

On the unusual IR spectra of the pentachlorophenol - trimethylamine complex in low temperature matrices.

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Rok wydania

2016

Czasopismo

Chemical Physics Letters

Numer woluminu

660

Strony

102-106

DOI

10.1016/j.cplett.2016.07.052

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Usually the stretching vibration of the A-H group in hydrogen-bonded complexes gives an intense, broad absorption in the IR spectrum. However in a few complexes it has proved difficult to detect this absorption in low temperature matrices. In this work the Ratajczak-Yaremko vibrational model of the hydrogen bond has been applied to simulate the IR spectrum obtained for one such complex: the pentachlorophenol-trimethylamine, PCP-TMA, hydrogen bonded complex isolated in an argon matrix. Quantum chemical calculations have also been carried out to gain further insight into this complex.

Słowa kluczowe

hydrogen bonds, Strong anharmonic coupling, infrared spectra, B3LYP

Adres publiczny

<http://dx.doi.org/10.1016/j.cplett.2016.07.052>

Strona internetowa wydawcy

<http://www.elsevier.com>