

Donor-acceptor and acid-base properties of complexes with hydrogen bonds and their participation in chemical reactions

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Abstract

Many chemical compounds are capable of forming homo- and heterocomplexes with hydrogen bonds (alcohols, amines, phenols, etc.) that are capable of acting as reagents. There are a number of data that indicate that complexes with hydrogen bonds are more active in chemical reactions than monomers. The reasons for this phenomenon, as a rule, remain unknown.

In this paper, based on the analysis of literature and own data obtained by quantum chemical calculations, it has been shown that complexes with hydrogen bonds have enhanced donor-acceptor and acid-base properties in comparison with monomers. This circumstance is the reason for the increased reactivity of complexes with hydrogen bonds. This leads to the fact that many transformations, which have traditionally been referred to as simple, prove to be complex, multichannel.

Each of these directions is characterized by its structures of pre- and postreaction complexes, transition states, thermodynamic parameters of activation and reactions.

Reactions involving complexes with hydrogen bonds can be regarded as autocatalytic. The complexes formed in the first stage of interaction from monomeric molecules react. During the transformation, a complex with a lower degree of association is formed, which, with the new molecules of monomers, forms a new associate with increased reactivity.

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