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## Molecular Structure of Benzene, Cyclohexane and Their Derivatives - A Study in X-Ray Diffraction

G. W. Stewart  
*State University of Iowa*

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## MOLECULAR STRUCTURE OF BENZENE, CYCLOHEXANE AND THEIR DERIVATIVES—A STUDY IN X-RAY DIFFRACTION

G. W. STEWART

An examination by the x-ray diffraction ionization method was made of benzene, toluene, *o*-, *m*- and *p*-xylene, mesitylene, ethyl benzene and isopropyl benzene; cyclohexane, methyl cyclohexane, *o*-, *m*- and *p*-dimethyl cyclohexane; phenol, aniline, cyclohexanol and cyclohexanone; 2 hydroxy 1-3 dimethyl benzene and three isomers, *o*-, *m*- and *p*-toluidine, and *o*-, *m*- and *p*-cresyl methyl ether. The diffraction peaks are taken to be caused by the semi-orderly space arrangement of the molecules in the liquid, or cybotactic condition, and the distances of separation of the planes containing diffraction centers are computed by Braggs' diffraction law. Both assumptions have been previously proved justifiable.

The structure of the benzene and cyclohexane rings are shown to be distinctly flat, having a thickness of 4.70 Å.u. and 5.10 Å.u. respectively. The proof of the flatness rests upon the effect of substitutions and the relative prominence of diffraction peaks. The general dimension in a plane perpendicular to the thickness is indicated by a diameter of approximately 6 Å.u., as indicated by an area of 31.4 (Å.u.)<sup>2</sup> for benzene and 35.2 (Å.u.)<sup>2</sup> for cyclohexane. These dimensions of the rings are based upon the direct measurements and are limited in reliability only by the correctness of the theory of the x-ray measurements and the space arrangement assumed.

The evidence is preponderately in favor of the maintenance of the general shape of the benzene and cyclohexane rings as units of structure. The similarity of the thickness to the diameter of *n*-paraffin and *n*-alcohols chain indicates the general correctness of the ring conception.

It is shown that the thicknesses of the benzene and cyclohexane "rings" depend upon the relative positions of the substituents. Four ortho, meta and para series, one with derivatives of cyclohexane and three with derivatives of benzene, show that the para substitutions give distinctly the least "thickness" of ring and that usually the meta gives less thickness than the ortho position. In a case of three substituents, variations caused by position were distinctly noticeable.

Six compounds having the substituent OH, with one a cyclohexane derivative, were found to show "double" molecules pro-

duced by the juxtaposition of the two OH groups. None of the others showed this type of orientation. This evidence was obtained by a second semi-orderly arrangement of molecules with diffraction centers in planes separated by a distance of the magnitude of two molecular lengths.

Ten compounds gave also an additional set of planes, caused more importantly by the positions than by the nature of the substituents. Of these ten, three, the hydroxy dimethyl benzenes, showed the three sets of planes; namely, one corresponding to the thickness of the ring, one to an arrangement in a perpendicular direction caused by the substituents, and one in a third direction perpendicular to the other two sets and corresponding to the double molecules of the polar groups.

The above conclusions are in harmony with current investigations from other view points and strengthen the theory of semi-orderly and temporary space arrangements of the molecules in a liquid, or the cybotactic condition.

STATE UNIVERSITY OF IOWA,  
IOWA CITY, IOWA.

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## DIFFRACTION OF X-RAYS IN LIQUIDS: EFFECT OF TEMPERATURE

E. W. SKINNER

Using an x-ray spectrometer similar to that used by G. W. Stewart, experiments are being carried out on the effect of varying temperature on liquid scattering, temperatures varying from room temperature to near the boiling points being used. To date, two liquids, cyclohexane (27°C and 83.5°C) and heptyl (heptylic) acid (28°C and 193°C) have been examined. Results and conclusions are as follows:

(1) The planar spacing giving the distance between molecules increases with increase in temperature (0.28 Å.u. for heptylic acid and 0.16 Å.u. for cyclohexane) change for temperatures noted. This change is attributed to the volume expansion of the liquid. In the case of heptylic acid, the dimension denoting the length of the molecule was not changed, which shows that expansion taken place in one direction only relative to the lengths of the molecules.

(2) The width of the peak increases at the higher temperatures. This is due to the disrupting of the molecular groupings due to thermal agitation, thus producing a more diffuse scattering.