

UV/Vis⁺ Spectra Data Base(UV/Vis⁺ Photochemistry Database)

EUV-VUV-UV-Vis-NIR Spectral Information (gas, liquid and solid phase) and related data (e.g. information concerning publications on quantum yield studies or photolysis studies) from published papers

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www.uv-spectra.de

Introduction:

The science-softCon "UV/Vis⁺ Spectra Data Base" is a non-profit project established in August 2000 and is operated in accordance to the "Open Access" definitions and regulations of the CSPR Assessment Panel on Scientific Data and Information (International Council for Science, 2004, ICSU Report of the CSPR Assessment Panel on Data and Information; ISBN 0-930357-60-4). The on-line database contains currently about 5,700 spectra (from low to very high resolution, at different temperatures and pressures) and data-sheets (metadata) of about 900 substances. In addition more than 250 links to on-line free available original publications are provided. The interdisciplinary of this photochemistry database provides a good interaction between different research areas. So, this database is an excellent tool for scientists who investigate on different fields such as physics and chemistry of planetary atmospheres, astrophysics, agriculture, analytical chemistry, environmental chemistry, medicine, remote sensing, etc.

Database quality assurance:

To ensure the high quality standard of the „UV/Vis⁺ Spectra Data Base“ an international Scientific Advisory Group (SAG) was established in 2004. The SAG members are in addition editors of the „UV/Vis⁺ Spectra Data Base“ CD-ROM series. The database contains spectral data and photochemical information from published papers.

Current SAG members:

Andreas Noelle (science-softCon, DE)

Askar Fahr (Howard University, US)

Stephane Le Calve (CNRS, FR)

F. Javier Martin-Torres (CAB, SP)

Farid Salama (NASA-Ames, US)

Richard P. Wayne (University Oxford, UK)

Gerd K. Hartmann (science-softCon, DE)

David Lary (NASA-GSFC, US)

Paulo Limao-Vieira (New University Lisbon, PT)

John J. Orlando (UCAR, US)

Ann Carine Vandaele (BIRA-IASB, BE)

C.Y. Robert Wu (University Southern California, US)

Database content:

The on-line database contains currently about 5700 spectra/data-sheets (gas, liquid, solid phase, at low to very high resolution, and at different temperatures and pressures); and data-sheets (metadata) of about 900 substances and related photochemical information (quantum yields, photolysis studies, etc...). Additional spectra/data-sheets are being added continuously. In addition more than 250 links to on-line free available original publications are provided. The database is subdivided into 27 substance groups:

Alkali Compounds	Aromatic Compounds	Carbon Oxides	Dyes
Halogenated Alkanes, Alkenes	Halogenated Aromatics	Halogenated Carbonyl Compounds	Halogenated Nitrogen Compounds
Halogens/Halogen Oxides	Hydrocarbons	Hydrogenhalides/Hypohalides	Nitrogen Acids
Nitrogen/Nitrogen Oxides	Noble Gases	Organic Acids/Esters	Organic Carbonyl Compounds
Organic Nitrogen Compounds	Organic Peroxy Compounds	Other Oxygenated Organics	Oxygen Hydrogen Compounds
PAHs	PBDEs	PCDDs	Pesticides/Herbicides
Radicals	Sulfur Compounds	Other Species (not yet categorized)	Related Data and Information

Database access:

The on-line „UV/Vis⁺ Spectra Data Base“ is subdivided into a „Literature Service“ and a „Spectra Service“. Via the „Literature Service“ all datasheets (meta data) as well as many quantum yields and photochemical information are available free-of-charge for all interested users. In addition the „Literature Service“ provides access to other related data like AutoChem software package (D. Lary, NASA-GSFC), Daily Solar Irradiances (J. Lean, NRL), MAS remote sensing data (G.K. Hartmann, MP Ae) or Solar Ultraviolet Measurements of Emitted Radiation data (W. Curdt, MPS). The „Spectra Service“ provides in addition full access to the digital spectra data. However, access to the „Spectra Service“ requires a very moderate utilization fee. This helps us not only to maintain the „Spectra Service“ but also to maintain the free-of-charge „Literature Service“ and is in accordance to the „Open Access“ definitions and regulations of ICSU/CODATA.

