Title:	Dynamics of the mixtures of fullerene-60 and aromatic solvents: A molecular dynamics approach
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Keywords:	fullerene molecular dynamics
Issue Date:	2020
Publisher:	John Wiley & Sons, Ltd.
Citation:	Journal of Physical Organic Chemistry, 33(11)
Abstract:	The dynamics of the fullerene molecule (C60) in the different aromatic solvents has been probed using all-atom molecular dynamics simulation. For this study, the four aromatic solvents, (1) 1-chloronaphthalene, (2) 1-methylnaphthalene, (3) 1,2,4-trimethylbenzene, and (4) chlorobenzene, have been used. The 1-chloronaphthalene is important due to the high solubility (51 g/L) of the fullerene in it. The rest of the three solvents have the decreasing order of solubility. In this work, the nature of diffusion of the fullerene and the solvents are studied. It is found that if the concentration of the fullerene molecule is same in different solvents, then the hydrodynamic radius of the fullerene molecules obeys a linear relation with solubility. Hydrodynamic radius of fullerene is found to increase with a decrease in solubility. The radial distribution function of fullerene and solvents is used to calculate their relative orientation. The free energy of solvation of fullerene in these four solvents is also calculated
URI:	https://onlinelibrary.wiley.com/doi/full/10.1002/poc.4103 (https://onlinelibrary.wiley.com/doi/full/10.1002/poc.4103) http://hdl.handle.net/123456789/3245 (http://hdl.handle.net/123456789/3245)
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