



Interaction energy decomposition analysis for formic acid complexes with argon and krypton atoms.

Autorzy

Jarosław J. Panek

Piotr Kornel Wawrzyniak

Zdzisław Latajka

Jan Lundell

Rok wydania

2006

Czasopismo

Chemical Physics Letters

Numer woluminu

417

Strony

100-104

DOI

10.1016/j.cplett.2005.09.129

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Interaction energy decomposition was performed for a series of HCOOH...Rg complexes, where Rg is either argon or krypton, and the formic acid molecule has trans or cis conformation. The decomposition, performed within Symmetry-Adapted Perturbation Theory framework, shows that even if the stability of the complexes is due to significant dispersion contribution, the role of induction and exchange should not be neglected. One of the complexes, which is the lowest energy minimum found, is a 'hydrogen bond-like' structure which, with respect to other complexes, exhibits visible changes in the relations between the interaction energy terms, particularly - much more pronounced induction contribution.

Adres publiczny

<http://dx.doi.org/10.1016/j.cplett.2005.09.129>

Strona internetowa wydawcy

<http://www.elsevier.com>