Vibrational spectroscopic properties of a $[C(NH_2)_3]_4Cl_2SO_4$ ferroelectric crystal : an experimental and theoretical study.

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Rok wydania

2014

Czasopismo

Acta Physica Polonica A

Numer woluminu

125

Strony

115-127

DOI

10.12693/APhysPolA.125.115

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Tetraguanidinium dichloride-sulphatecrystal, [C(NH2)3]4Cl2SO4,abbreviated as G4Cl2SO4was investigated.The vibrational infrared sp ectra of powdered G4Cl2SO4crystal in Nujol mull were studied in the wide range of temperature,from 298Kto377K.This temperature range contains all the phases in the crystal(namedI I I,I I,Ion heating,respectively).The temperature changes of wavenumb ers,centre of gravity,and intensity of the bands were analyzed to clarify the molecular mechanism of the phase transitions.It was shown that in cooling from 377 K to 313 K the phase II is the same as the room temperature phase.Information about hydrogen b onds was obtained.The time dependence of internal vibrations at 356 K was observed and it was connected with slow transitionI I I→I I.For more detailed band assignment Raman spectrum at room temperature,at ferro electric phase was carried out.Theoretical calculations were made based on density functional theory,with the B3LYP method using 6-311+G(d,p)basicset.Calculated normal vibrational mo des of the molecule,their frequencies and intensities were compared with the serecorded in exp eriment.Theoretical description of themolecule including hydrogen bonds were optimized and the bond parameters were obtained.The Mulliken charges p opulation analysis was performed.

Adres publiczny

http://przyrbwn.icm.edu.pl/APP/PDF/125/a125z1p22.pdf

Strona internetowa wydawcy

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