thoroughly revised, been the subject of Staff consultation and final versions published.

Customer Interface

- Maintain high levels of service to existing and prospective licensees of all products, including the effective follow-up of contacts made at external events
- Maintain close contact with all National Affiliated Centres, and work to resolve any issues concerning CSD availability that may arise
- Follow up mailings to prospective CSD subscribers in the USA and continue to develop this market in conjunction with the Applications and Marketing Group
- Assist, as required, with the promotion and distribution efforts for existing products and new releases, and in the development of educational initiatives

All of these tasks have been carried out successfully. The table below reports the total number of licences, including collaborators for CCDC products in 2006 and 2007.

	2007		2006	
	Academic	Industrial	Academic	Industrial
CSD	1057	137	1042	131
GOLD	269	62	221	64
DASH	81	11	69	10
Relibase+	23	40	23	41
SuperStar	26	26	29	26

Finance & Business

- Extend the reporting capabilities from the Access database
Additional system modules purchased for project but insufficient resource available for implementation
- Finish the new business database system
A working prototype has been developed and is currently under test
- Assign directed effort to business opportunities in developing countries, particularly China and India
CSD brochure text was translated into Chinese, but there was difficulty in finding suitable meetings and other opportunities for reaching potential customers and required more resource than was available in 2007

Group objectives for 2008

General Administration and Services

- Continue to maintain high levels of services in all areas of the group's responsibilities, these principally include:
 - Secretarial services
 - Assistance and support services for the Board of Governors
 - The personnel function
 - Accounting and payroll
 - Facilities management
 - Business development, contracting and invoicing
 - Conference registration and all travel arrangements for staff
 - Exhibition booking arrangements and shipping
 - Liaison with legal, financial and human resources consultants
- Conclude feasibility study on ventilation and heating improvements and implement agreed modifications
- Upgrade riser duct covers to current fire safety standards

Customer Interface

- Maintain high levels of service to existing and prospective licensees of all products, including the effective follow-up of contacts made at external events
- Maintain close contact with all National Affiliated Centres, and work to resolve any issues concerning CSD availability that may arise
- Follow up mailings to prospective CSD subscribers in the USA and continue to develop this market in conjunction with the Applications and Marketing Group
- Assist, as required, with the promotion and distribution efforts for existing products and new releases, and in the development of educational initiatives

Finance & Business

- Extend the reporting capabilities from the Access database
- Finish the new business database system and implement an Intranet interface
- Review wording of CSD licence terms and conditions
- Assign directed effort to business opportunities in developing countries, particularly China.

Annex 1 - CCDC Awards & Collaborating Institutions

CCDC Sponsored Awards and Prizes 2007

British Crystallographic Association Prize in Chemical Crystallography
Dr Andrew Parkin (University of Glasgow, UK)

Poster Prizes for Younger Scientists at 24th European Crystallography Meeting, Marrakech, Morocco
Laura Roces (Universidad de Oviedo, Spain)
Tia Jacobs (University of Stellenbosch, South Africa)
Dejan-Kresimir Bucar (University of Iowa, USA)

Principal Scientific Collaborations 2007

Department of Chemistry, University of Cambridge
Cavendish Laboratory, University of Cambridge
Department of Chemistry, University of Durham
Department of Chemistry, University of Bristol
Department of Chemistry, University of Bath
Chemical Crystallography Laboratory, University of Oxford
Department of Chemistry, University of Edinburgh
Department of Chemistry, University of Glasgow
Department of Pharmaceutical Chemistry, Philipps-Universität, Marburg, Germany
Department of Information Studies, University of Sheffield
Department of Chemistry, University of Sheffield
Department of Chemistry, University of Manchester
Department of Chemistry, University of Southampton
Department of Chemistry, University of Frankfurt, Germany
Department of Chemistry, Illinois State University, Normal, IL, USA
Astex Technology, Cambridge
AstraZeneca plc, Alderley Park, UK
Pfizer Institute for Pharmaceutical Materials Science, Cambridge
Pfizer Global R&D, Sandwich, UK, Groton & Ann Arbor, USA
Protein Data Bank, RCSB, Rutgers University, New Jersey, USA
Instituto de Quimica Medica, CSIC, Madrid, Spain
Rutherford Appleton Laboratory, Chilton, Oxfordshire

