Vibrational spectroscopy of 4-hydroxybenzhydrazide and its O,N-deuterated isotopologue accompanied by X-ray structure refinement.

Autorzy

Piotr Drożdżewski

Halina Zasłona

Maria Kubiak

Rok wydania

2009

Czasopismo

Vibrational Spectroscopy

Numer woluminu

50

Strony

185-192

DOI

10.1016/j.vibspec.2008.10.007

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The vibrations of crystalline 4-hydroxybenzhydrazide were investigated by IR and Raman spectroscopy. Spectral changes resulting from O,N-deuteration together with DFT calculations were employed for band assignment presented in terms of potential energy distribution. The characteristic absorptions of the hydrazide group were located at 1623 (CO stretching), 1588 (NH_2 bending) and 1532 cm^{-1} (NH bending). The greatest contributions of the NN and CN stretching vibrations were found in the 1208 and 1109 cm^{-1} modes, respectively. The predominant contribution of the CO stretching vibration was observed for the 1282 cm^{-1} absorption. The computations at the B3LYP level with 6-311++G(d,p) basis set were based on structural parameters taken from refined single crystal X-ray investigations. The details of hydrogen bonding and crystal packing are also presented.

Słowa kluczowe

4-Hydroxybenzhydrazide, 4-Hydroxybenzoic hydrazide, IR Raman spectra, DFT calculations, Deuteration, Crystal structure

Adres publiczny

https://doi.org/10.1016/j.vibspec.2008.10.007

Strona internetowa wydawcy

http://www.elsevier.com