



Original Article.

The Synthesis of Imine from the Reaction of (R)-2-((piperidin-1-yl) methyl) cyclohexanone with benzyl amine in Different Temperature Conditions by DFT method

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ABSTRACT

In this article, synthesis of the synthesis of Imine: phenyl-N-((R)-2-((piperidine-1-yl) methyl)cyclohexylidene)methanamine from the reaction of (R)-2-((piperidin-1-yl) methyl) cyclohexanone with benzylamine 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, 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: Imine, Synthesis, (R)-2-((piperidin-1-yl) methyl) cyclohexanone, Benzylamine

Introduction

At the moment, many scholars around the world are investigating on Imines. Because this compounds are very important in the synthesis of organic compounds. The most important application of these compounds is in medication chemistry. Imines are important as a medicine from analgesic and sedative agent and important mediator limit are in organic chemistry. That for example, the use of Imines in the provide of amin and amide can be mentioned. The compounds that there is in their structure piperidine ring along with factors such as alcohol, oxime, amine and acid that exhibit biological activity and are often sedative and effective the central nervous system.

As an example, alkaloidal family can be exemplified that they show biological properties with having piperidine ring. In this synthesis of Imine: Phenylene-N-((R)-2-((piperidino-1-yl)methyl)cyclohexylidene)methanamine from the reaction of (R)-2-(piperidine-1-yl)cyclohexanone with benzyl amine in different conditions of temperature by DFT method has been studied(Figure 1)

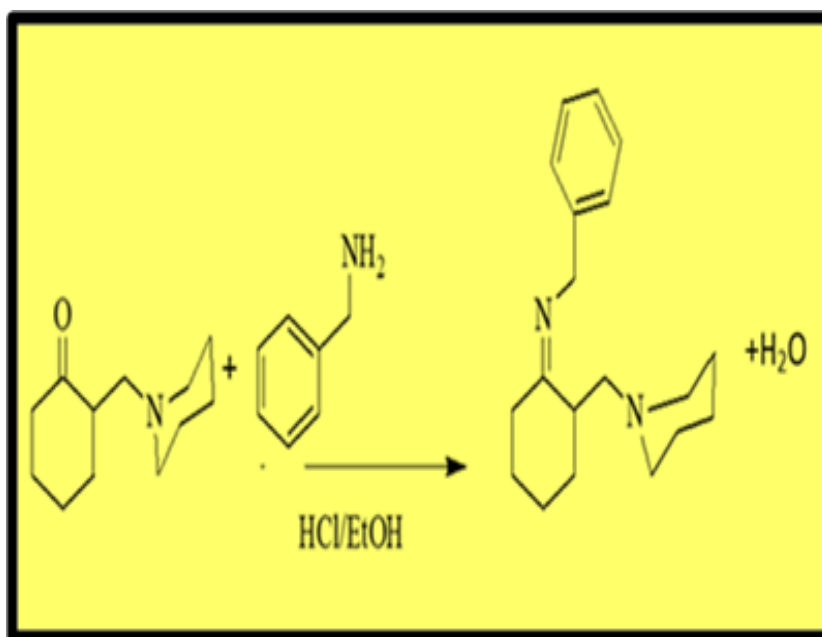


Figure 1. synthesis process Imine; phenyl-N-((R)-2-((piperidino-1-yl)methyl)cyclohexylidene)methanamine

Table(1). Some chemical properties calculated on the surface B₃LYP(6-31g) for Imine: Phenyl-N-((R)-2-((piperidino-1-yl) cyclohexylidene) metha namine (C₁₉H₂₈N₂) (Imine product) and (R)-2-(piperidine-1-yl)methyl) cyclohexanone and benzyl amine (primary materials).

