

Secondly, the  $^{19}\text{F}$  spectrum of the  $\text{CF}_3\text{COOH}$  derivative yields only a single resonance. Previous reports<sup>7,8</sup> have shown that the  $\text{CF}_3$  resonances for derivatives from the reaction of  $\text{CF}_3\text{COOH}$  and primary and secondary alcohols differ by about 0.5 ppm. Therefore, collectively the  $^1\text{H}$  and  $^{19}\text{F}$  spectra suggest a predominance of primary alcohols, >95%.

The  $^{13}\text{C}$  spectrum of sample A not only supports the above conclusions, but also yields additional data on the overall structure of the polymer chain. It is noteworthy that the spectrum is quite similar to that reported by Mochel<sup>4</sup> for polybutadiene polymerized with *n*-butyllithium. Nevertheless, extra peaks were observed in the alcohol, olefinic, and saturated  $\text{CH}_2$  and  $\text{CH}$  regions. Three primary alcohols, 64.83, 62.89, and 58.10 ppm from  $\text{Me}_4\text{Si}$  are clearly indicated and they were assigned to structures c, b, and a, respectively.

The assignments of the  $^{13}\text{C}$  resonances are substantiated by the chemical shifts of *cis*- and *trans*-3-methylalyl alcohols<sup>9</sup> and saturated primary alcohols.<sup>10</sup> The *cis* structure of this alcohol has a chemical shift of 57.9 ppm for the  $\text{CH}_2\text{OH}$  group while the *trans* structure gives rise to a value of 62.9 ppm for the corresponding group. In general, primary saturated alcohols produce resonances in the vicinity of 62 ppm. Any effect of the double bond in the vinyl structure should shift the peak downfield. Conse-

quently, the 64.83-ppm resonance was assigned to the alcoholic group of the vinyl structure.

The ratios of the three alcoholic  $^{13}\text{C}$  resonances, as determined from the uncoupled spectrum are: 24:58:18 (vinyl, *trans*, *cis*). They are in fair agreement with the  $^1\text{H}$  data and agree very well with the microstructure determined by infrared 25:55:20 (vinyl, *trans*, *cis*).

Since no other resonances are detectable in  $^{13}\text{C}$ ,  $^{19}\text{F}$ , or  $^1\text{H}$  alcohol regions, a reasonable limit of 5% secondary alcohol was established.

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- (8) G. Jung, W. Voelter, E. Breitmaier, and E. Bayer, *Anal. Chim. Acta*, **52**, 382 (1970).
- (9) J. B. Strothers, "Carbon-13 NMR Spectroscopy," Organic Chemistry—A Series of Monographs, Vol 24, Academic Press, New York, N. Y., 1972, p 188.
- (10) J. D. Roberts, F. J. Weigert, J. I. Kroschwitz, and H. J. Reich, *J. Amer. Chem. Soc.*, **92**, 1338 (1970).

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## CORRECTIONS

"Calculation of the Conformation of the Pentapeptide *cyclo*(Glycylglycylglycylprolylprolyl). III. Treatment of a Flexible Molecule," by Gregory C.-C. Niu, Nobuhiro Gō, and Harold A. Scheraga, Volume 6, Number 1, January-February 1973, page 91.

On page 93, Table ID, lines 5 through 8 in columns 2 through 6 should each be lowered by one line.

The first line at the top of the first column on page 95 should be replaced by the following: "values of  $K_\theta$  were determined from those used in the".

"Statistical Mechanics of Random-Flight Chains. IV. Size and Shape Parameters of Cyclic, Star-like, and Comb-like Chains," by Karel Šolc, Volume 6, Number 3, May-June 1973, page 378.

On page 379 the material between equations 3 and 4 should read:

Here  $\sigma^2$  is the mean square bond length and  $\mathbf{y}_k$  is the  $(N-1)$ -dimensional vector of the  $k$ th coordinates of the beads,  $\mathbf{y}_k \equiv \mathbf{x}_k^{(1)}, \mathbf{x}_k^{(2)}, \dots, \mathbf{x}_k^{(N-1)}$ . The normalization constant can be determined by integration over all coordinates: *e.g.*, for chains without any rings,  $\text{const} = 1$ , for chains containing one ring of  $N_r$  bonds,  $\text{const} = N_r^{3/2}$ ,

etc. The matrix  $\mathbf{V}$  can be set up easily for any definite structure without painful consideration of the individual bond probabilities  $p$  of eq 2 by observing the following rules. Designate the  $N-1$  freely moving beads of the macromolecule by integers from 1 to  $N-1$ , preferably in a way which results in a convenient form of the matrix  $\mathbf{V}$ . Then the matrix  $\mathbf{V}$  is made up of two kinds of contributions. (1) Each bond attached to the  $n$ th bead contributes  $1/2$  to the  $(n,n)$  element in the main diagonal of  $\mathbf{V}$  (*e.g.*, an end bead is represented by  $1/2$ , beads in the linear part of the chain by 1 and  $n$ -functional branch points by  $n/2$ ). (2) A bond connecting the  $n$ th and the  $m$ th beads contributes  $-1/2$  to the  $(n,m)$  and  $(m,n)$  elements of  $\mathbf{V}$ . The size of the symmetrical matrix  $\mathbf{V}$  is  $(N-1) \times (N-1)$  since only  $N-1$  freely moving beads have to be considered. Obviously one topological structure can be represented by many different matrices, depending upon the way of numbering the beads, and it is only the matter of convenience which way is chosen.

The symmetrical tensor of random orthogonal components  $X_{kl}$  of the square radius, referred to our coordinate system, is given by

Also on p 379 equation 10 should read:

$$\langle C^u C^v C^w \rangle = (1/6)(C_1^u C_2^v C_3^w + C_1^u C_3^v C_2^w + C_2^u C_1^v C_3^w + C_2^u C_3^v C_1^w + C_3^u C_1^v C_2^w + C_3^u C_2^v C_1^w) \quad (10)$$