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Abstracts presented in the original edition

APPLICABILITY OF IR SPECTRAL PARAMETERS FOR ESTIMATION OF THE STRENGTH OH···N HYDROGEN BONDS

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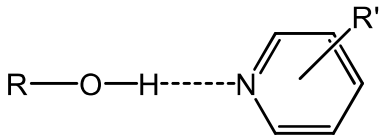
Non-covalent adaptive modern materials are often built from monomers, associated with hydrogen bonds. The properties of such materials are largely defined by the strength of these interactions. However, the evaluation of a single hydrogen bond strength is often a quite complicated task, especially for complexes with multiple hydrogen bonds. Thus it is necessary to use indirect methods – estimations of energies based on values of measurable spectral parameters (IR and NMR) [1,2].

In this work we investigated complexes ROH···NC_5H_4R' (where R = $CH_{3-n}F_n$, n = 0,…,3, R' = NO_2, F, C≡N, CH_3, OCH_3, see Figure 1) by means of quantum chemistry. We calculated equilibrium geometries of the model complexes, energy of complexation and spectral IR parameters at B3LYP/6-311++g(d,p) level.



R = $CH_{3-n}F_n$, n = 0,…,3;
R' = NO_2, F, C≡N, CH_3, OCH_3

Figure 1. Scheme of the studied complexes.

The sensitivity of IR parameters (stretching vibration frequencies and intensities) to the strength and geometry of hydrogen bonds were investigated. It was shown that the change of proton-donating group vibrational frequency is suitable for qualitative estimations of hydrogen bond properties.

References

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