CLUSTERS IN THE "SIMPLE" AND "NORMAL" FLUIDS

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It has been proposed relation for estimating the structural features of molecular liquids according to their thermophysical properties.

$$T\left(\frac{\partial p}{\partial T}\right)_V = B_0\left(1 - \frac{< n > -4/3}{Z^*}\right)\rho^3 + \frac{1}{< n >}\frac{RT}{M}\rho$$

It is shown that the origin of the liquid phase is accompanied by the dimer association of molecules.

In "simple" monoatomic liquids, when the temperature decreases, the number of particles in the associates (clusters) increases that leads to the formation of a "nearest order" in the liquid. This process is confirmed by x-ray investigation and measuring of isochoric heat capacity of argon, krypton, etc.

On the contrary, in liquids with polyatomic molecules, excluding liquids with hydrogen bonds, only dimeric association is observed practically on the entire equilibrium liquid-vapor curve of up to the crystallization region.

The obtained results indicate that, as in liquid hydrocarbons in "simple" liquids, in addition to dispersion forces (m=6) and repulsion forces (n=12) exhibit themself the long-range weak chemical bonds of the "Coulomb" type causing association of particles The character of association was determined by the symmetry of the molecules.

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1. Hobza P., Muller-Dethlefs K. Non-covalent Interactions: Theory and Experiment. Cambridge: Royal Society of Chemistry, 2010.