

# GROUP-THEORETICAL ANALYSIS OF THE TORSIONAL VIBRATIONS IN NON-RIGID MOLECULES HXYXH TYPE

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Here we present a very interesting group of molecules whose structure can be described by following general formula HXYXH. Different molecules appear if we connect in different combinations X=O, S, Se and Y=CH<sub>2</sub>, O, S, Se. Recently torsional spectra of the HOCH<sub>2</sub>OH and HOOOH molecules were studied [1,2]. All of these molecules have common structural properties. They all have two equivalent internal tops (hydroxyl groups) and have two stable conformations (trans- and cis-). Usually, the first conformer is energetically preferable than the second. Both conformers can exist in two configurationally-equivalent states as it is shown in Fig.1 for the HSSSH molecule.

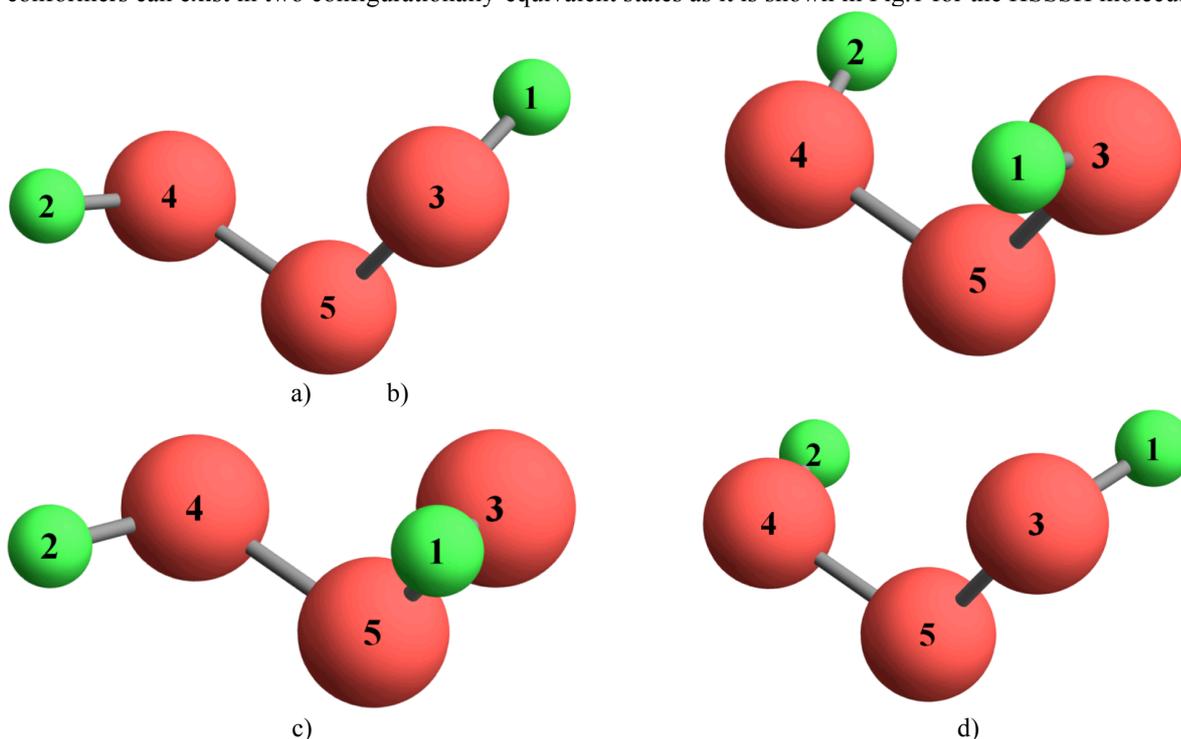


Fig. 1. Trans- (a, b) and cis- (c, d) conformers of the HSSSH molecule.

As we are dealing with non-rigid molecules to classify torsional states we have to use molecular symmetry groups. Even though different molecules from the analyzed group have different symmetry elements, all molecules belong to  $C_{2v}(M)$  molecular symmetry group which is isomorph to  $C_{2v}$  point symmetry group. It means that all torsional states of any molecule from HXYXH group belong to one of  $A_1$ ,  $A_2$ ,  $B_1$ ,  $B_2$  symmetry species. It is obvious if we consider trans- and cis-conformers of any molecule like a rigid object, their configurations will belong to  $C_2$  and  $C_s$  point groups respectively. It is interesting and important to find the correlation between irreducible representations of  $C_2$ ,  $C_s$  point symmetry groups and  $C_{2v}(M)$  molecular symmetry group. The performed analysis has showed that A and B irreducible representations of  $C_2$  point group split into  $A_1$ ,  $A_2$  and  $B_1$ ,  $B_2$  irreducible representations of the  $C_{2v}(M)$  molecular symmetry group respectively, while  $A'$  and  $A''$  irreducible representations of  $C_s$  point group split into  $A_1$ ,  $B_2$  and  $A_2$ ,  $B_1$  irreducible representations of  $C_{2v}(M)$  molecular symmetry group respectively. In addition, symmetry properties of the 2D PES, 2D dipole momentum components, 2D kinematic coefficients and torsional coordinates were analyzed too and will be discussed.

[1] G.A. Pitsevich, A.Ye. Malevich, V.V. Sapeshko, J.Mol.Spectr., 360 (2019) 31-38

[2] G.A. Pitsevich, A.E. Malevich, U.U. Sapeshka, Chem.Phys., 530 (2020) 110633.