

## Matrix-isolated hydrogen-bonded and Van der Waals complexes of hydrogen peroxide with OCS and CS<sub>2</sub>.

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### Streszczenie

Matrix isolation spectroscopy has been combined with ab initio calculations to characterize the 1:1 complexes of H<sub>2</sub>O<sub>2</sub> with OCS and CS<sub>2</sub>. The infrared spectra of the argon and nitrogen matrices doped with H<sub>2</sub>O<sub>2</sub> and OCS or CS<sub>2</sub> 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<sub>2</sub>O<sub>2</sub> complex and five for the CS<sub>2</sub>-H<sub>2</sub>O<sub>2</sub> 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<sub>2</sub>O<sub>2</sub> one with the OH group of H<sub>2</sub>O<sub>2</sub> 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<sub>2</sub>O<sub>2</sub> complex and the structure stabilized by the S⋯H and C⋯O interactions in the case of the CS<sub>2</sub>-H<sub>2</sub>O<sub>2</sub> complex. The solid nitrogen environment triggers the formation of the structures of C<sub>2v</sub> symmetry with a sulfur atom of OCS or CS<sub>2</sub> directed toward the center of O-O bond of H<sub>2</sub>O<sub>2</sub>, stabilized by S⋯O interactions.

### Słowa kluczowe

hydrogen bonding, infrared spectroscopy, Matrix isolation

### Adres publiczny

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### Strona internetowa wydawcy

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