Effect of electrical and mechanical anharmonicity on vibrational spectra of H-bonded complexes: phenol···B (B=acetonitrile, pyridine) systems.

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Streszczenie

The model of the anharmonic dipole moment function of the H-bonded complex AH.-.B is applied to C6HsOH(D) complexes with acetonitrile and pyridine. The frequencies and absolute intensities data for the overtones and the fundamental absorption bands in a wide spectral region (8000-50 cm <) and derivatives of the dipole moment function are presented and compared with ab initio calculation results on the Dk-T B3LYP/6-31G** level.

Słowa kluczowe

Hydrogen bond, Anharmonicity, Dipole moment function, Vibrational spectra Phenol

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