Spectral Databases

Jode Himann | Nemalux Research | 02.14.2015

The spectral databases are an important resource for Academic research, industrial research and in the field of education. Most of the spectral databases for the simple chemical compounds and monomers are freely available on the web. National Institute of Standards and Technology (NIST) website carries the largest collection of spectral data. NIST (1) is a U.S. federal agency, which maintains the measurement standards in science and industry. The spectral data from NIST are considered as the standard reference materials among researchers.

ChemSpider (3), an online chemical database supported by Royal Society of Chemistry is offering access almost 31 million unique chemical compounds sourced and linked out to almost 400 separate data sources on the Web. ChemSpider is also a search engine layered on terabytes of chemistry data; it is also a crowdsourcing community for chemists who contribute their data, skills, and knowledge to the enhancement and curation of the database. Internetchemistry.com (4) is another free website that acts as an intermediary between information seekers and almost all the free spectral databases in the world. A list of free spectral websites are given in the next page.

Bio-Rad and Sigma-Aldrich Corporation are the two of the well-known companies that sell spectral database libraries. Bio-Rad Laboratories (5) is a global provider of life science research and clinical diagnostic products with an annual sales of $2 billion. The company provides Infrared, Raman, NMR, Mass Spectroscopy and UV-Vis databases of Polymers, Organic, Inorganic, Industrial, Forensic, Environmental and Organometallic compounds. Bio-Rad offers spectral library collections with basic library for a cost of USD $3,465 and a comprehensive one for USD $26,120. Sigma-Aldrich Corporation (6) is a supplier of chemicals, biochemical and other related products with a company value more than $8 billion. Sigma-Aldrich's FT-IR spectral library software costs about USD $9,550.

There are many websites that provide and link spectral databases, but there are not many independent websites that provide spectral database of optical materials. Photonics industry is driven by optical materials, which is a $156 Billion industry with more than 2700 firms around the world and creating a database website of optical materials is practicable. Although, spectral data of materials are freely available in the websites of suppliers with the specification data of the product. A UK based company CRYSTRAN (7) has a list of transmission spectrums of optical materials they provide. The Sopra S.A. a company in France have optical database and also optical properties of materials as software, and it is not free.

1. http://www.nist.gov/srd/

   The website provides easy access to many (currently over 90) of the NIST scientific and technical databases. These databases cover a broad range of substances and properties from many different scientific disciplines. The Gateway includes links to free online NIST data systems as well as to information on NIST PC databases available for purchase.

2. http://hitran.iao.ru/

   HITRAN is an acronym for high-resolution transmission molecular absorption database. HITRAN is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in the atmosphere.

3. http://www.chemspider.com

   http://www.chemspider.com/DataSources.aspx, the link shows the data sources for chemspider

4. http://www.internetchemistry.com
5. http://www.bio-rad.com/en-ca/spectroscopy
6. http://www.sigmaaldrich.com

7. http://www.crystran.co.uk/optical-materials