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NOTES

Estimation of Densities of some Polymers Based on Bisphenol–A

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The densities and the volume expansion coefficients of some polymers based on bisphenol–A have been estimated by group counting method. A close agreement between the estimated and experimental values has been observed.

Barbari *et al*[1]. have reported the densities for films of a series of polymers based on bisphenol–A *viz.*, polycarbonate, polysulfone, polyarylate, polyetherimide and polyhydroxyether using density gradient column method at 35°C. In the present work, the author has estimated theoretically the densities of these polymers using empirical formulae based on group counting model[2] and compared them with the experimental values of Barbari *et al.*[1]

The density d of a polymer can be calculated[2] as:

$$d = (K_{av}M/N_A \Sigma\Delta v_i) \quad (1)$$

where K_{av} is the packing factor of polymers whose value is 0.68 when the polymer is taken in the bulk form and 0.695 when it is taken in the form of a film, M is the molecular weight of the repeating unit, $\Sigma\Delta v_i$ is the total van der Waals' volume of the repeating unit of the polymer and N_A is the Avogadro number.

Kitaigorodskj[3] has given the van der Waals' volumes of individual atoms in different environments. Using these values in Eq. (1), the densities of polymers[2] at a 15°C have been calculated. But barbari *et al*[1]. have reported the experimental density values at 35°C. In order to convert the density estimated at 15°C to the values at 35°C, the following relation is made use of:

$$d_{T_1} = d_{T_2} [1 + \gamma(T_2 - T_1)] \quad (2)$$

where d_{T_1} and d_{T_2} are the densities at the temperatures T_1 and T_2 respectively and γ is the volume thermal expansion coefficient of the polymer. As the γ values for these polymers are not available, the author has estimated these values also using the formula of Askadskii *et al.*[4]:

$$\gamma = [(\Sigma\gamma_i\Delta v_i + \Sigma\beta_i)/\Sigma\Delta v_i] \quad (3)$$

where γ_i is the partial thermal expansion coefficient of individual atoms in the repeating unit and β_i is the parameter characterizing strong intermolecular interactions in the polymer.

The chemical structures of the polymers based on bisphenol–A are available elsewhere[1]. The densities of these polymers have been estimated at 15°C and 35°C using Eqs. (1) and (2) respectively. The values have been estimated using Eq. (3). The values of Δv_i, γ_i and β_i have been taken from the literature[2–4]. The estimated d values at 35°C have been compared with the experimental values of Barbari *et al.*[1] These values are presented in Table 1. A close agreement between the estimated and experimental values has been observed (the average per cent deviation being 1.8) thus validitating Eqns. (1) and (2).

TABLE 1
ESTIMATED AND EXPERIMENTAL DENSITIES OF POLYMERS BASED ON BISPHENOL–A AT 15°C (d_{15}) and 35°C (d_{35}) AND THEIR VOLUME EXPANSION COEFFICIENTS (γ)

Polymer	d_{15} g/cc	$\gamma(10^{-4}\ K^{-1})$	d_{35}g/cc (Est.)	d_{35} g/cc (Expt.)	% of Deviation
PC	1.227	2.69	1.221	1.200	1.7
PSF	1.278	2.42	1.271	1.240	2.5
PA	1.242	2.35	1.236	1.210	2.1
PE_i	1.310	1.92	1.304	1.280	1.9
PH	1.175	3.51	1.167	1.180	1.1

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