Electronic Supplementary Information (ESI) for

From globule to crystal: a spectral study of poly(2-isopropyl-2-oxazoline) crystallization in hot water

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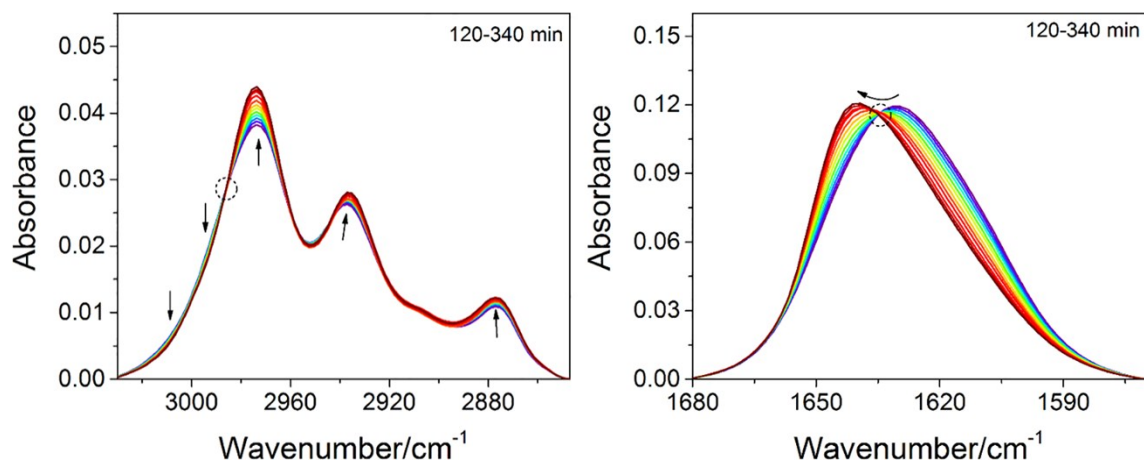
Fig. S1 Time-variable FTIR spectra of PIPOZ in D$_2$O (10 wt%) during annealing at 55 °C between

120 and 340 min. The dashed circles represent the positions of isosbestic points.

Operation Details of Sequence Order Determination from 2DCOS Results

Noda's rule can be summarized as follows: if the cross-peaks (v_1, v_2, and assume $v_1 > v_2$) in synchronous and asynchronous spectra have the same sign, the change at v_1 may occur prior to that of v_2, and vice versa. Thus, we firstly listed all the signs of cross-peaks in asynchronous spectra, then turned back to list the corresponding signs in synchronous spectra. Multiplication was performed in succession on these two signs of each cross-peak. To each final sign of cross-peaks, two corresponding wavenumbers can be found on the left and bottom respectively. Because all the signs are above the diagonal line ($v_1 = v_2$) in accordance with our spectra-reading habits, the wavenumber on the bottom is affirmatively larger than the one on the left. Therefore, according to Noda's rule, if the sign is positive (+), the larger wavenumber or the bottom wavenumber will respond to external perturbation earlier than the smaller wavenumber or the left wavenumber. Similarly, if the sign is negative (-), the left wavenumber will respond earlier than the bottom one. If the sign is zero (or blank), we cannot make an exact judgment.

The following are final results of multiplication on the signs of each cross-peak in synchronous and asynchronous spectra.

	3010	2991	2974	2937	2912	2881	2872	1655	1644	1630	1610
1610	+	+	-	-	+	-	+	+	+	-	
1630	+	+	+	+	-	+	+	+	+		
1644	+	+	-	-	+	-	+	+			
1655	+	+	-	-	+	-	-				
2872	+	+	-	-	+	-					
2881	+	+	-	-	+						
2912	+	+	-	-							
2937	+	+	+								
2974	+	+									
2991	+										
3010											

Thus we have the sequence order as follows:

3010 cm^{-1} → 2991 cm^{-1} → 2912 cm^{-1} → 1655 cm^{-1} → 2872 cm^{-1} → 1644 cm^{-1} → 1610 cm^{-1} →

2881 cm^{-1} → 2974 cm^{-1} → 2937 cm^{-1} → 1630 cm^{-1}