

***** science-softCon UV/Vis⁺ Photochemistry Database *****
“Spectra News“ (August 2019)

The “UV/Vis⁺ Photochemistry Database” has been available on-line for 19 years (2000 – 2019)

Dear Colleagues,

this is the 40th issue of the science-softCon *UV/Vis⁺ Photochemistry Database* “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 www.photochemistry.org. “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](mailto:helpdesk@photochemistry.org) (Subject: unsubscribe).

In this issue:

The 12th edition of the “UV/Vis⁺ Spectra Data Base” CD (ISBN 978-3-00-063188-7) has been published in August 2019

The 12th 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. Loch, J.F. Martin-Torres, K. McNeill, J.J. Orlando, F. Salama, A.C. Vandaele, R.P. Wayne and B.N. Rajasekhar) has been published in August 2019. The CD contains about 13500 spectra/datasheets and more than 5000 graphical representations for about 2800 substances and is available for 260 EURO (universities/governmental organizations 200 EURO). The CD is based on HTML and hence platform independent.

The purchase of the “UV/Vis⁺ Spectra Data Base” CD-ROM includes 12 months on-line access to the database. For details contact our [helpdesk](mailto:helpdesk@photochemistry.org).

Abstract

Spectral information (gas, liquid and solid phase from EUV-VUV-UV-Vis-NIR) and related data (e.g. information concerning publications on quantum yield studies or photolysis studies) from published papers. The 12th edition of the science-softCon "UV/Vis⁺ Spectra Data Base" CD-ROM series (ISBN 978-3-00-063188-7) contains about 13500 spectra/data sheets (ascii-format) as well as about 5000 graphical representations and additional photochemistry information from published papers for about 2800 substances. The database is subdivided into 28 substance groups. You will find more information at www.photochemistry.org.

Preface from the "Honorary Editor" Professor B.N. Rajasekhar, Bhabha Atomic Research Centre, Mumbai, India

It is a great honour to be invited to be the Honorary Editor of the 12th edition of the science-soft-Con UV/Vis+ Spectra Data Base. This data base has grown considerably over years and at present contain more than 13500 spectra/datasheets and above 5000 graphical representations for 2800 substances and it is updated regularly. The spectroscopic information available with this database is up to date and helpful for us for the last many years. Being a experimental Molecular spectroscopist and developer of experimental facilities for Atomic Molecular and optical Science research, I found UV/Vis+ Spectra Data Base is of immense value to my research programs and the Molecular Physics community visiting our experimental facilities at Indus synchrotron source in India. I am sure many molecular spectroscopic research programs around the world will be benefitted from this database project in the future especially for analysis of the different spectroscopic aspects of molecules. The accurate and reliable information available with this data base on molecules is fundamental in nature and helps in proceeding further to understand photon, electron and ion induced chemistry of molecules of interest not only in Astro-Chemistry, Astro-Physics, Environmental chemistry, plasma Physics but also in applied fields such as Medical Diagnostics, Agriculture, Bio-chemistry and catalysis. I strongly feel that this project, "science-softCon UV/Vis+ Spectra Data Base", requires continual updating as more data becomes available in future. This updating shall directly help the molecular research programs by providing vital information for understanding particle/photon induced processes in normal and extreme conditions. I urge the scientific community to support this important project and suggest to their students and colleagues to use this facility and get benefitted.

Review of the science-softCon UV/Vis⁺ Spectra Bata Base, Dr Nykola Jones, Beamline scientist on the AU-UV beamline at the ASTRID2 synchrotron ISA, Department of Physics & Astronomy, Aarhus University, Denmark

Now in its 12th edition, the full UV/Vis⁺ Spectra Database contains UV-Vis photoabsorption data for over 2800 molecules, ranging from the simplest inorganics, such as noble gases, to a wide variety of complex organics usefully categorised into groups.

For a molecule included in the database there is a compilation of relevant published papers containing UV/Vis data, including full reference details. These literature details are available free online, but with a subscription you can gain full access to the website. This enhanced access includes links to an online abstract or open access version of the paper and for many of the references there are also charts showing the data and text files containing the tabulated data. There is a summary document for each publication, containing selected important experimental details such as measurement range, resolution and the temperature and phase at which the spectrum was taken. This allows for easier comparison amongst the variety of experiments presented.

The accompanying CD, available with some subscriptions, is a duplication of the information available on the website. There is no search function on the on the CD, but instead an almost complete list of all molecules included in the database (Substance List), which can then be searched and has links to the more detailed information.

There are sometimes a hundred or more molecules grouped on a single page, so using the function on the website or in the browser is a must to help you find what you are looking for. CAS numbers for most molecules are also included, so that an unambiguous search term can be used.

One thing that is lacking in this great collection of spectra, is comparison of data for a single species. In a future update of the presentation of this collection, it would be nice to see figures where all of the available data for a molecule is plotted together.

It is clear that a large amount of work has gone into creating and keeping this database up-to-date with all the latest references and data for this large number of molecules. It is extremely useful to have an anthology of relevant papers containing UV-Vis spectra for a molecule, allowing for a quick check of the available data, and with many entries containing a link, it is quick and efficient to find the original source of the data.

Database maintenance

The on-line “UV/Vis⁺ Spectra Data Base” contains currently about 13600 spectra/datasheets and about 5100 graphical representations as well as other photochemical information for more than 2850 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](http://www.science-softcon.de/spectra/dev_1.png) (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 800 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 (12th edition 2019), 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 19 years and has grown continuously. The database will be updated weekly (see [development](http://www.science-softcon.de/spectra/dev_1.png)).

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.php) to the on-line database.

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)