CCLRC DARESBURY LABORATORY
EPSRC NATIONAL CHEMICAL DATABASE SERVICE

APPENDICES TO ANNUAL REPORT DOCUMENTS 2006/7

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2. Usage Statistics
3. CDS Use and RAE Grade for Chemistry Departments
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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.

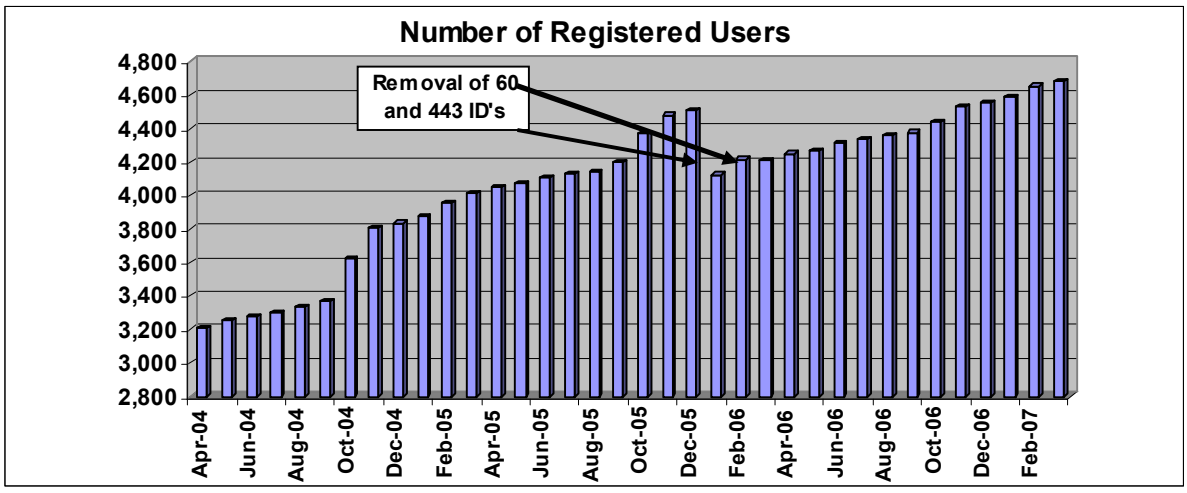
2. The full MAP will normally meet twice a year, and members may be asked to participate in additional meetings involving users or EPSRC as necessary.

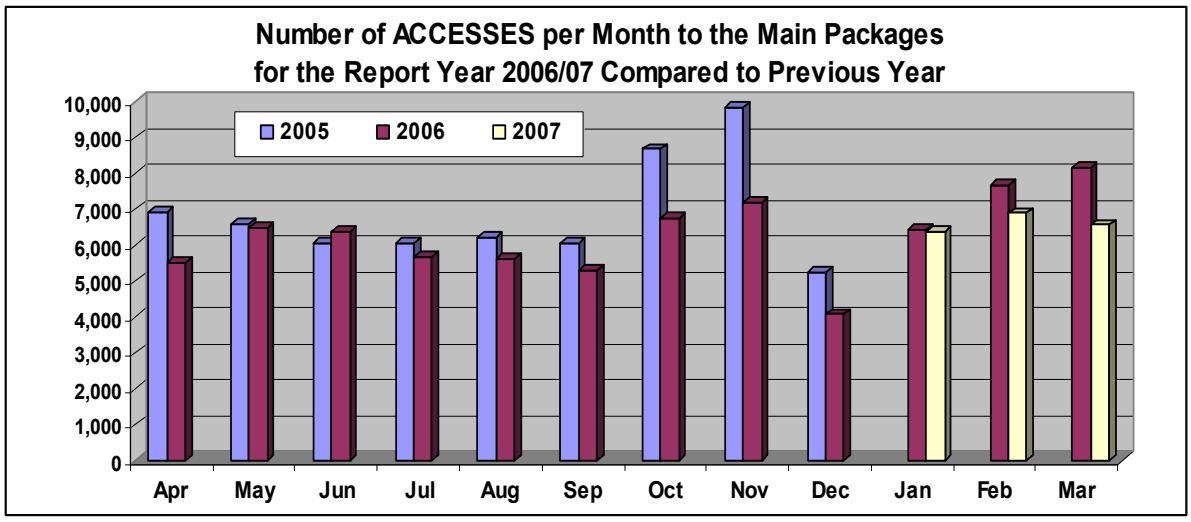
3. Members of the MAP should declare any personal interests and not participate in discussions where there would be a conflict of interest.

