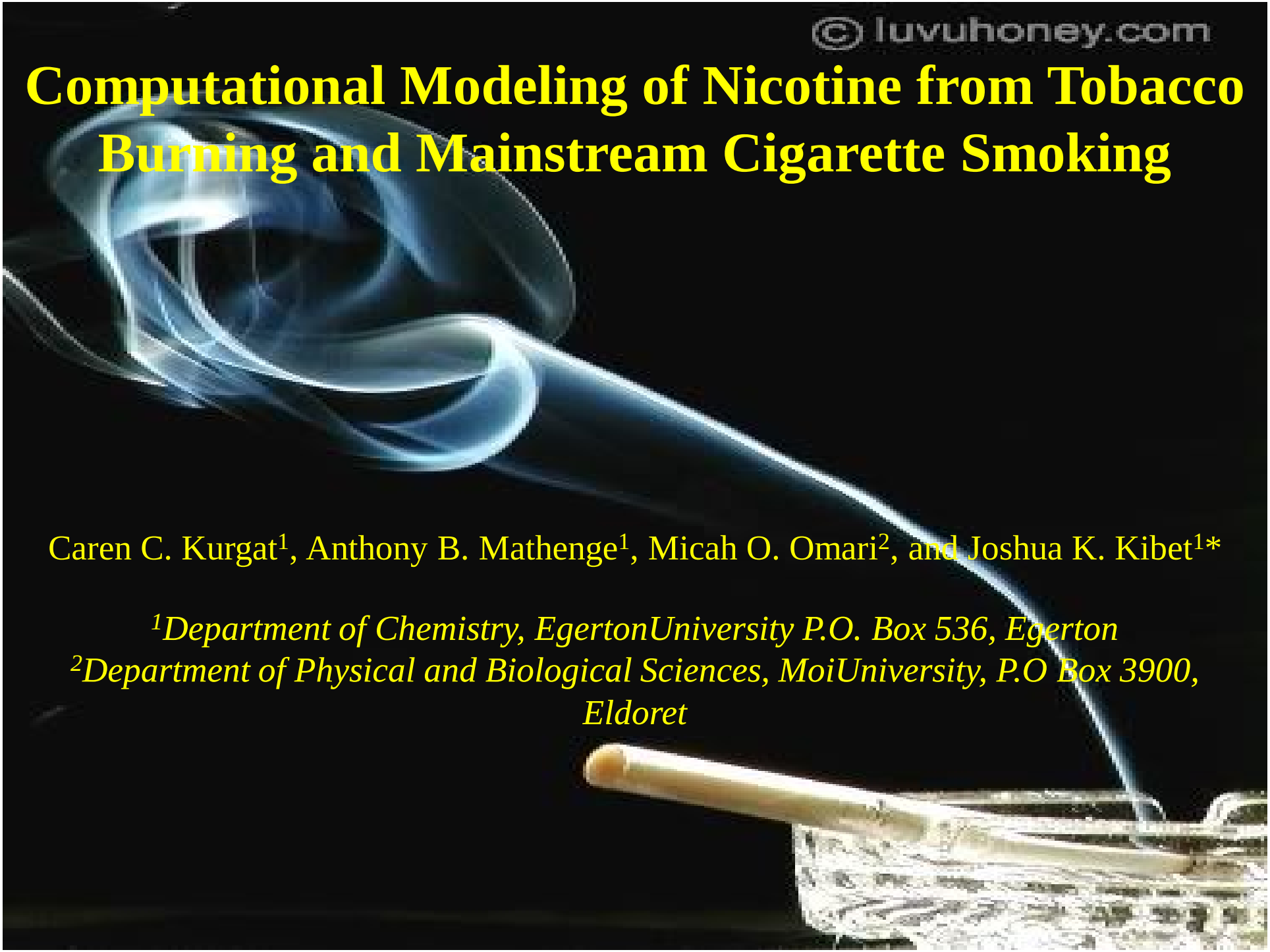

Computational Modeling of Nicotine from Tobacco Burning and Mainstream Cigarette Smoking

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Introduction

- It has been estimated that tobacco smoking causes around 4.9 million deaths per year worldwide (Jonathan Foulds, 2008).

- Studies have shown that **tobacco** smoke contains over **7,000** identified constituents, and its biological variety typified by the presence of carcinogens, toxicants, irritants, tumor promoters, co-carcinogens, and inflammatory agents.

