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Polarizability anisotropy relaxation in liquid binary mixtures of benzene and hexafluorobenzene BRANKA LADANYI, DOLORES ELOLA, Colorado State University — The relaxation of the many-body polarizability anisotropy in liquid binary mixtures of benzene and hexafluorobenzene was studied by molecular dynamics simulations at room temperature. Strong attractive intermolecular interactions between benzene and hexafluorobenzene molecules lead to the formation of relatively long-lived heterodimers. In this work we investigate the anisotropic nuclear response and orientational dynamics of benzene-hexafluorobenzene mixtures as a function of composition. The contribution to the collective polarizability from intermolecular interactions was included using first-order perturbation theory and calculated considering both molecule-centered and distributed site-polarizabilities. As a result of mixing, both benzene and hexafluorobenzene relaxation rates in mixtures are noticeably slower than those in the corresponding pure liquids, even at low mole fractions. The results are discussed and compared with experimental measurements performed by J. T. Fourkas and co-workers, using optical Kerr effect spectroscopy.

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