The complexes between CH_3OH and CF_4. Infrared matrix isolation and theoretical studies.

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Streszczenie

The complex formed between methanol and tetrafluoromethane has been identified in argon and neon matrixes by help of FTIR spectroscopy. Three fundamentals (ν(OH), ν(FCF), and ν(CO)) were observed for the complex isolated in the two matrixes, and the OH stretch was red shifted in a neon matrix and blue shifted in an argon matrix with respect to the corresponding vibration of the methanol monomer. The theoretical studies of the structure and spectral characteristics of the complexes formed between CH_3OH and CF_4 were carried out at the MP2 level of theory with the 6-311+G(2df,2pd) basis set. The calculations resulted in three stationary points from which two (I-1, I-2) corresponded to structures involving the O−H···F hydrogen bond and the third one (I-3) to the non-hydrogen-bonded structure. The topological analysis of the distribution of the charge density (AIM theory) confirmed the existence of the hydrogen bond in I-1, I-2 complexes and indicated weak interaction between the oxygen atom of CH_3OH and three fluorine atoms of CF_4 in the I-3 complex. The comparison of the experimental and theoretical data suggests that in the matrixes only the non-hydrogen-bonded complex I-3 is trapped. The blue/red shift of the complex OH stretching vibration with respect to the corresponding vibration of CH_3OH in argon/neon matrixes is explained by the different sensitivity of the complex and monomer vibrations to matrix material. The ab initio calculations performed for the ternary $CH_3OH{-}CF_4{-}Ar$ systems indicated a negligible effect of an argon atom on the binary complex frequencies.

Słowa kluczowe

Alcohols, Monomers, Oscillation, Chemical structure, Noncovalent interactions