Annex 2 – Research Publications 2007

Scientific Papers Published (19)

New software for searching the Cambridge Structural Database for solvated and unsolvated crystal structures applied to hydrates

J. van de Streek and S. Motherwell, *CrystEngComm*, **9**, 55-64, 2007. [DOI: [10.1039/b613332k](https://doi.org/10.1039/b613332k)]

Organic crystal hydrates: what are the important factors for formation?

L. Infantes, L. Fábíán and W. D. S. Motherwell, *CrystEngComm*, **9**, 65-71, 2007.

[DOI: [10.1039/b612529h](https://doi.org/10.1039/b612529h)]

Dichloro[(¹³C-cyclopentadienyl)dimethyl(¹³C-3-phenylindenyl)silane]hafnium(IV): a powder study

J.C. Burley, W.D.S. Motherwell, J. Maaranen, M. Ringwald, *Acta Cryst.*, **E63**, m238-m240, 2007.

[doi:[10.1107/S1600536806051269](https://doi.org/10.1107/S1600536806051269)]

Search for a Predicted Hydrogen Bonding Motif - A Multidisciplinary Investigation into the Polymorphism of 3-Azabicyclo[3.3.1]nonane-2,4-dione

A.T. Hulme, A. Johnston, A.J. Florence, P. Fernandes, K. Shankland, C.T. Bedford,

G.W.A. Welch, G. Sadiq, D.A. Haynes, W.D.S. Motherwell, D.A. Tocher, S.L. Price

J. Am. Chem. Soc., **129**, 3649 – 3657, 2007. [DOI: [10.1021/ja0687466](https://doi.org/10.1021/ja0687466)]

Importance of Molecular Shape for the Overall Stability of Hydrogen Bond Motifs in the Crystal Structures of Various Carbamazepine-Type Drug Molecules

A.J. Cruz Cabeza, G.M. Day, W.D.S. Motherwell, and W. Jones. *Crystal Growth & Design*, **7**, 100-107,

2007. [DOI: [10.1021/cg060504u](https://doi.org/10.1021/cg060504u)]

A strategy for predicting the crystal structures of flexible molecules: the polymorphism of phenobarbital

G.M. Day, W.D.S. Motherwell and W. Jones. *Phys. Chem. Chem. Phys.*, **9**, 1693-1704, 2007. [DOI:

[10.1039/b612190j](https://doi.org/10.1039/b612190j)]

Solvent inclusion in form II carbamazepine

A.J. Cruz Cabeza, G.M. Day, W.D.S. Motherwell, W. Jones, *Chem. Commun.*, 1600-1602, 2007. [DOI:

[10.1039/b701299c](https://doi.org/10.1039/b701299c)]

The Use of Crystallographic Databases in Structure-Based Drug Design,

S. Robertson, J. Liebeschuetz, *Advances in Structure-Based Design (CBI Japan Monograph Series and Solution Guide)*, 43-52, 2007.

All series of multiple solvates (including hydrates) from the Cambridge Structural Database

J. van de Streek, *CrystEngComm.*, **9**, 350-352, 2007. [DOI: [10.1039/b615938a](https://doi.org/10.1039/b615938a)]

Space group selection for crystal structure prediction of solvates

A.J. Cruz Cabeza, E. Pidcock, G. M. Day, W. D. S. Motherwell and W. Jones, *CrystEngComm*, **9**, 556-

560, 2007. [DOI: [10.1039/b702073b](https://doi.org/10.1039/b702073b)]

Database guided conformation selection in crystal structure prediction of alanine

