

Evolution of IR spectra of a weakly-bound $\text{OCO}\cdots\text{HCl}$ complex with increasing CO_2 density from the gas to liquid phase.

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Rok wydania

2001

Czasopismo

Journal of Molecular
Structure

Numer woluminu

598

Strony

205-211

DOI

10.1016/S0022-
2860(01)00634-2

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The IR spectra of HCl/CO_2 mixtures have been measured at CO_2 densities increasing from the gas to liquid phase at The spectroscopic data show a weakly bound $\text{OCO}\cdots\text{HCl}$ complex formation in the mixtures. The fundamental $\nu_{\text{c}}(\text{HCl})$ and first overtone $2\nu_{\text{c}}(\text{HCl})$ bands of the complex and the combination bands, originated from simultaneous excitation of the HCl and CO_2 subunits were studied. The spectral characteristics (frequencies, widths and intensities) of all the bands of the complex have been determined. Ab initio calculations utilizing the 6-311++G(3df,3pd) basis set with electron correlation at the MP2 level of approximation predict a potential energy minimum of $\sim 6.3 \text{ kJ mol}^{-1}$ for the H-bonded $\text{OCO}\cdots\text{HCl}$ linear structure and give reasonable values of red shift for the HCl fundamental frequency and of blue shift for the CO_2 fundamental asymmetric stretch frequency relative to free HCl and CO_2 molecules, respectively. The results obtained suggest anharmonic coupling between the stretching $\nu_{\text{c}}(\text{HCl})$ and high frequency bending $\nu_{\text{B}}(\text{ClH}\cdots\text{OCO})$ modes of the complex.

Słowa kluczowe

Complex, Hydrogen bond, HCl , CO_2 , Liquid phase, IR spectra

Adres publiczny

[https://doi.org/10.1016/S0022-2860\(01\)00634-2](https://doi.org/10.1016/S0022-2860(01)00634-2)

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-08-26 03:14:40

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/9Q2Yw_f.