

Eurospec goes live at Achema

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The International Spectroscopic Database (IS-DB) went live on 19 May 2003. Following over seven years fighting for funding and receiving the EU EuroSpec grant¹ in 2002 the team are pleased to announce that the first version of the international digital archive for spectroscopic data was switched on for data deposition in May.

One month ahead of schedule, the twin IS-DB Data Entry and IS-DB Archive Server systems were activated for access by authors of scientific publications for the deposition and review of supplementary digital spectroscopic data.

Now it is up to you!

In order to keep this resource up and running beyond the end of the initial funding period it is up to spectroscopists around the world to feed the system with good reference spectroscopic data. The system is also capable of being used to deposit older data collections to keep them available for posterity. The team will ensure that the files are always available to the scientific community in whatever is the current most widely used standard scientific data format.

Step one

You need to register in order to deposit spectra at the Data Entry server as well as to gain access to the Archive Server. The first step is to gain access to the Data Entry server by accessing the IS-DB homepage at www.is-db.org (see Figure 1). As you can see from the version number we are still improving the systems on a daily basis, so once you have tested the interface please let us have your thoughts through the "Contact IS-DB" option.

Step two

Registering yourself is simple—just follow the instructions you find there (Figure 2). Once logged in you will be greeted by a screen welcoming you to the system and informing you of your registration number. Make a note of this, as it will speed up the location of your own deposited data in the Archive Server in the future. If you forget it

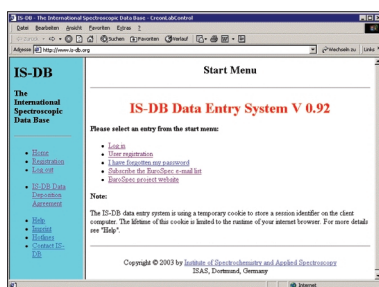


Figure 1. The IS-DB Data Entry system is used to administer users and as the portal through which spectroscopic data and associated metadata should be deposited in the archive.

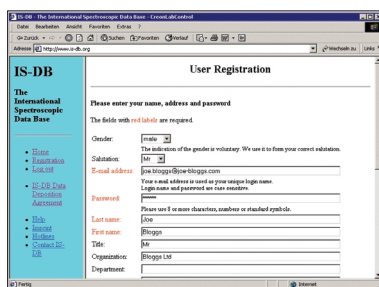


Figure 2. User registration is essential and the first step to depositing data or accessing the Archive Server.

don't worry, it will appear every time you log in to IS-DB.ORG.

Step three

Logged in users are now able to start depositing data in the archive, edit or modify information already on the system or change their user profiles and passwords. If you wish to submit a data file you may add it to a set of bibliographic information previously entered or you may want to start with new set of reference material. Let us suppose the bibliographic reference is new to IS-DB. Choosing this option will lead you to the screen in which you must decide whether your bibliographic information comes from one of a series of categories:

- Peer-reviewed paper
- Non-reviewed paper
- Proceedings contribution
- Book

- Book chapter
- Patent specification
- PhD thesis (or dissertation)
- Other university publication (e.g. master or diploma thesis)
- Project report
- Unpublished data

As the content of a reference varies with the thing it refers to different masks appear depending on your choice. Figure 3 shows the screen should you select a peer reviewed paper—mandatory fields are highlighted in red.

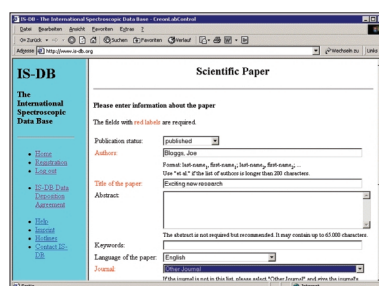


Figure 3. The various reference publication types have different requirements depending on type. This is the screen for peer-reviewed papers.

Step four

With the bibliographic data entered you will next need to enter information about the particular sample from which the spectrum arises in the Sample Description screen (Figure 4).

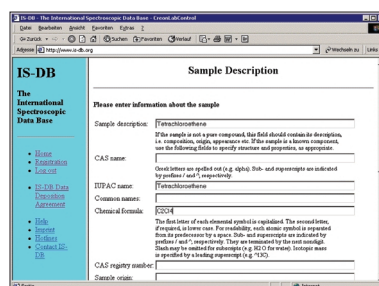


Figure 4. Each spectrum deposited needs to be accompanied by information about the sample which was measured.

This can be carried out many times for an individual publication reflecting the fact that a single paper may have many spectra.

