# CCLRC DARESBURY LABORATORY

# EPSRC NATIONAL CHEMICAL DATABASE SERVICE

## APPENDICES TO ANNUAL REPORT DOCUMENTS 2005/6

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# Appendix 1

## Management Advisory Panel

Prof. R.E. Hubbard, University of York &Vernalis (Chair)

Dr. N. Greeves, University of Liverpool

Dr. J.G. Frey, University of Southampton

Dr. W.G. Town, Kilmorie Consultants

Dr. M.J. Biggs University of Edinburgh

Prof. C.C. Wilson University of Glasgow

1. The Management Advisory Panel (MAP) exists to assist the Service Director in the effective operation of the National Service by:
*a)* Ensuring Service is fully utilised in supporting the highest quality science.
*b)* Advising on the special and changing research needs of the communities using the Service and how the Service might be developed to meet these needs.
*c)* Advising on how the Service is perceived both scientifically and organisationally by its user communities so that timely action may be taken to build on strengths and address weaknesses.
*d)* Assisting in the promotion of the Service to ensure that as many as possible of the researchers who might benefit from it are aware of its existence and technical capabilities.

2. The full MAP will normally meet twice a year, and members may be asked to participate in additional meetings involving users or EPSRC as necessary.

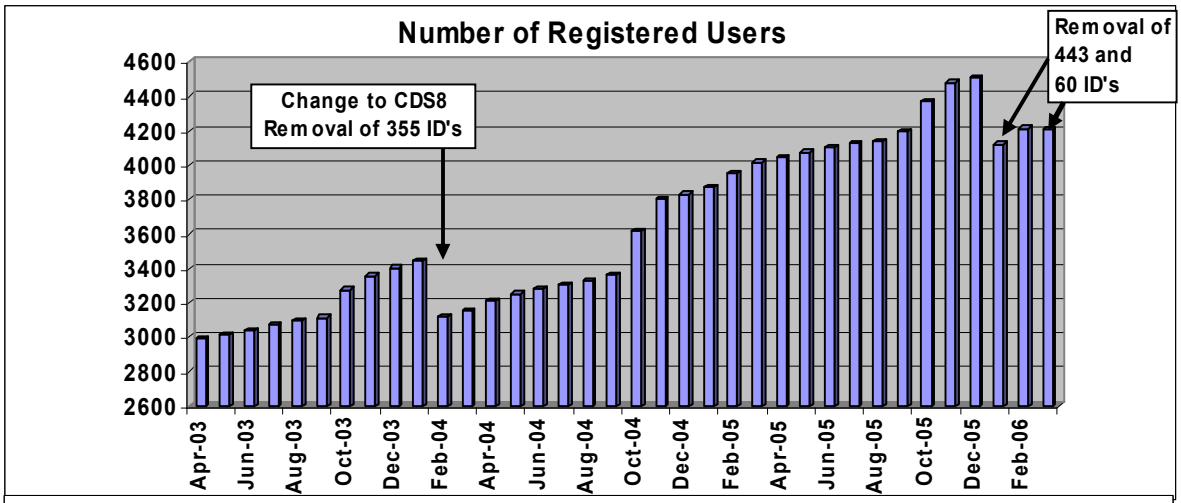
3. Members of the MAP should declare any personal interests and not participate in discussions where there would be a conflict of interest.

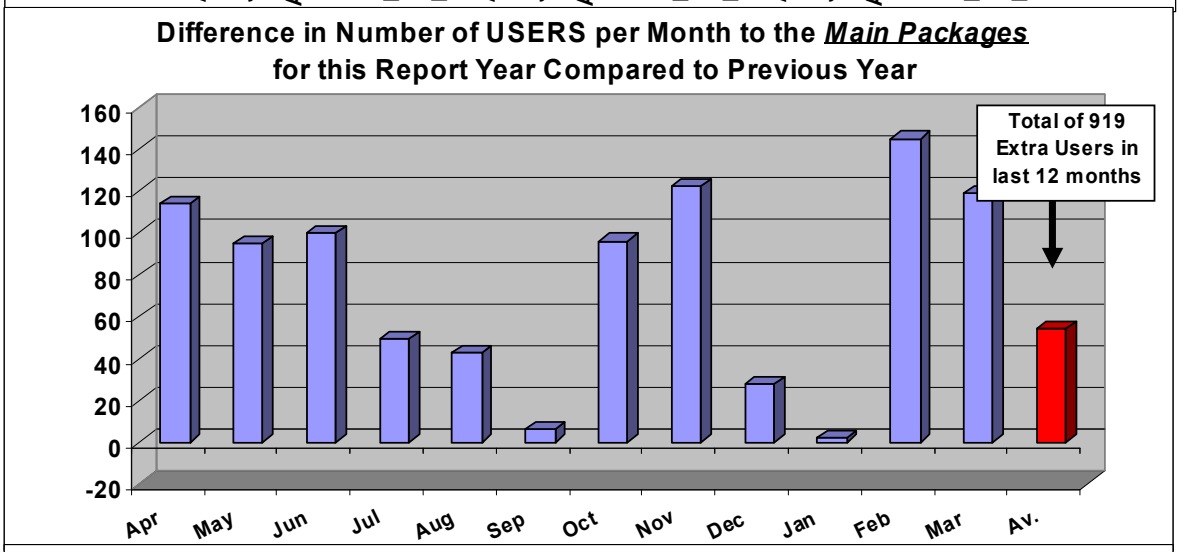
4. Membership of the Management Advisory Panel should ensure that the MAP has representatives from each main user community and should be reviewed on an annual basis to reflect changes in the user base.

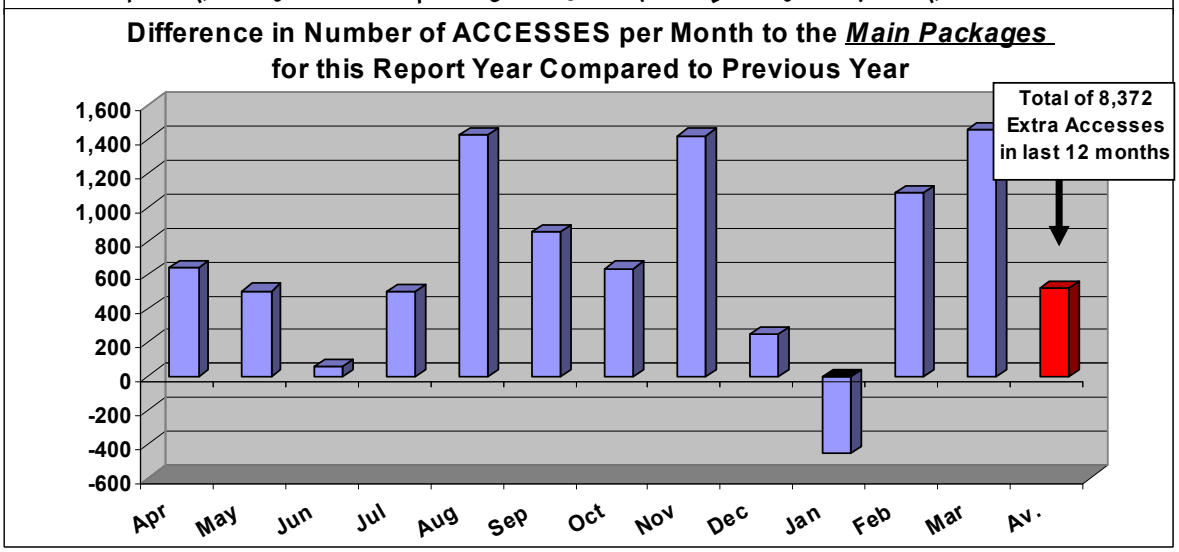
5. The composition of the MAP will be based on the following criteria:
*a)* MAP membership should be for a fixed three year term.
*b)* New MAP members to be chosen in consultation with EPSRC.
*c)* MAP to have at least one member from industry.
*d)* MAP to have at least one member who coordinates chemical information provision at a major UK university.
*e)* MAP to include no more than one member from any single institution.

