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The Study of dissolution Boric acid in different temperature conditions, the DFT method

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ABSTRACT

In this article, the dissolution of Boric acid in different temperature conditions, with density functional theory (DFT) is studied. the Boric acid with chemical formula H_3BO_3 (sometimes written $B(OH)_3$), and exists in the form of colorless crystals or a white powder that dissolves in water and produces Tetra hydroxy borate with the chemical formula $[B(OH)_4]^-$ in different conditions of temperature, with density functional theory method were studied. For this purpose, at first the material contained in the both sides of reaction were geometrically optimized, and then the calculation of the thermodynamic parameters performed on all of them. The amount of ΔH, ΔS and ΔG of this reaction at different temperatures in form of sum of parameters discrepancy in the products than reactants is obtained. And finally, the best temperature for the synthesis of explosive according to the obtained thermodynamic parameters were evaluated.

Keywords: Boric acid, dissolves, Tetra hydroxyl borate, Density Functional Theory.