

The model analysis of the effects of electrical and mechanical anharmonicity on vibrational spectra of H-bonded complexes.

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Streszczenie

The model of anharmonic dipole moment function is applied for the analysis of the hydrogen bridge $XH\cdots Y$ vibrations. The model allows to predict the characteristic features of the hydrogen bond formation in the intensities of $\nu(XH)$ and $\nu(XY)$ transitions. Three complexes of phenol with different proton acceptors (acetonitrile, pyridine and trimethylamine) are chosen as model systems. The experimental data and the model calculations are compared with the Density Functional Theory calculations at B3LYP/6-31G** level.

Słowa kluczowe

Hydrogen bond, Anharmonicity, Dipole moment function,
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