

Contradiction: the Thermodynamic Properties of the Model sp^3 Hybridization and Unexplored Specific Intermolecular Interaction and Their Energies

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The thermodynamic investigation of phase equilibrium of alkyl compounds 2-6 groups elements substantiated the regular alteration of enthalpies of vaporization at the groups elements and with changing of number carbon atom in alkyl ligands, which can not be understood using the model sp^3 hybridization. The idea of dative bond in alkyl compounds between carbon atom and central atom $A \leftarrow CH_3$ of complex AR_k clarifies this low-governed nature [1]. In the lecture we discuss the influence of this kind of bond on the dissociation energy $A-R$ with growing number of carbon atoms in the ligand.

Quantum-chemical calculation of electron structure of complex AR_k by the Restricted Hartree-Fock method and the B3LYP method showed that this kind bond is consistent [2]. It was established that bonds in complex AR_k and CH_4 never have model sp^3 -hybridization, and dative bond $C(2e) \rightarrow A(0e)$ may be formed with participation of a vacant electron pair of carbon atoms $2s^2(c)$ localized on atom (C) in basic and from another hand localized on atom A. In the lecture we bring substantiations of this very important problem in organic chemistry. Availability existence essentially non divided $2s^2(c)$ -electron pair forms specific intermolecular interaction with participation of pentacoordinated carbon atom. We motivate new kinds of specific intermolecular interactions in liquid non-electrolytes of elementorganic compounds. We analyzed functional solvents, gave proof different types of specific intermolecular interactions in the liquid state, and using novel approaches determined their energies.

[1] A.K.Baev, *Russian Journal Coordination Chemistry*, **22** (5), 399 (1996).

[2] A.K.Baev, D.V.Korolkov, *Book of Abstract 14th International FEChem Conference*. Zurich University, P.350 2003.