

Hanna Wilczura-Wachnik · Svava Ósk Jónsdóttir

Modeling of the phase equilibria of polystyrene in methylcyclohexane with semi-empirical quantum mechanical methods I

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Due to a mistake in the numerical calculations the graph shown on Figure 4 is incorrect. The correct graph is given below. This does not affect the main results and conclusions of this paper.

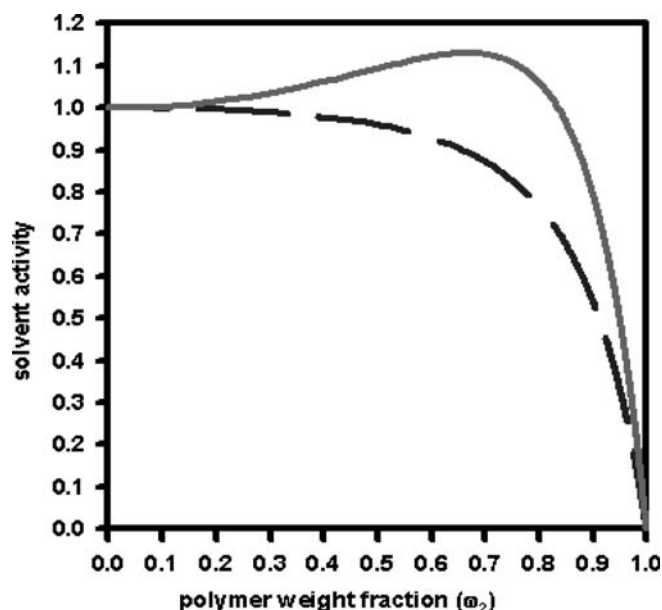


Fig. 4 Solvent activities for the methylcyclohexane(1) + polystyrene(2) system at 316K. — parameters a_{ij} obtained with the AM1 method; - - - parameters a_{ij} from VLE data for the ethylbenzene + methylcyclohexane system [28]. The abscissa is the polymer weight fraction defined as $\omega_2(x_1) = (1-x_1)M_2 / [x_1M_1 + (1-x_1)M_2]$ where x_1 is the solvent mole fraction and M_i are the molecular weights of the components

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H. Wilczura-Wachnik (✉)
The Faculty of Chemistry, Warsaw University,
Pasteura 1 Street, 02-093 Warsaw, Poland
E-mail: wilczura@alfa.chem.uw.edu.pl
Tel.: +4822 82200211

S. Ó. Jónsdóttir
Department of Chemistry,
Technical University of Denmark,
2800 Lyngby, Denmark