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Chemistry

SUB. CODE- BSCC2402

For B.Sc. 4th Semester

(Heterocycles)

Module-IV

Indole: Structure elucidation

By

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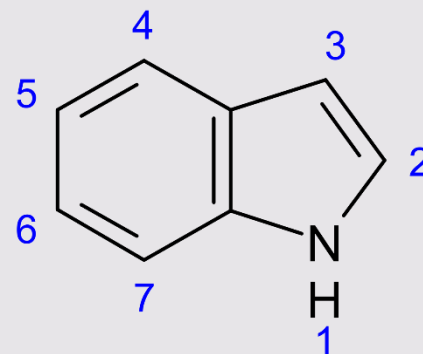


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Indole

Indole is an aromatic heterocyclic organic compound with formula C_8H_7N . It has a bicyclic structure, consisting of a six-membered benzene ring fused to a five-membered pyrrole ring. Indole is widely distributed in the natural environment and can be produced by a variety of bacteria.





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Indole: structure elucidation

1. Molecular formula is C_8H_7N deduced from analytical and molecular weight determinations

2. Nature of carbon skeleton

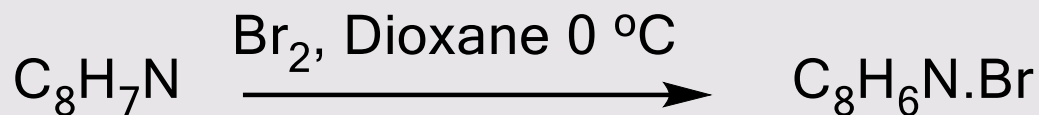
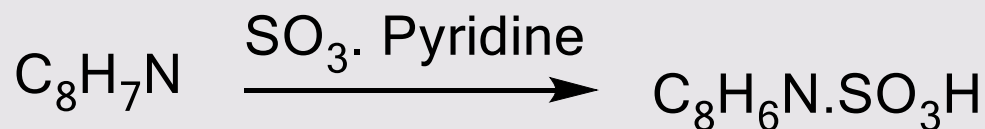
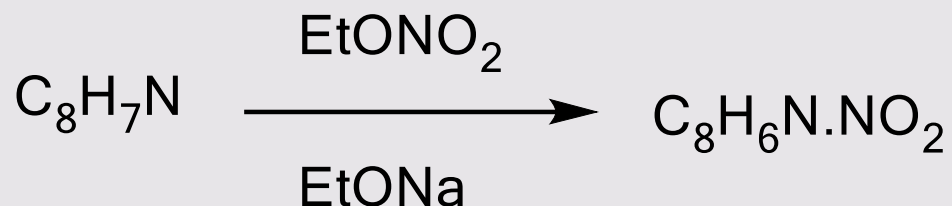
- i. It does not undergo addition reaction with halogens, halogen acids.
- ii. It does not decolorise alk. $KMnO_4$ solution.
- iii. A very stable compound
- iv. It undergoes electrophilic aromatic substitution reactions like nitration, sulphonation, halogenation etc. which indicates its aromatic nature as benzene.



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Indole: structure elucidation

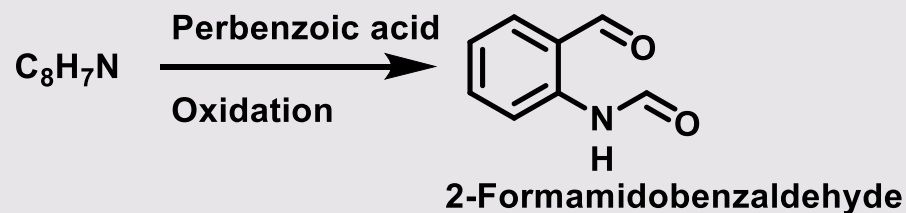




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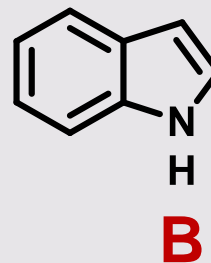
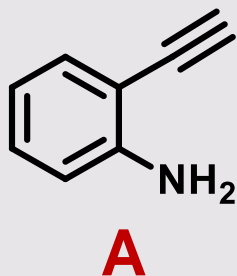
Indole: structure elucidation

3. On oxidation with perbenzoic acid, it gives 2-formamidobenzaldehyde.



This indicates the presence of a benzene ring with 2 side chains or a fused ring on two adjacent carbons.

4. From the reactions, the two possible structures for Indole are proposed as A or B:





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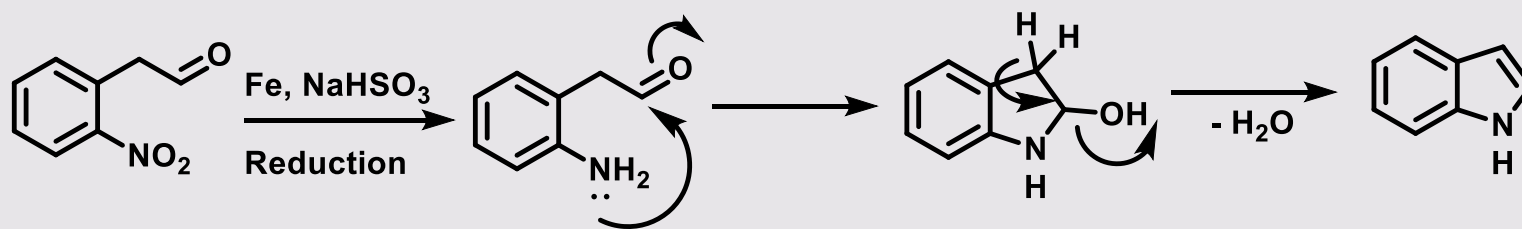
Indole: structure elucidation

Structure A does not give properties of acetylene and primary amino group, hence discarded.

Also indole on reduction gives octahydroindole, showing the presence of four double bonds.

Structure B with a benzene ring fused with a pyrrole ring accounts for all the above properties.

This structure of indole is further confirmed by its synthesis from o-nitrophenyl acetaldehyde.





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References

1. K.D Sharma and Y. R. Sharma, Kalyani Publishers, Unit-III page-278;
2. University Chemistry, Vol-IV, Dr. U. N. Dash, Dr. K. K. Ojha, Himalaya Publishing house, Unit IV, page-378