Goals of the Study

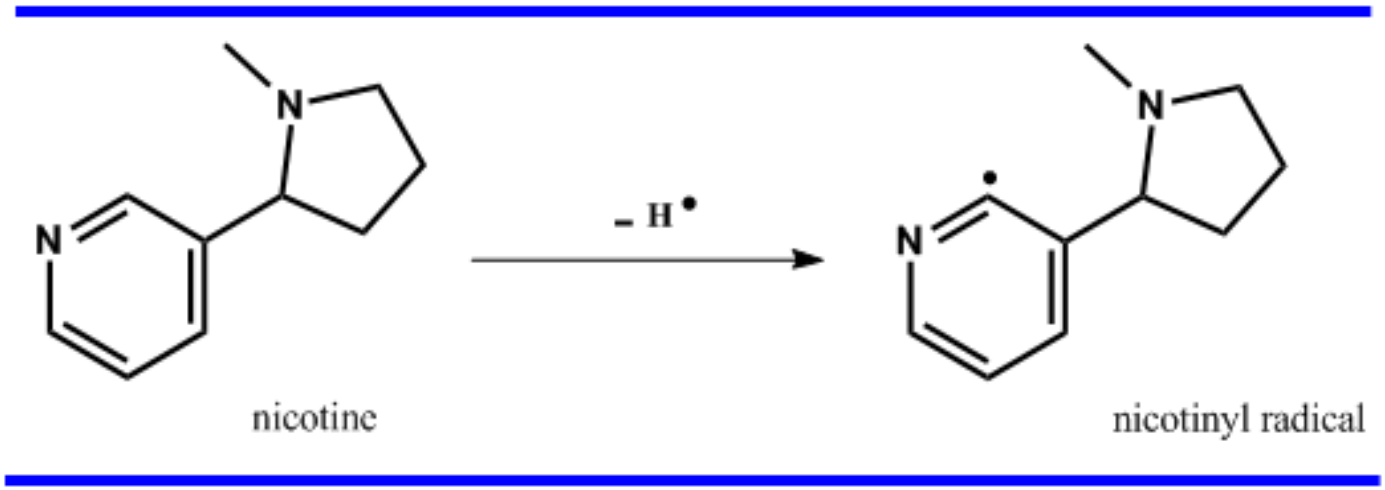
1. To probe the thermodynamic stability of nicotine from quantum theory
2. To determine the change in enthalpy between molecular nicotine and its corresponding free radical
3. To estimate toxicity indices for nicotine and its corresponding free radical using HyperChem computational code
4. To present experimental product evolution of nicotine between 200 and 700 ˚C

Computational Methods

- All calculations were performed using ***Gaussian 03*** program with DFT, in combination with 3-21G
- DFT (Density Functional theory) uses the knowledge of the Schrödinger Equation
- DFT maps the many-body problem into a single body problem and takes into account inter-electronic correlations
- DFT is computation intensive, too many approximations, but works well for short time scales and gives excellent results, even better than experimental data

Free Radical Formation

- At high temperatures a hydrogen atom may be abstracted from nicotine leading to the formation of a reactive free radical
- Free radicals are associated with oxidative stress and carcinogenicity

