EFFECT OF DENSITY AND TEMPERATURE ON THE INFRARED SPECTRA OF FLUID ETHENE BY MOLECULAR DYNAMICS SIMULATIONS

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A study of the influence of density and temperature on the dynamical behavior of ethene molecules in liquid and gas phases is performed by classical molecular dynamic simulation technique. The simulations were carried out for the density of the system in the range from 600 to 900 kg.m^{-3} and at 1.26 kg.m^{-3} in the gas phase at 123K and for the temperature in the range from 73K to 143K at 750 kg.m^{-3}. The analysis of the infrared spectra shows strong modifications upon the increasing of the density and no significant effect of the temperature. Firstly, going from gas to liquid phase, the change in rotational motion of the molecules modifies the shape of the infrared bands and secondly, the frequencies of the bands shift upwards while the pressure increases in the liquid phase.