Hyperpolarizabilities of some model hydrogen-bonded complexes: PM3 and*ab initio* studies.

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Streszczenie

The polarizability and first hyperpolarizability value of the F–H···NH_3 hydrogen-bonded complex has been calculated using the *ab initio* method with different basis sets. In addition, the first hyperpolarizability values of the hydrogen-bonded complexes formed by nitrosubstituted phenols with trimethylamine have been calculated using PM3 and *ab initio* (STO-3G) methods. It has been shown that enhancement of the first hyperpolarizability ($\Delta\beta$) of the complex arises from the hydrogen bond interaction between the phenol derivative and trimethylamine.

Słowa kluczowe

NLO, Hyperpolarizabilities, Hydrogen bond, Ab initio, PM3

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