# Appendix 2

## CDS Usage Statistics

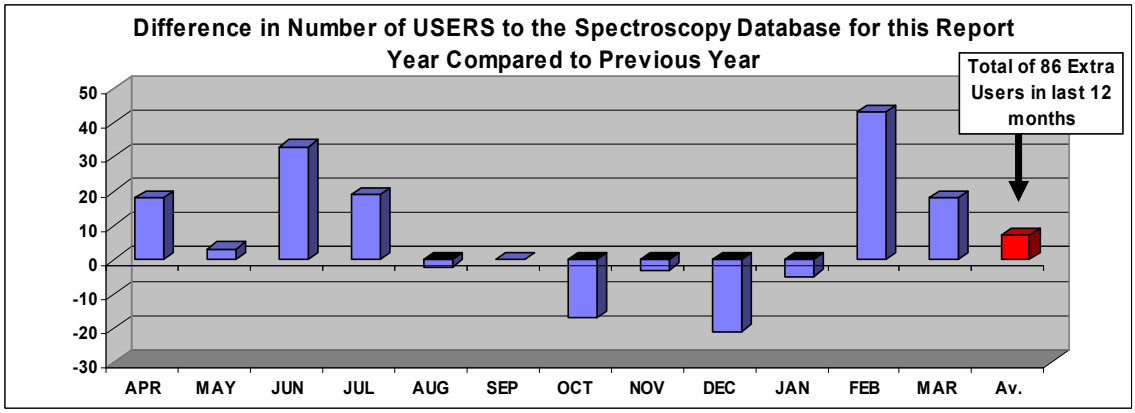


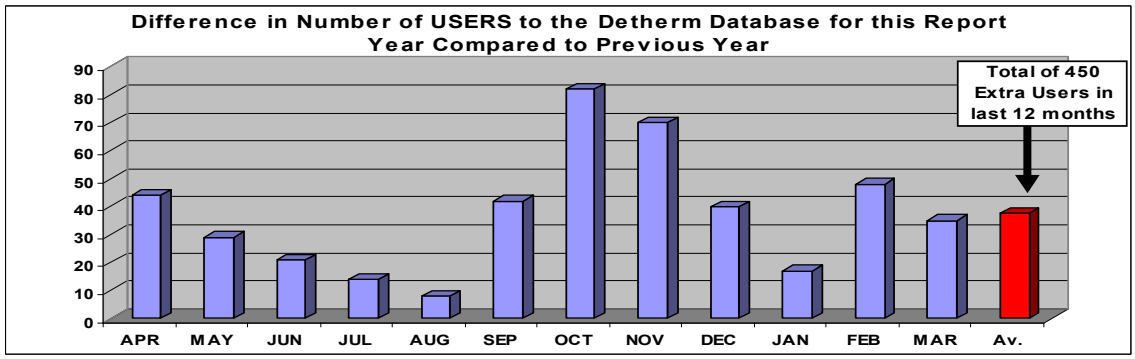



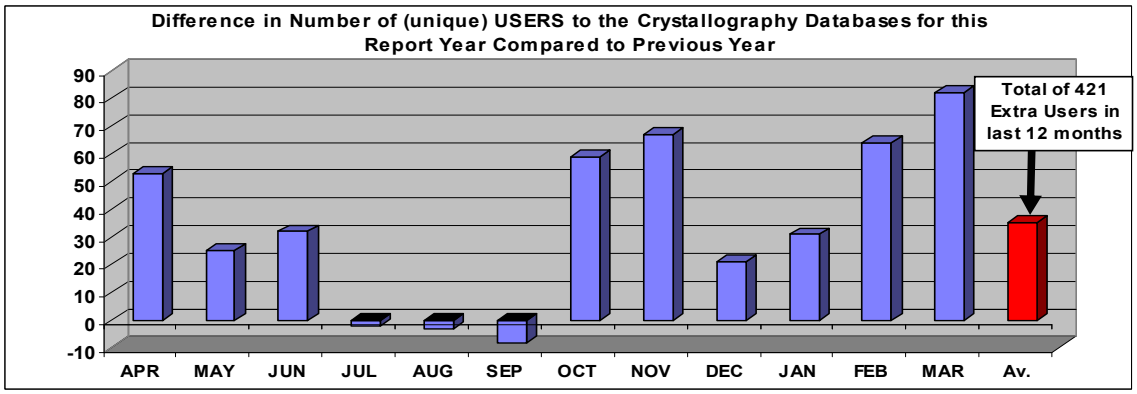



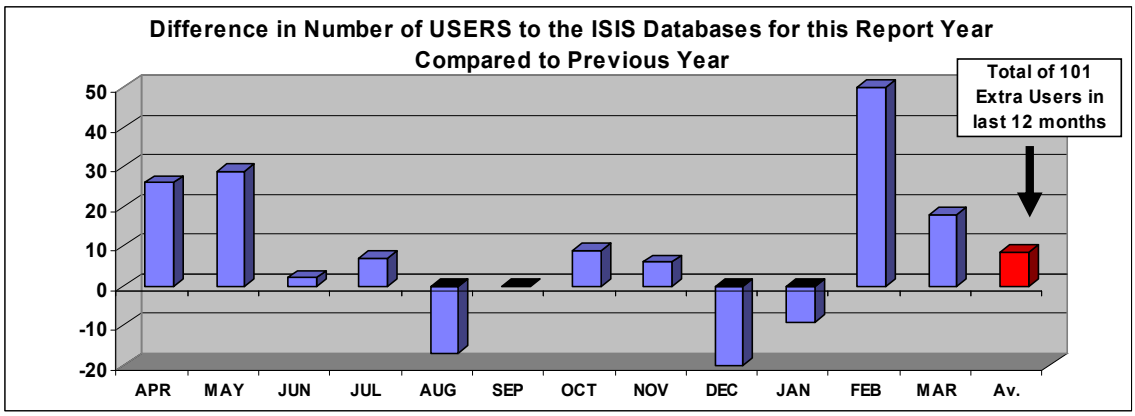
# Appendix 2 (cont.)