Temperature=298.15K, pressure=1 atm			
	Reactant		Product
	C ₁₂ H ₂₁ NO	C ₇ H ₉ N	C ₁₉ H ₂₈ N ₂
ENERGY	-592.661757 au	-322.952201 au	-839.989978
ENERGY(aq)	-592.663957 au	-322.959381 au	-839.989978 au
SOLVATION ENERGY	-5.78kJ/mol	-18.85 kJ/mol	-3.13 kJ/mol
E HOMO	-9.10eV	-8.77 eV	-8.85 eV
E LUMO	4.48 eV	-4.22 ev	4.17 ev
Dipole Moment	2.65 debye	1.57 debye	2.14 debye
weight	195.306 amu	107.156 amu	284.447 amu
volume	224.33 Å ³	127.23 Å ³	330.85 Å ³
Area	242.71 Å ²	147.38 Å ²	346.62 Å ²
POLARIZABILITY	56.38	48.64	65.16
ZPE	900.53 KJ/mol	412.68 KJ/mol	1247.05 KJ/mol
H°	-592.306904 au	-322.787893 au	-839.499067 au
CV	204.18 J/mol	103.90 J/mol	294.92 J/mol
S°	426.43 J/mol	331.04 J/mol	503.36 J/mol
G°	-592.355329 au	-322.825 au	-839.556228 au

Calculation and results

Computational survey of Imine synthesis; phenyl-N-((R)-2-((piperidino-1-yl)methyl) cyclohexylidene)methanamine from the reaction of (R)-2-(piperidine-1-yl)methyl) cyclohexanone with benzyl amine was studied in different conditions of temperature, the DFT method.

This operation was performed using Gaussian 98 and Gausswave software. The compounds were initially optimized with DFT method in the base series(6-31g), then, studies IR were carried out to calculate thermodynamic parameters related to the process.

All computation at level B₃LYP (6-31g) were carried out at a temperature of (300 to 400 Kelvin degrees) and one atmospheric pressure.

The reaction reviewed case as follows:



Calculate and review the amounts of ΔH changes:

With using the Gaussian 98 program, the ΔH amounts for primary materials and products in the synthesis process were calculated. For the calculation and obtaining of ΔH changes in reactions $\text{A} + \text{B} \rightarrow \text{AB}$ from the following equation is used[1-8].:

$$\Delta\text{H} = \text{H}_{\text{end}} - \text{H}_{\text{primary}} \quad (1)$$

Now with regard to the reaction:



The formed ΔH amounts obtained by calculating Gaussian software are as follows:

$$\Delta\text{H}_f = [\text{H}_{\text{C}_{19}\text{H}_{28}\text{N}_2} + \text{H}_{\text{H}_2\text{O}}] - [\text{H}_{\text{C}_{12}\text{H}_{21}\text{NO}} + \text{H}_{\text{C}_7\text{H}_9\text{N}}] \quad (2)$$

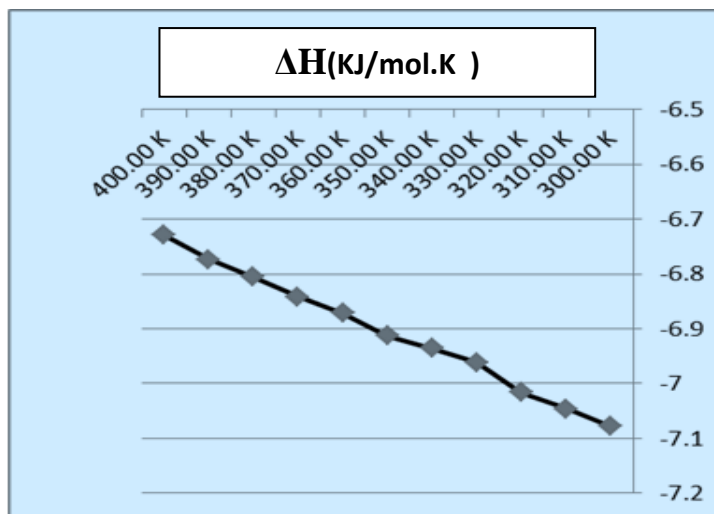


Figure 2. the formed ΔH changes diagram for Imine synthesis; phenyl-N-((R)-2-((piperidino-1-yl)methyl)cyclohexylidene)methanamine from the reaction of (R)-2-(piperidine-1-yl)methyl)cyclohexanone with benzyl amine at different temperatures.

The value of ΔH_f shows that the Imine synthesis process:

phenyl-N-((R)-2-((piperidino-1-yl)methyl)cyclohexylidene)methanamine from the reaction of (R)-2-(piperidine-1-yl)methyl)cyclohexanone with benzyl amine at different temperatures, the

heat dissipates and with increasing reaction temperature the amount of released heat is reduced shape(2).

