MOLECULAR DYNAMIC SIMULATION OF THE STRUCTURE OF LIQUID CHLOROBENZENE, *ortho*-CHLOROTOLUENE, AND THEIR MIXTURES

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The molecular dynamics method is used to simulate the structure of liquid chlorobenzene, *ortho*-chlorotoluene, and their mixtures with concentrations of 0.03 ppm, 0.05 ppm, 0.1 ppm, 0.5 ppm, and 0.95 ppm chlorobenzene. Radial angular distribution functions (RADFs) were found for the distances between benzene ring planes and the angle between them in pure components and solutions. The data obtained from RADFs indicate that in the nearest environment of molecules the parallel orientation of benzene rings is the dominant configuration, while the fraction of perpendicular contacts is relatively small. In a concentration range of 0.03 ppm, 0.05 ppm, and 0.95 ppm chlorobenzene, conglomerates form with structural characteristics close to those of the dissolved substance. At a concentration of 0.1 ppm chlorobenzene, solute molecules start to agglomerate. In a concentration range from 0.15 ppm to 0.9 ppm chlorobenzene, both agglomerates and conglomerates of the same size are present in the mixture. The radial distribution functions of chlorine–chlorine distances calculated in pure components and mixtures indicate the presence of chlorine aggregates. The results obtained are compared with molecular light scattering data.

Keywords: liquid chlorobenzene, liquid *ortho*-chlorotoluene, molecular dynamics, radial angular distribution function, homo- and heteromolecular agglomerates, chlorine aggregates.