

Roles of Conformational Flexibility in the Crystallization of Stereo-irregular Polymer

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Table S1. T_{1C} values for all carbons for *s*-, *i*- and *a*-hPNBs at 117, 155, and 117 °C, respectively.

	C1,4	C2,3	C5,6	C7
<i>s</i> -hPNB (117°C)	291±91 (0.41±0.03) ¹	255±27 (0.37±0.12) ¹	243±23 (0.70±0.07) ¹	279±85
<i>i</i> -hPNB (155°C)	7.20±0.29 (0.85±0.06) ¹	0.52±0.02 (0.58±0.02) ¹	4.75±0.15 (0.81±0.03) ¹	7.20±0.29 (0.78±0.12) ¹
<i>a</i> -hPNB (117 °C)	1.55±0.03	1.10±0.05 (0.35±0.01) ¹	0.69±0.03	1.55± 0.03

1) T_{1C} for the amorphous region.

Table S2. ¹³C CSA principal values and isotropic chemical shift values for all carbons for *a*-hPNB at 25 °C.

	σ_{11} / ppm	σ_{22} / ppm	σ_{33} / ppm	σ_{iso} / ppm
C5,6	49.0	32.0	15.0	32.4
C2,3	51.0	44.0	17.0	37.1
C1,4	60.0	46.0	22.0	42.5
C7	64.0	45.0	23.0	44.2