## CDS Usage Statistics



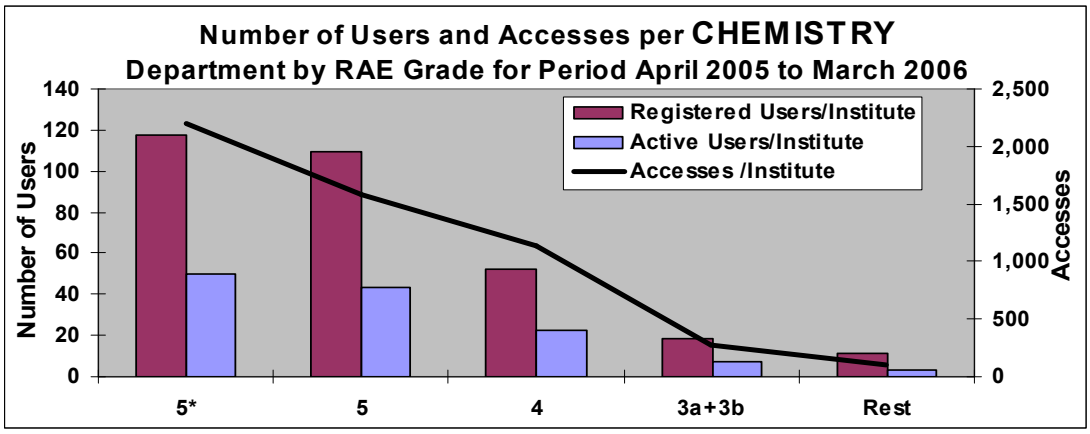



# Appendix 3

## CDS Usage and RAE Grade for *Chemistry Departments* (April 2005 - March 2006)

| Institution CHEMISTRY Department | RAE Grade | Acesses | Registered Users | Active Users | Accesses per Reg User | Accesses per Active User | %Active vs Reg.User |
|---|---|---|---|---|---|---|---|
| University of Oxford | 5* | 3401 | 118 | 65 | 29 | 52 | 55.1% |
| University of Cambridge | 5* | 3393 | 147 | 65 | 23 | 52 | 44.2% |
| Imperial College, London | 5* | 2970 | 135 | 46 | 22 | 65 | 34.1% |
| University College London | 5* | 1757 | 68 | 36 | 26 | 49 | 52.9% |
| University of Durham | 5* | 1036 | 122 | 50 | 8 | 21 | 41.0% |
| University of Bristol | 5* | 592 | 114 | 36 | 5 | 16 | 31.6% |
| University of Southampton | 5 | 3714 | 241 | 81 | 15 | 46 | 33.6% |
| University of St Andrews | 5 | 2679 | 82 | 47 | 33 | 57 | 57.3% |
| University of Manchester | 5 | 2566 | 178 | 59 | 14 | 43 | 33.1% |
| University of Liverpool | 5 | 1719 | 115 | 59 | 15 | 29 | 51.3% |
| University of Birmingham | 5 | 1511 | 68 | 45 | 22 | 34 | 66.2% |
| University of Warwick | 5 | 1326 | 89 | 39 | 15 | 34 | 43.8% |
| University of York | 5 | 1318 | 84 | 37 | 16 | 36 | 44.0% |
| University of Edinburgh | 5 | 1278 | 72 | 32 | 18 | 40 | 44.4% |
| University of Sussex | 5 | 1225 | 39 | 18 | 31 | 68 | 46.2% |
| University of Leeds | 5 | 1151 | 105 | 26 | 11 | 44 | 24.8% |
| University of Nottingham | 5 | 1040 | 191 | 62 | 5 | 17 | 32.5% |
| University of Sheffield | 5 | 649 | 98 | 32 | 7 | 20 | 32.7% |
| University of East Anglia | 5 | 282 | 56 | 27 | 5 | 10 | 48.2% |
| University of Reading | 4 | 4597 | 100 | 39 | 46 | 118 | 39.0% |
| University of Bath | 4 | 2058 | 66 | 39 | 31 | 53 | 59.1% |
| Heriot-Watt University | 4 | 2043 | 50 | 28 | 41 | 73 | 56.0% |
| University of Wales, Cardiff | 4 | 1897 | 104 | 58 | 18 | 33 | 55.8% |
| University of Glasgow | 4 | 1183 | 49 | 19 | 24 | 62 | 38.8% |
| University of Strathclyde | 4 | 1124 | 56 | 24 | 20 | 47 | 42.9% |
| University of Hull | 4 | 762 | 73 | 16 | 10 | 48 | 21.9% |
| University of Exeter | 4 | 606 | 31 | 11 | 20 | 55 | 35.5% |
| The Queen's University of Belfast | 4 | 540 | 44 | 21 | 12 | 26 | 47.7% |
| Loughborough University | 4 | 463 | 73 | 29 | 6 | 16 | 39.7% |
| University of Newcastle upon Tyne | 4 | 395 | 47 | 15 | 8 | 26 | 31.9% |
| University of Leicester | 4 | 194 | 12 | 6 | 16 | 32 | 50.0% |
| Kings (London) | 4 | 52 | 13 | 3 | 4 | 17 | 23.1% |
| University of Wales, Swansea | 4 | 44 | 11 | 6 | 4 | 7 | 54.5% |



# Appendix 4

# Components Available during Report Period

**CRYSTALLOGRAPHY**

CSD Cambridge Structural Database. Crystal structure data for over 368,000 organic and organo-metallic compounds. 3D geometric search capabilities are available for this data. Accessed via Quest, ConQuest and CSSR.

ICSD Inorganic Crystal Structure Data File. Over 89,000 inorganic structures, searchable via a web interface. Available via the ICSD-WWW web browser interface.

CRYSTMET Crystal structure data for over 81,000 metals, alloys and intermetallics.

CDIF The NIST Crystal class and unit cell data for over 237,600 structures.

*All crystallographic databases are also accessible via the CrystalWeb interface.*

**SPECTROSCOPY**

SPEC SpecInfo is a multi-technique spectroscopic database system designed to aid the chemist in interpretation and structure elucidation problems. The associated database currently contains over 146,000 $^{13}C$, $^{15}N$, $^{17}O$, $^{19}F$ and $^{31}P$ NMR spectra, 117,000 $^{1}H$ NMR spectra, 21,000 Infra-Red spectra and 138,000 Mass Spectra.

*Accessed via SpecSurf, a web browser based interface.*

**PHYSICAL CHEMISTRY**

DETHERM One of the world's largest collections of thermophysical properties databases of pure components and compound mixtures. It contains around 5 Million datasets for over 122,000 systems (25,166 pure substances and 97,046 mixtures) covering more than 500 property fields.