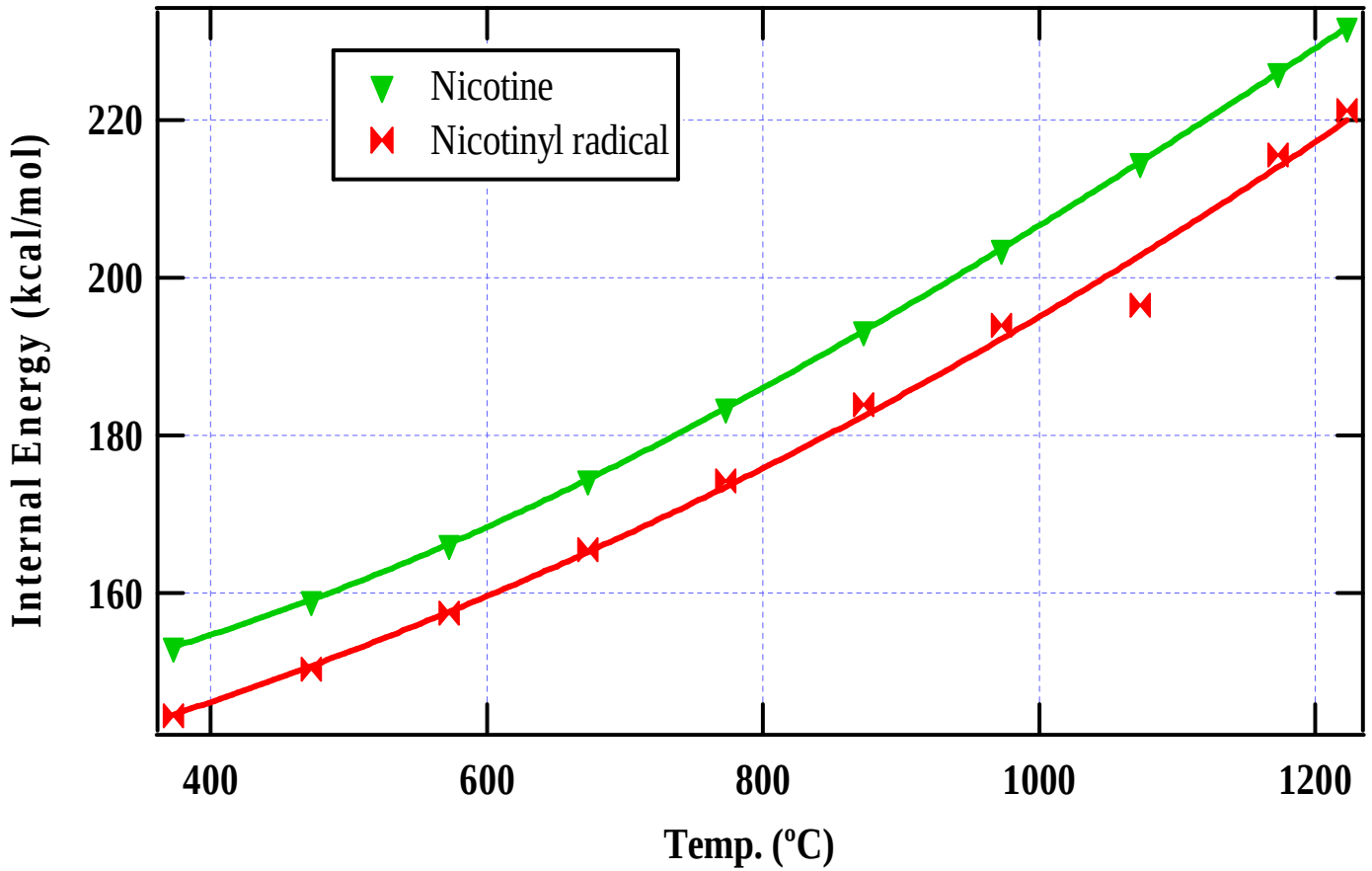


RESULTS

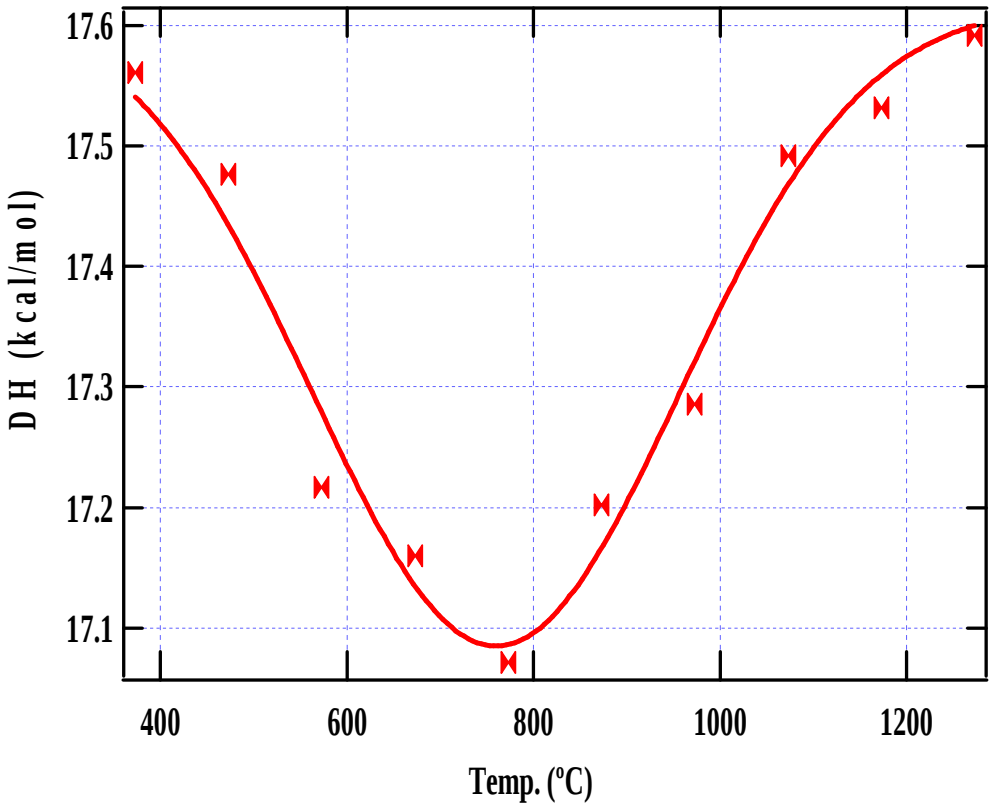
- Internal energies for nicotine and its radical calculated using the density functional theory (DFT) with 3-21G basis set were recorded and the variation with temperature plotted on a graph.