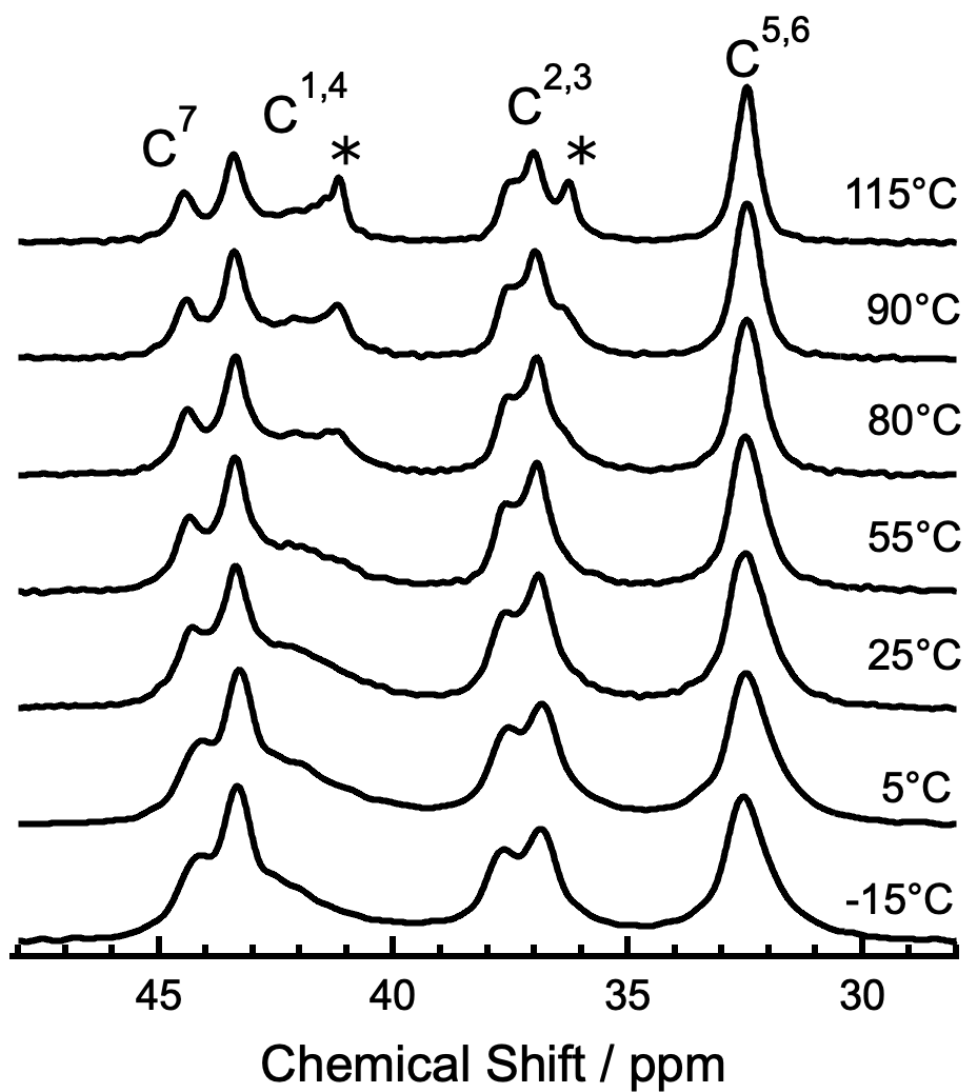


Figure S1. ^{13}C CPMAS NMR spectra for *s*-hPNB at various temperatures. * indicates signals from amorphous region.

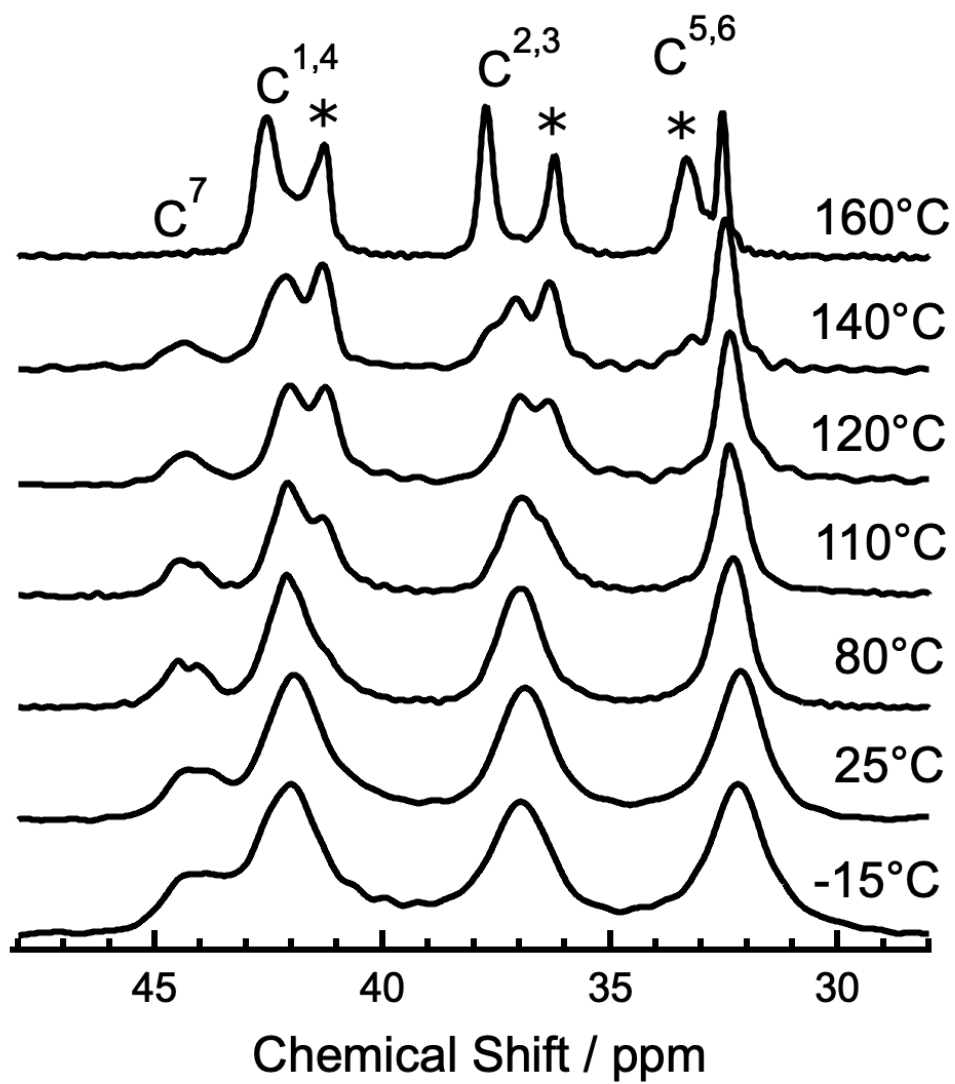


Figure S2. ^{13}C CPMAS NMR spectra for *i*-hPNB at various temperatures. * indicates signals from amorphous region.