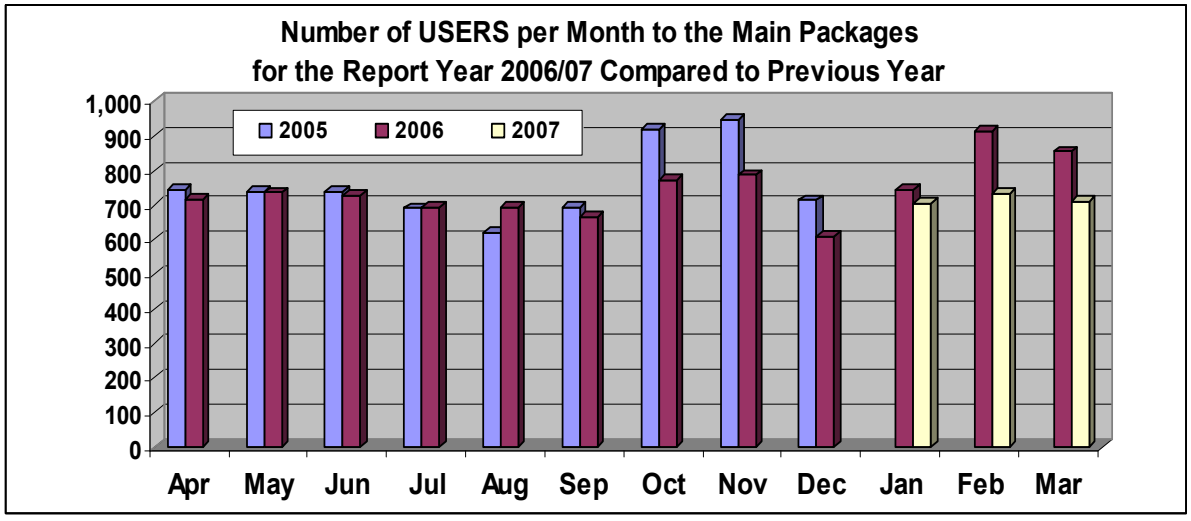
4. Membership of the Management Advisory Panel should ensure that the MAP has representatives from each main user community and should be reviewed on an annual basis to reflect changes in the user base.

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.

