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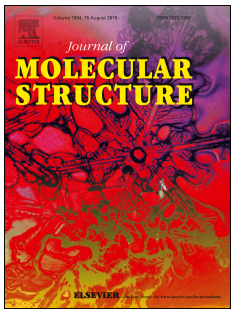

Structure, vibrations and quantum chemical investigations of hydrogen bonded complex of bis(1–hydroxy–2–methylpropan–2–aminium)selenate

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Structure, vibrations and quantum chemical investigations of hydrogen bonded complex of bis(1–hydroxy–2–methylpropan–2–aminium)selenate

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Abstract

The hydrogen bonded molecular complex bis(1–hydroxy–2–methylpropan–2–aminium)selenate ($C_8H_{24}N_2O_6Se$) has been prepared by the reaction of 2–amino–2–methyl propanol and selenic acid. The X–ray diffraction analysis revealed that the intermolecular proton transfer from selenic acid (SeO_4H_2) to 2–amino–2–methylpropanol results in the formation of bis(1–hydroxy–2–methylpropan–2–aminium)selenate (HMPAS) salt and the fragments are connected through H–bonding and ion pairing. The N–H···O and O–H···O interactions between 2–amino–2–methylpropanol and selenic acid determine the supramolecular arrangement in three–dimensional space. The salt crystalises in the space group P121/n1 of monoclinic system. The complete vibrational assignments of HMPAS have been performed by FTIR and FT–Raman spectroscopy. The experimental data are correlated with the structural properties namely the energy, thermodynamic parameters, atomic charges, hybridization concepts and vibrational frequencies determined by quantum chemical studies performed with B3LYP method using 6–311++G*, 6–31+G* and 6–31G** basis sets.