Thermodynamic Phase and Chemical Equilibrium of Involved Systems Aluminum Alkyls and their Derivatives

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Investigation of liquid-vapor equilibrium and chemical process realized in vapor phase in system of alkyl compounds and their derivatives were conduced in a wide interval of temperature and, pressure in saturated and unsaturated vapor. The results illustrate the possibility of a static method with zero-manometer to study complicated systems. Discussed are thermodynamic properties of evaporation, dimerization process, dissociation in vapor phase with formation C_4H_{2n}, temperatures of stable existence, decomposition process and its mechanism of alkyl compounds and their derivatives. Investigation of unsaturated vapor showed that $Al(CH_3)_3$(100), $Al(C_2H_5)_3$.(60), $Al(n\text{-}C_3H_7)_3$(~3%), $Al_2O(CH_3)_4$, $Al_2O(C_2H_5)_4$, $AlH(C_2H_5)_2$ form dimers in the vapor phase. We determined partial pressures and calculated thermodynamic properties. In the lecture we discuss thermodynamic properties of different process and reactions:

$$AR_3 = AlHR_2 + 0.5C_2H_{2n}$$
$$R_2Al\text{-}O\text{-}AlR_2 = RHAl\text{-}O\text{-}AlHR + C_2H_{2n}$$
$$R_2Al(OR_2) = RHAl(OR_2) + 0.5C_2H_{2n}$$

Thermodynamic properties showed that presence of an oxygen bond Al-O-Al in alumoxane lower the energy of the Al-C_2H_5-Al dimerization process. The regularities in the change of thermodynamic properties lead to dative (reverse) bond Al←C or A←C [1] in complex AR_k. In the lecture we present results of quantum chemical calculations of electron configuration in complex AR_k and substantiate that this kind of bond really exists. We discuss specific intermolecular interactions realized in liquid alkyl compounds. This kind of bond formed by essential non-divided $2s^2$(c) -electron pair of carbon atom localized on central atom (A) of complex AR_k [2] is basic. Only two electrons from four valence electrons of carbon atom form four bonds (one C - A and three C – H) for expanse the same electrons on three valence AO 2px, 2py and 2pz. Using thermodynamic properties we determined energy specific intermolecular interactions.

[1] A.K. Baev, *Russian Journal Coordination Chemistry* **22** (5), 399 (1996).
[2] A.K.Baev and D.V. Korolkov, *Book of Abstract, 14th International FECHEM Conference*, Zurich University, 2003, P. 350.