FTP-Server for exchange, interpretation, and database-search of ion mobility spectra, literature, preprints and software

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ABSTRACT

To assist current discussion in the field of ion mobility spectrometry, at the Institut für Spektrochemie und angewandte Spektroskopie, Dortmund, start with 4th of December, 1994 the work of an FTP-Server, available for all research groups at universities, institutes and research worker in industry. We support the exchange, interpretation, and database-search of ion mobility spectra through data format JCAMP-DX as well as literature retrieval, pre-print, notice and discussion board.

We describe in general lines the entrance conditions, local addresses and main code words. For further details monthly a news report will be prepared for all common user directly. To organise the first call, please contact BAUMBACH@HELIOS.ISAS-DORTMUND.DE or VONIRMER@HELIOS.ISAS-DORTMUND.DE. We send the password and account soon as possible.

EXCHANGE, INTERPRETATION, AND DATABASE-SEARCH OF SPECTRA

To assist peak assignment in ion mobility spectrometry it is important to have quality reference data. The reference collection should be stored in a database system which is capable of being searched using spectral or substance information. We propose to build such a database customized for ion mobility spectra. To start off with it is important to quickly reach a critical mass of data in the collection. We wish to obtain as many spectra combined with their IMS parameters as possible. Spectra suppliers will be rewarded for their participation with access to the database. To make the data exchange between users and system administration possible, it is important to define a file format specially made for the requirements of ion mobility spectra. The format should be computer readable and flexible enough for extensive comments to be included. In this document we propose a data exchange format, and we would like you to give comments on it.

For the international data exchange it is important, to have a standard data exchange format. We propose to base the definition of this format on the JCAMP-DX protocol, which was developed for the exchange of infrared spectra. This standard made by the **J**oint **C**ommittee on **A**tomic and **M**olecular **P**hysical Data is of a flexible design. The aim of this paper is to adopt JCAMP-DX to the special requirements of ion mobility spectra.

For further details see: "Exchange, interpretation, and database-search of ion mobility spectra supported by data format JCAMP-DX" by J.I.Baumbach, A. Davies, A.v.Irmer, P.Lampen.

FTP-SERVER & DATABASE

The main structure of the FTP-Server and Database is given in figure 1: The input includes ion mobility spectra themselves for pure components or mixtures and the different IMS configurations used in the experiments, commercial or home-made. Special boards for questions and answers and discussions are available. The retrieval system includes different literature databases from the IMS research community as well as news from the laboratories. A main point is the IMS-Preprint service. Please send pre-prints in your own word-processing system and pictures as TIFF files attached to the DATASERVER. Thus, very short

distributions time can be reached. The newest information will be available. Comments on papers are possible as well deep discussion on special topics to later main papers and publications.