T. G. Cooper, W. Jones, W. D. S. Motherwell and G. M. Day, *CrystEngComm*, **9**, 595-602, 2007, [DOI:

[10.1039/b702136d](https://doi.org/10.1039/b702136d)]

Screening for Pharmaceutical Cocrystal Hydrates via Neat and Liquid-Assisted Grinding

S. Karki, T. Friscic, W. Jones, and W.D.S. Motherwell, *Molecular Pharmaceutics*, **4**, 347-354, 2007, [DOI:

[10.1021/mp0700054](https://doi.org/10.1021/mp0700054)]

3-Hydroxysalicylaldoxime

P. A. Wood, R. S. Forgan, S. Parsons, E. Pidcock, P. A. Tasker, *Acta Cryst.*, **E63**, o3131.

[doi:[10.1107/S1600536807020922](https://doi.org/10.1107/S1600536807020922)]

3-Fluorosalicylaldoxime

P. A. Wood, R. S. Forgan, S. Parsons, E. Pidcock, P. A. Tasker, *Acta Cryst.*, **E63**, o3132.

[doi:[10.1107/S1600536807020776](https://doi.org/10.1107/S1600536807020776)]

Powder X-ray diffraction as an emerging method to structurally characterise organic solids
S. Karki, L. Fabian, T. Friscic, W. Jones, *Organic Letters*, **9**, 3133-3136, 2007. [DOI: [10.1021/ol07](https://doi.org/10.1021/ol07)]

A Knowledge-based Model of Hydrogen Bonding Propensity in Organic Crystals
P.T.A. Galek, L. Fábíán, W.D.S. Motherwell, F.H. Allen, N. Feeder., *Acta Cryst.*, **B63**, 768-782, 2007
[doi:10.1107/S0108768107030996]

Supramolecular chemistry in metal recovery; H-bond buttressing to tune extractant strength
R. S. Forgan, P. A. Wood, J. Campbell, D. K. Henderson, F. E. McAllister, S. Parsons, E. Pidcock, R. M. Swart, P. A. Tasker, *Chem. Commun.* 4940-4942, 2007 [DOI: [10.1039/b712278k](https://doi.org/10.1039/b712278k)].

The Crystal structure of pigment yellow 181 from laboratory powder diffraction data
E. Pidcock, J. van de Streek, M. U. Schmidt, *Z. Krist.*, **222**, 713-717, 2007.
[DOI: [10.1524/zkri.2007.222.12.713](https://doi.org/10.1524/zkri.2007.222.12.713)]

Userscripts for the life sciences

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The CSD – 450,000 answers but what are the questions?
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Evaluating Docking Programs: Keeping the Playing Field Level:
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Conformational variability of molecules in different crystal environments: a database study
Z. F. Weng, W. D. S. Motherwell, F. H. Allen, J. M. Cole, *Acta Cryst., B*, In Press.

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P. A. Wood, S. J. Borwick, D. J. Watkin, W.D. S. Motherwell, F. H. Allen, *Acta Cryst., B*, In Press.

Pybel: a Python wrapper for the OpenBabel cheminformatics toolkit.
N.M. O'Boyle, C. Morley and G. R. Hutchison., *Chem. Cent. J.*, In Press.

Annex 3 – External Conferences, Meetings and Visits, 2007

Scientific and Technical Conferences

Drug Design VI, London, UK, 28 February – 1 March [Invited Lecture: *Robin Taylor*, Exhibition: *Robin Taylor, John Liebeschuetz, Peter Carlqvist*]

233rd ACS National Meeting, Chicago, IL, USA, 25-29 March [Exhibition: *Susan Robertson, Peter Carlqvist, Jason Cole*]

BCA Spring Meeting, University of Kent, Canterbury, UK, 17-19 April [Exhibit: *Stephen Salisbury, Stephen Holgate*, Posters: *Laszlo Fabian, Peter Galek*]

