LOW TEMPERATURE IR SPECTROSCOPIC AND THEORETICAL STUDY OF UNSTABLE COMPLEXES BETWEEN ACYLHALIDES AND ALUMINUM HALIDES - INTERMEDIATES OF C-H BOND ACTIVATION IN ALKANES

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The system aluminum halide - acylhalide is used for alkane activation under mild condition. The method of low temperature IR spectroscopy was used in order to understand the mechanism of this activation The interaction of dimeric aluminum chloride or bromide with acylhalides was studied using successive condensation of the components at 77 K on a cold support in a specially designed low temperature IR cell. The obtained film was gradually warmed directly in the spectrometer; the processes were monitored by IR spectra. Several types of unstable complexes between aluminum halides and acylhalides were fixed, which finally transformed to a stable complex where the aluminum atom is bound to the oxygen atom of acylhalides. Upon further temperature increase the halide atom transfers to aluminum halide to give acylium ion. The structure of complexes will be discussed on the basis of DFT calculation and comparison of the experimental data to the results of calculations.