MP2 STUDY OF THREE TOP INTERNAL ROTATIONS IN $B(OH)_3$ MOLECULE.

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Boric acid $B(OH)_3$, as a boron containing molecule, is of interest due to being essential micronutrient for a plant growth. In addition, it is a molecule containing three equivalent internal tops which are hydroxyl groups. As a rigid object, this molecule belongs to $C_{3H}$ point group, but due to internal rotation $B(OH)_3$ is actually a non-rigid molecule. Therefore, belongs to $D_{3H}(M)$ molecular symmetry group. High symmetry of this molecule lets us reduce the volume in 3D($\gamma_1$, $\gamma_2$, $\gamma_3$) phase space (here $\gamma_i$ is a torsional coordinate for $i$-hydroxyl group) in which potential energy and kinematic coefficients have been calculated. Then the entire 3D($\gamma_1$, $\gamma_2$, $\gamma_3$) phase space was filled by using symmetry operations. All calculations were performed at the MP2/cc-pVQZ level of theory. The calculated 2D PES projections on $\gamma_2$, $\gamma_3$ plane of the boric acid molecule are shown in Fig. 1. One can observe that for the $\gamma_1 = 0^\circ$ global minimum located near $\gamma_2 = \gamma_3 = 0^\circ$ while for $\gamma_1 = 180^\circ$ global minimum appears near $\gamma_2 = \gamma_3 = 180^\circ$. The values of the energies of the stationary torsional states were calculated too.

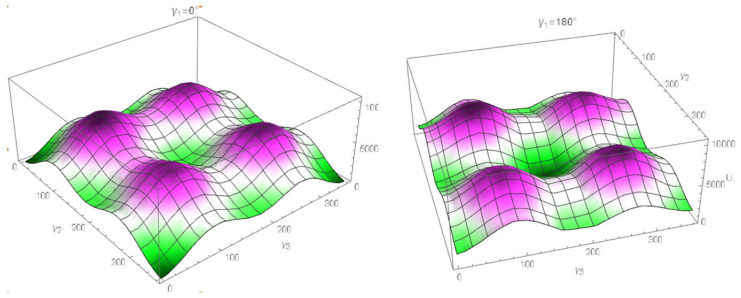


Fig. 1 Calculated at MP2/cc-pVQZ level of theory 2D PES for $\gamma_1 = 0^\circ$ on the left and $\gamma_1 = 180^\circ$ on the right.