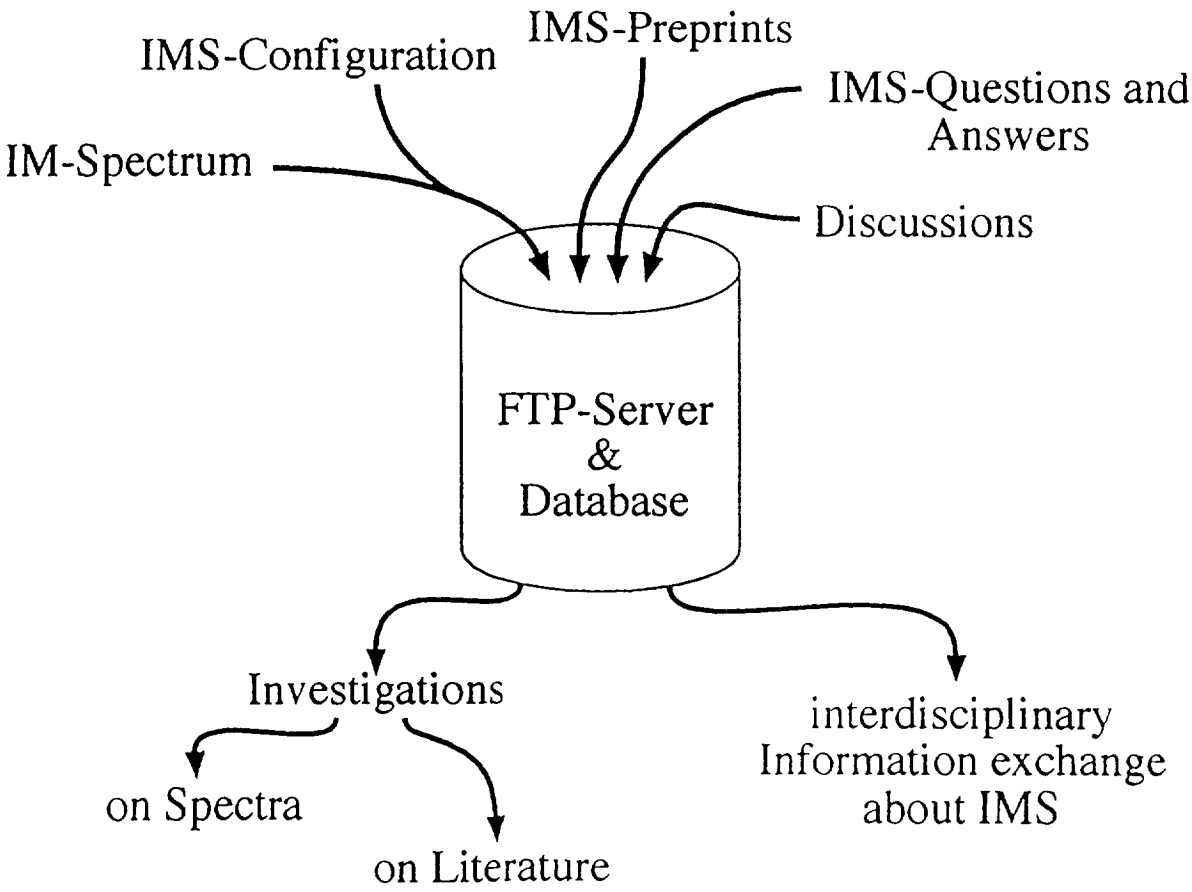

Figure 1: Main structure of FTP-Server & Database

ACCOUNT, PASSWORD AND FURTHER INFORMATION

The details of the server account are given in Table 1. This includes the FTP- oder TELNET-ACCOUNT to DATASERVER.ISAS.DE with the main password IMSDATA and the private password sended on request to the E-Mail addresses:

Table 1:
General pass line to DATASERVER at the Institut für Spektrochemie und angewandte Spektroskopie, Dortmund

TELNET	DATASERVER.ISAS.DE
FTP	DATASERVER.ISAS.DE
general password	IMSDATA
private password	will be sended on request
User	IMS

BAUMBACH@HELIOS.ISAS-DORTMUND.DE or VONIRMER@HELIOS.ISAS-DORTMUND.DE soon to the participants. The USER name is IMS. All details are readable on the page or will be sended on request.

HELPLINE AND SUPPORT

If an open question occurs, please don't hesitate to contact: Dr. Jörg Ingo Baumbach, Insitut für Spektrochemie und angewandte Spektroskopie, Bunsen-Kirchhoff-Str. 11, D-44139 Dortmund, Telefon +49-231-1392-238, FAX +49-231-1392-120.

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Basic research in ion mobility spectrometry has given rise to rapid advancement in hardware development and applications. The Third International Workshop on Ion Mobility Spectrometry (IMS) was held October 16-19, 1994, at Johnson Space Center to provide a forum for investigators to present the most recent results of both basic and applied IMS research. Presenters included manufacturers and various users, including military research organizations and drug enforcement agencies. Thirty papers were given in the following five sessions: Fundamental IMS Studies, Instrument Development, Hyphenated IMS Techniques, Applications, and Data Reduction and Signal Processing. Advances in hardware development, software development, and user applications are described.

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