POLAR (ACYCLIC) ISOMER OF FORMIC ACID DIMER: RAMAN SPECTROSCOPY STUDY

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Formic (methanoic) acid spectral range of 575–1150 cm^{-1} has been studied by gas-phase Raman spectroscopy method. A weak Raman-active vibration of polar (acyclic) HCOOH dimer has been found at 864±2.1 cm^{-1} and assigned using quantum chemistry data. The temperature-dependence of intensity ratios of Raman lines was used to evaluate the thermodynamic parameters of polar dimer. Its experimental dimerization enthalpy ($\triangle$H) was found to be -8.6±0.2 kcal mol^{-1}. Entropy of dimerization has been evaluated using theoretical (MP2) Raman scattering activities. Its value ($\triangle$S) is estimated as -36±2 cal mol^{-1} K^{-1}. The results are compared with the published experimental data and calculations. The presented results can be used for molecular dynamics simulations, hydrogen bond energy estimation, and analysis of CH_2O_2 vapor density measurements.