

Investigation of Liquid-Liquid Phase Transition for *Trans*-1,2 dichloroethylene

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A single component liquid, contrary to common belief, may have more than one kind of isotropic liquid state, and the transition between these states is called the liquid-liquid phase transition (LLPT). Evidence of such a transition in *trans*-1,2-dichloroethylene (TDCE) has already been reported by Kawanishi et al. [1, 2]. By applying the NMR technique they found that temperature dependences of spin-lattice relaxation times (T_1) exhibited a "jump" at -16 °C which indicated the presence of the liquid-liquid phase transition. Specific volume measurements showed a change in V-T curve at the singular point of -16 °C.

IR vibrational spectroscopy has been employed to study liquid-liquid phase transitions of *trans*-1,2-dichloroethylene (TDCE). Temperature dependence of the vibrational frequency, band absorbance and band broadening has been analyzed in the temperature range 293 K to 237 K. All peaks show distinct increases of their absorbancies at the temperature 246.7 K accompanied by frequency shift and bandwidth changes. Weak H...Cl hydrogen bonding is suggested as the explanation of the overall behavior in a wide temperature range, whereas the significant changes of the spectrum at 246.7 K are probably due to molecular ordering originating from electrostatic interactions. The transition is regarded as a nucleation growth-type and is well described by the model of the cooperative formation of locally favored structures.

The TDCE molecule is non polar itself therefore no dipolar distribution of charge is expected for dimers. However, for one configuration of dimers structure, the resultant dipole moments is about 0.25 D. Recent our measurements of the non-linear dielectric effect (NDE) for TDCE strongly support such a concept. They show a positive sign of the NDE signal that dramatically increases on approaching 247 K. This is most probably due to the increase of the local polarity of the system.

[1] S. Kawanishi, T. Sasuga, M. Takehisa, J. Phys. Soc. Jpn. 48 (1980) 1307.

[2] S. Kawanishi, T. Sasuga, M. Takehisa, J. Phys. Soc. Jpn. 50 (1981) 3080.