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

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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 = N_2, CO, H_2O, NH_3); 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-N_2, 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-H_2O, NH_3 complexes the (C=)O···H(OH) and (C=)O···H(NH_2) 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-H_2O, DMF-NH_3 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

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