



On the nature of bonding in HCOOH...Ar and HCOOH...Kr complexes.

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Streszczenie

The chemical interaction in HCOOH...Ng (Ng=Ar, Kr) complex was analyzed by topological analysis of the electron density based on Atoms-In-Molecules theory. For all computationally stable equilibrium structures of 1:1 HCOOH...Ng complexes, an intermolecular bond path with a "bond" critical point was found and perturbation of formic acid (FA) atomic basins and electron density was observed. The intermolecular interaction between the two complex subunits can be classified, according to its nature, as a closed-shell van der Waals type of interaction. However, one of the computed structures (complex II), pictures a noble gas atom attached linearly to the acidic O-H tail of FA. In this particular case, the electron density at the intermolecular bond critical point was found to resemble a hydrogen-bonded system and thus, may be termed a hydrogen-bond-like interaction. This change in the nature of the interaction is also shown by large perturbations of the FA properties found for this complex structure. The structural and vibrational perturbations are larger than for the other three structures and they increase for the Kr complexes compared to the Ar complex.

Słowa kluczowe

Complex, Computational chemistry, Electron density, Formic acid, Noble gas

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