Matrix-isolated hydrogen-bonded and Van der Waals complexes of hydrogen peroxide with OCS and CS_2.

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Streszczenie

Matrix isolation spectroscopy has been combined with ab initio calculations to characterize the 1:1 complexes of H_2O_2 with OCS and CS_2. The infrared spectra of the argon and nitrogen matrices doped with H_2O_2 and OCS or CS_2 have been measured and analyzed. The geometries of the complexes were optimized at the MP2/6-311++G(3df,3pd) level of theory. Four structures were found for the OCS-H_2O_2 complex and five for the CS_2-H_2O_2 one; every pair of the corresponding structures showed close correspondence. For every optimized structure the interaction energy was partitioned according to the SAPT Scheme and the topological distribution of the charge density (AIM theory) was performed. The SAPT analysis and AIM results indicate that only one complex among the nine optimized ones is stabilized by the hydrogen bonding, namely the OCS-H_2O_2 one with the OH group of H_2O_2 bonded to an oxygen atom of OCS. The other structures are stabilized by van der Waals interaction. The spectra analysis evidences that at least two types of the complexes are trapped in the argon matrices including the most stable ones: hydrogen bonded structure in the case of the OCS-H_2O_2 complex and the structure stabilized by the S⋯H and C⋯O interactions in the case of the CS_2-H_2O_2 complex. The solid nitrogen environment triggers the formation of the structures of C_{2v} symmetry with a sulfur atom of OCS or CS_2 directed toward the center of O□O bond of H_2O_2, stabilized by S⋯O interactions.

Słowa kluczowe

hydrogen bonding, infrared spectroscopy, Matrix isolation

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