TORSIONAL VIBRATIONS IN THE HOSOH MOLECULE

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HOSOH belongs to the interesting group of molecules which is specified by the HXYXH formula, where Y and X are allowed to be identical. Recently we analyzed symmetry properties and the torsional spectra of the $HOCH_2OH$ [1] and HOOOH [2] molecules that belong to that group. Calculation technics of the data preparation, numerical solution of the vibrational Schrödinger equation, using DVR and Fourier methods in the case of very small splitting of the lowest torsional states due to tunneling, was discuss [2]. It was found that tunneling frequencies in the ground state of the $HOCH_2OH$ and HOOOH: of the order of 10^{-6} cm^{-1} and 10^{-10} cm^{-1}, respectively. As in the case of hydrogen peroxide molecule, it is very interesting how substitution of the oxygen atoms for the sulfur ones in the HOOOH molecule effects the height of the potential barriers and the values of the splitting of the torsional states. For example, possibility to detect the parity violation effect in HSSSH molecule [3]. 2D PES of the HOSOH molecule was calculated at the MP2/cc-pVQZ level of theory. The energies of the stationary torsional states were found by numerical solution of the vibrational Schrödinger equation. It was found that the tunneling frequency in the ground state of the HOSOH molecule is order of 10^{-11} cm^{-1}. Differences in the potential barriers of the $HOCH_2OH$, HOOOH and HOSOH molecules were discussed.

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[3] C. Fabri, L. Horny, M. Quiack, ChemPhysChem 16 (2015) 3584-3589