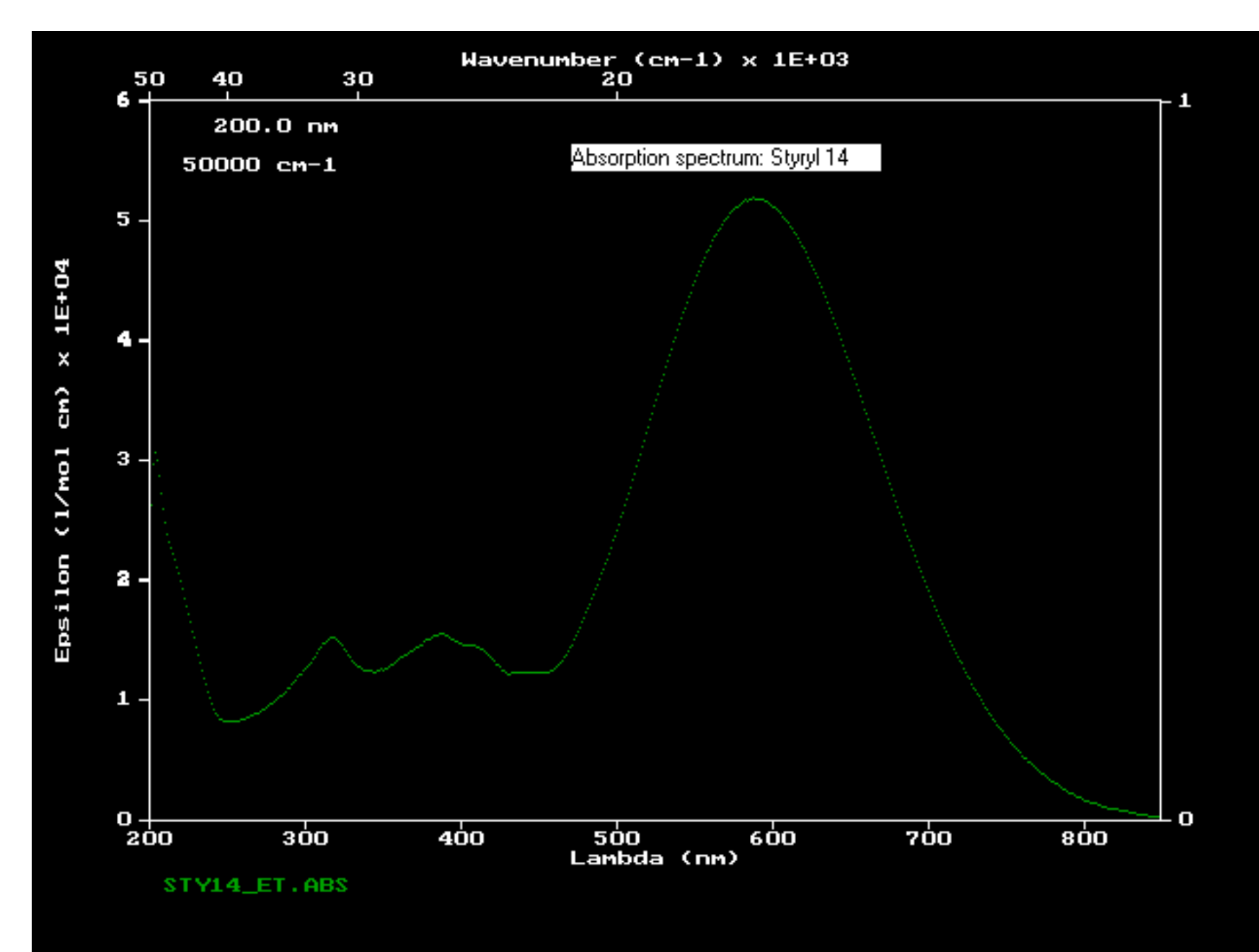


Fig.1 Graphics are available for some of the spectra, specially the dyes

Database formats:

