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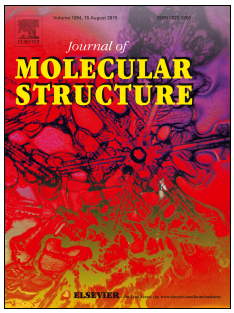

Crystal structure, vibrational spectra and DFT studies of hydrogen bonded 1,2,4–triazolium hydrogenselenate

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Crystal structure, vibrational spectra and DFT studies of hydrogen bonded 1,2,4–triazolium hydrogenselenate

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Abstract

The new hydrogen bonded molecular complex 1,2,4–triazolium hydrogenselenate (THS) is prepared by the reaction of 1H–1,2,4–triazole and selenic acid. This complex is stablised by N–H···O and C–H···O hydrogen bonding and electrostatic attractive forces between 1H–1,2,4–triazolium cations and hydrogen selenate anions. The XRD studies revealed that intermolecular proton transfer occur from selenic acid to 1H–1,2,4–triazole molecule, results in the formation of 1,2,4–triazolium hydrogenselenate which contains 1,2,4–triazolium cations and hydrogenselenate anions. The molecular structure of THS crystal has also been optimised by using Density Functional Theory (DFT) using B3LYP/cc–pVTZ and B3LYP/6–311++G** methods in order to find the whole characteristics of the molecular complex. The theoretical structural parameters such as bond length, bond angle and dihedral angle determined by DFT methods are well agreed with the XRD parameters. The atomic charges and thermodynamic properties are also calculated and analysed. The energies of frontier molecular orbitals HOMO, LUMO, HOMO–1, LUMO+1 and LUMO–HUMO energy gap are calculated to understand the kinetic stability and chemical reactivity