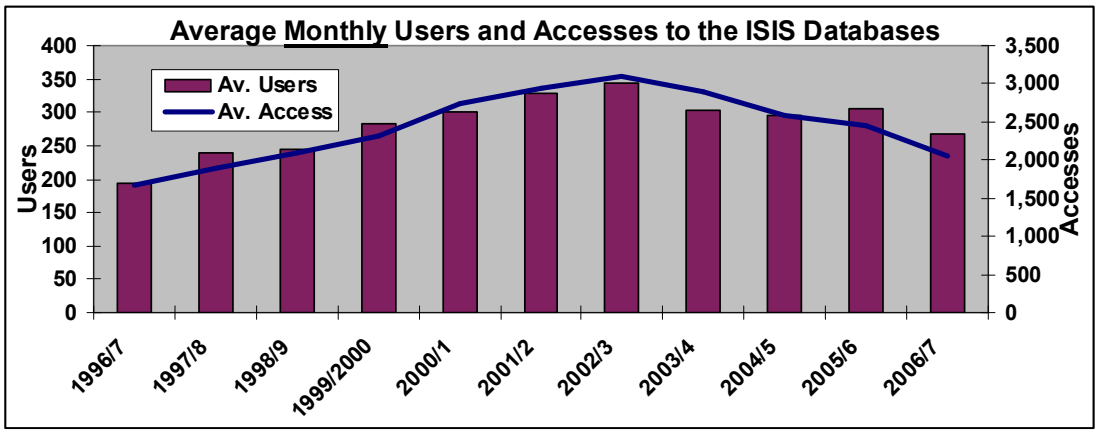
Appendix 2
CDS Usage Statistics

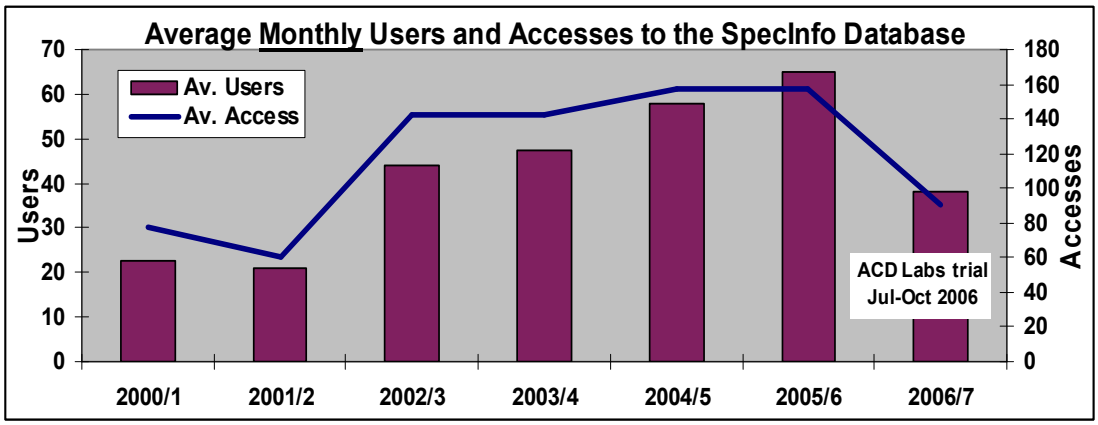


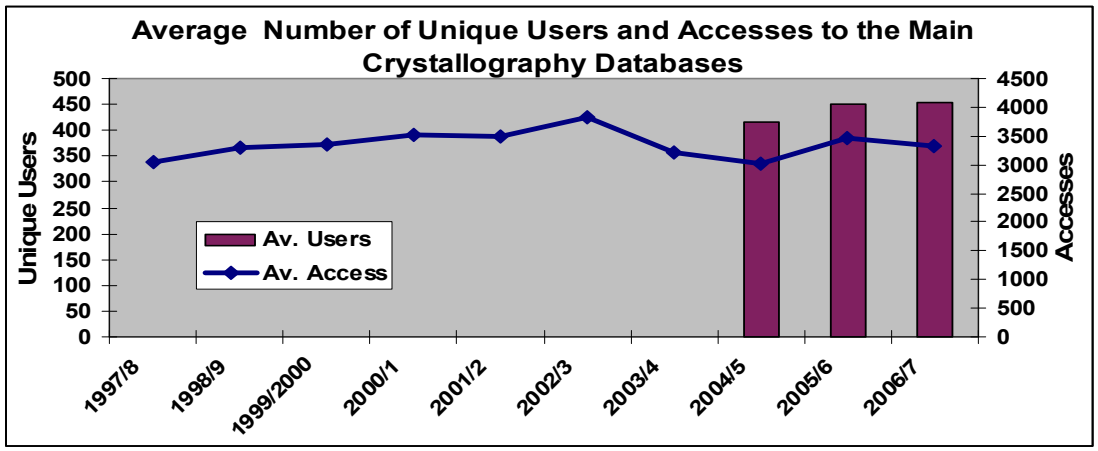


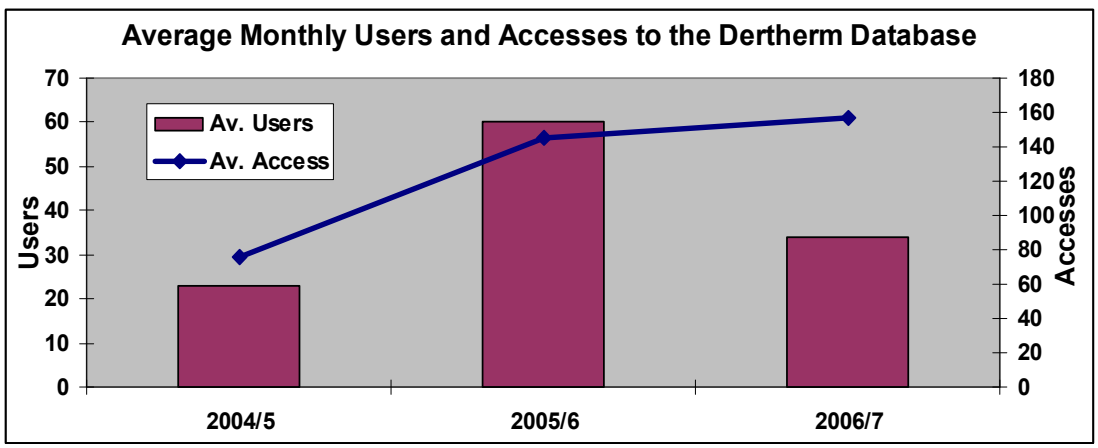