Calculate and review the amounts of ΔS changes:

With using the Gaussian 98 program, the ΔS amount for primary materials and products in the synthesis process were calculated. For the calculation and obtaining of ΔS changes in reaction $A+B \rightarrow AB$ the following equation is used:

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

Now with regard to the reaction



The formed ΔS amount obtained by calculating Gaussian software are as follows:

$$\Delta S_f = [S_{C_{19}H_{28}N_2} + S_{H_2O}] - [S_{C_{12}H_{21}NO} + S_{C_7H_9N}] \quad (4)$$

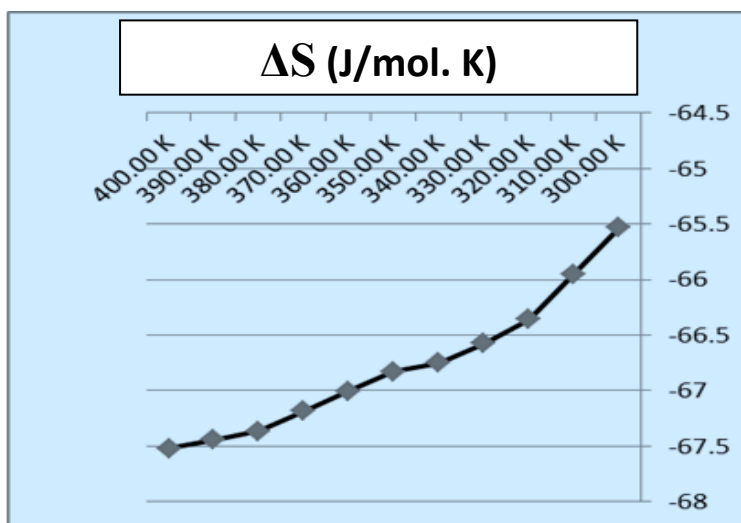


Figure 3. the formed ΔS changes diagram for Imine synthesis: phenyl-N-((R)-2-((piperidino-1-yl)methyl)cyclohexylidene)methanamine from the reaction of (R)-2-(piperidine-1-yl)methyl)cyclohexanone with benzyl amine at different temperatures

The value of ΔS_f shows that the Imine synthesis process: phenyl-N-((R)-2-((piperidino-1-yl)methyl)cyclohexylidene)methanamine from the reaction of (R)-2-(piperidine-1-yl)methyl)cyclohexanone with benzyl amine at different temperatures it has a negative ΔS that with increasing temperatures, ΔS becomes less negative shape(3).

Calculate and review special heat capacity C_v :

With using the Gaussian 98 program, the special heat capacity amounts C_v for primary materials and products in the synthesis process were calculated.

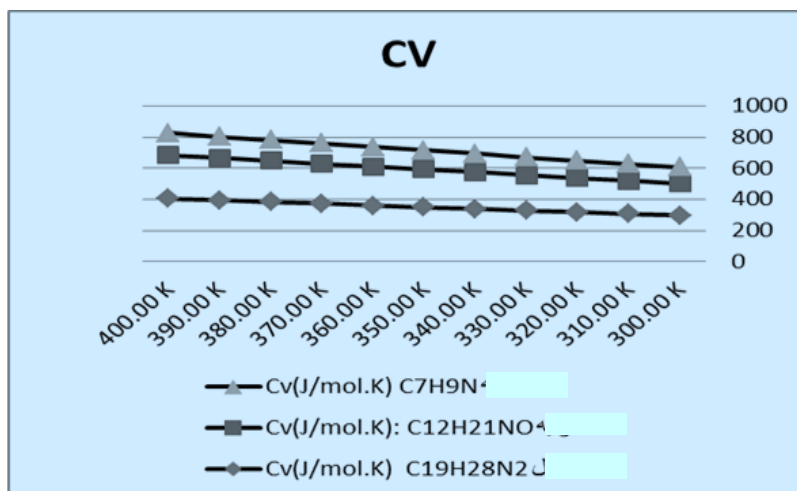


Figure (4) the special heat capacity C_v changes diagram in the product of Imine and primary materials (R)-2-(piperidine-1-yl) methyl) cyclohexanone with benzyl amine at different temperatures

The special heat capacity C_v changes amounts in the product of Imine; phenyl-N-((R)-2-((piperidino-1-yl) methyl) cyclohexylidene) metha namine from the reaction of (R)-2-(piperidine-1-yl)methyl) cyclohexanone with benzyl amine at different temperatures, it shows that the product has a lower specific heat capacity, that is, In the same conditions it's increases temperatures with getting less heat relative to the primary material Figure (4) [9-11].

