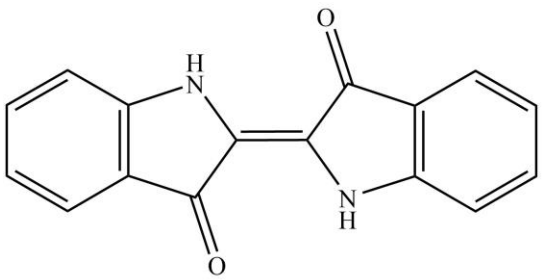
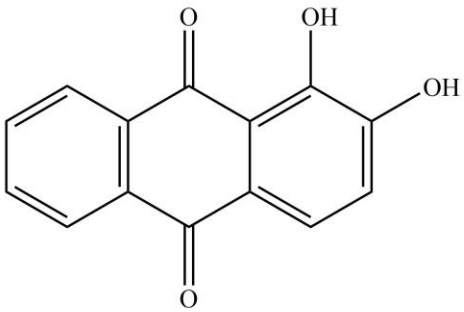
❖ Structure Elucidation of Indigo and Alizarin

Two of the most popular examples of natural dyes are indigo and alizarin which have a cultural history all across the globe. In this section, we will discuss the general method of structure elucidation of alizarin and indigo as well.



Indigo



Alizarin

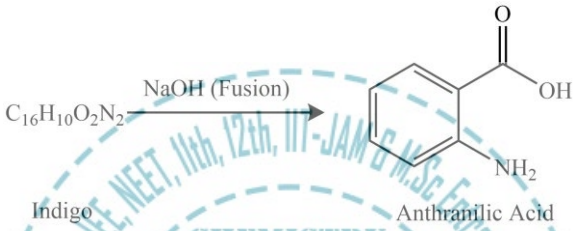
➢ ***Structure of Indigo***

Indigo is a naturally occurring blue dye whose molecular structure can be elucidated by the general method as given below.

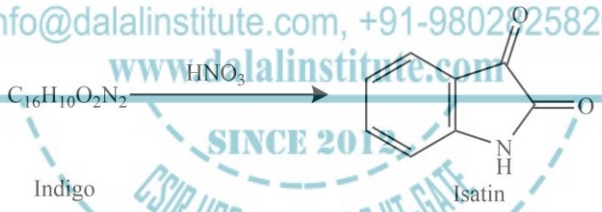
1. The combined study of elemental analysis and mass spectrum suggested that $C_{16}H_{10}O_2N_2$ is the molecular formula of indigo.

2. The double bond equivalent (D.B.E) for indigo was found to be 13 suggesting that there must be more than one benzene ring.

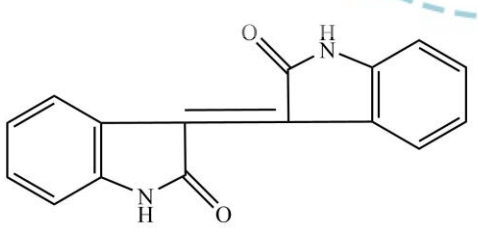
3. Indigo's fusion at low-temperature results in anthranilic acid suggesting that there must be at least one ortho-substituted benzene ring where one position is bind by nitrogen and the other by carbon.



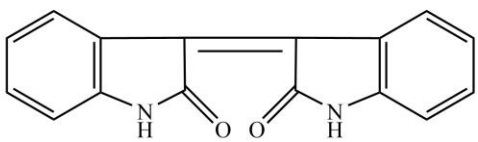
4. Indigo's oxidation with nitric acid results in two moles of isatin indicating two identical units in indigo that are connected with each other such that one molecule of isatin is generated from each unit.



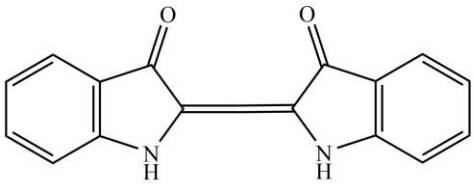
5. Three possible structures can be concluded from the isatin structure.