Appendix 2 (cont.)
CDS Usage Statistics



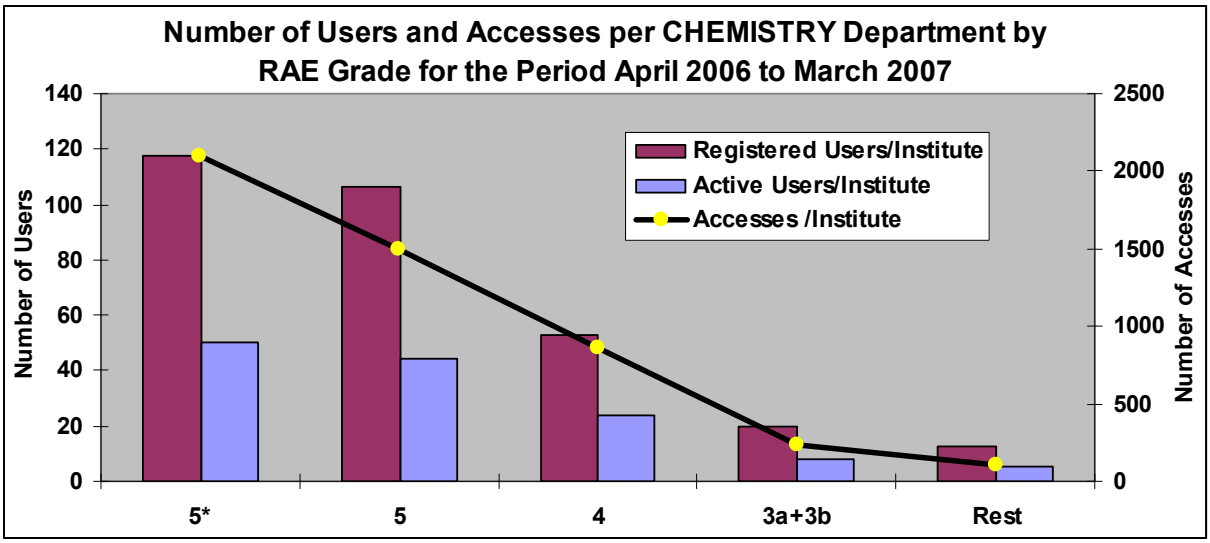






Appendix 3
CDS Usage and RAE Grade for Chemistry Departments
(April 2006 - March 2007)

