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Dimensions of Carbon Chains

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DETERMINATION OF PURITY OF LIQUID ISOMERS BY X-RAY DIFFRACTION

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Previous contributions have been made by the writer and Professor Skinner on the isomers of primary normal alcohols and by the writer on normal paraffins. The difference between the normal compounds and isomers are shown by displacements of the chief diffraction peak in amounts indicated by increases in the mean diameter of the molecule. The diameters of the normal alcohols and of the normal paraffins have been found and published. The former diameter increases linearly 4.3Å with propyl to 4.5Å, n-lauryl alcohol. The values for n-methyl and ethyl are 3.8Å and 4.2Å respectively. With the n-paraffins the diameter is constant from pentane to tetradecane at 4.6Å. A branch with either chain shows at once a displayed diffraction peak. As an illustration of the reliability of the method may be cited experiments with n-pentane and n-decane. These compounds were obtained from a research laboratory but were found to have diffraction peaks which were over a degree displaced from that of the normal paraffins. But later when synthetic normal compounds were obtained they were found to have diffraction peaks at the same place as the other normal paraffins. This shows that the original samples were not normal compounds. All these experiments point to the fact that the x-ray diffraction method has an important place in distinguishing between isomers and in testing the purity of chain compounds.

DIMENSIONS OF CARBON CHAINS

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There seems to be no doubt in reference to the existence of carbon chains in organic compounds, but the arrangements of the carbon atoms and the dimensions of the chains are much in doubt. In connection with x-ray diffraction in liquids it has been possible to make measurements of interest on the paraffin, the alcohol and the fatty acid chains, and these may be summarized as follows:

1. The chain widths in the three cases are almost the same, i.e. 4.6Å.

2. The primary normal alcohols show a small but steady increase in width from a content of three to a content of eleven carbon atoms.

The normal fatty acids from four carbon atoms to eleven carbon atoms show either a smaller increase or none at all.

The rapid decrease in width of both fatty acids and alcohol chains is similar from a content of about three carbons or four carbons to that of one carbon.

The width of the paraffin series is the same with a content from five to fourteen carbon atoms.

3. The carbon atom may occupy approximately 1.3Å along the length of the chain in all three cases of the normal compounds, but satisfactory measurements are not yet made on this point.

4. When a branch is attached the chain molecules alter either their shape or their orientation or both. This is indicated by the facts that follow.

5. The addition of two CH_3 groups to the paraffin chain causes a much greater alteration in diameter than in the case of the alcohols.

6. The attachment of an OH group as a branch of an alcohol molecule (and its removal from the end) causes approximately the same change as the attachment of a CH_3 branch. Likewise, when attached to the same atom simultaneously with the CH_3, it produces approximately the same change as the attachment of two CH_3 branches.

7. In cases of three like branches at an end of the chain, none of these three branches lies in the median straight line of the chain.

8. The attachment of branches in the alcohols shortens the molecules but not without change of shape or of orientation.

9. The removal of the OH group from the end carbon or the next adjacent atom of an alcohol changes the molecule from a double to a single one.

10. The attachment of branches in the paraffins seems to increase the volume much more rapidly than can be accounted for without change of shape or of orientation.

11. The general conclusion is that evidence favors (1) a close similarity between the chains of the primary normal alcohols, the saturated normal fatty acids and the normal paraffins. (2) A difference between the first and last chains which appears in evidence when branches are attached to the chains.

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