

Review of the science-softCon UV/Vis+ Spectra Database 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 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.