Institution CHEMISTRY Department	RAE Grade	Acesses	Registered Users	Active Users	Accesses per Reg User	Accesses per Active User	%Active vs eg.User
University of Cambridge	5*	147	74	3601	24	49	50.3%
University of Oxford	5*	106	55	3477	33	63	51.9%
Imperial College, London	5*	138	55	2232	16	41	39.9%
University College London	5*	68	38	1516	22	40	55.9%
University of Durham	5*	130	48	1201	9	25	36.9%
University of Bristol	5*	117	30	558	5	19	25.6%
University of St Andrews	5	64	45	2892	45	64	70.3%
University of Southampton	5	170	75	2713	16	36	44.1%
University of Liverpool	5	104	58	2291	22	40	55.8%
University of Manchester	5	192	74	2214	12	30	38.5%
University of Nottingham	5	244	71	1736	7	24	29.1%
University of Edinburgh	5	78	32	1202	15	38	41.0%
University of Birmingham	5	71	43	1160	16	27	60.6%
University of Warwick	5	76	39	1052	14	27	51.3%
University of Leeds	5	127	44	1016	8	23	34.6%
University of Sussex	5	31	11	986	32	90	35.5%
University of York	5	76	35	977	13	28	46.1%
University of Sheffield	5	98	30	781	8	26	30.6%
University of East Anglia	5	48	17	414	9	24	35.4%
Heriot-Watt University	4	54	31	2537	47	82	57.4%
University of Wales, Cardiff	4	96	42	1518	16	36	43.8%
University of Reading	4	140	58	1415	10	24	41.4%
University of Bath	4	69	38	1401	20	37	55.1%
University of Strathclyde	4	72	40	1261	18	32	55.6%
University of Exeter	4	31	10	1133	37	113	32.3%
University of Glasgow	4	51	20	840	16	42	39.2%
University of Hull	4	55	25	599	11	24	45.5%
Loughborough University	4	59	30	438	7	15	50.8%
The Queen's University of Belfast	4	44	20	364	8	18	45.5%
University of Newcastle upon Tyne	4	38	11	238	6	22	28.9%
University of Leicester	4	11	3	140	13	47	27.3%
Kings (London)	4	8	4	78	10	20	50.0%
University of Wales, Swansea	4	11	5	19	2	4	45.5%



Appendix 4

Components Available during Report Period

CRYSTALLOGRAPHY

CSD Cambridge Structural Database. Crystal structure data for over 403,000 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 97,000 inorganic structures, searchable via a web interface. Available via the ICSD-WWW web browser interface.

CRYSTMET Crystal structure data for over 105,000 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.

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 nearly 1.6M 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 0.7M *unique compounds from* 719 *different suppliers and SCD (Screening Compounds Database) that contains over 5.6 Million compounds from 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

Papers Citing the Chemical Database Service JCICS review paper in 2006/2007 (data retrieved from the ISIS Web of Science)