- The graph was linear suggesting that high temperatures favours formation of these compounds.

Variation of Internal Energies with Temperature



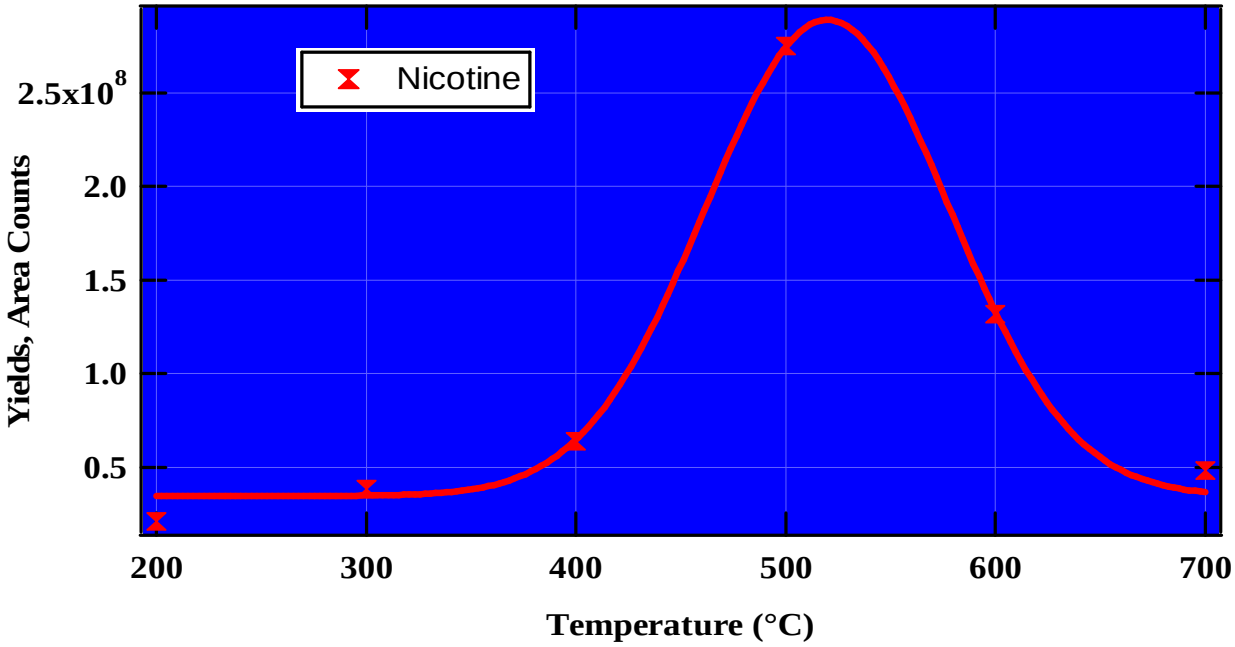
Enthalpy Change (ΔH)



- The enthalpy decreased steadily between 373 to 873 K before rising to 1223 K
- This may suggest magic stability between molecular nictoine and nicotyl radical at certain Temps.

