MULTIPLE NONCOVALENT BONDING IN HALOGEN COMPLEXES WITH OXYGEN TERTIARY AMIDES

Burakov N. I., Kanibolotsky A. L.

L. M. Litvinenko Institute of Physical Organic and Coal Chemistry NAS of Ukraine

n_burakov@ukr.net

The present work describes the structure and binding of adducts of N,N′-diacetylpiperazine with halogens and interhalogens based on combination of different experimental methods and quantum chemical calculations. On the basis of conductometric and spectro-photometric experimental results, behavior of complexes in the acetonitrile solution was described.

Fig. Formation of DAP···halogen adduct via simultaneous via C=O···I and C−H···I interactions

The iodine adduct with N,N′-diacetylpiperazine fully degrades into components. Adducts of interhalogens I−X (X = Cl or Br) with N,N′-diacetylpiperazine in acetonitrile partially dissociate to anionic [X−I−X]− and cationic species. In the solid state, molecules are connected via C=O···I, C−H···I, and Cl···Cl (or Br···Br) attractive interactions. N,N′-diacetylpiperazine···dihalogen complex is stabilized by simultaneous C=O···I and C−H···I interactions. Such binding mode allows to explain the problems of the direct halogenation of acetyl-containing compounds with molecular halogens as reagents. We believe that the observed binding pattern can be used as prototypical for future design of halogeno complexes.