*The full DETHERM service was made available on 1/4/04. Accessed via Client/server interface*

**SYNTHETIC ORGANIC CHEMISTRY**

ISIS Chemical reaction information management system allowing search, retrieval and display of molecules, reactions and their associated data. Currently ISIS can access around 1.4M searchable reactions from the following databases:

REFLIB (Reference Library of established literature)
DERWENT-JSM (Journal of Synthetic Methods)
CHEMINFORM (Current awareness database - updated every 6 months)
ORGSYN (Organic Synthesis)
SPG (Synopsys Protecting Groups)
SPS (Solid Phase Synthesis)
BioCatalysis (Biomolecules as catalysts)
ChirBase (Chiral Separations by Chromatography)
NCI (National Cancer Institute Database.

*ISIS also allows access to ACD (Available Chemicals Directory), which is a database of suppliers of chemicals that contains around* 0.5M *unique compounds from* 664 *different suppliers and SCD (Screening Compounds Database) that contains over 4.5 Million compounds from around 24 suppliers.*

*Both client/server and web browser interfaces are available for all ISIS components.*

# Appendix 5

## CDS Service Levels

Any service levels which involve people do not apply during a holiday period such as Christmas - New Year. The computers are left running over this period and can be accessed by users. Any serious faults reported will be investigated, with staff being called out if necessary.

### 1. Database Services

1. New database releases available to users within one working week of reception 95% of the time. Any failures to meet this service level will be recorded as a cumulative total number of days and reported (with full details) to the Management Advisory Panel.
2. Advice on use of chemical information systems, not available in the database service, to be given within two working days with 95% availability in a calendar month.

### 2. Support

1. Chemist available to answer queries during office hours with 95% availability in any calendar month.
2. General computing queries ( high priority ) responded to within two working hours during office hours with 97% availability in any calendar month.
3. All other computing queries responded to within two working days with 95% availability in any calendar month.
4. Registration of new users complete within one working week with 95% availability within a calendar month.
5. Bugs and errors in online documentation to be corrected within 2 working days of notification 95% of the time.

### 3. System Performance

1. Service availability 99% in any calendar month excluding scheduled down time.
2. Scheduled down time less than 4 hours per quarter.
3. At least two working days warning of scheduled down time via login messages.
4. a) Daily incremental back up of user discs on main machine with 99% successful completion.
   b) Weekly full disc back up on main machine with 99% successful completion.

### 4. Network Access

1. 99% Availability of Daresbury campus network (JANET packet switched exchange (JPSE) and campus packet switched exchange (CPSE) and associated on site network) excluding the JNT specified 'at risk' periods (when scheduled maintenance may occur) which are confined to Tuesdays from 8 am to 10 am.
2. We can not guarantee the availability of the academic network (JANET) but will give assistance in tracing network access difficulties within one working day during office hours with 95% availability in any calendar month.

# Appendix 6

# CDS Site Visits and Training

| Site | Date | New users Registered | No. at Training Course |
|---|---|---|---|
| East Anglia Chemical Sciences and Pharmacy | 29-Sep-05 | 17 | |
| Birmingham Chemical Engineering | 11-Oct-05 | 12 | |
| Nottingham Pharmacy | 20-Oct-05 | 7 | |
| Newcastle Chemistry | 27-Oct-05 | 20 | |
| Liverpool John Moores Biosciences | 10-Nov-05 | 12 | |
| Aberdeen Biomedical Sciences | 17-Nov-05 | 4 | |
| Cardiff Chemistry | 29-Nov-05 | 30 | 55 |
| Belfast Chemistry | 06-Dec-05 | 8 | 10 |
| London School of Pharmacy | 26-Jan-06 | 5 | |
| Sunderland Bioscience and Chemistry | 08-Feb-06 | 5 | 10 |
| Cranfield BioScience and Technology | 16-Feb-06 | 4 | 20 |
| Liverpool John Moores Biosciences | 17-Feb-06 | 4 | 12 |
| Liverpool Chemistry | 24-Feb-06 | 16 | 27 |

**Training by Local Representatives**

**We have supplied 14 Universities with their own training ID's. The following training courses have been run by the local representative.**

| Department | Training Course |
|---|---|
| Brighton Pharmacy and Biomolecular Sciences | ISIS |
| Cambridge Chemistry | ISIS |
| Cranfield Biotechnology | ISIS |
| Exeter Chemistry | ISIS |
| Heriot-Watt Chemistry | Crystallography |
| Leeds Materials & Ceramics | Crystallography |
| Queen Mary & Westfield Library | Crystallography |
| Strathclyde Chemistry | Crystallography |
| UCL Chemistry | Crystallography |
| Warwick Chemistry | ISIS |

