

***** science-softCon UV/Vis⁺ Spectra Data Base *****
“Spectra News“ (December 2016)

The “UV/Vis⁺ Spectra Data Base” has been available on-line for 16 years (2000 – 2016)

Dear Colleagues,

this is the 38th issue of the science-softCon *UV/Vis⁺ Spectra Data Base* “Spectra News”. To regularly 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 3-4 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).

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The 11th edition of the “UV/Vis⁺ Spectra Data Base” CD will be published in January 2017

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) is in press and will be 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 (academic users 200 EURO; make your preorder until 31. December 2016 and get a 20% deduction).

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](#).

Starting with the 7th Edition of the CD-Series the SAG has decided to nominate a scientist who had made significant contributions in the research areas Spectroscopy and/or Photochemistry as “Honorary Editor”. The “Honorary Editor” will change for each issue.

It’s a pleasure and honour for us to announce that Michael Brunger from Flinders University, Australia, has accepted the invitation of the SAG to become “Honorary Editor” of the 11th edition CD.

Please find hereinafter the Laudatio written by Paulo Limao-Vieira from Universidade Nova de Lisboa (member of the “UV/Vis⁺ Spectra Data Base” SAG) and the Preface for the 11th edition CD written by Michael Brunger.

Laudatio to the Honorary Editor of the 11th Edition of the “UV/Vis⁺ Spectra Data Base” (written by Paulo Limao-Vieira)

Professor Michael Brunger from the School of Chemical and Physical Sciences, Flinders University, Adelaide, South Australia, is internationally well-known as an experimentalist researcher with interests in positron and electron scattering from a range of molecular species and radicals that are of medical, technological and atmospheric importance. Over the years he has also developed a modelling faculty that enables the role of electron-driven processes in our atmosphere and that of other planets to be simulated. He has made several unprecedented contributions within the electron and positron scattering communities with more than 300 papers published in international peer reviewing journals, with several of them as landmark contributions and serving as benchmark data for different communities, e.g. plasma processing, modelling the transport of electrons in gases or liquids, charged-particle track studies of radiation damage in matter, among many others. He serves as associate dean in the School of Chemical and Physical Sciences at Flinders and holds several relevant national and international recognition awards for his active and relevant roles in academia and in science.

Preface for the 11th Edition of the “UV/Vis⁺ Spectra Data Base” (written by Michael J. Brunger)

It is a real honour to be invited to be the Honorary Editor of the 11th edition of the science-softCon UV/Vis⁺ Spectra Data Base. This data base has grown to currently contain more than 10000 spectra/datasheets and about 3400 graphical representations for about 2000 substances, and it is updated regularly. For an electron and positron spectroscopist, and part-time computational modeller for the role of electron-driven processes in planetary atmospheres and comets, such as myself, the UV/Vis⁺ Spectra Data Base is invaluable to my research. For example, the interpretation of our lower-resolution electron energy loss spectra (EELS), from which scattering cross sections (collision probabilities) are ultimately derived, is significantly assisted by the higher-resolution photoabsorption spectra contained within the data base. Specifically, the spectral assignments for the optically allowed transitions in the EELS rely critically on the photoabsorption data, which goes right to the crux for the validity of the electron scattering cross sections we ultimately report. Those cross sections, in turn, are finding increased application as a vital sub-set of the data inputs needed for modelling the transport of electrons in gases or liquids, under the influence of applied (external) electric and/or magnetic fields, as well as being employed in charged-particle track studies of radiation damage in matter. Without accurate and reliable input data, the results obtained from these modelling studies might be unphysical and so it is no exaggeration to state that UV/Vis spectra, such as contained within this data base, are fundamental to not only my investigations but to many others that might not initially be apparent to the reader.

If I might quote my predecessor (Dr. D. P. M. Holland) as Honorary Editor, “the science-softCon UV/Vis⁺ Spectra Data Base is an on-going project which requires continual updating as more data becomes available, and I urge the scientific community to support this important work”. I fully endorse that sentiment, and as a consequence hope you all ‘get on board’!

Database maintenance

The on-line “UV/Vis+ Spectra Data Base” contains currently about 10500 spectra/datasheets and about 3500 graphical representations as well as other photochemical information for ~ 2000 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](http://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 \(www.science-softcon.de/spectra/permanent.htm\)](http://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 develop 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)