

Discrepancy between Model sp^3 -hybridization and Natural Chemical Interactions and the Chemistry of Liquid Non-electrolytes

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The discrepancy between the model sp^3 -hybridization and the electron configuration of carbon atoms, involving intramolecular and intermolecular interactions in organic and organometallic compounds has a phenomenological and fundamentally significant consequence for non-electrolyte solutions. Well founded conclusions about the dative bond $A \leftarrow CH_3$ in alkyl complexes [1] and the existence of an essential non-divided $2s2(c)$ -electron pair localized on the contacted carbon atom of the alkyl ligand with central atom (A) in the complex [2,3] opened a new perspective in the development of the theory of solutions. The same essential non-divided $2s2(c)$ -electron pair is responsible for intermolecular interactions with the participation of a penta-coordinated carbon atom which forms a dative mechanism. The experimentally determined effective intermolecular interactions in liquid alkyl complexes are mediated by the same pseudo-atomic $2s2(c)$ -electron pair. This exact electron pair takes part in the formation of intermolecular interactions which were not considered, specifically, in liquid functional solvents. That has been determined to be the integral value specific to intermolecular interactions regarded as hydrogen bonds. In this lecture, we substantiate different types of specific intermolecular interactions in liquid functional solvents with perspiration of all vacated groups, penta-coordinated carbon atoms and we discuss the methodology for the determination of their energy using thermodynamic properties. Different types of specific energies of intermolecular interactions and hydrogen bonds of liquid solvents including alcohols, ketones and ethers are considered. We will discuss the results of quantum-chemical calculations of the electron configuration of the alkyl complex, methane, and regularities of change in energies of hydrogen bonds in liquid solvents.

- [1] A.K. Baev, *Russian Journal Coordination Chemistry*. **22** (5), 399 (1996).
- [2] A.K. Baev and D.V. Korolkov, *Book of Abstracts. 14th International FEChem Conference. Zurich University*. P.350 (2003).
- [3] A.K. Baev, *Book of Abstracts. Sixth. International Symposium on Carbanion Chemistry. Germany. Marburg*. P.75 (2001).