Thematic course: Kinetics and mechanism of acyl transfer reactions. Part IV.

Quantum chemical simulation of the mechanism of benzoyl chloride and benzenesulphonyl chloride interactions with amino compounds of different classes

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Abstract

Potential energy surfaces are calculated for reactions of ammonia and a number of amino compounds with benzoyl chloride and benzenesulfonyl chloride in gas phase, as well as for ammonia interaction with benzoyl chloride in water by using the polarized continuum model. It is shown that all the reactions proceed by the concerted mechanism, and benzoylation occurs by the pathway with frontal nucleophilic attack, whereas arensulfonylation – by the pathway with varying attack angle. Non-specific solvation by water decreases activation energy of ammonia acylation as compared to gas phase reaction.