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Original Research Article

The Study of Dissolution Boric Acid in Different Temperatures: A DFT study

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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.

Introduction

Boron is Metalloid and semiconductor. It can be sorted in to non –metals, chemically. The boron chemistry is different from other members of 3rd Group and is mostly similar to silicon. $B(OH)_3$, cos an example, is specifically acidic and doesn't have amphoteric attribute while $Al(OH)_3$ is a base. Boron Hybrids are volatile and enflame spontaneously [1-11].

Boron halides except BF_3 an easily hydro listed. In Boric acid, the B $(OH)_3$ units as connected through hydric links, forming unlimited sheets or layers which have Hexagon metallic symmetry. The layer distances as 3/18 angstrom and this explains the simplicity of crystal delamination [12-23].

Boric acid is used as disinfection. Boric acid is an important combination used in fabric productions. The boric iodine existing in count oil causes extreme fizzy attribute in abundance co count oil [23-25].

Boric Acid and borax as also used can sub meter, in metal welding. In order to elute the eyes, the lotion at Boric Acid and water is the best in BX_3 combinations, Boron Atoms octagonal structure doesn't complete due to a sense of law energy orbital in the link and lack of electron [26-28].

In addition to that, Boron atoms can't make BBr_4^- and Bcl_4 combinations will big atoms such cons cl and Br because of its it is Small size.

But since F is small, the BF_4 is entirely stable. In this way, a dative band is formal between Boron and F^- ion and in this link; Boron gets to sp^3 approximate hybridization.

In this study, $B(OH)_3$ Boric Acid dissolution process in water result to $B(OH)_4^-$ and hydronium ion and have been studied in range of 300-500 kelvin degree in density function theory [29-35].

Boric Acid mostly dissolves in water and its dissolvability increases by increasing temperature. This acid is single bas and weak and not only does not work as proton donator but also as acid Lewis (hydroxide ion receiver)

$$B(OH)_3 + 2H_2O \leftrightarrow B(OH)_4^- + H_3O^+ (aq)$$

$$(K = 7.3x10^{-10};\ pK = 9.14)$$

Table (1). Some chemical properties calculated at level B3lyp/6-31g for B $(OH)_4^-$ and B $(OH)_3$

	Temperature=298.15K , pressure=1 atm	
	reactant	Product
	$B(OH)3$	$B(OH)4^-$
ENERGY	-249.8094 au	-324.8425 au
E HOMO	-13.16	-5.53 eV
E LUMO	6.84 eV	-13.07 ev
Dipole Moment	0 debye	0 debye
weight	61.832 amu	78.839 amu
volume	55.76 A^3	65.95 A^3
Area	79.37 A^2	92.35 A^2
POLARIZABILITY	41.25	42.39
ZPE	133.52 KJ/mol	167.63 KJ/mol
H°	-249.7533 au	-324.771655 au
CV	61.26 J/mol	90.18 J/mol
S°	268.99 J/mol	307.65 J/mol
G°	-249.7839 au	-324.8066 au

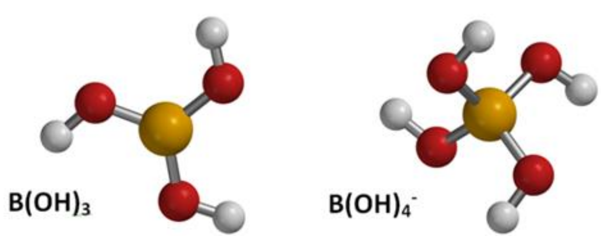

Fig1: pictures B $(OH)_4^-$ and B $(OH)_3$ calculated in B3lyp/6-31g computation ad results

Calculation and Results

The calculative study of Boric acid desolation process in water which its Production is B $(OH)_4^-$ and hydronium ion in 300-500 kelvin range has been Study in density functional theory. This study has been done by Gaussian application 98. The primary combination in density functional theory in basic series (6-31g) has been optimized then IR studies have been done in order to compute thermodynamic parameters regarding couriered process. All calculations have been done in B3lyp/6-31g level and the temperature at 300-500 kelvin degree and are atmosphere pressure. The following is the considered reaction:

$$B(OH)_3 + H_2O \rightarrow B(OH)_4^- + H_3O^+$$

Computation and examination of amount at enthalpy changes (ΔH)

By using the Gaussian application 98 the amounts of enthalpy for raw material and productions in synthesis process have been computed. The following (1) is used in order to compute the enthalpy changes. A+B→AB Relation (1):

$\Delta H_f = H_{final} - H_{initial}$

Now According to reaction $B(OH)_3 + 2H_2O \rightarrow B(OH)_4^- + H_3O^+$, the forming enthalpy amounts resulted from Gaussian application computation is:

