

MULTIPLE NONCOVALENT BONDING IN HALOGEN COMPLEXES WITH OXYGEN TERTIARY AMIDES

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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.

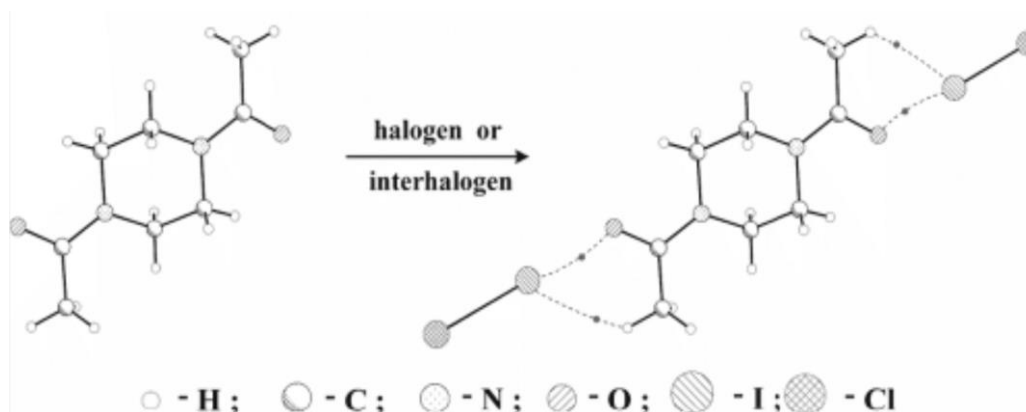


Fig. Formation of DAP...halogen adduct via simultaneous via C=O...I and C-H...I interactions

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.