



Inelastic neutron scattering studies on dichloro-1,4-benzoquinones.

Autorzy

Andrzej Pawluko

I. Natkaniec

Grażyna Bator

Eugeniusz Grech

Lucjan Sobczyk

Rok wydania

2004

Czasopismo

Spectrochimica Acta Part A-
Molecular and Biomolecular
Spectroscopy

Numer woluminu

60

Strony

2875-2882

DOI

10.1016/j.saa.2004.01.022

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Inelastic neutron scattering (INS) spectra of 2,6-dichloro- and 2,5-dichloro-1,4-benzoquinone were compared with Raman and infra-red (IR) spectra and analysed in detail below 1800 cm^{-1} . The analysis was based on calculations tending towards simulation of spectra by using GAUSSIAN (HF, DFT/B3LYP and BLYP/6-31G(d,p)), and auctiCLIMAX programs. The correlations between calculated and experimental (either INS or Raman and IR) frequencies enabled to analyse the problem of scaling factors (SFs). The advantages of INS technique was shown in studies of low frequency vibrations with participation of H-atoms. The macroscopic lattice effect at low temperatures on INS spectra is discussed.

Adres publiczny

<http://dx.doi.org/10.1016/j.saa.2004.01.022>

Strona internetowa wydawcy

<http://www.elsevier.com>