Calculate and review the amounts of Gibbs free energy changes (ΔG):

With using the Gaussian 98 program, the Gibbs free energy amounts (ΔG) for primary materials and products in the synthesis process were calculated. for the calculation and obtaining of Gibbs free energy changes (ΔG) in reactions $A+B \rightarrow AB$ the from following equation is used:

$$\Delta G_{AB} = [G_{AB}] - [G_A + G_B] \quad (5)$$

Now with regard to the reaction:



The formed Gibbs free energy amounts obtained by calculating Gaussian software are as follows:

$$\Delta G_f = [G_{C_{19}H_{28}N_2} + G_{H_2O}] - [G_{C_{12}H_{21}NO} + G_{C_7H_9N}] \quad (6)$$

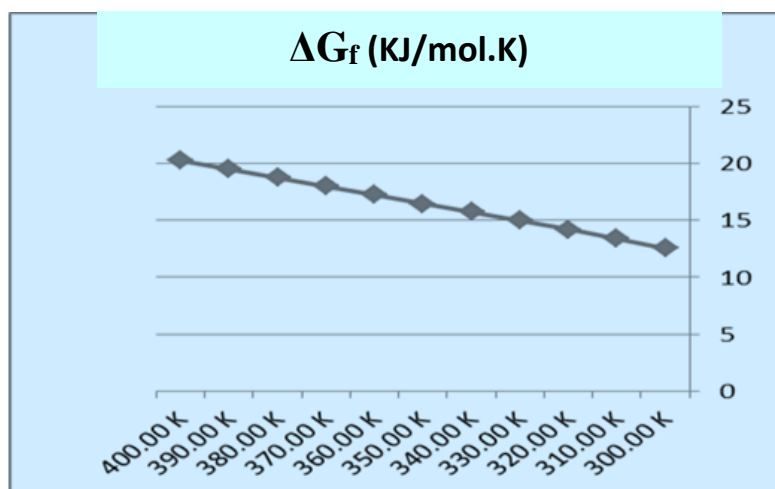


Figure 5. the formed Gibbs free energy ΔG_f amounts diagram for Imine synthesis: phenyl-N-((R)-2-((piperidino-1-yl) methyl) cyclohexylidene) metha namine from the reaction of (R)-2-(piperidine-1-yl)methyl cyclohexanone with benzyl amine at different temperatures

The value of ΔG_f shows that the Imine synthesis process: phenyl-N-((R)-2-((piperidino-1-yl) methyl) cyclohexylidene) metha namine from the reaction of (R)-2-(piperidine-1-yl)methyl cyclohexanone with benzyl amine at different temperatures, it's not spontaneous and with

temperature increases, Gibbs free energy changes process become more positive. So, the reaction at lower temperatures is done better shape (5).

Discuss and conclusion:

The results of the calculation show that in the synthesis of Imine process: phenyl-N-((R)-2-((piperidino-1-yl) methyl) cyclohexylidene) methanamine from the reaction of (R)-2-((piperidino-1-yl)methyl) cyclohexanone with benzyl amine at different temperatures, ΔH reaction is a negative that shows in the process indicates is heat dissipates and with increasing the reaction temperature, the amount of released heat is released and the amount of ΔS_f is negative that shows in the process disorder is low and with increasing temperature the ΔS becomes less negative.

The special heat capacity (C_v) changes values in the product of matter phenyl-N-((R)-2-((piperidino-1-yl) methyl) cyclohexylidene) methanamine from the reaction of (R)-2-((piperidino-1-yl)methyl) cyclohexanone with benzyl amine at different temperatures it shows that the product has less specific heat capacity values. that is, In the same conditions it's increases temperatures with getting less heat relative to the primary material.

Finally, values ΔG_f show that the process of synthesis is of a non-existent nature and with increasing process temperature Gibbs free energy changes is more positive. So, the reaction at lower temperatures is better.

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