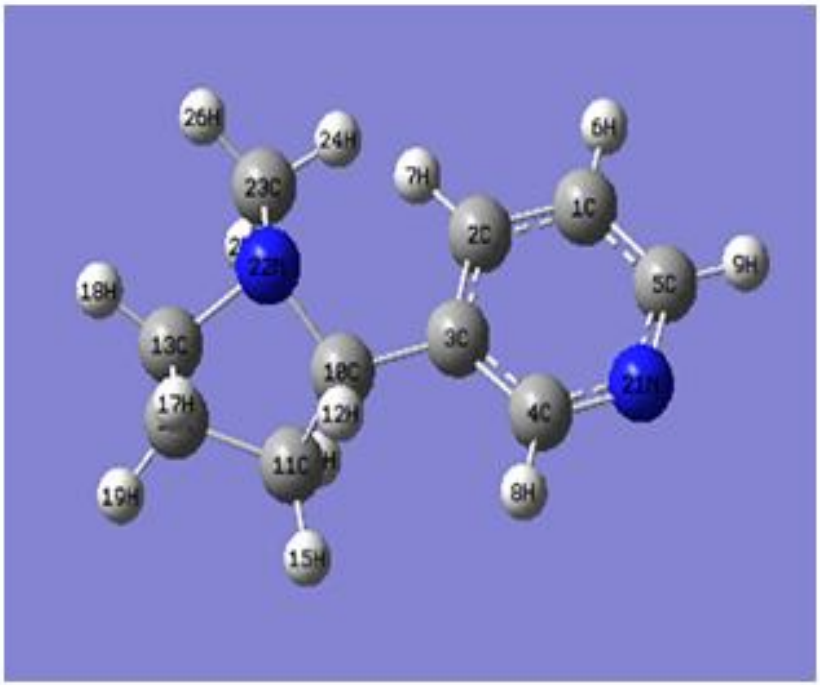
Experimental Product Evolution

Evolution of nicotine at different temperatures was investigated using **GC-MS.**



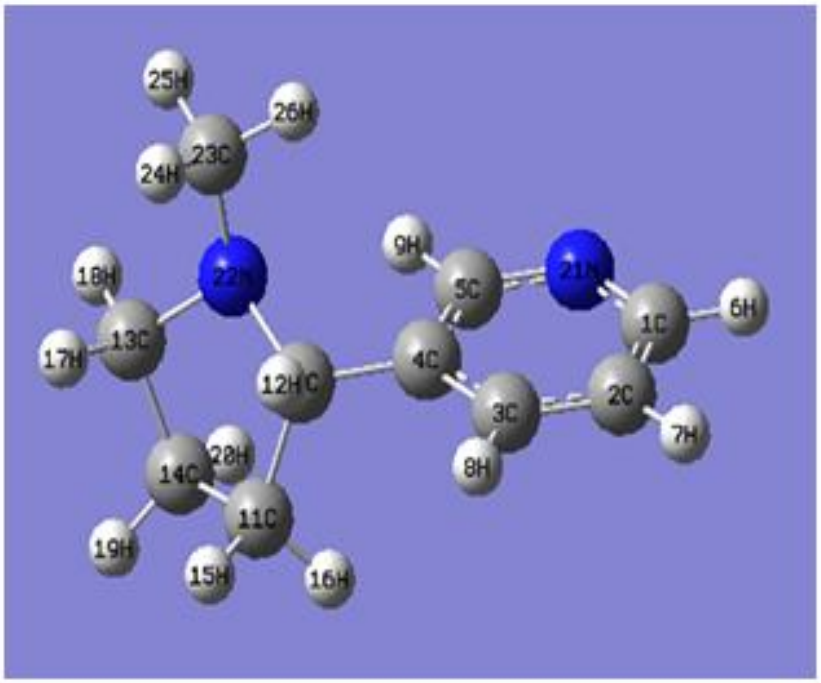
Geometry Optimization

Input structure



B=1.45722(N22, C10)
B=1.50327(N22, C13)
A=121.465(C4, N21, C5)

