THE DETERMINATION OF MOLECULAR STRUCTURE OF 2−METHYLCYCLOHEXANONE

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The atomic and molecular structure of 2−methylcyclohexanone at 293 K was investigated using the X-ray diffraction method [1]. Monochromatic radiation MoK_α enabled determination of the scattered radiation intensity between S_{min} = 0.430 Å^{-1} and S_{max} = 14.311 Å^{-1}. The curves of reduced radiation intensity were analysed by the reduction method of Blum and Narten [2].

The aim of the study was to establish the role of the cyclohexane ring and the functional groups ($-CH_3$, $=O$) attached to it of the molecule of the liquid studied. The numbering scheme is defined in Fig. 1.

The bond distances used were: C(1)−O = 1.22 Å; C(1)−C(2) = C(2)−C(3) = C(3)−C(4) = 1.53 Å; C(2)−H = = C(3)−H = 1.09 Å. The mean least inter- and intramolecular distances were determined with the following accuracy: for $1.0 < r \leq 2.0$ Å: $\Delta r = \pm 0.01$ Å, for $2.0 \leq r \leq 3.0$ Å: $\Delta r = \pm 0.02$ Å, for $3.0 \leq r \leq 4.0$ Å: $\Delta r = \pm 0.05$ Å [3].

The results permitted the determination of the intermolecular and intramolecular distances, the coordination numbers and the packing coefficient [1].

The packing coefficient of molecules in liquid 2−methylcyclohexanone is approximately 58%.

In the liquid 2−methylcyclohexanone the neighbouring molecules assume the arrangement in which their dipole moments are antiparallel [1]. The methyl group $-CH_3$ shows the C_{3V} symmetry (Fig. 1).

Because of the supposed role of the cyclohexyl ring and the functional groups: $=O$ and $-CH_3$ attached to it at the *equatorial* position, for mutual configurations of molecules in liquid 2−methylcyclohexanone, it seems very probable that the proposed model of local arrangement can also hold for other derivatives of cyclohexane in the liquid phase.

References

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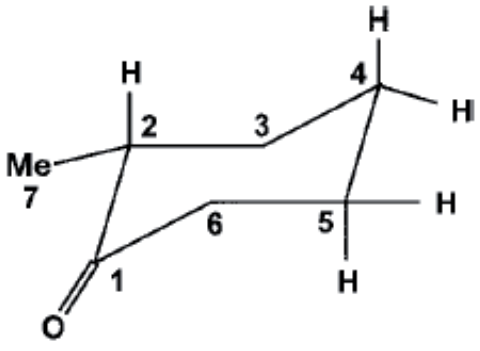

Figure 1. Definition of structural parameters for 2−methylcyclohexanone.

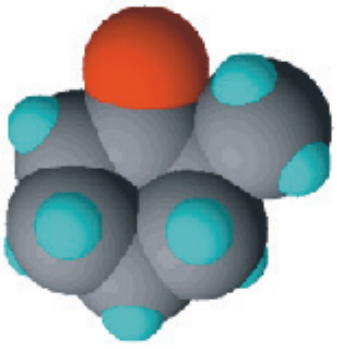

Figure 2. A model of 2−methylcyclohexanone molecule structure.