Structure 1

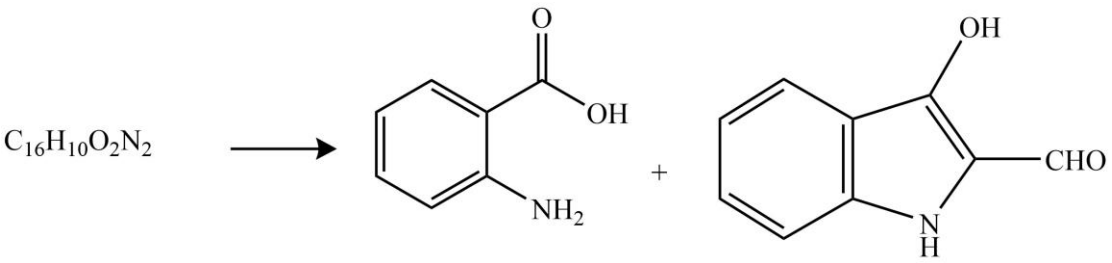


Structure 2



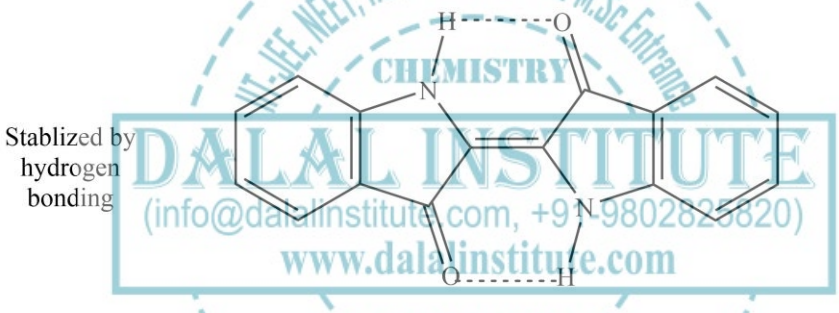
Structure 3

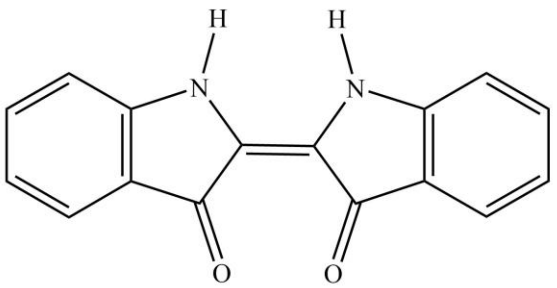
6. The treatment of indigotin with dilute alkali results in the formation of indoxyl-2-aldehyde and anthranilic acid.



Indigo Anthranilic Acid Indoxyl-2-aldehyde

7. Finally, we may conclude that two identical units must be joined via the second position of the indoxyl fragment, and an oxygen-containing functional group must be present at position 3. All this suggests following two structures for indigotin.





cis-Indigo

Now since trance configuration is stabilized by H-bonding, it must be the primary choice. Similar results were obtained by qualitative analysis of mass spectra and NMR data.

➢ ***Structure of Alizarin***

Indigo is a naturally occurring blue dye whose molecular structure can be elucidated by the general method as given below.

1. The combined study of elemental analysis and mass spectrum suggested that $C_{14}H_8O_4$ is the molecular formula of alizarin.

2. The double bond equivalent (D.B.E) for alizarin was found to be 11 suggesting that there must be at least one benzene ring.

