Towards better understanding of NIR spectra

(DESCRIPTION FOR THE GENERAL PUBLIC)

NIR spectra are more complex as compared with MIR or Raman spectra, even for relatively simple molecules. In the NIR range appear numerous bands due to overtones and combination modes. All these bands heavily overlap with each other, and therefore the spectral envelopes are complex. For this reason the band identification and correct assignment is a challenging task. Classical methods of analysis of NIR spectra have limited usefulness since they do not provide the complete information on all spectral features. Previous analysis of NIR spectra focused mainly on the band assignment and was based on the observed peak positions. In contrast, the other band parameters like intensity and half-width were not systematically studied. It is of particular note that the overtones of many important bands like C=N or C≡N were not identified yet. Above facts evidence that the satisfactory understanding of NIR spectra still requires numerous studies, but realization of this project is expected to advance this understanding.

The main aim of the proposed project is better understanding of NIR spectra of all studied samples. In addition, we expect to obtain more general information on this spectral region. During realization of this project, for the first time, we plan to undertake comprehensive study of all spectral parameters of the overtones and combination bands. To ensure a general character of the obtained conclusions we intend to study various kinds of chemical compounds with different structure and functionalities. In addition, several deuterated derivatives will be examined. We plan to measure NIR, MIR and Raman spectra of the neat samples and the diluted solutions. To obtain information on the hydrogen bonding, the spectra of selected samples will be recorded as a function of the concentration. From the experimental spectra we determine the spectral parameters like position, intensity or half-width for the fundamental transitions as well as for the overtones and combination modes. These parameters will be a subject of detailed analysis. Using advanced theoretical methods, we calculate the anharmonic vibrational spectra for all studied samples. The results of these calculations will be applied for the reconstruction of NIR spectra. The comparison of the experimental and reconstructed NIR spectra should provide important information on the structure and interactions as well as on the anharmonicity and possible resonances between different vibrational modes. We expect that realization of this project will be an important step towards better understanding of complex NIR spectra, and in future may stimulate new applications in the field of the physical and analytical chemistry.