Developments of X-Ray Scattering Apparatus and Analytical Method for Determination of Liquid Structures and Their Application to Several Neat Liquids and Liquid Mixtures

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Information on liquid structure is significantly important in discussing chemical reactions in solution microscopically. Various methods have been used to investigate the structure of molecular liquids. X-Ray scattering method can provide direct information on intermolecular structures. The X-ray scattering apparatus of transmission mode using a CCD detector was developed, and the data reduction procedure was established. The time of measurement with the CCD detector was reduced to about 1/100 of that with the reflection type apparatus. The quality of data by the present apparatus was comparable with or higher than that by the reflection type one.

Analysis of liquid structure by the X-ray scattering method is to make up a local structure model. A simple approach for determining a liquid structure without constructing any plausible structure models is suggested. Polar coordinates and Euler's angles are introduced as intermolecular structural parameters. The intermolecular structure parameters were refined by using a least-squares calculation. The applicability of the present method was checked by examining the liquid structure of acetonitrile. The liquid structures of acetone, cyclohexane, benzene, and its derivatives were then successfully analyzed by this method.

The liquid structure of mixture is more complex than that of neat liquid because that consists of plural pairs of the intermolecular interactions. The liquid structures of binary mixtures with various mole fractions were investigated. The extent of intermolecular interactions and the structure parameters of intermolecular interactions of unlike pairs formed by mixing were estimated by using the least-squares calculations. From the extent of the water-water interaction, the number of water-water hydrogen bonds in liquid mixtures was experimentally determined for the first time.