AUTHOR	JOURNAL	IMPACT FACTOR 2005
Blake AJ, Li WS, Lippolis V, et al.	**ACTA. CRYSTALLOGR. B**., 63, 81-92, Part 1, FEB 2007	1.91
Pritchard RG, Ali M, Munim A, et al.	**ACTA. CRYSTALLOGR. C**, 62, M467-M468, Part 10, OCT 2006	0.777
Coyle JL, Fuller A, Mckee V, et al.	**ACTA. CRYSTALLOGR. C**, 62, M472-M476, Part 10, OCT 2006	0.777
Pritchard RG, Ali M, Munim A, et al.	**ACTA. CRYSTALLOGR. C**, 62, M507-M509, Part 11, NOV 2006	0.777
McClain JM, Maples DL, Maples RD, et al.	**ACTA. CRYSTALLOGR. C**, 62, M553-M555, Part 11, NOV 2006	0.777
Skakle JMS, Wardell JL, Wardell SMSV	**ACTA. CRYSTALLOGR. C**, 62, O312-O314, Part 6, JUN 2006	0.777
Skakle JMS, Wardell JL, Wardell SMSV	**ACTA. CRYSTALLOGR. C**, 62, O476-O477, Part 8, AUG 2006	0.777
Pritchard RG, Moreland L	**ACTA. CRYSTALLOGR. C**, 62, O656-O658, Part 11, NOV 2006	0.777
Harding MM	**ACTA. CRYSTALLOGR. D**, 62, 678-682, Part 6, JUN 2006	1.401
De Vivar MEDA, Baggio S, Baggio R	**ACTA. CRYSTALLOGR. E**, 62, M986-M988, Part 5, MAY 2006	0.581
Najafpour MM, McKee V	**ACTA. CRYSTALLOGR. E**, 62, O1365-O1368, Part 4, APR 2006	0.581
Skakle JMS, Wardell JL	**ACTA. CRYSTALLOGR. E**, 62, O1402-O1404, Part 4, APR 2006	0.581
de Oliveira CD, et al.	**ACTA. CRYSTALLOGR. E,** 62, O1492-O1493, Part 4, APR 2006	0.581
Costa MS, Boechat N, Ferreira VF, et al.	**ACTA. CRYSTALLOGR. E**, 62, O1925-O1927, Part 5, MAY 2006	0.581
Costa MS, Boechat N, Ferreira VF, et al.	**ACTA. CRYSTALLOGR. E**, 62, O2048-O2050, Part 5, MAY 2006	0.581
Boechat N, Lages A, Kover WB, et al.	**ACTA. CRYSTALLOGR. E**, 62, O2563-O2565, Part 6, JUN 2006	0.581
Mckee V, Grace G, Nelson M, et al.	**ACTA. CRYSTALLOGR. E**, 62, O3747-O3749, Part 9, SEP 2006	0.581
Silversides JD, Sparke AE, Archibald SJ	**ACTA. CRYSTALLOGR. E**, 62, O5944-O5946, Part 12, DEC 2006	0.581
James L, Maguire GEM, et al.	**ACTA. CRYSTALLOGR. E**, 63, O153-O155, Part 1, JAN 2007	0.581
de Oliveira CD, et al.	**ACTA. CRYSTALLOGR. E.**, 62, O1494-O1495, Part 4, APR 2006	0.581
Givaja G, Volpe M, Edwards MA, et al.	**ANGEW. CHEM. INT. ED.**, 46 (4), 584-586 2007	9.596
Brown LJ, Bouvet DR, Champion S, et al.	**ANGEW. CHEM. INT. ED.**, 46 (6), 941-944 2007	9.596
