



Chemical Database Service

NEWSLETTER

Issue 6

November 1996

A paper describing the Chemical Database Service has been published in the Journal of Chemical Information and Computer Science. Publications stemming from the use of the service should acknowledge such usage by citing the following reference:

The United Kingdom Chemical Database Service, Fletcher, D.A., McMeeking, R.F., and Parkin, D., J. Chem. Inf. Comput. Sci. (1996), 36, 746-749.

A CHEST deal for five year access to the **Beilstein and Gmelin** databases via the CrossFire system has been finalised. Sites which subscribe to the deal will be able to use their CDS ids to access the data as during the trial period (see page 2 for more details). Non CDS ids will also be available from your local CHEST representative. The CrossFire system will be run by the CDS staff at Daresbury for the first year of the service.

The **REACCS** service has now ended. The organic reaction databases and the available chemicals database are now only accessible via ISIS.

ISIS - new data and software available. See the article on page 3 for details of how these changes may affect you.

The chiral separation database, **Chirbase**, is now on extended trial until the end of June 1997. See page 6 for details of how to access the database.

A **scratch disk** is now available for temporary storage of large user files. See page 5 for details of how to access it.

Thanks to everyone who responded to our online **survey** in October. Results from the survey are presented on page 8.

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The Chemical Database Service is funded by the Engineering and Physical Sciences Research Council



Access to the Beilstein and Gmelin Databases

A CHEST deal has been announced for 5 years of access to the Beilstein and Gmelin databases. For the first year the service will continue to be run by the CDS staff at Daresbury. During this period you can use your CDS id to access the Beilstein and Gmelin Databases through the CrossFire system, provided that your site has signed up for the Beilstein/CrossFire CHEST deal. Your local CHEST representative (usually a librarian) will be able to tell you if your site has subscribed to this service.

Getting your Beilstein password

Your Beilstein id is the same as your CDS id, though a separate password is required. To get your Beilstein password, logon to cds1 using your CDS id and password and type **cpass**. This will give you your Beilstein password. If you wish to change the password use the command **npass**.

Getting the client software

The CrossFire system, which you use to access the Beilstein and Gmelin Databases, consists of two parts. The client software, called the Beilstein Commander, runs on your PC or Mac and this communicates with the CrossFire Server running at Daresbury. If you do not have the client software on your computer you can download it from cds1. You will need a file transfer (FTP) program on your computer. You use this to logon to cds1 using your CDS id and password. Change to the directory /ftp/beilstein/ibm (for the PC version of the software) or /ftp/beilstein/mac (for the Mac version). Get the file called beilstein_download.txt. This file gives instructions for downloading and installing the Commander software.

Documentation

Documentation for the Crossfire system is available to download from cds1. It is stored in the directory /ftp/beilstein/docs. Manuals, including a tutorial introduction, produced by Beilstein, are stored in compressed MS Word 6 (and Word 5 for Mac) format. In addition there are some plain text (.txt) files which provide a quick guide to using the system. These quick guides can also be viewed on the World Wide Web from the CDS site at URL <http://www.dl.ac.uk/CDS/cds.html>. The CDS web site also contains some training exercises with solutions.

Help

Apart from the documentation mentioned above, there is an online help system within the Beilstein Commander program. In addition, there is a listing of solutions to common problems available through the Online Information Server on cds1 (type ois on cds1 and follow the Beilstein links). Queries can also be addressed to the CDS support staff (see page 12 for contact details).

ISIS update

There have been a number of improvements to the ISIS service in the last few months which may affect users. These are detailed below.

ISIS/Client 2.0 now available

ISIS/Client 2.0, previously called ISIS/Desktop and containing both ISIS/Base and ISIS/Draw, is now available (see the article later in this newsletter for more details) for PCs and Macs. The SGI version is expected at the start of next year. All users are encouraged to upgrade from version 1.2.

ChemInform RX 96.2 database installed

The ChemInform RX 96.2 database has been installed, adding a further 33,000 reactions from recent literature.

ALL ISIS USERS WILL NEED TO UPDATE THEIR DATABASE REMOTE ACCESS FILES IN ORDER TO ACCESS THIS NEW DATA.

SGI users should simply download the file all.db from /ftp/isis/sgi on cds1 and use this to replace their current all.db file.

PC and Mac users can either update their RXL Browser file as follows:

- Start ISIS/Base.
- Select 'Configure Database' or 'Change Hview in Database' from File menu
- Choose the RXL Browser file.
- Add +cirx97 to the end of the list of databases.
- Click on OK.

