OPTICA APPLICATA online
open access
A quarterly of the Institute of Physics, Wroclaw University of Technology
Wroclaw University of Technology
INSTITUTE OF PHYSICS

Optica Applicata 2006(Vol.36), No.4, pp. 587-591

Ab initio study of formic acid monomer, dimer and trimer

Leszek ZIEMCZONEK, Tomasz WROBLEWSKI, Grzegorz P. KARWASZ

Keywords

formic acid, clusters, electron affinity

Abstract

Configurations of the formic acid monomer, dimer and trimer are presented. The total energies for these structures have been calculated while the negatively charged clusters were considered and the possible pathways of interaction of low energy electrons with monomers and clusters were discussed. Calculations have been executed using 6–311*G*** and 6–311++*G*** basis sets. The electron affinities of monomer and clusters are presented. Influence of choice of the molecular basis set is also discussed. Only such systematic studies allow to explain values observed experimentally, for example, in electron attachment experiments on formic acid (Martin I. *et al*., Phys. Chem. Chem. Phys. 7(10), 2005, p. 2212).

644.8 kB