



Influence of substituents on the anharmonicity of $\nu_s(\text{OH})$ vibration in phenol derivatives explored by experimental and theoretical approach.

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Streszczenie

Very good reproducibility of the first five vibrational transitions of phenol in the gas phase by the MP2/ 6-31G** potential for O-H bond stretching was found. The vibrational levels were calculated by a program for variational solving of the time-independent Schrödinger equation in one dimension. Relative intensities of particular transitions were determined on the basis of the function of the dipole moment. The substituent effects on the $\nu_s(\text{OH})$ transitions and on the intensity of these transitions, as well as on the structure of eleven phenols, was analyzed as a function of the pK_a values.

Słowa kluczowe

Aromatic compounds, Chemical calculations, Energy levels, Oscillation, Reaction products

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