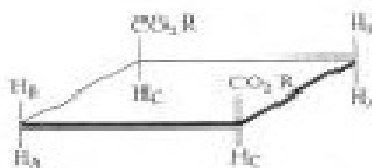


"High Resolution NMR of Macromolecules" by Frank A. Bovey, Academic Press, NY, London (1972)

SHEET-02

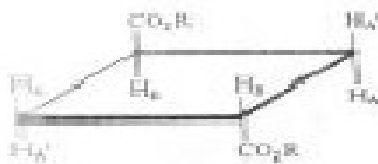


In such polymer chains (but see p. 140). Spectrum (b) in Fig. IV-1 was calculated using this model and the following parameters:

$$\begin{aligned} \tau_A &= 8.31 & \tau_B &= 7.86 & \tau_C &= 7.42 \\ J_{AB} &= -14.0 \text{ Hz} & J_{AC} &= 6.0 \text{ Hz} & J_{BC} &= 7.5 \text{ Hz} \end{aligned}$$

Line width at half-height: 2.4 Hz

In spectrum (d) the α methylene resonance appears as a poorly resolved multiplet centered at 8.16 τ . A residual resonance occurs in nearly this same position in spectrum (n). This multiplet can be satisfactorily reproduced with the following spin model parameters:



$$\begin{aligned} \tau_A &= 8.16 & \tau_B &= 7.42 \\ \frac{1}{2}(J_{AB} + J_{AB'}) &= 7.0 \text{ Hz} \\ \text{Line width at half-height} &= 2.4 \text{ Hz} \end{aligned}$$

The case of polystyrene: Experimental & simulated CH & CH₂ peaks: from the book of Bovey cited above (top of this sheet-02)

Experimental styrene PMR from SDBS database:
http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

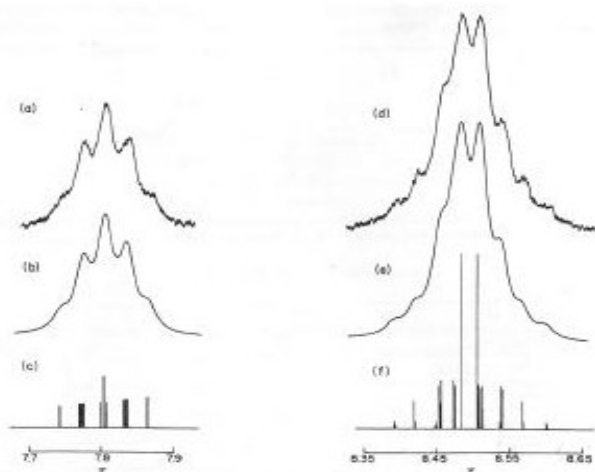
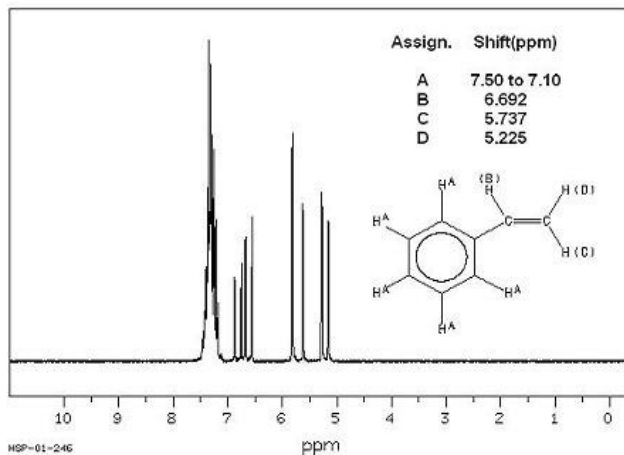


FIG. VI-3. 220 MHz backbone proton spectrum of isotactic polystyrene, 2% in *o*-dichlorobenzene at 130°. (a) and (d) are the experimental spectra of the α - and β -protons, respectively; (b) and (e) are spectra calculated with the parameters shown in Table VI-1 (for 130°); (c) and (f) are "stick" spectra corresponding to (b) and (e) (Heatley and Bovey⁷).



SDBS-1H NMR SDBS No. 3044HSP-01-246 89.56 MHz
 C8 H8 0.04 ml : 0.5 ml CDCl₃
 styrene