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[E0005]

Spectroscopy on-line

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At the University of Potsdam, Chemistry Department the following teaching and working material is on-line available (http://www.chem.uni- potsdam.de/tools):

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NMR- Spectroscopy

Incremental calculation of ^{13}C chemical shifts of substituted benzenes, pyridines, pyridazines, biphenyls, 2,2´-bipyridyls, naphthalines, quinolines with and without ortho correction and numerical as well as graphical output, a ^{1}H-Wizard for interpretation of ^{1}H NMR spectra, a small ^{13}C NMR data bank and a Complete Line Shape Analysis simulation of the non-coupled AB-case. Further, a number of surveys concerning chemical shifts (^{1}H, ^{13}C, ^{11}B, ^{15}N, ^{17}O, ^{31}P, ^{19}F), $^{n}J_{H,H}$ coupling constants, NMR solvents (physical data and $^{1}H/^{13}C$ NMR spectra) and the Periodical Table of the NMR elements (nucleus data, NMR characteristics) can be employed for structural search.

In addition, but still in German (http://www.chem.uni-potsdam.de/tools/index_de.html), an on-line introduction into NMR spectroscopy together with an number of exercises concerning spectroscopy (NMR as a special) and a small dictionary of NMR termini (the latter two under permanent extension) can be recommended to teach the method in graduated courses or themselves in an interactive way. A english version of of the Introduction to the ^{1}H- NMR spectroscopy is in preparation. the first working modell ist available at http://www.chem.uni-potsdam.de/1hbuch/english/index.html.

Picture 1 shows the startpage of your site. On the left hand site you have some navigation tools and you can access the wizard directly. All other services are available under the point tools.

IR- Spectroscopy

For the intrepretation of IR Spectra a IR- Wizard is available. You can enter the wavenumber of a interesting vibration and the program gives you some possible structurals fragments to you. The following picture shows a sample output of this wizard.

MS- Spectrometry

In addition to the NMR and IR Wizards we have also a MS- Wizard available here!

All comments on this poster should be sent by e-mail to (mailto:ecsoc@listserv.ariz ona.edu) ecsoc@listserv.arizona.edu with **E0005** as the message subject of your e-mail.
