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EXPERIMENTAL AND AB INITIO CHARACTERIZATION OF THE ANHARMONICITY OF ν_S(OH) VIBRATION IN PHENOL DERIVATIVES

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An anharmonicity is a fundamental quantity shaping the potential for stretching OH vibration in phenol and its derivatives. The phenomenon is examined both by experimental and theoretical methods. FT-IR and NIR spectra of series of phenols derivatives were measured in the range of fundamental and first two overtones of $_s$(OH) vibrations in CCl_4 solutions.

The electronic influence of substituents on the analyzed frequencies is discussed and correlated with pK_a parameters. *Ab initio* MP2/6-31G(d,p) and B3LYP/6-31G(g,p) calculations of the potential for proton movement in OH group were performed. Equilibrium structures were also determined. The frequencies of fundamental and overtones were calculated by Numerov-type procedure.

The results of calculations are compared with the experimental data. The best linear correlations were obtained for the results of MP2/6-31G(d,p) calculations. It was shown that some structural parameters are especially sensitive on substitution. The linear correlations were found between those parameters and spectroscopic data.

The results of calculation are compared with available crystallographic data.