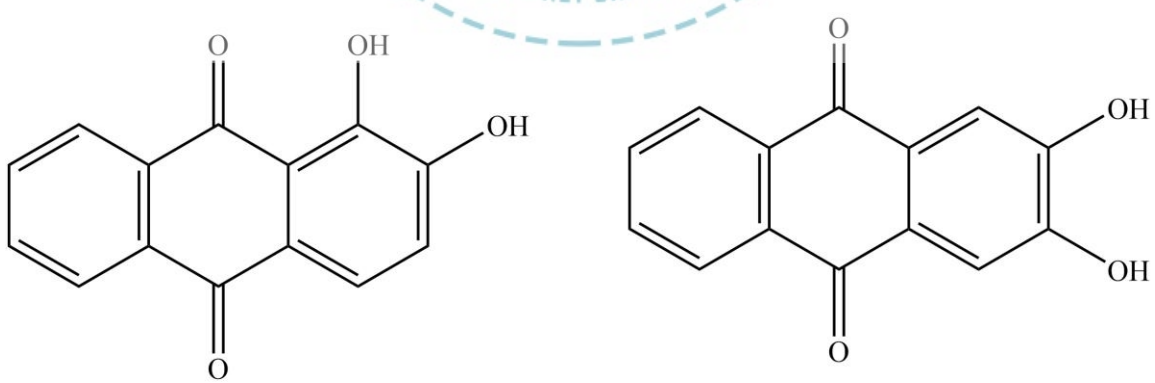
3. The reduction of alizarin with zinc at 675K results in anthracene indicating that alizarin must a derivative of the anthracene molecule.

4. The reaction of alizarin with acetic anhydride results in diacetate showing two hydroxyl groups are expected in the alizarin molecule.

5. Since the condensation of phthalic anhydride with catechol at 455K results in alizarin, it can be concluded that this dihydroxy derivative of anthraquinone must be having OH groups in the same cycle.

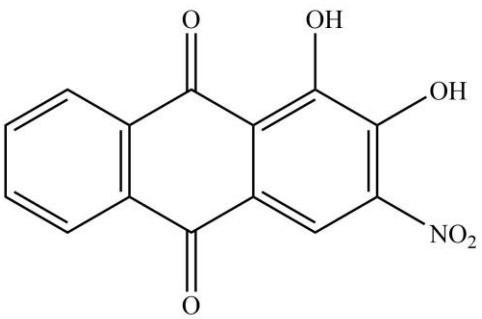
Phthalic Anhydride Catechol Alizarin

6. Therefore, following structures can be proposed for alizarin molecule.

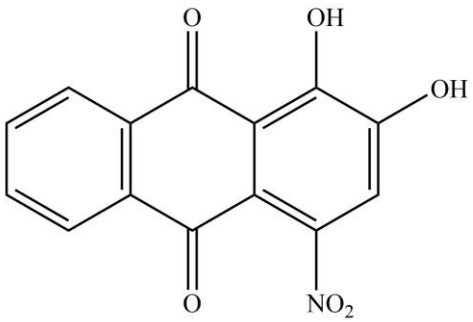


Structure I Structure II

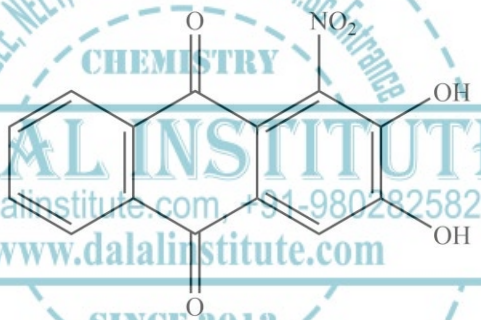
7. The nitration of alizarin results in two isomers of mono-nitro derivative, which in turn produce phthalic acid upon oxidation; indicating the presence of the nitro group in the same cycle as the hydroxy group. Now since structure I can give two mono-nitro derivatives but the second structure can produce only one mono-nitro derivative, the correct answer should be structure I.



Structure IA



Structure IB



Structure IIA

Now since trance configuration is stabilized by H-bonding, it must be the primary choice. Similar results were obtained by qualitative analysis of mass spectra and NMR data

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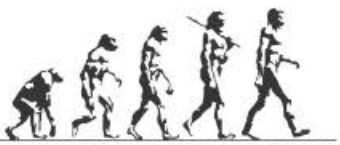

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