

Hydrogen bonding in coordination compounds containing homoconjugated bis-dimethylsulfoxide cation. Ab initio and IR studies.

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DFT calculations of vibrational spectra and structural parameters of dimethylsulfoxide (DMSO) molecule, its hydrogen bonded complex with HCl, mono- and bis-dimethylsulfoxide cations DMSOH^+ and DMSOHOSDM^+ have been performed at B3LYP/6-31G** level. The results obtained for free DMSO and DMSO+HCl complex are in good agreement with the known experimental data. For free homoconjugated cation $(\text{DMSOHOSDM})^+$, an extremely short and a practically linear hydrogen bond with nearly central position of the bridging proton have been found. The addition of a counterion leads to lengthening and bending of the hydrogen bond. A solid $[(\text{DMSO})_2\text{H}]_2[\text{PtCl}_6]$ compound has been synthesized and the IR spectrum of this salt has been investigated. The structural parameters and vibrational frequencies calculated for $[(\text{DMSO})_2\text{H}]^+\text{X}^-$ complexes were found to be in good agreement with experimental X-rays and IR data for solid $[(\text{DMSO})_2\text{H}]_2[\text{PtCl}_6]$. The most important feature of vibrational spectrum of homoconjugated bis-dimethylsulfoxide cation is the essential involvement of proton stretching and bending coordinates in different normal modes, resulting in mixing of proton vibrations with vibrations of sulfoxide moiety, particularly with νSO , νCS , δCH .

Słowa kluczowe

Hydrogen bond, Homoconjugated cation, Vibrational spectrum, Dimethylsulfoxide

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