



Magdalena Sałdyka, Zofia Mielke, Karolina Haupa

PII: S1386-1425(17)30773-4
 DOI: doi: [10.1016/j.saa.2017.09.046](https://doi.org/10.1016/j.saa.2017.09.046)
 Reference: SAA 15480

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 24 June 2017
Revised date: 14 September 2017
Accepted date: 16 September 2017

Please cite this article as: Magdalena Sałdyka, Zofia Mielke, Karolina Haupa , Structural and spectroscopic characterization of DMF complexes with nitrogen, carbon dioxide, ammonia and water. Infrared matrix isolation and theoretical studies, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2017), doi: [10.1016/j.saa.2017.09.046](https://doi.org/10.1016/j.saa.2017.09.046)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Structural and spectroscopic characterization of DMF complexes with nitrogen, carbon dioxide, ammonia and water. Infrared matrix isolation and theoretical studies

Magdalena Saldyka*, Zofia Mielke, Karolina Haupa

Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland

Abstract

An infrared spectroscopic and MP2/6-311++G(2d,2p) study of the complexes between *N,N*-dimethylformamide (DMF) and nitrogen, carbon dioxide, water, ammonia trapped in solid argon matrices is reported. The 1:1 molecular complexes have been identified in the DMF/B/Ar matrices (B = N₂, CO, H₂O, NH₃); their structures were determined by comparison of the spectra with the results of calculations. The analysis of the experimental and theoretical data indicate that the DMF-N₂, CO complexes present in the matrices are stabilized by (C=)O...N and (C=)O...C van der Waals interactions. In turn, in the DMF-H₂O, NH₃ complexes the (C=)O...H(OH) and (C=)O...H(NH₂) hydrogen bonding is present in which the carbonyl group of DMF acts as a proton acceptor. In all systems studied the C-H...X (X = N, C, O) bonding is a second intermolecular force stabilizing the planar complexes. Some spectral features indicate that for DMF-H₂O, DMF-NH₃ systems the nonplanar structures with the C=O...H interaction are also present. The study demonstrated the strong sensitivity of the CH stretching wavenumber to an involvement of the C-H and/or C=O groups of DMF in an intermolecular interaction.

Keywords: *N,N*-dimethylformamide; hydrogen bond; van der Waals interaction; matrix isolation; *ab initio* calculations; molecular complexes

*Corresponding author

E-mail: magdalena.saldyka@chem.uni.wroc.pl

Download English Version:

<https://daneshyari.com/en/article/5139346>

Download Persian Version:

<https://daneshyari.com/article/5139346>

[Daneshyari.com](https://daneshyari.com)