Alternately they can redownload the RXL Browser files from cds1. PC users should get the file /ftp/isis/ibm/rxl13.db and Mac users should get the file /ftp/isis/mac/RXL_Browser.sea.hqx.

Users who have downloaded their copies of ISIS from cds1 after 20/9/96 do not need to make any changes, since the downloadable database files have been modified.

Synopsys Protecting Groups database now accessible via ISIS

The Synopsys Protecting Groups database, previously only available via REACCS, has now been converted to run under ISIS. It contains some 23,000 protecting group reactions, with data on stability and lability. An example screen with a typical retrieved reaction is shown on page 7.

A separate remote access file is available to access this database. PC users should get the file /ftp/isis/ibm/spg.db, SGI users should get the file /ftp/isis/sgi/spg.db and Mac users should get the file /ftp/isis/mac/spg.sea.hqx.

Chiral separation database trial

A trial of the chiral separation database Chirbase is under way. It is accessible using ISIS. See the article later in this newsletter for more details.

Login messages via ISIS

A test version of the RXL Browser file for PCs and Macs is available which displays the login messages when you first access the databases. We would like people to try it out and would welcome comments on its usefulness.

PC users should get the file `/ftp/isis/ibm/testrxl.db` and Mac users should get the file `/ftp/isis/mac/testrxl.sea.hqx`. The testrxl file needs to be put into the RXL Browser directory (or folder) in order for it to work correctly.

SpecInfo 3.1.5

SpecInfo now has a number of new features and some enhancements which make it easier to use (see below), since the update to version 3.1.5 has been installed. The associated database of spectra is unchanged.

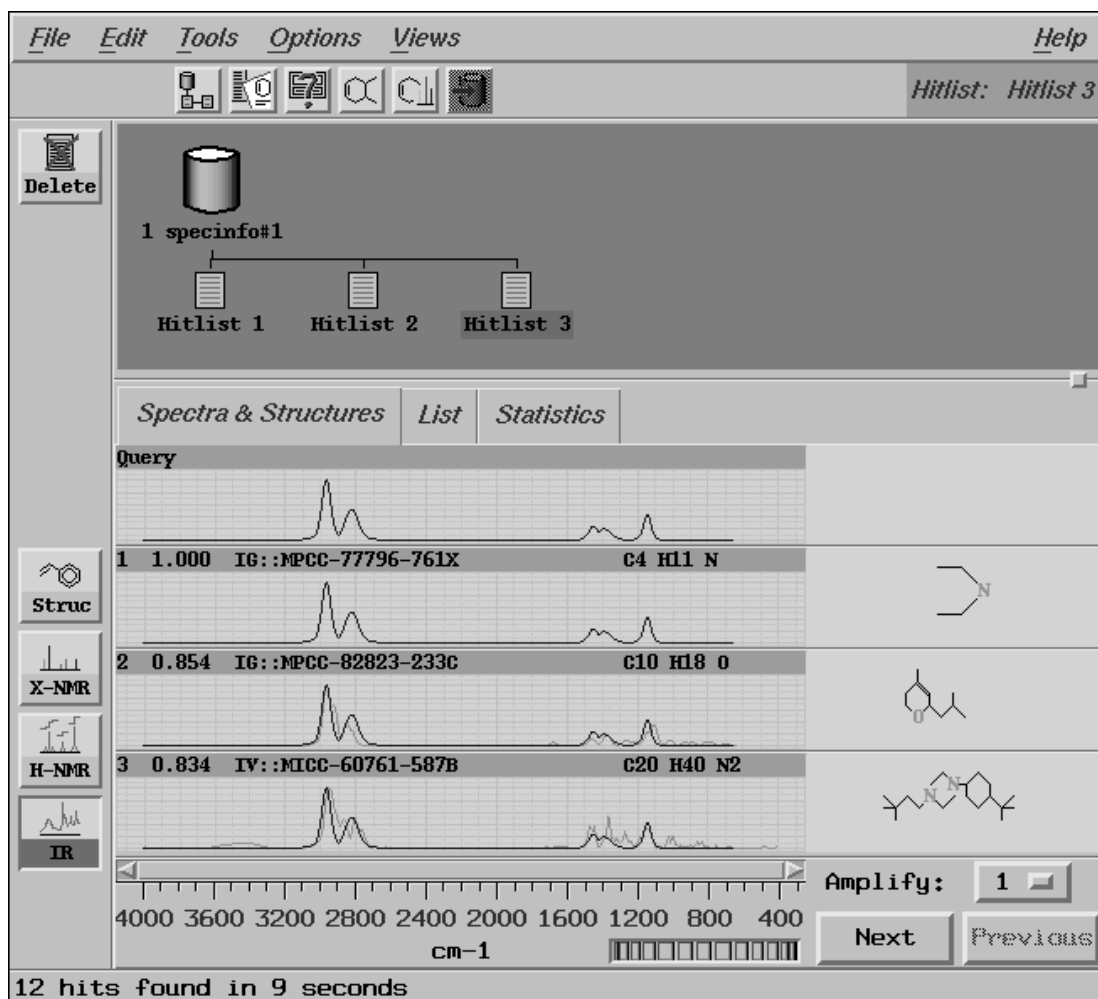
The guide to using the program has been updated for the new version and is available to download from the directory `/ftp` on `cds1`.

