acta phys. slov. 43 (1993), No. 1, 27–29

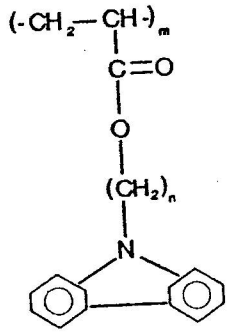
ESTIMATION OF GLASS TRANSITION TEMPERATURES OF POLYACRYLATES WITH PENDANT CARBAZOLE GROUP

A.V. Rajulu
Polymer Physics Laboratories, Sri Krishnadevaraya University, Anantapur - 515 003, India

The glass-transition temperatures of carbazole containing polyacrylates with different spacers in the side chains have been estimated using an empirical formula based on a group counting model. A good agreement between the estimated and experimental values has been observed.

Hu et al.[1] have synthesized a series of new carbazole containing polyacrylates with a different spacers in the side chains. They have determined the glass-transition temperature (T_g) of these polymers with increase in the number (n) of methylene groups and found that T_g decreases as n increases. In the present work, the author has estimated the glass-transition temperatures of these polymers using an empirical formula proposed by Askadski [2] which is based on a group counting model. The author has selected these polymers as they find wider applications in electrophoto-
graphy [1].

The structure of the polymer under study is presented below:



where n is varied from 2 to 8. The polymers with varying n are as $\underline{n}$. Films of these polymers have been cast from solutions of dichloroethane.

The glass-transition temperature (T_g) of a polymer is given [2] by:

$$T_g = \frac{\sum \Delta v_i}{\sum (a_i \Delta v_i) + \sum b_i}, \qquad (1)$$

where $\sum \Delta v_i$ is the total van der Waals volume of the repeating unit of the polymer, a_i is the coefficient characterizing the van der Waals interaction of each atom in the repeating unit and b_i is the coefficient characterizing.specific interactions such as dipolar, hydrogen bonding, para-substitution in the back-bone of the repeating unit of the polymer.

Kitaigorodski [3] has given the van der Waals volumes of individual atoms in different environments. The values of a_i and b_i have been taken from literature [2,4]. Using Eq. (1), the T_g values of the polymers 2, 3, 4, 5, 6 and 8 have been estimated. The $\sum \Delta v_i$ and $\sum a_i v_i$ values and the estimated and experimental [1] T_g values have been presented in Table 1.

Table 1

Total van der Waals volume $\sum \Delta v_i$, $\sum a_i v_i$, specific interactions $\sum b_i$ of the repeating unit, estimated (Est) and experimental (Expt.) glass transition temperature (T_g) of polyacrylates with carabazole group

$\sum \Delta v_i$ (A^3)	$\sum a_i \Delta v_i$ ($\times 10^3$ K^{-1} A^3)	$\sum b_i$ ($\times 10^3$ K^{-1} A^3)	T_g(K) Est.	Exptl.	% Deviation
250	690	-55.4	394	378	4.2
267	769	-55.4	374	352	6.2
284	849	-55.4	358	341	4.7
301	929	-55.4	345	319	8.1
319	1009	-55.4	334	315	6.0
353	1169	-55.4	316	285	10.8
				Average	6.7

Though a close agreement between the estimated and experimental values has been observed (average % deviation being 6.7), the individual % of deviation varies from 4.2 to 10.8. Generally very close agreement between the estimated and experimental values has been observed (deviation < 3%) when the polymer is taken in the bulk or melt pressed film form [5]. But in the present case, the films have been cast from dichloroethane solutions [1]. The moderately larger deviations may be due to the solute-solvent interaction as the polymer is having polar groups. Recently similar explanation has been given by Askadski and Rajulu [6] in the case of some heat resistant polymer films cast from solutions.

REFERENCES

[1] C. Hu, R. Oshima, S. Sato, M. Seno: J. Polym. Sci. Polym. Letters. *26* (1988), 441.

[2] A.A. Askadskii: in Polymer Year Book 4 Ed. R.A. Pethrick, Harwood Academic Publ., London 1987.

[3] A.I. Kitaigorodski: Organic Crystallochemistry, Academy of Science Publ., Moscow 1955.

[4] A.A. Askadskii, L.K.Kolmakova, A.A.Tager: Visokomolek. soedin Ser. A. *19* (1977), 1004.

[5] A.V. Rajulu: Chinese Chemical Society J. *(in press)*.

[6] A.A. Askadskii, A.V. Rajulu: Acta Polymerica *42* (1991), 407.

Received July 10th, 1992
Accepted for publication September 22nd, 1992