# Appendix 7

## Papers Citing the Chemical Database Service JCICS review paper in 2005 (data retrieved from the ISIS Web of Science)

| AUTHOR | JOURNAL | IMPACT FACTOR 2004 |
|---|---|---|
| Edwards DJ, et al. | **ACTA. CRYSTALLOGR. B.** 61: 335-345 Part 3 JUN 2005 | 5.42 |
| Aucott SM, et al. | **ACTA. CRYSTALLOGR. C.** 61: O112-O113 Part 2 FEB 2005 | 0.73 |
| Dale SH, et al. | **ACTA. CRYSTALLOGR. C.** 61: O411-O413 Part 6 JUN 2005 | 0.73 |
| Howie RA, Wardell JL, | **ACTA. CRYSTALLOGR. E.** 61: M1701-M1704 Part 9 SEP 2005 | 0.49 |
| Barker J, et al. | **ACTA. CRYSTALLOGR. E.** 61: M748-M750 Part 4 APR 2005 | 0.49 |
| Nagaraj B, et al. | **ACTA. CRYSTALLOGR. E.** 61: O1041-O1042 Part 4 APR 2005 | 0.49 |
| de Souza MVN, et al. | **ACTA. CRYSTALLOGR. E.** 61: O1347-O1349 Part 5 MAY 2005 | 0.49 |
| Nagaraj B, et al. | **ACTA. CRYSTALLOGR. E.** 61: O1609-O1610 Part 6 JUN 2005 | 0.49 |
| Nagaraj B, et al. | **ACTA. CRYSTALLOGR. E.** 61: O1757-O1759 Part 6 JUN 2005 | 0.49 |
| Lynch DE, McClenaghan I, | **ACTA. CRYSTALLOGR. E.** 61: O2347-O2348 Part 8 AUG 2005 | 0.49 |
| Smith JH, et al. | **ACTA. CRYSTALLOGR. E.** 61: O2499-O2501 Part 8 AUG 2005 | 0.49 |
| Narasegowda RS, et al. | **ACTA. CRYSTALLOGR. E.** 61: O849-O850 Part 4 APR 2005 | 0.49 |
| Nagaraj B, et al. | **ACTA. CRYSTALLOGR. E.** 61: O884-O885 Part 4 APR 2005 | 0.49 |
| Boag NM, Clapham S, et al. | **ACTA. CRYSTALLOGR. E.** M2172-M2173 Part 10 OCT 2005 | 0.49 |
| Ward BD, et al. | **ANGEWANDTE CHEMIE-INT. ED.** 44 (11): 1668-1671 2005 | 9.16 |
| Cheung KMJ, et al. | **BIOORG MED CHEM LETT.** 15 (14): 3338-3343 JUL 15 2005 | 2.33 |
| Williams GD, et al. | **CHEM. COMMS** (37): 4735-4737 2005 | 4.00 |
| Sosa-Sanchez JL, et al. | **CHEM-EUR. J.** 11 (14): 4263-4273 JUL 4 2005 | 4.52 |
| Dunn SC, et al. | **CHEM-EUR. J.** 11 (7): 2111-2124 MAR 18 2005 | 4.52 |
| Beltran HI, et al. | **CHEM-EUR. J.** 11 (9): 2705-2715 APR 22 2005 | 4.52 |
| Skakle J, | **CHEMICAL RECORD** 5 (5): 252-262 2005 | 2.71 |
| Holmes KE, et al. | **CRYSTENGCOMM** 7: 202-205 MAR 14 2005 | 2.60 |
| Grossel MC, et al. | **CRYSTENGCOMM** 7: 279-283 APR 7 2005 | 2.60 |
| Burrows AD, et al. | **CRYSTENGCOMM** 7: 388-397 JUN 15 2005 | 2.60 |
| Deeth RJ, Hearnshaw LJA, | **DALTON TRANSACTIONS** (22): 3638-3645 2005 | 2.93 |
| Fontecha JB, et al. | **DALTON TRANSACTIONS** (5): 923-929 2005 | 2.93 |
| Boa AN, et al. | **EUR. J. INORG. CHEM.** (5): 872-878 MAR 4 2005 | 2.34 |
| Drew MGB, et al. | **INORG. CHEM. COMMUN.** 8 (3): 239-241 MAR 2005 | 3.45 |
| Frampton PPC, et al. | **INORGANIC CHEMISTRY** 44 (20): 7138-7142 OCT 3 2005 | 1.68 |
| Grandjean D, et al. | **J. AM. CHEM. SOC.** 127 (41): 14454-14465 OCT 19 2005 | 6.90 |
| Etok SE, et al. | **J. MATER. SCI.** 40 (21): 5627-5633 NOV 2005 | 0.86 |

| | | |
|---|---|---|
| Dascombe MJ, et al. | **J. MED. CHEM**. 48 (17): 5423-5436 AUG 25 2005 | 5.08 |
| Ghuman J, et al. | **J. MOL, BIOL.** 353 (1): 38-52 OCT 14 2005 | 5.54 |
| Davis CJ, et al. | **J. ORG. CHEM.** 70 (11): 4414-4422 MAY 27 2005 | 3.46 |
| Davies JR, et al. | **J. ORG. CHEM.** 70 (18): 7305-7316 SEP 2 2005 | 3.46 |
| Xu YJ, et al. | **J. ORG. CHEM.** 70 (20): 8079-8087 SEP 30 2005 | 3.46 |
| Gonzalez-Outeirino J, et al. | **J. ORG. CHEM.** 70 (7): 2486-2493 APR 1 2005 | 3.46 |
| Cheung FK, et al. | **J. ORG. CHEM.** 70 (8): 3188-3197 APR 15 2005 | 3.46 |
| Brewster AG, et al. | **LETT. ORG. CHEM.** 2 (1): 21-24 FEB 2005 | |
| Jones JW, et al. | **LIQUID CRYSTALS** 32 (11-12): 1465-1481 NOV 2005 | 1.06 |
| Mitchell RJ, et al. | **MATER. SCI. TECH-LOND.** 21 (1): 125-132 2005 | 0.64 |
| Bailey EH, et al. | **MINERALOGICAL MAGAZINE** 69 (5): 563-575 OCT 2005 | 1.27 |
| Bailey EH, et al. | **MINERALOGICAL MAGAZINE** 69 (5): 563-575 OCT 2005 | 1.27 |
| Rogers K, et al. | **NUCL. INSTRUM. METH A.** 548 (1-2): 123-128 AUG 11 2005 | 1.35 |
| Cohen HM, et al. | **ORG. BIOMOL. CHEM.** 3 (1): 152-161 2005 | 2.19 |
| Rejzek M, et al. | **ORG. BIOMOL. CHEM.** 3 (1): 73-83 2005 | 2.19 |
| Bentz EL, et al. | **ORG. BIOMOL. CHEM.** 3 (15): 2872-2882 2005 | 2.19 |
| Palmer FN, | **ORG. BIOMOL. CHEM.** 3 (20): 3805-3811 OCT 21 2005 | 2.19 |
| Cooper TS, et al. | **ORG. BIOMOL. CHEM.** 3 (7): 1252-1262 2005 | 2.19 |
| Leung LMH, et al. | **ORGANIC LETTERS** 7 (23): 5183-5186 NOV 10 2005 | 4.20 |
| Matharu DS, et al. | **ORGANIC LETTERS** 7 (24): 5489-5491 NOV 24 2005 | 4.20 |
| Boyd CL, et al. | **ORGANOMETALLICS** 24 (10): 2347-2367 MAY 9 2005 | 3.20 |
| Ward BD, et al. | **ORGANOMETALLICS** 24 (10): 2368-2385 MAY 9 2005 | 3.20 |
| Tredget CS, et al. | **ORGANOMETALLICS** 24 (13): 3136-3148 JUN 20 2005 | 3.20 |
| Aspinall HC, et al. | **ORGANOMETALLICS** 24 (14): 3458-3467 JUL 4 2005 | 3.20 |
| Skinner MEG, et al. | **ORGANOMETALLICS** 24 (23): 5586-5603 NOV 7 2005 | 3.20 |
| Morales F, et al. | **PHYS. CHEM. CHEM. PHYS.** 7 (4): 568-572 2005 | 2.08 |
| Glatzel P, et al. | **PHYSICAL REVIEW B** 72 (1): Art. No. 014117 JUL 2005 | 3.08 |
| Alexandrou I, et al. | **REV. ADV. MATER. SCI.** 10 (5): 467-472 DEC 2005 | |
| Johnson C, et al. | **SOLID STATE NUCL. MAG.** 27 (3): 155-164 MAY 2005 | 1.70 |
| Hussaini SR, Moloney MG, | **SYNTHETIC COMMUNICATIONS** 35 (8): 1129-1134 2005 | 0.97 |
| Coles SJ, et al. | **TETRAHEDRON** 61 (18): 4447-4452 MAY 2 2005 | 2.64 |
| Jacob AM, | **TETRAHEDRON LETTERS** 46 (51): 8823-8825 DEC 19 2005 | 2.48 |
| Boucheron C, et al. | **TETRAHEDRON-ASYMMETRY** 16 (10): 1747-1756 MAY 23 2005 | 2.39 |
| Leung LMH, et al. | **TETRAHEDRON-ASYMMETRY** 16 (14): 2449-2453 JUL 18 2005 | 2.39 |

# Appendix 7

## CDS Survey Results (Autumn 2005)

This was a web form based survey, users being alerted by email with an appropriate link to the survey form. A total of 3,621 emails were sent out and 195 forms filled out. This is a 5.4% response rate.