File	Format
<code>spec315manual.ps</code>	PostScript
<code>spec315manual.rtf</code>	Rich Text Format (for MS Word)
<code>spec315manual.asc</code>	ASCII (i.e. plain text)

It is also accessible from the Online Information Server on `cds1`.

New Features in SpecInfo 3.1.5

- The main window now displays up to 5 structures and/or spectra from a hitlist.
- Structures can be imported in MDL molfile format.
- Both NMR and IR spectra can be imported.
- Graphical spectra can be printed.
- IR spectra can be displayed overlaid with a query spectrum.
- Dragging of structures and spectra between modules has been improved.
- The structure editor has been improved and a set of functional group buttons added.
- It is now possible to restrict a search within a previous hitset.
- Structure searches can be restricted to certain spectroscopic techniques.
- Individual user configurations of paths and display options are now possible.



Main window of SpecInfo showing the first three hits from an infra-red spectrum search. The query spectrum is shown at the top and is also overlaid on the hit spectra. This display of hits can be changed using the options from the Options and Views menus as well as the buttons to the top and left of the hitlist display area.

Scratch disk

An area of scratch disk space has been created on cds1 for users to temporarily store large files (e.g. PostScript files for printing). This filespace can be accessed from the directory /scratch. Users should create their own subdirectory within /scratch and store their files within this subdirectory. To do this type:

```
cd /scratch
mkdir cxxx
```

where cxxx is your userid. You can then store your temporary files in /scratch/cxxx. Currently files in the scratch area will be automatically deleted after 24 hours.

Chiral separation database

The Chirbase database provides a powerful information system for chiral separations of enantiomers by chromatography. There are currently over 23,000 chiral separations with 10,000 molecular structures in the database.

The Chirbase Project is coordinated by Professor Roussel at the University of Marseille. It results from the recent development of chiral chromatographic methods using more than 1000 chiral stationary phases (CSP) and thousands of examples of enantiomer separations for HPLC and GC. Some 20% of these stationary phases are commercially available and new developments are still underway. Since there are so many CSPs available to the end-user, the selection of the appropriate system (CSP and operating conditions) often remains difficult to find by trial and error and might be highly expensive in terms of time, material and labour. The Chirbase molecular database project was initiated in Marseille, France for HPLC and in Tübingen, Germany for GC to fill this gap. Data available in the database include molecular structures (enantiomer and CSP), chromatographic data, experimental conditions and source. In addition, a database of commercially available CSPs is available on the Chirbase web pages and can be accessed through the Online Information Server on cds1 or via the CDS web pages.

The Chirbase database is currently accessible through ISIS, and we have arranged an extended trial to run until the end of June 1997. To access the data users need to download a database remote access file from cds1.

PC users should download the file (in binary format):
/ftp/isis/ibm/chirbase.db

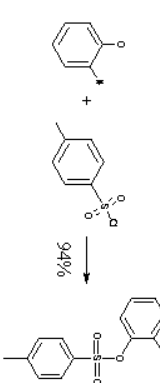
Mac users should get the file (in ASCII format):
/ftp/isis/ibm/chirbase.sea.hqx

This file needs to be 'unbinhexed' and the resulting .sea file run in order to produce the required remote access file.

SGI users should download the file (in binary format):
/ftp/isis/sgi/chirbase.db

Comments are invited from users about the value of this database and whether it should become a permanent part of the service.