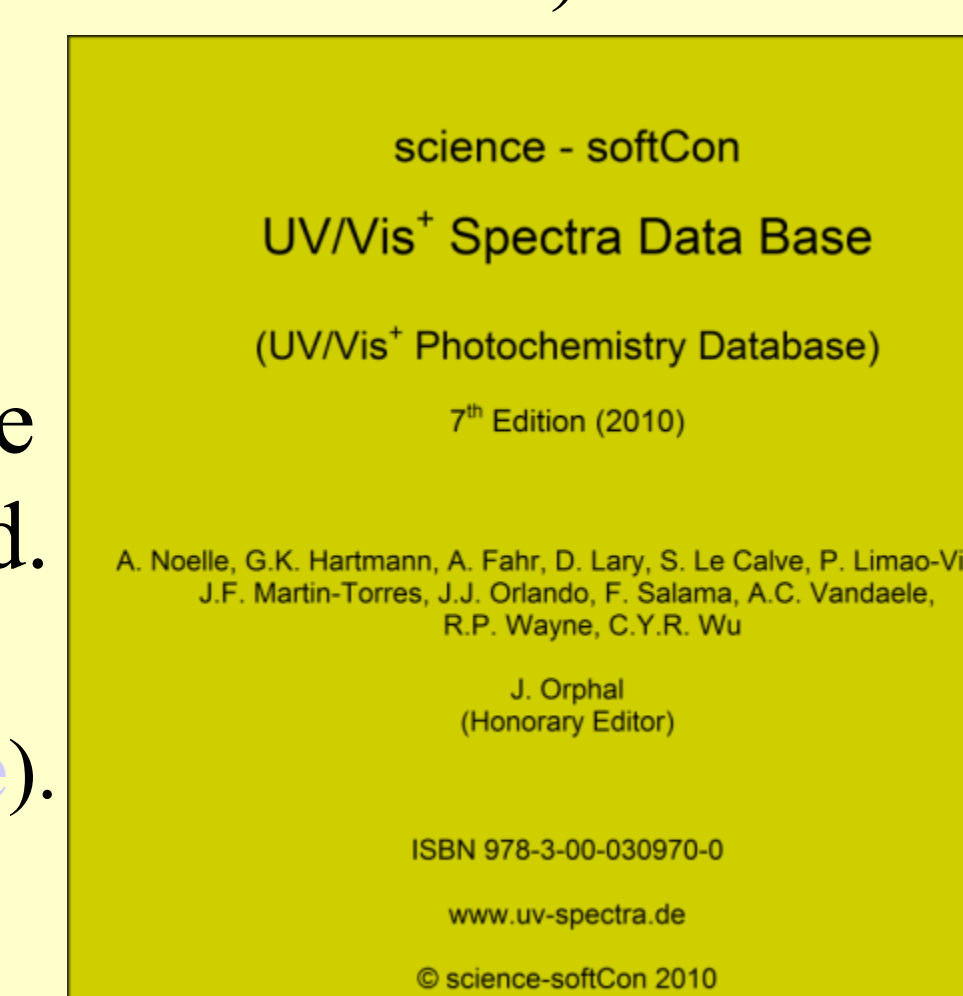
All datasheets (meta data) as well as the spectral data (2 column tables) are in plain ascii format.

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"Dyes" data file: E. S. Orlandi et al., 2007  
Title: Dyes with different substituents: absorption and fluorescence spectra  
Absorption: 200.0-800.0 nm (200.0-800.0 nm)  
Fluorescence: 200.0-800.0 nm (200.0-800.0 nm)  
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206 0.000  
208 0.000  
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Outlook:

The database is not static, additional spectra/datasheets and related photochemical information (quantum yields, photolysis studies etc.) will be added continuously. The 7th edition „UV/Vis⁺ Spectra Data Base“ CD-ROM (ISBN 978-3-00-030970-0) is now available (May 2010). The CD is a mirror of the on-line database as of March 2010 and contains about 5600 spectra/datasheets of about 900 substances.

An application for a CODATA Task Group „UV/Vis⁺“ to support the future development of the „UV/Vis⁺ Spectra Data Base“ is envisaged. If you are interested in joining this initiative or if you have any questions/suggestions please contact us (helpdesk@science-softcon.de).



For more information visit our web-site at www.uv-spectra.de