

## IS IT POSSIBLE TO IMPROVE THEORETICAL PREDICTION OF THE FREQUENCIES OF THE TORSIONAL VIBRATIONS BY ACCOUNTING ZPVE? TESTING MOST SIMPLE MOLECULES

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Torsional vibrations and internal rotation are the one kind of large amplitude motion in polyatomic molecules and clusters. It is well known that the standard approach within the frame of harmonic approximation to calculating the frequencies of torsional vibrations is unworkable. In this case, one must calculate full potential energy surface (PES) while varying torsional coordinates throughout all intervals of their determination. Recently, when calculating PES, some authors took into account zero-point vibrational energy (ZPVE). Sometimes it leads to an improvement in the agreement between calculated and experimental data, and sometimes it rather worsens the agreement between them [1,2]. To obtain more complete information on the efficiency of taking into account ZPVE, we have made a calculation of energy of stationary torsional states for hydrogen peroxide and methyl alcohol molecules with and without taking into account ZPVE. It is well known that there is much more experimental data about the energy of excited torsional states for these molecules than for any others. The calculations were performed on several levels of theory.

[1] S. Dalbouha, M.L. Senent, N. Komiha *J.Chem.Phys.*, 142(7) 2015 074304.

[2] G.A. Pitsevich, A.E. Malevich, U.V. Lazicki, U.U. Sapeshka *Journal of the Belarusian State University. Physics.* 2021 15.