Motherwell Symposium, BCA Spring Meeting, University of Kent, Canterbury, UK, 19-20 April [Speakers: *Frank Allen, Robin Taylor, Sam Motherwell, Elna Pidcock, James Chisholm, Clare Macrae, Peter Wood*]

'Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design and Application', 39th Erice Crystallography Meeting, Erice, Sicily, 7-17 June [Attendance, Posters and Workshop: *Laszlo Fabian, Peter Galek*]

4th Joint Sheffield Conference on Chemoinformatics (MGMS and CSAT), University of Sheffield, UK 18-20 June [Attendees: *Simon Bowden, Noel O'Boyle*]

ACA Annual Meeting, Salt Lake City, Utah, USA, 21-26 July [Lecture: *Robin Taylor*, Exhibition: *Gary Battle, Peter Wood, Robin Taylor*]

234th ACS National Meeting, Boston, MA, USA, 19-23 August [Lecture: *John Liebeschuetz*, Exhibition: *Ian Bruno, Peter Carlqvist, Noel O'Boyle, John Liebeschuetz*]

24th European Crystallography Meeting, Marrakech, Morocco, 22-27 August [Session Organiser: *Frank Allen*, Lectures: *Peter Galek, Laszlo Fabian*, Session Chair: *Laszlo Fabian*, Exhibition: *Gary Battle, Peter Wood, Jenny Field*]

CPOSS Open Meeting, UCL, London, UK, 7 September [Attendees: *James Chisholm, Peter Wood, Laszlo Fabian, Peter Galek*]

IQPC Conference on Pharmaceutical Materials, Amsterdam, The Netherlands, 25-26 September [Attendees: *Robin Taylor, James Chisholm*]

Applications of Cheminformatics & Chemical Modelling to Drug Discovery, Bryn Mawr, PA, USA, 15-19 October [Lecturers: *Robin Taylor, John Liebeschuetz*]

Spanish Crystallographic Association Intensive Course in Crystallography, Jaca, Spain, 22-24 October [Lectures, Demonstrations and Workshop: *Frank Allen, Lourdes Infantes (CSIC, Madrid)*]

BCA Industrial Group Meeting, AstraZeneca, Macclesfield, UK, 7-8 November [Lecture: *James Chisholm*, Attendee: *Elna Pidcock*]

Pfizer Inst. Symposium, Sandwich, Kent, UK, 14-16 November [Presentations: *Laszlo Fabian, Peter Galek*]

QSAR Symposium, Kyoto University, Japan, 15-16 November [Lecture: *John Liebeschuetz*, Exhibition: *Stephen Salisbury*]

Structure Solution from PXRD/ DASH Symposium, JAICI, Tokyo, Japan, 20 November [Lecture and demonstration: *Jacco van de Streek*, CCDC Representatives: *John Liebeschuetz, Stephen Salisbury*]

Polymorphism & Crystallisation, Clearwater, FL, USA, 29-30 November [Exhibition: *Susan Henderson, Peter Wood*]

MCMG Young Modellers Forum, London, UK, 30 November [Attendees: *Elna Pidcock, Peter Carlqvist*]

Scientific Research and Collaboration Visits

American Chemical Society, Washington DC, USA, 7 February [Conference call discussion, Journals issues: *Frank Allen, Robin Taylor, Jenny Field, Matthew Towler*]

Astex Ltd, Cambridge, UK, 8 March [Collaborative visit: *Simon Bowden, Jason Cole, John Liebeschuetz, Noel O'Boyle*]

Accelrys Inc., Cambridge, UK, 19 March [Collaborative visit: *Robin Taylor, Clare Macrae, James Chisholm*]

Royal Society of Chemistry, Cambridge, UK, 8 August [Collaborative Visit: *Frank Allen, Steve Salisbury, Jenny Field*]

Pfizer Global Research, Sandwich, Kent, UK 13-15 August [Collaborative Visit: *Peter Galek*]