Step five

With the sample information logged into the system, you need to provide information about the data set to be deposited with the archive. You need to accept the deposition agreement and provide information about the file in the Submit a File screen (Figure 5). The more relevant information you can provide at this stage the greater the likelihood that your data will be found and will be of use to the scientific community in the future.

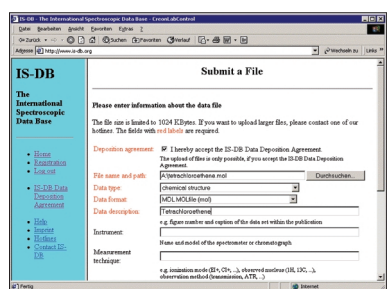


Figure 5. The data sets also need to be annotated with relevant information about the deposited file.

Step six

With the data entered and the user logged out, the automation takes over. The relevant metadata from the screens you have entered are automatically transferred using XML data files from the Data Entry system to the Archive Server. The files are re-numbered to ensure consistency but the Archive is also searchable by the old file number should you wish to use this as a key.

You should have received your Archive Server username and password by this time (depending on workload this may take up to a couple of days) and providing all the systems are up and running your spectra should be viewable through the Archive Server front end (Figure 6).

The Archive Server can be accessed either via www.is-db.org or through www.eurospec.org. The Archive Server is currently a customised version of the Q-DIS/PANDA electronic record management system.

The Archive can be searched by any of the keywords used during deposition, deposition date or a variety of other search fields (Figure 7). All data and metadata XML files associated with a particular bibliographic reference are stored under the same IS-DB ID num-



Figure 6. Accessing the Archive Server is by use of the Archive Server access information you will be mailed after registering.

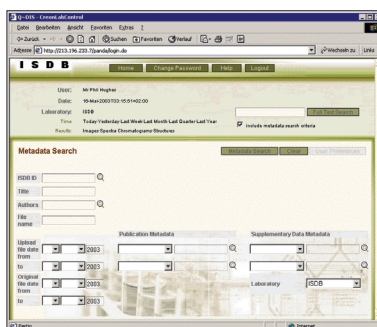


Figure 7. Locating data on the Archive Server is through a wide variety of search keys and metadata fields.

ber and can shown together by clicking on the Publication Overview button of the search result screen (Figure 8).

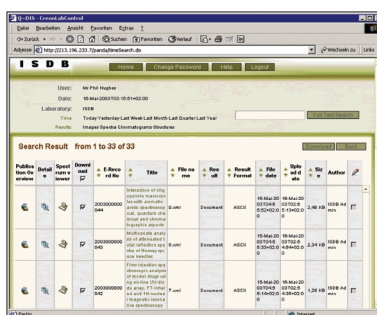


Figure 8. The results can be sorted.

Step seven

Having located that vital piece of spectroscopic data you can view it by clicking on the Spectrum Viewer icon next to the located entry. With luck and good judgement you may well get a display such as that in Figure 9!

Summary

Well after all the efforts, we are live with the first version of the

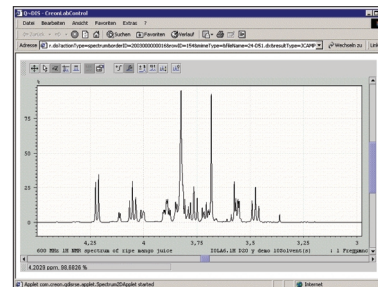


Figure 9. Finally, the spectra can be reviewed.

International Spectroscopic Database! This is, however, just the beginning. We need your data to give the whole system a much need trial under load, and we are very, very keen to get as much constructive criticism as possible in order to meet any improvements or demands for additional features in the next release.

Please bear with us and help us to make this into a key resource for spectroscopists and service providers for spectroscopists alike.

Depositors should be aware that in the initial test phase data depositions are being passed straight to the Archive Server for public access. In a later release features such as “retain hidden until publication” will be switched on as well as access to the hidden data for named reviewers of the submitted scientific papers to enhance the peer review process.

The consortium would like to thank all the publishers that are helping to make the International Spectroscopic Database happen.

The EuroSpec Consortium comprises of:

- ISAS, Institute of Spectrochemistry and Applied Spectroscopy, Dortmund, Germany
- CreonLabControl AG, Frechen, Germany
- LGC, Runcorn, United Kingdom
- INA P-G, Institut National Agronomique Paris – Grignon, Paris, France
- ICT, Institute of Chemical Technology, Prague, Czech Republic
- SPECS and BioSPECS BV, Rijswijk, The Netherlands
- IM Publications, Chichester, United Kingdom
- University of Aveiro, Aveiro, Portugal

References

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