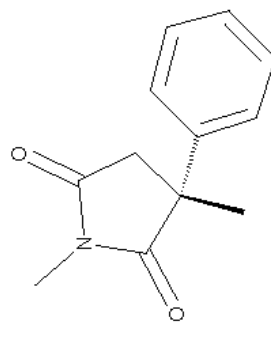
An example screen from an ISIS session showing a typical retrieved separation is shown on page 7. Some examples of searching the database are available through the Online Information Server on cds1 or via the CDS web pages.

Synopsis Protecting Groups		1	
Ref	Kurita K, Chem Ind (London), () p.345, 1974		
Title	Selective tosylation of o-aminophenol		
Comments	 <p>Replacing NEB3 with pyridine afforded the N-tosyl isomer in 93% yield. No isomerization of the above product occurred on heating in pyridine/KOH. The product was also protected by heating with 0.5M KOH in MeOH. No other examples are given.</p>	Conditions	NEB3 CH2Cl2 20 C 1 h
		Yield	94
		Exp:	n
		Substrate	n
Functional Group & Protected	Alcohol (benzyl)	PG	4-Toluenesulphonate
Keyword	Phenol protection, Chemoselective, O-Protection, O-Sulphonation		
Reaction Condition Keys	Amine base		
<i>Tolerated Groups - serve format as Functional Groups & Protected Groups</i>			
No. 1	Tolerated Group: Amine (primary, benzyl)	Associated functional group: -	
Stability - use cataly/si or solvent display name to search for			
Stability conditions	NABH4P/Pyridine/MeOH/20 C/45 m	Stability citations	J Biol Chem, p.107, 1955
Stability keywords	Borohydride reductant, Amine base		
Lablity - use cataly/si or solvent display name to search for			
Lablity conditions	Et4NI/e-DMF	Lablity citations	J Gen Chem USSR (Engl Transl), p.2615, 1971
Lablity keywords	Electrolytic, Ammonium		

Stability, Lablity, and Catalyst & Solvent information can also be searched and viewed on the STABILITY, LABLITY and CATALYST forms respectively - select 'Open Form' from the 'File' menu.

Remember to use @ wildcard delimiters for keyword searching.

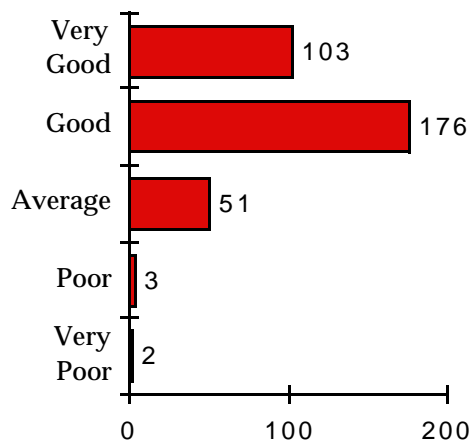
Example ISIS screens showing retrieved data from the Synopsis Protecting Groups database (above) and the Chirbase chiral separation database (below).

CHIRBASE		Standard Form		version 2.00		ENS/PL/AM 1996				
Sample				CSP						
RXN	lit	1st	2nd	K1	K2	K2/K1	Res	RI1	RI2	
1000	1	(+)	(-)	2.33	6.24	2.66	7.80			
1001	1	(S)	(R)	3.01	3.53	1.17				
1002	1	(R)	(S)	7.41	8.30	1.12				
1003	1	(R)	(S)	5.08	5.54	1.09				
1004	1	(R)	(S)	3.47	4.45	1.26				
reference	Shibata, T.; Ichida, A.; Fukui, Y.; Mori, K.; Int Symp. Chiral Sep. Guilford, 1989.								refno	8387
sample_name	Methsuximide			sample_chirality						
method	HPLC			detection	scale		amount			
mobile_phase	96:4 EtOH / H2O			Analytical						
csp_name	Cellulose tris-(4-methylphenylbenzoate)/macroporous silica			csp_trade_name		csp_supplier				
type_of_column	One (250*4.6 mm)			CHIRALCEL OU		DAICEL				
				csp_particle_size		cspno				
						55				
Res. reported in "Chiral Separations by HPLC", Ed. A.M. Krsulovic, Ellis Horwood 1989.										

