********** science-softCon UV/Vis$^+$ Spectra Data Base **********
"Spectra News" (October 2017)

The "UV/Vis$^+$ Spectra Data Base" has been available on-line for 17 years (2000 – 2017)

Dear Colleagues,

this is the 39th issue of the science-softCon *UV/Vis$^+$ Spectra Data Base* "Spectra News". To regulary obtain "Spectra News", which provides important information concerning the on-line *UV/Vis$^+$ Spectra Data Base*, register at no cost for our mailing list or visit our web-site (http://www.uv-spectra.de/). "Spectra News" will be sent out periodically, about every 6 months.

The on-line *UV/Vis$^+$ Spectra Data Base* is a non-profit project and is operated in accordance with the **"Open Access"** definitions and regulations of the CSPR Assessment Panel on Scientific Data and Information (International Council for Science, 2004).

We welcome your suggestions, comments, questions, etc. To unsubscribe, send an E-Mail to helpdesk (Subject: unsubscribe).

In this issue:

The 11th edition of the "UV/Vis$^+$ Spectra Data Base" CD-ROM (Editors: A. Noelle, G.K. Hartmann, A. Fahr, D. Lary, Y.-P. Lee, P. Limao-Vieira, R. Locht, J.F. Martin-Torres, K. McNeill, J.J. Orlando, F. Salama, A.C. Vandaele, R.P. Wayne and M. Brunger) has been published in January 2017. The CD contains about 10500 spectra/datasheets and more than 3500 graphical representations for about 2000 substances and is available for 240 EURO (universities/governmental organizations 200 EURO).

The purchase of the "UV/Vis+ Spectra Data Base" CD-ROM includes 6 months on-line access to the database. For details contact our helpdesk.

Review of science-softCon "UV/Vis$^+$ Spectra Database" (UV/Vis$^+$ Photochemistry Database), 11th Ed., 2017 (ISBN 978-3-00-055351-6)

As anyone who is engaged in scientific research today knows, before tackling a new problem, it is essential to have all the existing literature and information about the particular topic/species to be studied at hand. In this context, the science-softCon "UV/Vis$^+$ Spectra Data Base" is indeed a boon to researchers, not only in molecular spectroscopy and photochemistry, but also several other diverse fields where spectral information

pertaining to molecules/radicals is desired. As a researcher in the area of VUV molecular spectroscopy I have personally referred to this database quite extensively and found it extremely useful. Ever since this project was initiated in 2000, there have been constant efforts by the editors to improve, expand and upgrade the database which has now grown into a large and comprehensive collection of spectroscopic data and literature covering a vast spectral region from IR to extreme UV. The latest (11th) edition of the database contains fairly exhaustive spectroscopic information on a wide range of molecules, conveniently classified, both by CAS numbers as well as different chemical groups like alkali compounds, aromatic compounds, pharmaceuticals, sulphur compounds, radicals, etc. for ease of searching. A unique feature of this particular database is that it has practically all the available published spectroscopic data (graphical as well as ASCII data) on a particular molecule in gas/liquid and solid phases as well as related photochemical information like quantum yields, millimetre wave data, free software package for atmospheric modelling, etc. Additionally there is an updated bibliography of all relevant papers right from early 1900's to the latest ones, pertaining to each molecule, arranged chronologically and with links to download the ones that are available online. The graphical interface is user friendly and self-explanatory and for further convenience, a short user manual and commonly used photochemical conversion factors are also provided. It may be noted that the database has both CD-ROM and online versions which are identical in their appearance and functions. In view of the costs that would be incurred in compiling and maintaining such a database it seems fair enough that access to the spectral data (in the form of a CD along with 6 months free access to online data) is charged, but access to the bibliography is free for all. Moreover, scientists who have contributed their data to the database have lifetime free access to the entire online database and there is a provision for permanent institutional access against a one-time payment. All in all, I find it to be currently one of the best databases available for molecular spectral data, comparable to the NIST database for atomic data.

Aparna Shastri, Atomic & Molecular Physics Division, BARC, Mumbai, India (May 2017)

Database maintenance

The on-line "UV/Vis^{+} Spectra Data Base" contains currently about 11700 spectra/datasheets and about 4000 graphical representations as well as other photochemical information for more than 2300 substances. Additional spectra/datasheets will be added continuously. In addition to the spectral data, links to abstracts of listed publications as well as links to on-line available original publications are available. For more details concerning the database development see development www.science-softcon.de/spectra/dev_1.png).

One-time registration for university libraries and governmental organizations

To minimize the bureaucratic expenditure and to benefit from future development of the database a one-time registration for university libraries and governmental organizations is possible. However, we do charge a one-time registration fee of 950 EURO for such institutions which is necessary to help us to maintain the database and provide this non-profit service to the scientific community. Thus, a one-time charge, which includes the latest issue of the "UV/Vis+ Spectra Data Base" CD-ROM series (11th edition 2017), will provide your institution permanent access to this fast growing

database (Literature Service and Spectra Service) via IP-number authentication. Please note that the database has been on-line for more than 16 years and has grown continuously. The database will be updated weekly (see development).

This type of subscription is available since January 2011 and there are already several universities/governmental organizations which have made use of this convenient and helpful opportunity. You can check if your organisation has already permanent and full access (www.science-softcon.de/spectra/permanent.htm) to the on-line database.

Become permanent user and join our initiative:

"Share Spectral Data & Information, Find Answers"

This initiative should develope the spectral (photochemical) database towards a spectral (photochemical) data sharing platform. The advantage of such a spectral data sharing platform is that the more scientists provide their data for inclusion into the database the better is the chance for all users to find specific spectral data within the database. In addition the spectral database gets more and more interdisciplinary usable. So every user can benefit from the database especially if their University/Governmental Organisation has permanent access to the database

For more information please contact your librarian or our helpdesk@science-softcon.de.

The support of the scientific community is required

The support of the scientific community is of utmost importance for such a data compilation project. We would be grateful to have your opinion on the database in its present form. Any criticism will be just as welcome as your positive comments and suggestions, since all considerations will be very helpful in improving the database.
To support us in maintaining the database, we would be grateful for your assistance in supplying any missing or new spectra data as well as other related data and information (e.g. quantum yield studies, photolysis studies) for inclusion into the database. Our database philosophy is that those scientists who support us in maintaining the database will get free access to the database. Currently more than 90% of its users have free-of-charge access to the database.

Yours sincerely,
Andreas Noelle (mail to: andreas.noelle@science-softcon.de)