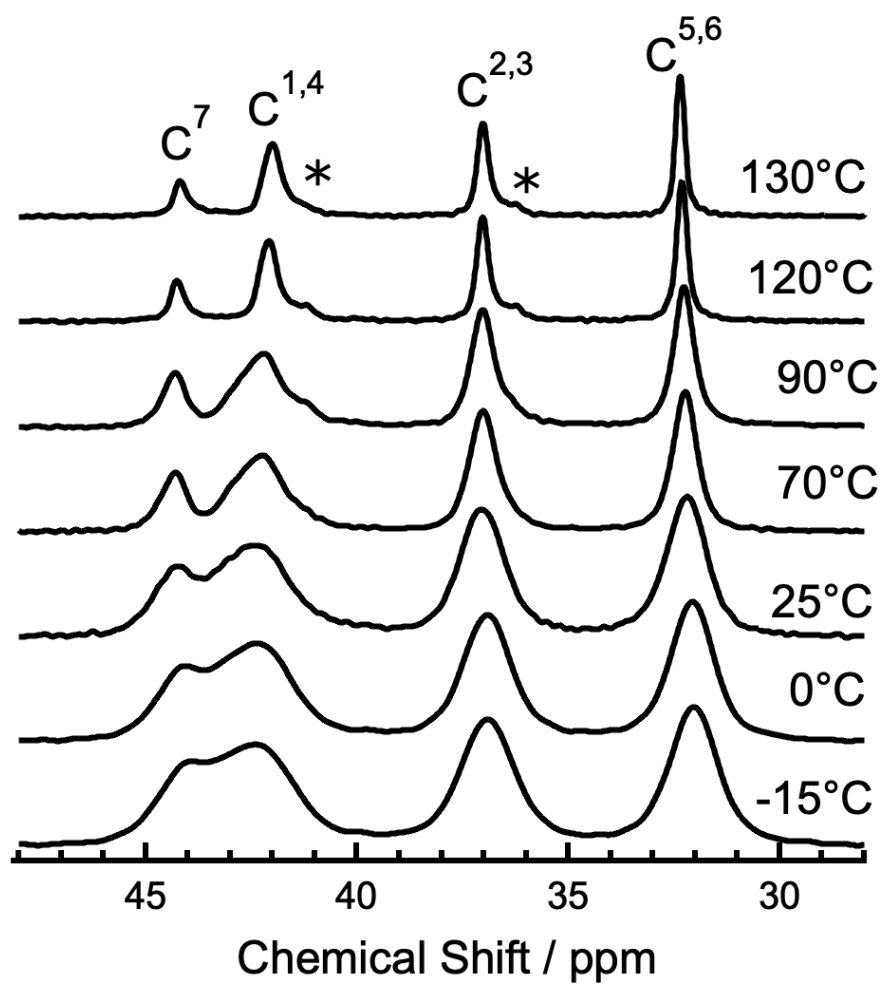


Figure S3. ^{13}C CPMAS NMR spectra for α -hPNB at various temperatures. * indicates signals from amorphous region.