Lawrence NJ, Patterson RP, Ooi LL, et al.	**BIOORG. MED. CHEM. LETT.**, 16 (22), 5844-5848, 15, NOV 2006	2.478
Morley JO, Matthews TP	**BIOORG. MED. CHEM.**, 14 (23), 8099-8108, 1, DEC 2006	2.286
Proisy N, Sharp SY, Boxall K, et al.	**CHEM. BIOL.**, 13 (11), 1203-1215, NOV 2006	6.138
Morton D, Pearson D, Field RA, et al.	**CHEM. COMMUN.**, (17), 1833-1835 2006	4.426
Matharu DS, Morris DJ, Clarkson GJ, et al.	**CHEM. COMMUN.**, (30), 3232-3234 2006	4,426
Allan DR, Blake AJ, Huang DG, et al.	**CHEM. COMMUN.**, (39), 4081-4083 2006	4,426
O'Leary J, Wallis JD	**CHEM. EUR. J.**, 12 (29), 7724-7732, 10, OCT 2006	4.907
Mead RN, Mountjoy G	**CHEM. MATER.**, 18 (17), 3956-3964, 22, AUG 2006	4.818
Johnson CD, Mallon AJ, Worrall F	**CLAYS CLAY MINER.**, 54 (6), 678-688, DEC 2006	1.364
Grossel MC, Dwyer AN, et al.	**CRYSTENGCOMM**, 8 (2), 123-128 2006	3.508
Hillier S, Lumsdon DG, Brydson R, et al.	**ENVIRON. SCI. TECHNOL.**, 41 (6), 1921-1927, 15, MAR 2007	4.054
Beard CD, Carr L, Davis MF, et al.	**EURO. J. INORG. CHEM.** (21), 4399-4406, 6, NOV 2006	2.514
Bigmore HR, Zuideveld MA, et al.	**INORG. CHEM.**, 45 (16), 6411-6423, 7, AUG 2006	3.851
Ward BD, Risler H, Weitershaus K, et al.	**INORG. CHEM.**, 45 (19), 7777-7787, 18, SEP 2006	3.851
Griffith GA, Hillier IH, Moralee AC, et al.	**J. AMER. CHEM. SOC.**, 128 (40), 13130-13141, 11, OCT 2006	7.419
Bolton PD, Clot E, Cowley AR, et al.	**J. AMER. CHEM. SOC**., 128 (46), 15005-15018, 22, NOV 2006	7.419
Dalby KJ, Ellis D, Erhardt S, et al.	**J. AMER. CHEM. SOC.**, 129 (11), 3302-3314, 21, MAR 2007	7.419
Pickup DM, Ahmed I, FitzGerald V, et al.	**J. NON-CRYST. SOLIDS**, 352 (28-29), 3080-3087, 15, AUG 2006	1.264
Mead RN, Mountjoy G	**J. CHEM. PHYS.**, 125 (15), 154501, 21, OCT 2006	3.138
Pierloot K, Vancoillie S	**J. CHEM. PHYS.**,125 (12), 124303, 28, SEP 2006	3.138
Howell JAS	**J. CHEM. SOC., DALTON TRANS.**, (11), 1104-1114 2007	3.003
Foreman MRS, Hudson MJ, et al.	**J. CHEM. SOC., DALTON TRANS.**, (13), 1645-1653, 7, APR 2006	3.003
Fey N, Howell JAS, Lovatt JD, et al.	**J. CHEM. SOC., DALTON TRANS.**, (46), 5464-5475 2006	3.003
Burrows AD, Dodds D, Kirk AS, et al.	**J. CHEM. SOC., DALTON TRANS.**, (5), 570-580 2007	3.003

