Structural Isomers of benzene

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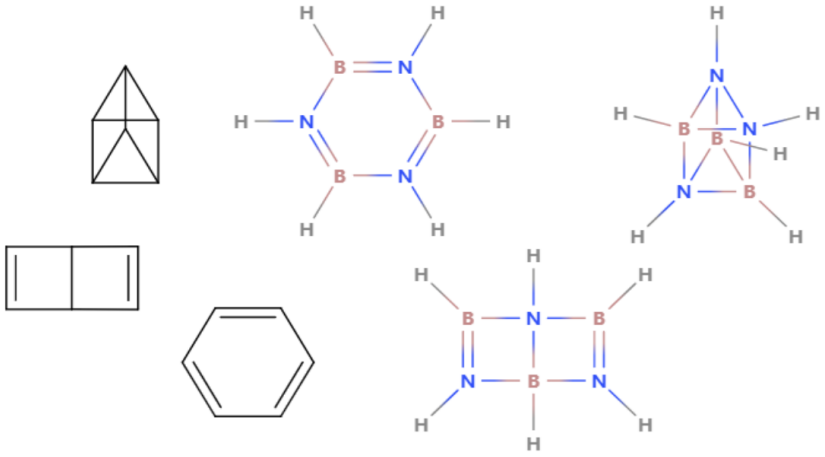
Abstract:

The structure and free energy differences of the isomers of benzene element, namely, benzene element, dewar benzene and alkane were studied. At the same time, the structural and free energy differences of inorganic benzene, (borazine analogue of dewar benzene) and (borazine analogue of dewar alkane) were further studied.

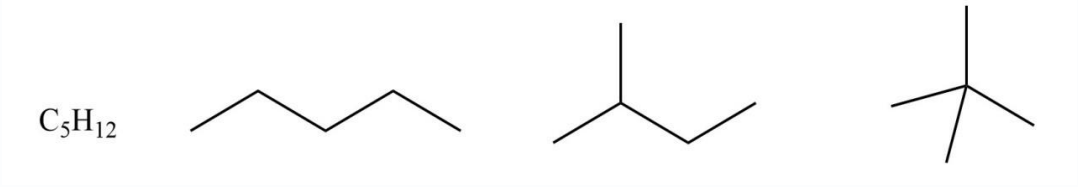


Introduction：

Recently, my downstairs was being renovated, and I would sometimes smell paint when I went upstairs, so I became curious about the composition of the paint. After some inquiry I realized that one of the harmful substance called benzene element, so I started a study of benzene. At first I just searched some information on the Internet and looked up my textbook about benzene. While looking up the materials, I found a picture of benzene elements with the same molecular formula but different structures, so I started my research.

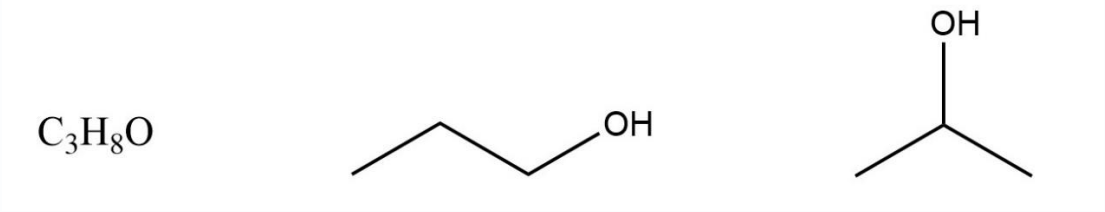
In organic chemistry, compounds with the same molecular formula but different structures are called isomers, also known as structural isomers. The phenomenon of having the same molecular formula but different structures is called isomerism(1). Silver fulminate and silver cyanate were the first isomers discovered by man.

As far as I know, in 1830, Bochilias came up with a new concept of chemistry called "homodifferentiation." This means that the same chemical composition can form compounds with different properties. He gives the example of cyanic acid and fulminic acid, which are "homodifferentiated" compounds with the same chemical composition but different properties. Until then, chemistry had assumed that a compound had one component, and that no two different compounds had the same chemical component.(2)



carbon frame isomers

(1)(2) Refer to Baidu Baike



position isomers

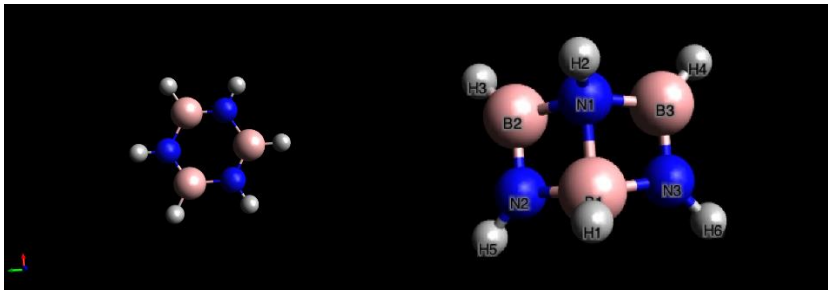
As the picture shows, isomers are divided into several types, such as carbon frame isomers, position isomers, and so on.

Method：

I first asked my chemistry teacher and constructed the structure of benzene elements on the website Molview. Then I downloaded Avogadro and Gaussian from the Internet. Then I downloaded the model I built and put my model into Avogadro for the first initial optimization using Optimize Geometry. Then, Gaussian is used to calculate his free energy. When I used Gaussian, density functional theory has been used, level of calculation is B3LYP/6-31g(d,p).

I did the same thing for the next five different compounds. However, when dealing with Borazine analogs of dewar, some problems occurred in the calculation of Gaussian. At the end of the calculation, the software displayed an error. At the beginning, I went to the Internet to find a solution to the problem. At last, the code of Gaussian calculation was changed and "opt=(Cartesian,calcall)" was used. After 20 minutes of calculation, I successfully concluded the Borazine analogue of dewar benzene free energy. I think it's because the material is so unstable that it can't be calculated.

Then I divided the six data into two groups and made a data comparison.



Result:

Sum of electronic and thermal Free Energy differences

	Benzene (kcl/mol)	BN1 (kcl/mol)
Benzene	0	0
dewar benzene	88.1	120.0
prismane	127.6	185.0

prismane has a number of three/four membered rings， so it have a bigger ring tension. Dewar benzene is geometrical strain with only two member rings， so it is more stable than prismane. Benzene little geometric strain delocalisation

Conclusion:

After studying these six compounds, I found that the more stable a substance is, the less free energy it has. Benzene was more stable than dewar benzene and prismane. The conclusion is the same for borazine and its derivatives.