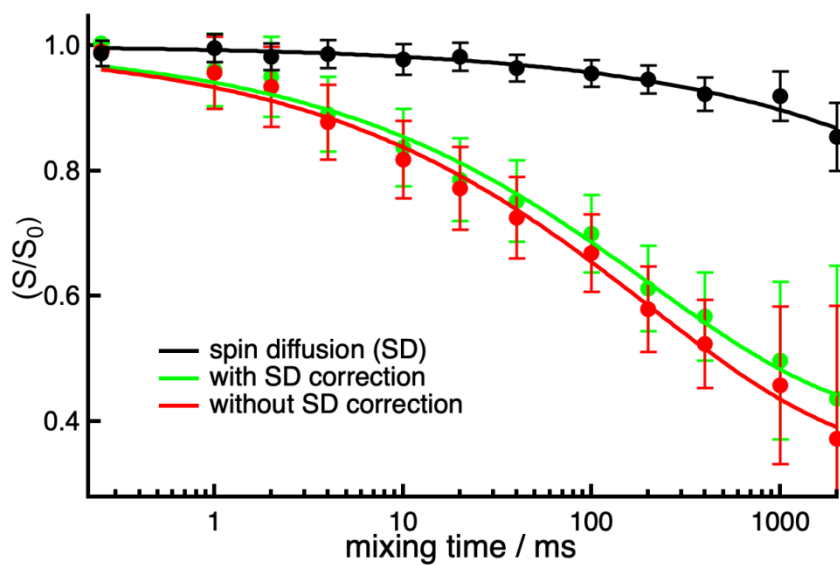


Figure S4. CODEX t_{mix} dependence for (S/S_0) for the C5,6 carbons for α -hPNBs with t_{evo} of 4.5 ms at -5°C (green circles) and at 110°C (red circles) and $(S/S_0)^*$ for the C5,6 carbons for α -hPNB after spin-diffusion correction (black circles).

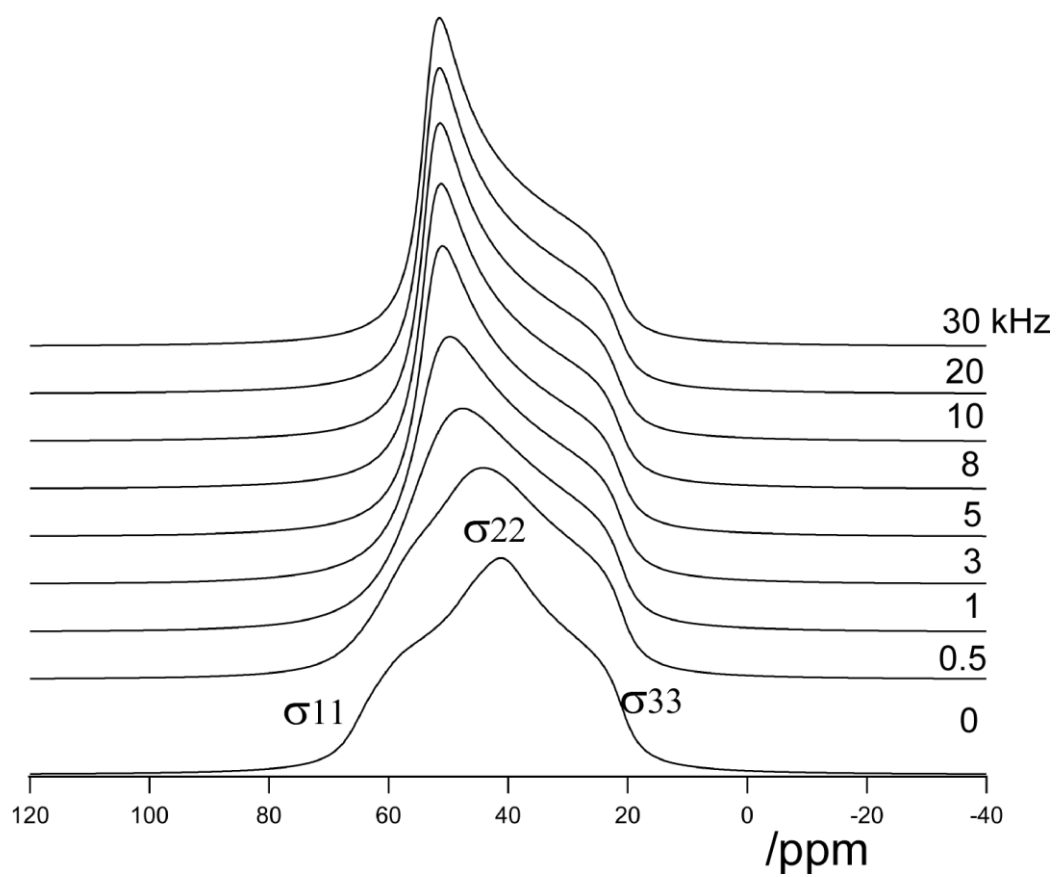


Figure S5. ^{13}C simulated CSA patterns for uniaxial rotation of C7 carbon around σ_{33} axis as a function of rotation rate, k .