Dept. of Information Studies, U. Sheffield, UK, 9 November [Collaborative Visit: *Robin Taylor*]

Takeda Co., Japan 16 November [Collaborative visit: *John Liebeschuetz*]

CCDC Product Presentations, Training and Marketing

Wyeth Inc., USA, WebX video conference, 24 January [Customer training: *Gary Battle, Susan Robertson*]

Biofocus, Saffron Walden, UK, 22 February [Customer Visit: *John Liebeschuetz, Susan Robertson*]

UCB, Belgium, WebX video conference, 30 March [Customer training: *Gary Battle, Frank Allen*]

GSK (Harlow, Stevenage, Zagreb, Verona), WebX video conference presentation from the CCDC, 5 July [GOLD/Relibase Training Session: *John Liebeschuetz, Gary Battle, Peter Carlqvist*]

GSK (Harlow, Stevenage, Zagreb, Verona), SameTime presentations from the CCDC, 18 July [CSD System Training Update: *Gary Battle, Susan Robertson*]

Amgen Corp., Cambridge, MA, USA, 24 August [Site Visit: *John Liebeschuetz, Peter Carlqvist*]

UCB, Granta Park, Cambridge, UK, 9 Nov. [Customer visit: *Gary Battle, Susan Henderson, Peter Carlqvist*]

Medivir, UK and Swedish sites, 13 November [Webinar: *Gary Battle, Susan Henderson, Peter Carlqvist*]

Kyoka Hakko, Kyoto, Japan, 14 November [Company visit: *John Liebeschuetz*]

DASH Users' Meeting, JAICI, Tokyo, Japan, 21 November [Demonstrations: *Jacco van de Streek (U. Frankfurt)*], CCDC Representatives: *John Liebeschuetz, Stephen Salisbury*]

Astellas Co., Tokyo, Japan, 22 November [Company visit: *John Liebeschuetz, Stephen Salisbury*]

External Advisory Boards and Professional Organisations

Pfizer Institute Board Meeting, Sandwich, UK, 19 March [Board member: *Frank Allen*]

Pfizer Institute Board Meeting, Cambridge, UK, 18 June [Board Member: *Frank Allen*]

Pfizer Institute Board Meeting, Cambridge, UK, 10 December [Board Member: *Frank Allen*]

Training Courses and Technical Presentations attended by CCDC staff

VAT Seminar, Peters Elworthy & Moore, Cambridge, UK, 18 January [Attendee: *Stephen Salisbury*]

University First Aid conference, Cavendish Laboratory, Cambridge, 12 June [*Owen Johnson*]

Workshop on virtualisation, London, 15 June [*Keith Taylor, Matthew Burling*]

MySQL & PHP courses, Robinson College, Cambridge, 4 & 25 July [*David Bardwell*]

Hewitsons Breakfast Seminar, Cambridge, UK, 1 November [Attendee: *Stephen Salisbury*]

Annex 4 – CCDC Product Distribution

Table 4.1 Distribution summary for all CCDC products 2001-2007

<i>Product</i>	<i>Year</i>	<i>Total</i>	<i>Industrial</i>	<i>Academic</i>	<i>Collaborators</i>
<i>CSD System</i>	2007	1263	138(15)	1070 (69)	55
	2006	1227	131(15)	1042 (69)	54
	2005	1228	124 (15)	1053 (68)	51
	2004	1140	124 (15)	980 (63)	36
	2003	1070	125 (15)	912 (62)	33
	2002	1021	122 (13)	865 (60)	34
	2001	970	108 (12)	829 (58)	33
	<i>GOLD</i>	2007	360	65	282
2006		300	64	221	15
2005		236	59	164	13
2004		180	56	116	8
2003		132	45	81	6
2002		98	41	50	7
2001		67	30	34	3
<i>SuperStar</i>		2007	75	26	48
	2006	76	26	49	1
	2005	78	27	49	2
	2004	82	33	48	1
	2003	65	25	40	1
	2002	41	23	16	2
	2001	37	18	15	4
	<i>Relibase+</i>	2007	75	40	25
2006		74	41	23	10
2005		62	33	20	9
2004		49	29	14	6
2003		42	25	11	6
2002		27	15	6	6
2001		17	12	1	4
<i>DASH</i>		2007	113	14	85
	2006	92	10	69	13
	2005	65	8	44	13
	2004	50	6	34	10
	2003	39	3	28	8
	2002	25	3	15	7
	2001	12	2	6	5