**1. How useful is the CDS to your work ?**

| | | |
|---|---|---|
| No answer 5 (3%) | Slightly useful 10 (5%) | Very useful 69 (35%) |
| No use at all 0 (0%) | Sometimes useful 21 (11%) | Vital 49 (25%) |
| | Useful 41 (21%) | |

**2. What other electronic chemical information sources do you use ?**

| | | |
|---|---|---|
| SciFinder 79 (41%) | NIST (chemistry webbook or | Scopus 12 (6%) |
| CrossFire Beilstein/Gmelin 93 (48%) | other web resource) 43 (22%) | CD-ROMs 19 (10%) |
| | Web of Science 160 (82%) | Other 28 (14%) |

**3. Are there any other specific databases that you would like to see CDS acquire ?**

Chemical safety data
MDDR
Electron diffraction data/3D reciprocal space representations of crystal structures
SciFinder (x2) Chemical Abstracts
ACD/Labs NMR Spectral Databases
Patent database
LiqCryst Database (LCI Publishers, Hamburg)
SciGlass
Surface structure database
More less common phases suh as columbite, baddeyrite, etc in TiO2, high pressure Fe Surface data for solids and morphology
NMR (15N) & Mass Spectra
Green synthetic methods database
Polymers/ materials both synthesis and characterisation and properties
Register of Toxic Effects of Chemical Substances (RTECS)
JCPDS x3
Phase diagrams
Binary Alloy Phase Diagrams database
Ternary Alloy Phase Diagrams database
Magnetic structures database
Physical and thermochemical data of materials
Aldrich libraries of rare compounds and chiral compounds
Materials properties, especially electronic materials
Raman spectra from materials
Protein structure determination

**4. As a central service, CDS has made available a number of specialist databases, such as Chirbase and Solid Phase Synthesis, which have limited appeal but tend to be very useful to a subset of users. Should CDS continue to acquire and support such databases ?**

| | | |
|---|---|---|
| No answer 7 (4%) | No 4 (2%) | Probably 52 (27%) |
| Don't know 35 (18%) | Possibly 19 (10%) | Yes 78 (40%) |

**5. CDS currently sends out news about the Service via a number of mechanisms. Please could indicate how useful these are to you.**

**Our six monthly Newsletter**

| | | |
|---|---|---|
| No answer 6 (3%) | Slightly useful 45 (23%) | Very useful 13 (7%) |
| No use at all 16 (8%) | Sometimes useful 68 (35%) | Vital 0 (0%) |
| | Useful 47 (24%) | |

**Broadcast e-mail - generally with a link to further information on the Web**

| | | |
|---|---|---|
| No answer 6 (3%) | Slightly useful 23 (12%) | Very useful 37 (19%) |
| No use at all 7 (4%) | Sometimes useful 56 (29%) | Vital 4 (2%) |
| | Useful 62 (32%) | |

**News banners when you logon to the CDS server**

| | | |
|---|---|---|
| No answer 12 (6%) | Slightly useful 49 (25%) | Very useful 15 (8%) |
| No use at all 29 (15%) | Sometimes useful 47 (24%) | Vital 0 (0%) |
| | Useful 43 (22%) | |

**The messages posted on the CDS web homepage**

| | | |
|---|---|---|
| No answer 10 (5%) | Slightly useful 52 (27%) | Very useful 10 (5%) |
| No use at all 28 (14%) | Sometimes useful 58 (30%) | Vital 0 (0%) |
| | Useful 37 (19%) | |

**Checking the CDS News section directly**

| | | |
|---|---|---|
| No answer 16 (8%) | Slightly useful 54 (28%) | Very useful 6 (3%) |
| No use at all 48 (25%) | Sometimes useful 41 (21%) | Vital 0 (0%) |
| | Useful 30 (15%) | |

**The CDS Roadshow**

| | | |
|---|---|---|
| No answer 23 (12%) | Slightly useful 39 (20%) | Very useful 8 (4%) |
| No use at all 71 (36%) | Sometimes useful 26 (13%) | Vital 4 (2%) |
| | Useful 24 (12%) | |

**6. CDS is looking at producing a simple global interface to all of the databases we run. The idea is that you would search for a molecule and retrieve all of the data (or possibly links and/or meta-data) about this molecule held in the other CDS databases. Do you think such a system would be useful ?**

No answer 4 (2%)
Don't know 11 (6%)
No 3 (2%)
Possibly 19 (10%)
Probably 36 (18%)
Yes 122 (63%)

**7. Please can you tell us the approximate number of papers you have published in the last 3 years which cite or acknowledge use of the CDS**

A total of 211 papers. This would imply around 1300 papers per year (excluding duplications).

**8. Please can you tell us the approximate number of papers you have published in the last 3 years which do not cite or acknowledge, but do make some use of the CDS**

A total of 489 papers. This would imply around 3000 papers per year (excluding duplications).
**Comments**

**Comments about value of the Service**

The crystallographic databases are of vital importance to me. I have just finished a book on introductory crystallography, in press by Wiley. It would not be possible to produce such a book without your help. [I have acknowledged this fully - see Donald Parkin for more info.]

The most useful part of the service for my group by far is chirbase. It is a great shame if this is under threat. Some of the interfaces are very difficult.....(NMR etc., so we have never really managed to get them to work....It would be good if they were all run from ISIS draw type packages.

The ISIS ACD is extremely useful, as are the others, although I seem to be the only person in my office who uses ACD.

Inorganic crystal structure database is essential to my work

Although I have not used the service directly as a resource for my recent papers, is essential for checking speculative ideas for grant applications.

The service provided is excellent. It forms an important part of our teaching and research effort. Long may it remain so.

ICSD is indispensable

As a biochemist/molecular modeller I find the CDS to be an extremely useful resource, despite my rather occasional use of the service. In the particular area of protein-ligand interactions, and of force-field development, the CDS provides one of the "bedrock" sets of data on which we draw information. The tools provided to retrieve data are excellent and continually improving. My message to the EPSRC is that it is vitally important that the UK continues to support this resource of truly international importance.

Although my use of CDS is sporadic, it is an extremely useful source of 3D structures.

The CDS should continue and it is an essential service especially for many of us researching in an ever increasing multidisciplibnary field

The Cambridge Crystallographic Database, and equally the various associated visualisation tools, are a very important and helpful asset to my research activity.

I think it is a wonderful service to the practicing organic chemist and long may it continue.

CDS is now my only means of access to the Cambridge Structural Database. Up till March 2005 this was available to me 'in house'. It is essential for a part of the work I have been doing.

A very necessary structural database service.

