

Specific Intermolecular Interactions of Pentacoordinated Carbon Atom and Hydrogen-Bonding in Liquid Alcohols of Acetylene Series and of Vitamin E Synthesis Components

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Acetylene alcohols are a remarkable example for the study of hydrogen-bonding and specific intermolecular interactions, for example the influence of C-C bond on the energy of a realized interaction in liquid state of these compounds. Although the acetylene alcohols $C_{15}H_{28}O$, $C_{20}H_{38}O$, isophitol ($C_{20}H_{40}O$) and dihydrolinalool ($C_{10}H_{16}O$ -3,7-dimethyloctaen-6-in-1-ol-3) are probably common examples of formation of hydrogen-bonding in compounds which have double and triple bonds of carbon atom and are very important compounds for practical purposes, their fundamental thermodynamic properties have not been determined

We conducted investigations of liquid-vapor equilibrium of saturated and unsaturated vapors of these compounds with high purity by a static method with a zero-manometer and calorimetric vaporization method, and established the monomer form of the molecule in the vapor phase and thermodynamic properties of the vaporization process, which are coordinated with thermodynamic characteristics of aliphatic series alcohols.

Practically invariable of the evaporation enthalpy of acetylene alcohols, isophitol are, firstly, a classical example of an absurdity of the existing principle that molecular mass is determined from the value of the vaporization enthalpy and, secondly, that these data do not depend on the number of CH_2 -groups, but are determined by the number and energy of realized specific intermolecular interactions and hydrogen-bonding.

In this lecture we use the novel approaches of structure-energetic analysis [1,2] of liquid alcohols, which established four bonding vacancies of their molecules which form two hydrogen-bonding and two specific intermolecular interactions with the participation of a pentacoordinated carbon atom of the functional CH_3 -group. This kind of specific intermolecular interaction is formed essentially by a non-divided $2s^2(c)$ -electron pair localized on a carbon atom of a methyl group [3,4] which takes part effectively at formation of the discussed type of specific interaction. We determined their energies and hydrogen-bonding in liquid aliphatic series alcohols and acetylene alcohols, and discuss their values and the regularities of their variation.

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- [4] A.K. Baev and D.V. Korolkov, *XVth FECHM Conference on Organometallic Chemistry*, University of Zurich, 2003, P. 350.