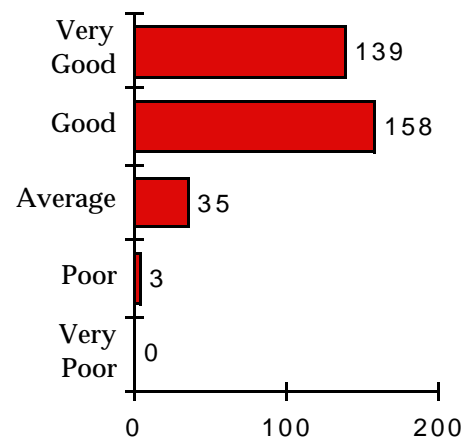
Online survey

Thanks to everybody who took part in the online survey which we ran in October. The results were very favourable to the service and the comments will help us to maintain and improve the quality of the service.

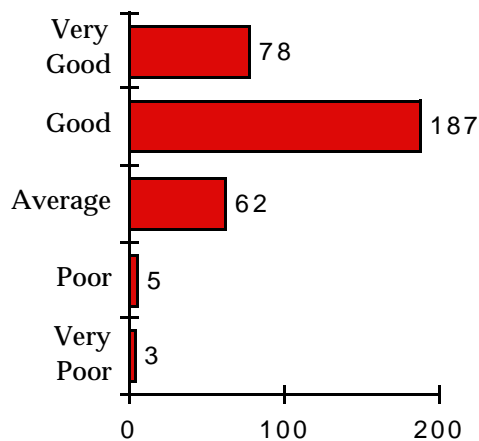
A total of 335 (82%) out of 408 users asked completed the survey. The results are illustrated below together with the most common comments.



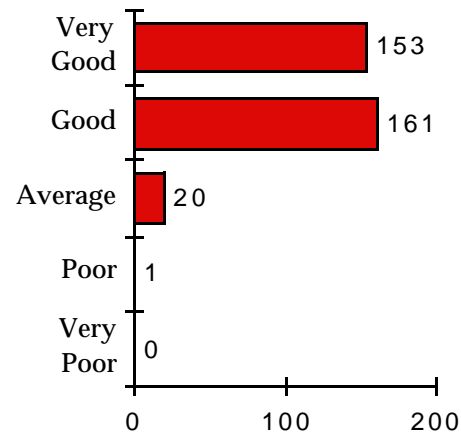
How would you rate the quality of help/support you receive ?



How would you rate the availability of the service ?



How would you rate the online response time ?



How would you rate the Chemical Database Service overall ?

Most people (83%) found our recent practice of sending important login messages to users via email useful and therefore we intend to continue with this. However, a significant minority (7%) found it irritating, so we will set up a mechanism for people to opt out of email messages.

A total of 34 comments were received, most of which related to the three areas discussed below.

Delete key does not work:

A number of people commented on problems with the delete key not working. The simplest solution is to add the following line to your .login file
stty erase "*"
where * represents pressing your delete key.

X-window difficulties:

Most of these comments related to the cost and setup of X-Windows emulation software. We cannot help with the cost of the software, but we endeavour to give what help and advice we can for setup problems (see page 12 for contact details).

Manuals/documentation:

We received a number of requests for ISIS manuals and for access to the online CDS manuals via the world wide web (WWW).

There are no printed ISIS manuals. The ISIS/Client software contains a comprehensive online help system. In addition we provide introductory training material on the CDS WWW pages.

Web access to online CDS manuals is currently only possible through the Online Information Server whilst logged on to cds1. However, we plan to run a web server on cds1 in the future and these manuals will then be accessible via the web.

ISIS/Client 2.0

Version 2.0 of the ISIS/Client software (previously called ISIS/Desktop and containing both ISIS/Base and ISIS/Draw) is now available for the PC and Mac. The SGI version is expected next January. All users are encouraged to upgrade to the new version, which has major enhancements to the ISIS/Draw interface and the online help system.

Major changes

- Macintosh users no longer require the VersaTerm Telnet Tool.
- You can interrupt searches and retain interim hit lists.
- Innovative and completely redesigned online help.
- The ISIS/Draw interface has been significantly changed and improved.

Other changes to ISIS/Base

- Browsing speed has been improved.
- Form building has been simplified and improved.
- Reaction highlighting is now supported.
- List handling and list logic have been enhanced.
- Improvements have been made in local searching performance.