We are very grateful to have access to CDS as we have great difficulty accessing electronic chemical information/literature as we do not have an "ac.uk" email and do not have Athens access and so although we do not make huge use of the CDS it is a very valuable facility and the only reason that we do not make more use of it is because of the very variable nature/timescale of our work

I used to take the CDS for granted, but after working in the States where there is no equivalent to the CDS I have realised just how valuable the CDS is.

The MDL ISIS synthesis databases are vital to my work, and should be maintained at all costs!
The service is great - it makes the difference between finding the run of the mill information, and actually finding the stuff that makes a credibility difference for top-level science.

**Comments about publications**

I have only used ICSD, but found it very useful in my teaching. I have only started using it recently, but I expect it will be useful in my research, and will lead to some publications. The issue of citation and acknowledging use of the service is quite complex. I often use it to 'check' on a small bit of information, which might in some form or other get through to inclusion in a paper. However this snippet of information generally would only comprise a minute fraction of the paper and its provenance would be lost or deemed not significant enough. Indeed, if it were to be cited then the likelihood is that it would be the ORIGINAL paper reporting the information that gets into the reference list and not one citing the CDS. Only in a paper where there was a significant amount of searching or data mining involved would I cite the CDS.

For the purposes of accounting (and accountability) to EPSRC I would suggest an alternative mechanism to 'register' the usage of your service. How about a data 'hits counter'? This could be run like an honesty box where the user checks a tick box to indicate that some information gleaned from searching the CDS will contribute in some part to a publication? SciFinder is extremely useful but very very expensive. Even the better UK chemistry departments struggle to provide it. Could the CDS look into some sort of arrangement where it is available to all users, maybe on a one free session per month basis or similar.

The reason for the lack of acknowledgement is that for a substantial amount of the last 3 years I worked in the Republic of Ireland and thus could not access (I believe!) the CDS services

The absence of any acknowledgement of CDS in the two papers referred to in (8) above was an oversight (apologies!). I use the CDS databases (REACCS, ACD) on such a regular basis that all my work benefits from their availability. They are essential tools now.

CDS is particularly useful for background work, e.g., finding cheapest chemicals (via ACD), analysing NMR spectra, getting literature on thermodynamic parameters (DETHERM) etc. This background information rarely gets published but is absolutely essential for research. This probably explains the low rate of CDS citations.

I do not publish papers myself, but support a number of people who do. As a group we have probably published about 3 papers in the past year which have used information held on the CDS and about 6 others that have made some use but not been reliant on information. We mainly use it for sourcing chemicals on the ACD, and finding melting points and CAS registry numbers to enable us to search for the compounds elsewhere.

RE: Q's 7 and 8- now you ask the specific question, I am sure that I. like many authors, look up data in the CDS during the research and then unless in the manuscript one cites data extracted from the CDS, it is easy to forget one has done it or role it into the usual acknowledgement to EPSRC for "funding" or "support". I am sure this is not intentional - just in the pressure of work one does not always remember.

I use CDS to look up bond distances etc quickly, but these never seem enough to justify a full acknowledgment. I hope I'm not letting you guys down by doing this.

Sorry I never thought to cite the service. I will in future

I would only cite the CDS if it has made a crucial difference to a piece of work - which is very rare. After all I do not cite WOK, SciFinder, our library, on-line journal providers, the Aldrich catalogue etc and would not cite the use of well known reactions, the NMR software we use, Mac OS X etc. These are part of the infra structure of doing research.

I do strongly support the CDS, and am very happy to show that support in other ways (letters of support etc) but do not feel that references in a paper are the appropriate mechanism (at least for reaction searching which is my main use). Thanks a lot!

I principally use CCSD, ISDS and Chirbase which are all extremely useful if not vital to our work. I have not tended to cite use of CDS because I did not realise how important it maybe to its future existence and because I do not tend to cite any other information source. However there is no reason not to cite the CDS and in future I will do so. I beleive I am not alone as most publications in my field, for example, that deal with single crystal structure descriptions tend to cite the primary literature and not that the citation was found via the CCSD/CDS

The problem is what is making use of CDS. The only data bases I use on CDS are CSSR and ICSD. When for example I cite the literature values of the cell parameters for one compound it seems over the top to cite CDS as well, but when I want to make a systematic comparison of series of compounds then of course CDS should be cited.

To be honest almost every crystallograhic paper will make some use of the CDS, and should really be cited every time. There is a lot of CDS derived background data that is thought of in the community as general knowledge, but is really from the CDS

Reason for 0 papers, is that I am haven't published any papers, but the ACD database has been very helpful in my first year of PhD study, however one of my friends was struggling to find sugars, which he knew where available on the database, which could be something to look at in the future.

For me, one of the most useful databases in the whole of CDS is the available chemicals directory. As a means of sourcing specific compounds or finding which structural variant are sold, it is invaluable. I am sure that I (and many others) overlook the use of this database when writing up the work. The CDS probably deserves many more citations arising from use of this database alone. I have 1 paper in preparation where I intend to acknowledge the CDS, as I have used results from the crystallographic database, but this is more obvious than using the ACD.

It is difficult to say what use has been made of CDS in any one paper when it is one of a number of different sources of background information. The importance of such background information needs to be stressed to the funding bodies.

The reason for the answers to 7 and 8 is that the use of the CDS tends to come at the very early planning or execution stages of a project, whereas paper preparation relies on the primary literature.

Sorry, I should have cited the use of CDS. We use it especially as the route to the Cambridge Structural Database. This is vital for our work on structural chemistry, and I am happy to be quoted on that.
I took it for granted that one would not have to cite the use of databases such as scifinder or Reaccs in publication. As I am typically only using acdfind and rxnbrow I did not see it as necessary. Was I wrong - Probably partly also that I have never read any publication where others have done this in my field.

As a technical editor for a science publisher, I don't author papers myself but I occasionally use the CDS to check references. I also encourage authors to cite it correctly in papers I handle.

It is very difficult to be specific about the "use" of CDS in a particular publication. I use almost exclusively Reaction searching and ACD. It is very rare that a reaction carried out and described in a paper will have arisen directly and exclusively from a CDS search. The search will form part of the overall preparation, planning and execution of a synthetic scheme and the planning will also involve other databases (e.g. Beilstein, Web of Science), books and consultation with colleagues. It would be unfair and unrepresentative to cite CDS exclusively as the information source and impractical to cite all sources of information and inspiration. I do not see an easy way round this problem except to give feedback through questionnaires like this that CDS is at least as vital a resource to my work as the University Library or access to the internet - and just as difficult to acknowledge.
Also organic chemists in general tend not to cite the databases they use for searching reactions, as the database is not considered part of the science. This is especially true for ACD, which I think is the most widely used CDS database in my lab. People would regard this in the same light as citing the Aldrich catalogue. Perhaps suggesting the routine use of the CDS citation as part of the experimental section of synthetic organic chemistry papers might help increase citation rates.

