

Quantum chemical study of the bimolecular complex of HONO.

Autorzy

Robert Wieczorek

Zdzisław Latajka

Jan Lundell

Rok wydania

1999

Czasopismo

Journal of Physical Chemistry
A

Numer woluminu

103

Strony

6234-6239

DOI

10.1021/jp990610p

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Structures, energetics, and vibrational properties for the bimolecular complex of HONO have been studied by ab initio methods. Ten stable complexes of (HONO)₂ were found. Four of the complexes are formed between two *trans* isomers, three between two *cis* isomers, and three complexes are found between one *trans* and one *cis* isomer. All complexes involve a hydrogen bond from the OH tail of one of the subunits. The calculated interactions energies at the MP2/6-311++G(2d,2p) level vary between -10 and -20 kJ mol⁻¹ representing a relatively strong interaction. The structural properties of the subunits were found strongly perturbed upon complexation, and the vibrational spectra of the various (HONO)₂ complexes are predicted to show large vibrational shifts compared with the monomer spectra.

Słowa kluczowe

Energy, Interaction energies, Monomers, Noncovalent interactions, Oxygen

Adres publiczny

<https://doi.org/10.1021/jp990610p>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>