



Strong intermolecular OH...N hydrogen bond as a source of polymorphism in the complex of pentachlorophenol with 4-methylpyridine

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Streszczenie

For the first time the polymorphism connected with the proton transfer in strong intermolecular hydrogen bond was presented. The structure of a new polymorph of the complex of pentachlorophenol with 4-methylpyridine was compared to the structure known for a long time. The new polymorph is characterized by an elongation of the distance between the proton donor and acceptor and a change of the OH...N angle. The differences between the degree of proton transfer for both polymorphs are visible in the IR spectrum, in which the continuous proton absorption, typical for very strong hydrogen bonds, disappears. The results of theoretical calculations show that in the case of strong hydrogen bonds, due to the low energy barrier for proton transfer and the arrangement of donor and acceptor orbitals, the existence of polymorphs related to the degree of proton transfer is possible.

Słowa kluczowe

Complex of pentachlorophenol with 4- methylpyridine, IR, QTAIM, NLBO

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