Notes

- The *CSD System* comprises the CSD, ConQuest, Mercury, Vista, IsoStar & Mogul
- Academic distribution of the CSD System and SuperStar is via (a) 33 National Affiliated Centres (Table 4.2, below) or (b) directly from the CCDC. The number of countries served is in parentheses following the number of subscribers.
- All industrial distribution of the CSD System and SuperStar, and all distribution of GOLD, Relibase+ and DASH, is from the CCDC, except in Japan, where the Japan Association for International Chemical Information is our agent.
- Complimentary licences are issued to institutions or companies carrying out collaborative research and development with the CCDC, or carrying out specific testing on our behalf.

Table 4.2**CSD System - Academic Distribution by Country 2003-2007**

The number of industrial subscribers supplied by the CCDC in 2007 is given in parentheses after the country name where appropriate.

<i>Country</i>	<i>National Affiliated Centre</i>	2003	2004	2005	2006	2007
	<i>Countries served:</i>	62	63	68	69	69
Argentina	<i>Instituto Rocasolano-CSIC, Madrid</i>	7	8	8	9	9
Armenian Rep.	<i>Academy of Sciences of Russia</i>	1	-	-	-	-
Australia	<i>Aust. Nuclear Science & Technology Org.</i>	22	23	22	22	22
Austria (1)	<i>Universität Graz</i>	7	7	7	8	8
Azerbaijan	<i>Academy of Science of Russia</i>	-	-	-	-	1
Belarus	<i>Academy of Science of Russia</i>	1	1	1	1	1
Belgium (3)	<i>Katholieke Universiteit Leuven</i>	8	8	8	8	7
Brazil	<i>Instituto Rocasolano-CSIC, Madrid</i>	13	14	17	16	17
Canada (3)	<i>University of Guelph</i>	27	30	30	31	35
Chile	<i>Instituto Rocasolano-CSIC, Madrid</i>	2	5	5	5	6
China (1)	<i>Chinese Academy of Sciences</i>	6	6	13	13	14
Colombia	<i>Instituto Rocasolano-CSIC, Madrid</i>	4	4	3	3	3
Congo	CCDC	-	-	-	-	1
Costa Rica	<i>Instituto Rocasolano-CSIC, Madrid</i>	1	1	1	1	1
Croatia (2), Slovenia	<i>Rudjer Boskovic Institute, Zagreb</i>	4	4	4	4	4
Cuba	<i>Instituto Rocasolano-CSIC, Madrid</i>	3	2	2	2	2
Cyprus	CCDC	-	1	1	1	1
Czech Rep., Slovakia	<i>Czech & Slovak Crystallographic Association</i>	4	4	4	3	3
Denmark (2)	<i>Aarhus University</i>	7	7	7	7	7
Egypt	CCDC	-	-	-	1	1
Eire	CCDC	2	3	2	3	4
Estonia	<i>Academy of Science of Russia</i>	-	1	1	1	2
Finland (1)	<i>Centre for Scientific Computing (CSC)</i>	16	16	17	18	18
France (6)	<i>INIST, Paris</i>	50	53	77	85	99
Germany (13)	<i>Inst. für Anorg. und Analyt. Chemie, Braunschweig</i>	65	63	64	67	69
Greece	<i>University of Crete</i>	1	1	1	1	1
Hong Kong	<i>Hong Kong Univ. Science & Technology</i>	1	4	3	4	-
Hungary (1)	<i>Hungarian Academy of Sciences</i>	4	5	4	5	5
India	CCDC	13	12	20	20	28
Iran	CCDC	-	-	-	1	1
Israel	<i>Weizmann Institute of Science</i>	15	20	23	22	20
Italy (4)	<i>Università di Parma</i>	34	37	38	38	40
Ivory Coast	<i>Univ. Witwatersrand, Johannesburg</i>	-	-	1	1	-
Japan (26)	<i>Osaka University</i>	88	94	104	100	105
Kazakhstan	<i>Academy of Science of Russia</i>	1	1	1	1	1
Kenya	<i>Univ. Witwatersrand, Johannesburg</i>	-	-	-	1	-
Korea	<i>Chungnam National University</i>	15	19	23	23	24
Kyrgystan	<i>Academy of Science of Russia</i>	1	-	-	-	-
Latvia	<i>Academy of Science of Russia</i>	2	2	2	2	2

