Defects in high pressure rotator phase of n-tridecane, pentadecane and heptadecane: an FT-IR study

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The effect of pressure on phase transition behavior and defect populations of n-tridecane, pentadecane and heptadecane has been investigated by using Fourier transform infrared spectroscopy at 25°C. The transition between the high pressure ordered (HPO) and high pressure rotator (HPR) phase has been observed in the pressure ranges of 270–220, 106–95 and 152–181 MPa for C_{13}, C_{15} and C_{17}, respectively, and the transition between the HPR and liquid phase was observed in the pressure ranges of 171–112, 73–47 and 43–70 MPa for C_{13}, C_{15} and C_{17}, respectively. The populations of the -gtg- + -gtg’, -gg- and gt- defects determined from the methylene wagging mode are smaller in the HPR phase than in the liquid phase and are smaller under higher pressure in both of the HPR and liquid phases. A relationship has been found between the conformation and the intensity of the 890 cm\(^{-1}\) band, which has been assigned as the methyl rocking mode and has been considered as insensitive to conformation.