MOLECULAR DYNAMICS SIMULATION OF LIQUID MIXTURES OF BENZENE WITH CHLOROBENZENE

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A molecular dynamics method is used to simulate liquid mixtures of benzene and chlorobenzene at different concentrations. Radial angular distribution functions (RADFs) for distances between the benzene ring planes and the angle between them were calculated to analyze the structure of pure components and mixtures. In chlorobenzene, the highest RADF maximum at a distance between the mass centers of the benzene rings of about 4 Å corresponds to the stacked configurations of molecules, and at 5-7 Å the number of stacked contacts are much less than that at 4 Å and is comparable with the orthogonal ones. In liquid benzene, the number of stacked and orthogonal configurations is approximately equal in a range from 4 Å to 7 Å. RADF for benzene reveals extended regions of correlation, which gives evidence of the occurrence of agglomerates bound by specific interactions between the benzene rings. These agglomerates are not characteristic of chlorobenzene, but the presence of maxima on the radial distribution function for the distances between chlorine atoms indicates chlorine aggregation. The effect of halogen aggregation on the structure of benzene–chlorobenzene mixtures is considered. The obtained results are compared with the data on molecular light scattering.

Keywords: molecular dynamics simulation, radial angular distribution function, liquid benzene, liquid chlorobenzene, liquid benzene–chlorobenzene mixtures, chlorine aggregation.