Macedonian Rep	<i>Rudjer Boskovic Institute, Zagreb</i>	1	1	1	1	1
Malaysia	<i>Unioersiti Sains Malaysia</i>	3	2	3	2	2
Mexico	<i>Instituto Rocasolano-CSIC, Madrid</i>	12	13	13	13	13
Moldova	<i>Academy of Science of Russia</i>	2	2	2	3	3
Namibia	<i>Unio. Witwatersrand, Johannesburg</i>	-	1	1	-	-
Netherlands (3)	<i>CMBI, Nijmegen</i>	4	4	5	4	4
New Zealand	<i>University of Waikato, Hamilton</i>	7	7	7	7	7
Norway	<i>University of Oslo</i>	6	6	6	6	5
Pakistan	CCDC	-	-	1	1	2
Peru	<i>Instituto Rocasolano-CSIC, Madrid</i>	1	1	1	1	1
Poland	<i>Institute of General Chemistry, Lodz</i>	38	40	45	46	55
Portugal	<i>Centro de Quimica Estrutural, Lisbon</i>	9	8	8	9	9
Romania	<i>Babes-Bolyai University</i>	1	1	1	1	2
Russia	<i>Academy of Science of Russia</i>	58	62	62	56	59
Saudi Arabia	CCDC	1	1	1	1	1
Senegal	<i>Unio. Witwatersrand, Johannesburg</i>	-	-	1	1	1
Serbia	CCDC	-	-	-	1	1
Singapore (1)	CCDC	-	-	2	3	4
South Africa	<i>Unio. Witwatersrand, Johannesburg</i>	10	11	11	12	13
Spain (3)	<i>Instituto Rocasolano-CSIC, Madrid</i>	42	46	48	50	51
Sweden (2)	<i>University of Stockholm</i>	8	7	7	9	9
Switzerland (5)	<i>ETH Zentrum, Zurich (National facility)</i>	1	1	1	2	3
Taiwan	<i>Nat. Ctr. High-Performance Computing</i>	14	12	12	12	12
Thailand	<i>Suranaree University of Technology</i>	1	-	1	1	1
Tunisia	CCDC	1	1	1	1	1
Turkey	CCDC	-	-	1	1	1
Ukraine	<i>Academy of Science of Russia</i>	5	5	5	4	5
United Arab Emirates	CCDC	-	1	1	-	1
Uruguay	<i>Instituto Rocasolano-CSIC, Madrid</i>	1	1	1	1	1
UK (20)	CCDC	19	41	37	38	37
USA (55)	<i>Wavefunction Inc, Irvine, CA</i>	239	267	281	259	243
Uzbekistan	<i>Academy of Science of Russia</i>	1	2	2	2	2
Venezuela	<i>Instituto Rocasolano-CSIC, Madrid</i>	3	3	3	3	3
West Indies	CCDC	1	1	1	1	1
Zimbabwe	<i>Unio. Witwatersrand, Johannesburg</i>	2	2	2	-	-