

## HYDROXYL GROUPS TORSIONAL MOTION IN CATECHOL MOLECULE.

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Catechol molecule  $C_6H_4(OH)_2$  is the representative of a separate class of aromatic hydrocarbons. It is an important component of biochemical, industrial and commercial products. In a recently published article [1] rotationally resolved Fourier Transform far-infrared spectrum of the free and bonded  $O - H$  groups forming the intramolecular hydrogen bond was recorded. The authors were also able to measure pure rotational spectrum in the 70–220 GHz frequency range using a millimeter-wave spectrometer. Splitting due to tunneling was resolved for free  $O - H$  torsional state. Having this solid experimental background, we have performed extensive calculations of the kinetic parameters and 2D potential energy surfaces formed by variation of the  $O - H$  torsional coordinates of the catechol molecule at few levels of theory. It was found that almost all used levels of theory very well predict the frequency value of the fundamental torsional vibration of the free hydroxyl group: 224–227  $cm^{-1}$ , while experimental value is 221.9  $cm^{-1}$ . At the same time calculated frequencies of the  $H$ -bonded hydroxyl group torsional fundamental vibration is higher (422–425  $cm^{-1}$ ) than experimental one (415  $cm^{-1}$ ). We associate this difference with overestimating intramolecular  $H$ -bond energy in the frame of used levels of theory. It is also worth noting that there was a good agreement between calculated and experimental tunneling splitting of the first excited torsional state of free  $O - H$  group ( $3.6 \times 10^{-6}$  and  $1 \times 10^{-5}$  respectively). Besides, complete information about the second conformer of the catechol molecule with  $C_{2V}$  symmetry has been obtained.

[1] J. Bruckhuisen and etc, *Molecules* 26 (2021) 3645