Optimized structure

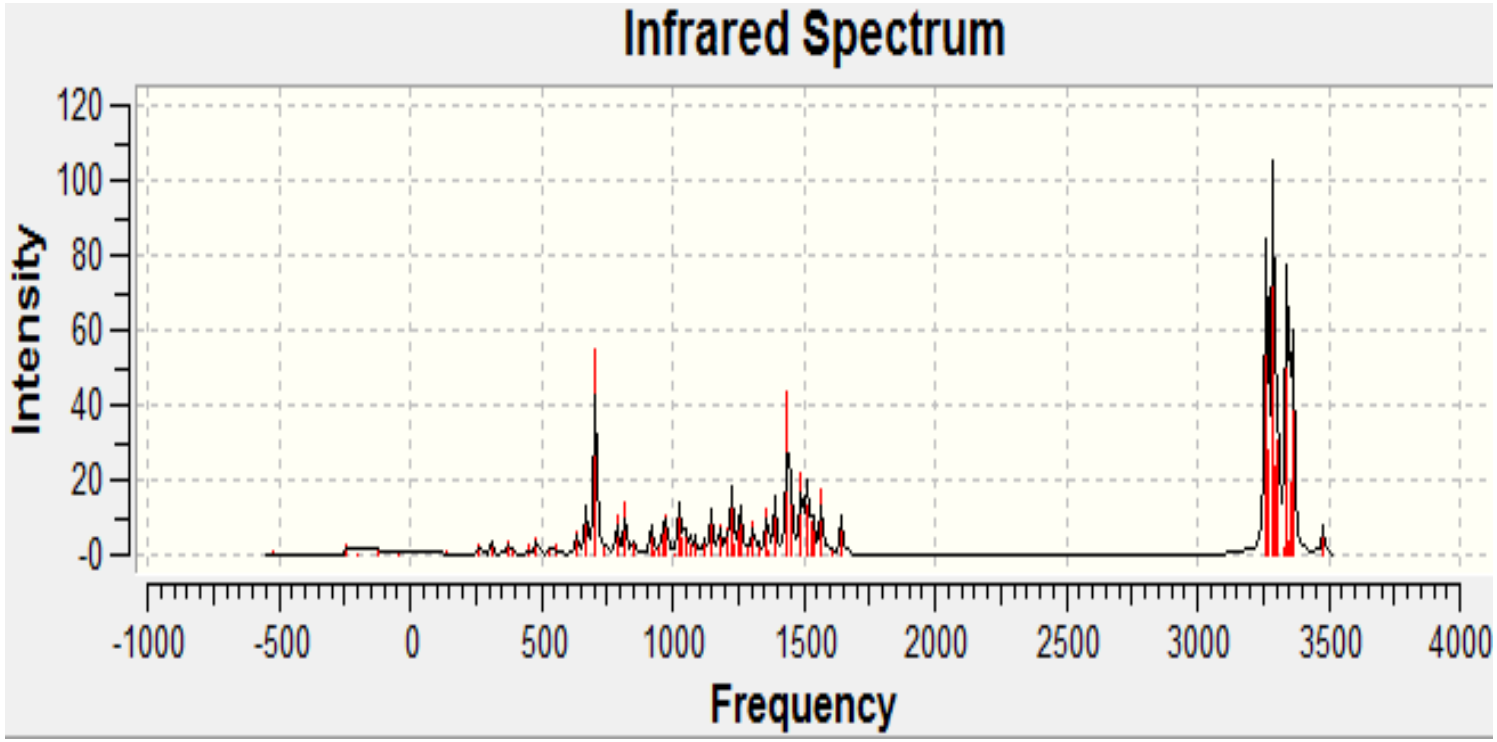


B=1.48231(C13, N22)
B=1.35063(C5, N21)
A=117.672(C1, N21, C5)

Toxicity Indices

- ✓ The estimated toxicity indices for nicotine and its corresponding free radical were 0.22 and 0.74 respectively.
- ✓ These values suggest that nicotine and its respective radical are lyophilic.
- ✓ High Lipophilicity correlates more strongly with biological activity which translates to more oxidative stress and extensive cellular assault

Vibrational Spectrum



Conclusion

1. Thermochemical data has shown interesting results between nicotine and nicotinyl radical between 600 and 800 ˚C.
2. Experimental results have shown that the yield of nicotine in cigarette smoke peaks at about 500 ˚C.
3. The lethal temperature region for cigarette smokers is between 400 and 600 ˚C.
4. Toxicity indices indicate that both nicotine and its radical are lipophilic hence soluble in biological fluids.

Recommendations

1. The unique stability exhibited by nicotine and its corresponding free radical between 600 and 800 ˚C is remarkable and needs further investigation to examine this behavour.
2. In the development of modern cigarettes, emphasis should be towards developing cigarettes that can be smoked at optimum temperatures where formation of toxins are not favoured

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My fellow authors in this study

Thank you!