$\Delta H_f = [H_{B(OH)4^-} + H_{H3O^+}] - [H_{B(OH)3} + H_{H2O}]$

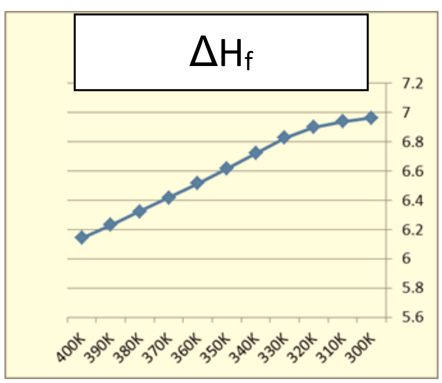

Fig (1) is the diagram of enthalpy changes of boric acid dissolution process in water result in B $(OH)_4^-$ and hydronium ion in different temperature

The amount of ΔH_f shows that the boric acid dissolution in water (B $(OH)_3$) product B $(OH)_4^-$ and hydronium ion is endothermic so this done better by increase temperature. (fig2)

Computation and examination of entropy change amounts (ΔS) [2]

The amount of entropy for primary material and productions in kinetic

Process has been done by Gaussian program 98. The following is used in order to compute the entropy changes.

Relation (3): $\Delta S_{AB} = [S_{AB}] - [S_A + S_B]$

Now according to $B(OH)_3 + 2H_2O \rightarrow B(OH)_4^- + H_3O^+$ the amount of formed entropy computed with Gaussian application is done like the following.

Relation (4): $\Delta S_f = [S_{B(OH)_4^-} + S_{H3O^+}] - [S_{B(OH)_3} + S_{H2O}]$

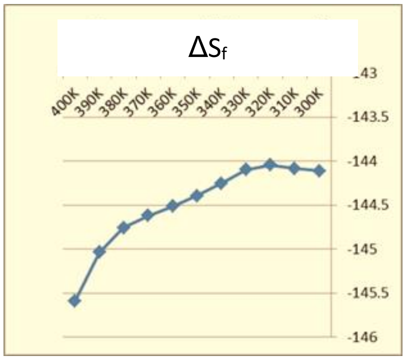

Fig (2) the diagram of entropy changes of boric acid desolation process in water result in $B(OH)_4^-$ and hydronium ion.

The amount of ΔS_f displays that the boric acid desolation process in water product $B(OH)_4^-$ and hydronium ion hos negative entropy so it is clear because the combination of three particles in the first side causes the reaction of two particle in the second side fig3.

Computation and examination of C_V:

The C_v has been computed for the primary material and products in synthesis process by Gaussian program 98.

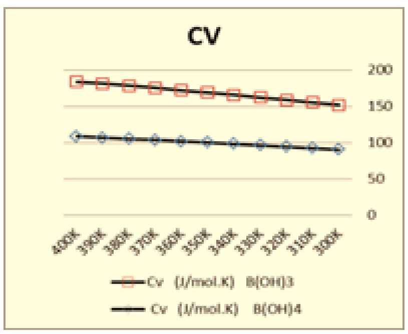

Fig (3) the diagram of C_V changes in $B(OH)_4^-$ and Boric acid $B(OH)_3$ in different temperatures

The amounts of C_V changes in B $(OH)_4^-$ and Boric acid B $(OH)_3$ in different temperatures shows that the product has lower C_V .

This means in the same condition by gettis less therm, its temperature increases in comparison to raw material. The raw material reported in table1 restarts this too. (fig3)

Computation and examination of the changes amount of (ΔG):

The amount ΔG for raw material and products in synthetics has been computed with Gaussian program 98. The following is used in order to measure the ΔG Changes.

Relation (4): $\Delta G_{AB} = [G_{AB}] - [G_A + G_B]$

Now according to $B(OH)_3 + 2H_2O \rightarrow B(OH)_4^- + H_3O^+$

The amount of ΔG computed with Gaussian program is

Relation (5): $\Delta G_f = [G_{B(OH)_4^-} + G_{H3O^+}] - [G_{B(OH)_3} + G_{H2O}]$

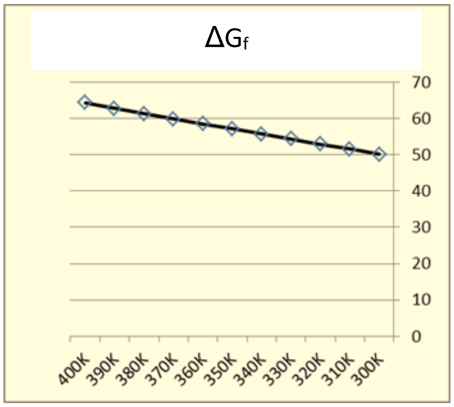

Fig (4) diagram of ΔG_f amounts of Boric acid desolation process in water result in B $(OH)_4^-$ and hydronium ion.

The amount of ΔG_f shows that the dissuasion process of Boric acid in water Product B $(OH)_4^-$ and hydronium in different temperatures con not be done spontaneously.

Discussion and conclusion

The results taken from computation show that in Boric acid desolation

Process in water product B $(OH)_4^-$ and hydronium ion in different temperature, the amount of ΔH_f is possible in all the temperature which means that process is endothermic so by increase temperature, the desolation is done much better.

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