Changes to ISIS/Draw

- A chem check feature verifies that the molecules and reactions as drawn are valid items for searching a database using ISIS/Base.
- Can double-click objects to edit their properties (the Style menu has been eliminated)
- Molecule and sketch tools combined into one tool bar.
- Pop-up help for tools (can be turned on and off)
- Context-sensitive help for dialog boxes.
- Simpler method to apply atom-atom maps to reactions.
- Simpler method to build reactions.
- Create DNA, RNA, or amino acid sequences and other molecules that are larger than 255 atoms.
- Print preview feature added.
- New tools for selection, chain creation and arrows.
- Simpler customisation of default tools, template tools and menus, and preferences.

Getting ISIS/Client 2.0

The ISIS/Client software is stored on cds1 in the directories /ftp/isis/ibm (for the PC version) and /ftp/isis/mac (for the Mac version). It can be downloaded by all CDS users who have signed the ISIS/Desktop usage memorandum. You can check whether you are authorised to download the software by logging on to cds1 and typing **auth**.

Users should first download the file Getting_ISIS2 from the mac or pc directory. This file gives instructions for downloading and installing the ISIS/Client software.

Summary of databases available from the Chemical Database Service

A brief description of all the databases currently available from the CDS at Daresbury.

- ISIS** A chemical reaction information management system allowing search, retrieval and display of molecules, reactions and their associated data. Currently contains 665,000 searchable reactions and supplier information on 200,000 different compounds.
- SPEC** SpecInfo is a multi-technique spectroscopic database package intended to cover NMR, IR and mass spectra. The package is designed to aid the chemist in spectral interpretation and structure elucidation problems. The database currently contains 99,059 ¹³C NMR; 999 ¹⁵N NMR; 856 ¹⁷O NMR; 2,183 ³¹P NMR; 1,825 ¹⁹F NMR and 20,898 infra-red spectra. It does not, at present, contain any mass spectra.
- CSD** The Cambridge Structural Database. Crystal structure data for 160,000 organic and organometallic compounds. Currently available under both Cambridge's QUEST retrieval software and our in-house software (CSSR). The QUEST software has a number of features not available in CSSR, such as 3D searching.
- ICSD** Inorganic Crystal Structure Data File. About 41,500 inorganic structures - the companion file to the Cambridge organic file.
- MDF** Metals Data File. Crystal structure data for nearly 56,000 metals, alloys and intermetallics.
- PDB** The Brookhaven Protein Data Bank containing bibliographic and coordinate details for proteins and other biological macromolecules. There are currently over 4,900 coordinate sets.
- CDIF** Crystal Data Identification File. Crystal class and unit cell data for over 200,000 crystal structures.
- FNMR** A databank of 6,000 ¹⁹F NMR spectra and coupling constants.
- ELYS** Electrolyte Solutions Database. Thermodynamic and transport property data such as density, viscosity and diffusion coefficients. Currently contains about 10,000 entries.

Information

General queries and registration of new accounts:

Computer Help Desk/User Interface Group (UIG)
Daresbury Laboratory
Daresbury, Warrington
WA4 4AD
(01925) 603351
Email uig@dl.ac.uk

Hours are:
Mon-Thur 9:00-12:00, 13:00-17:00
Fri 9:00-12:00, 13:00-16:00

Otherwise 24 hour answer phone.

General database queries:

Chemical Database Service (CDS)
Room C18, Daresbury Laboratory
Daresbury, Warrington
WA4 4AD
(01925) 603162
Email cdsbb@dl.ac.uk

For ISIS specific problems:

Dr. D. Parkin
Email D.Parkin@dl.ac.uk
(01925) 603162

For SpecInfo specific problems:

Dr. D.A. Fletcher
Email D.A.Fletcher@dl.ac.uk
(01925) 603162

For QUEST specific problems:

Dr. R. F. McMeeking
Email R.F.McMeeking@dl.ac.uk
(01925) 603162

World Wide Web Server

Information about CDS is available over the World Wide Web at URL:
<http://www.dl.ac.uk/CDS/cds.html>

Online help and information:

Online help and information, including documentation, is available via the Online Information Server on cds1. Type 'ois' to access it.

Documentation:

Most documentation is available online and some can be downloaded from the directory /ftp on cds1. Printed manuals can still be ordered through the online orderdoc utility or from UIG at the above address.

Access:

The service is available free of charge to UK academic research groups for non-commercial work. Each individual user will be issued with a unique ID. It is not our policy to allow shared IDs.

cds1 (main service machine):

Internet number: 148.79.160.113
Internet name: cds1.dl.ac.uk

Comments:

All comments, questions and suggestions about this newsletter should be sent to:

Dr. D.A. Fletcher
Email D.A.Fletcher@dl.ac.uk