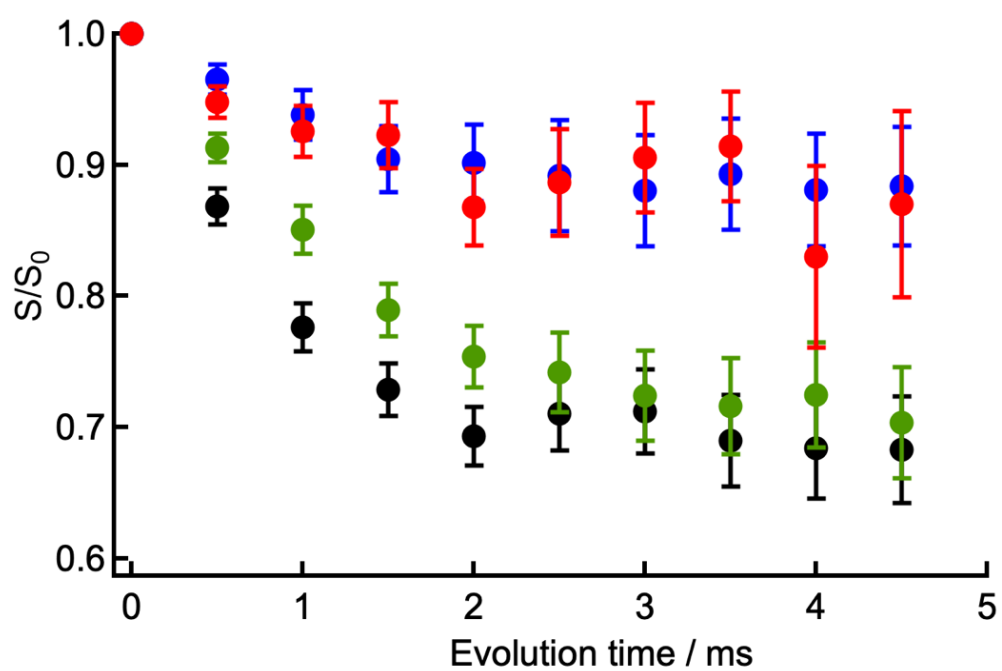


Figure S6. CODEX t_{evo} dependence of S/S_0 for C5,6 (black filled circle), C1,4 (blue), C2,3 (green), and C7 (red) of *i*-hPNB with t_{mix} of 200 ms at 135°C.

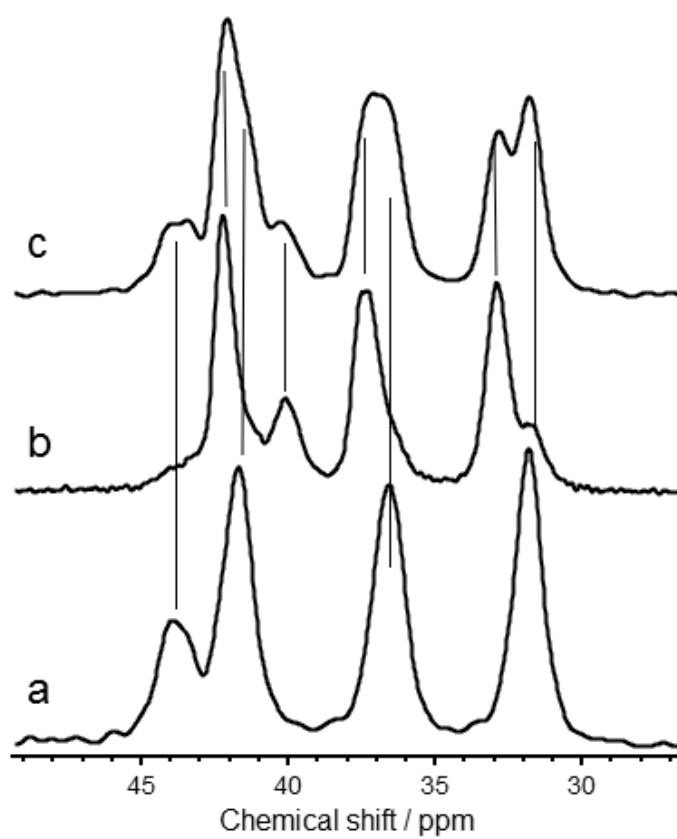


Figure S7. ^{13}C CPMAS NMR spectra with $T_{1\rho\text{H}}$ filter of 20 ms for *i*-hPNB (a) in fresh powder, (b) cooled from 155 °C, and crystallized from (c) the melt. All were measured at 25 °C.