Silversides JD, Allan CC, Archibald SJ	**J. CHEM. SOC., DALTON TRANS.**, (9), 971-978 2007	3.003
Ok KM, Doran MB, O'Hare D	**J. MATER. CHEM.**, 16 (33), 3366-3368 2006	3.688
Johnson CD, Worrall F	**J. MATER. CHEM.**, 17 (5), 476-484 2007	3.688
Morris DJ, Hayes AM, Wills M	**J. ORG. CHEM.**, 71 (18), 7035-7044, 1, SEP 2006	3.675
Randell K, Stanford MJ, Clarkson GJ, et al.	**J. ORGANOMET. CHEM.**, 691 (16), 3411-3415, 1, AUG 2006	2.025
Morales F, Grandjean D, Mens A, et al.	**J. PHYS. CHEM. B**, 110 (17), 8626-8639, 4, MAY 2006	4.033
Mead RN, Mountjoy G	**J. PHYS. CHEM. B**, 110 (29), 14273-14278, 27, JUL 2006	4.033
Grandjean D, Castricum HL, et al.	**J. PHYS. CHEM. B**, 110 (34), 16892-16901, 31, AUG 2006	4.033
Thomas BWM, Mead RN, Mountjoy G	**J. PHYS. CONDENS. MATTER**, 18 (19), 4697-4708, 17, MAY 2006	2.145
Clark EB, Mead RN, Mountjoy G	**J. PHYS. CONDENS. MATTER**, 18 (29), 6815-6826, 26, JUL 2006	2.145
Skinner LB, Barnes AC, Crichton W	**J. PHYS. CONDENS. MATTER**, 18 (32), L407-L414, 16, AUG 2006	2.145
Guillaume C, Morniroli JP, Frost DJ, et al.	**J. PHYS.: CONDENS. MATTER**, 18 (37), 8651-8660, 20, SEP 2006	2.145
Heng JYY, Williams DR	**LANGMUIR** 22 (16), 6905-6909, 1, AUG 2006	3.705
Merroun M, Rossberg A, Hennig C, et al.	**MAT. SCI. ENG. C**, 27 (1), 188-192, JAN 2007	1.599
Clark GNI, Haslam AJ, Galindo A, et al.	**MOL. PHY.**, 104 (22-24), 3561-3581, NOV-DEC 2006	1.351
Hussaini SR, Moloney MG	**ORG. BIOMOL. CHEM.**, 4 (13), 2600-2615 2006	2.547
Moloney MG, Panchal T, Pike R	**ORG. BIOMOL. CHEM.**, 4 (21), 3894-3897 2006	2.547
McErlean CSP, Proisy N, Davis CJ, et al.	**ORG. BIOMOL. CHEM.**, 5 (3), 531-546 2007	2.547
Cheung FK, Hayes AM, Morris DJ, et al.	**ORG. BIOMOL. CHEM.**, 5 (7), 1093-1103 2007	2.547
Linclau B, Jeffery MJ, Josse S, et al.	**ORGANIC LETTERS** 8 (25), 5821-5824, 7, DEC 2006	4.368
Owen CT, Bolton PD, Cowley AR, et al.	**ORGANOMETALLICS** 26 (1), 83-92, 1, JAN 2007	3.473
Bolton PD, Clot E, Adams N, et al.	**ORGANOMETALLICS**, 25 (11), 2806-2825, 22, MAY 2006	3.473
Mountford AJ, Lancaster SJ et al.	**ORGANOMETALLICS**, 25 (16), 3837-3847, 31, JUL 2006	3.473
Adams N, Arts HJ, Bolton PD, et al.	**ORGANOMETALLICS**, 25 (16), 3888-3903, 31, JUL 2006	3.473
Bolton PD, Adams N, Clot E, et al.	**ORGANOMETALLICS**, 25 (23), 5549-5565, 6, NOV 2006	3.473
Wong DM, Simpson SJ	**POLYHEDRON,** 25 (11), 2303-2317, 31, JUL 2006	1.957
Howell JAS	**POLYHEDRON**, 25 (15), 2993-3005, 3, NOV 2006	1.957
Biswas M, Rosair GM, Pilet G, et al.	**POLYHEDRON,** 26 (1), 123-132, 2, JAN 2007	1.957
Yamada K, Honda H, Yamazaki T, et al.	**SOLID STATE NUCL. MAG. RES.**, 30 (3-4), 162-170, OCT 2006	1.41
Yamada K, Nemoto T, Asanuma M, et al.	**SOLID STATE NUCL. MAG. RES.**, 30 (3-4), 182-191, OCT 2006	1.41
Tsami A, Grillo F, Bowker M, et al.	**SURFACE SCIENCE**, 600 (17), 3403-3418, 1, SEP 2006	1.78
Nicholson G, Silversides JD, Archibald SJ	**TET. LETT.**,47 (37), 6541-6544, 11, SEP 2006	2.477
Morris DJ, Docherty G, Woodward G, et al.	**TET. LETT.**,48 (6), 949-953, 5, FEB 2007	2.477
Needs PW, Kroon PA	**TETRAHEDRON** 62 (29), 6862-6868, 17, JUL 2006	2.61
Tamanini E, Watkinson M, Todd MH	**TETRAHEDRON ASYMMETRY**, 17 (15), 2235-2239, 11, SEP 2006	2.429
Xu YJ, Docherty GF, Woodward G, et al.	**TETRAHEDRON ASYMMETRY**, 17 (20), 2925-2929, 6, NOV 2006	2.429
Johnson CD, Feldmann J, Macphee DE	**WASTE MANAGE.**, 27 (3), 375-379 2007	1.123

Average Impact Factor = 2.75