We use CDS primarily for ACD finder, but should use it for RXN finder too, at the moment we just use Beilstein. It seems a little excessive to cite CDS for the use of ACD finder in general research, it would be more appropriate to acknowledge CDS in ackowledgments, as we do for the MS service at Swansea.

Haven't published any papers in the last three years! Just returned to experimental science after four years working on databases.

I will ensure that CDS is cited in future!

I use crystallographic databases (organic and inorganic) as the useful reference tools in the routine job. In my case the obtained information is not normally used for publications, but allows to avoid duplicate time-consuming experiments and saves me a lot of time.

This is not the best way to judge the service - who gets the citation CDS or ICSD?? CDS is for the use of UK academics and is very good BUT its ICSD who have generated the database. The service has actually become less use to me, due to the availability of local access to Beilstein, SciFinder, Web of Science. My NMR needs are satisfied via ACD/Labs software that I pay for from Grants. SpecInfo is less vital to me than it was. In reality I do not make much use of the service now. Notwithstanding I think it should continue. For example can you set up an agreement to have access to all the ACD/Labs software.

7 and 8 look odd, but a lot of my use is running something, sometimes solving and refining with difficulty, only to find some0ne else has already done it, or something so similar as to make my stuff pointless. Thus the database is INVALUABLE to me inasmuch as stops me wasting time effort etc and to back up me shouting at people 'why didn't you check first!', but won't appear in print

I did go through a phase a few years ago of citing the service on every paper, but I stopped. It seems strange having to cite something that is so integral and essential to our work...it is used completely routinely for work in organic synthesis, especially rxnbrowser, acd; also often (but less so) chirbase I find the ACD useful for structure and substructure searches. I am not sure that this merits an acknowledgement in a paper though.

Our primary (daily) use of the CDS is to check for known phases - thus the high number of entries under 8 above. Although this does not give rise directly to publications or citations it makes a vital contribution to all our work as it allows us a rapid means to avoid needlessly duplicating published results. Overall it increases the efficiency of chemical research, and has direct benefits for 25-30 academic staff and their projects.

**Comments about Mac support**

It is crucially important that CDS continues to support interfaces with Apple computers

Web-based services are generally the most useful for cross-platform access (I write as a Mac user...)

As a Mac user I am appalled there there appears to have been a complete discontinuation of support for Mac OS. When are OSX versions of ISIS, Chime for Safari etc going to be produced ? If they are not then I can guarantee that all Mac users in my department will simply use Scifinder all the time and forget all about CDS. Sorry to have to say this but it is essential that something is done if you want people to use you and cite you. Otherwise you will drift into obscurity and redundancy.

Please Please make the service work with Macs. The majority of my colleagues are Mac users and it is frustrating that the web interfaces require chime pro which is not available for Mac OSX users. This is where scifinder and the like win out in popularity, even though they are technically inferior to CDS services.

The low use of CDS is simply a mater of access. I use a Mac and the access eg to ACD requires I load classic and an old version of Netscape. There are similar problems with reaction browser (or were when I last looked). If access was simpler than I suspect i would make more use of it and might even show my students how to use it - they probably are not even aware of its existence

**Other comments**

I think the service is excellent

CDS needs to be more informative, like accessing journal from that particular crystal structure itelf (link to the journal).

Determination of Protein X-Ray structures will be useful.

If it is a same crystal structure, then repetition should be excluded and the sequence should be in order of good crystal structures, then the rest.

For some crystals, the coordinates are unavailable, which is meant to be available.

I have no Could do with more data relating to materials properties (all sorts). CRC 'Rubber book' can be useful but often has little data.

Maybe Daresbury would consider becoming the 'home' for all published papers arising from publicly funded research. Papers would be in .pdf format for download. This free access would fit in with the trend towards open access as mooted by Wellcome

Re the simple global interface. It would be good only if it worked. As an example of what I mean; currently you get different results using the CrystalWeb search page to search CrystMet than if you use the older command line system. A global interface will only work if it will definately find all references to the compound in question. My answers seem contradictory, but my main use of the CDS has been to identify possible impurity phases present in our samples by Rietveld refinement. So far I've had no positive identifications so I havn't cited the CDS. I think we should rectify this in
future.

Note - I am retired, but still continue with my work. It would be a disaster if the serive is withdrawn and one fear I have is that as I am no longer full time I will loose rights of use.

Since we gained access to Beilstein both myself and my students have stopped using CDS in the perhaps mistaken belief that the former database was larger and more comphrehensive. Following a recent e-mail by Nick Greaves I decided to start using CDS again. I was pleasently surprised that my username and password still worked and was able to download the data base. However I failed to get it to work-- and I have limited time to play around with these things. Perhaps there are others in my position who would like to use the facility but cannot overcome the initial barrier.

The usefulness of the global searching facility referred to in question 6 is dependent upon it interfacing properly with the CCDC, which for my work is the truely vital part of the CDS.

We're not heavy users, but occasionally find the CDS useful when exploring new areas, searching for model systems etc.

I use the crystallographic databases, which I find very useful

The no use at all are due to the fact that I have not used them!

In general Crystal Web is what I need and would like 1 'portal' to get ANY 3D structure
I'm not an academic, I'm a service manager and I haven't published anything in the last 3 yrs. I do find the NMR databases very useful on occasions when I need to look something up though.

Making the thermal parameters available along with the coordinates on downloaded structures would be really useful - especially when preparing pictures for reviews and teaching purposes!!
i am actually making a PhD... CDS is sometimes useful for me... but because I am working mainly with organic compound and I am just using the CDS for running CONQUEST, I do not log often on the CDS website..

The database is terrible!!!

I very rarely use the CDS service. My original registration dated from the time when you hosted the CrossFire database, but I have still used your service on occasion to access small molecule crystal data.

The CDS database I use most frequently is the ACD, hence 'some use' of the CDS is true for all of the synthetic work we do. Student feedback from the CDS Roadshow was that the leaflet is informative and useful, but that the effectiveness of the presentation could be vastly improved (e.g. it would be good to see the databases actually in use - run through an example on each one?).

I am only an occasional user, as a biochemist. I am sure that the service is far more valuable to Physical Scientists and Chemists.

Use of the ICSD would have been invaluable at my previous jobs, but these were not in the UK, so I didn't have access to the CDS.
I am registered since 1 year and have not done new structures calculations. I am interested in uncommon phases (for example in TiO2) but they are not refered so CDS is not useful at the moment and my articles in progress had not needed those data. However, I think that a such database is very useful for the community. I hope that you will include new structures and new data such as exposed surfaces in solids, morphology, IR, TPD, etc.

I noticed that the reaction databases don't get as much use by our group members as they might. People tend to default to Beilstein, even though I find the reaction browser is better for very common synthetic reactions.

I'm not sure if it comes under the CDS remit but a chemical electronic notebook would be very useful.

When I have had problems with the service I have always found the helpdesk staff to be prompt with their response and really helpful.

I'm now retired (but still almost active as normal), and have tended to use the longer established facilities.