

Supporting Information for

Spectral Interpretation of Thermally Irreversible Recovery of Poly(*N*-isopropylacrylamide-co-acrylic acid) Hydrogel

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S1: Determination of the Sequence Order of Major Bands for 2D Analysis

As mentioned above, the sequence of major bands in hydrogel can be summarized from the multiplication of correlation intensities in 2D synchronous and asynchronous spectra according to Noda's rule.⁴³⁻⁴⁴ When the cross-peak $\{\Phi(\nu_1, \nu_2)\}$ (assuming $\nu_1 > \nu_2$) in synchronous spectra has the same symbol to the cross-peak $\{\Psi(\nu_1, \nu_2)\}$ in asynchronous spectra, the response at band ν_1 should be prior to or earlier than that at band ν_2 and vice versa.

	2987	2970	2943	2931	2927	2899	2883	2873	1728	1720	1713	1691	1687	1684	1653	1624	1601
2987	-	+	+	-	-	+	-	-	-	-	-	+	+	+	-	+	+
2970		+	+	-	-	+	+	+	+	+	+	+	+	+	+	+	+
2943			+	-	-	+	-	-	-	-	-	-	+	+	-	+	+
2931				-	-	-	-	-	-	-	-	-	-	-	-	-	-
2927					+	+	+	+	+	+	+	+	+	+	+	+	+
2899						+	+	+	+	+	+	+	+	+	+	+	+
2883							-	-	-	-	-	-	-	-	-	-	-
2873								-	-	-	-	+	+	+	+	+	+
1728	2927	2899	2970	2873	2987	2943	2883	2931		+	+	+	+	+	+	+	+
1720										+	+	+	+	+	+	+	+
1713											-	+	+	+	+	+	+
1691												+	+	+	+	+	+
1687													+	+	-	+	+
1684														+	-	+	-
1653									1728	1713	1720	1691	1687	1684		+	+
1624																	-
1601																	
															1653	1601	1624
	2927	2899	2970	1728	1713	1720	2873	1653	2987	1691	2943	1687	1601	1684	1624	2883	2931

Figure S1. Operation details of the sequence order determination in PNIPAM-co-AA hydrogel based on calculated results of 2D spectra during heating.

	2989	2974	2968	2943	2939	2931	2926	2893	2885	2873	2848	1728	1714	1705	1699	1693	1687	1684	1655	1643	1639	1622	1605				
2989	+	-	+	+	+	+	+	+	+	-	+	+	-	+	-	-	+	+	-	+	+	-	+				
2974		-	-	-	-	-	+	-	-	-	+	-	-	-	-	-	-	-	-	+	-	-	-				
2968			+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+				
2943				+	+	+	+	+	+	-	+	+	-	-	-	-	-	-	-	+	-	-	-				
2939					+	+	+	+	+	-	+	+	-	-	-	-	-	-	-	+	-	-	-				
2931						+	-	-	-	-	+	-	-	-	-	-	-	-	-	+	-	-	-				
2926							-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-				
2893								-	-	+	-	-	-	-	-	-	-	-	-	+	-	-	-				
2885									-	+	+	-	-	-	-	-	-	-	-	+	-	-	-				
2873											+	+	+	+	+	+	+	+	+	+	+	+	+				
2848	2968	2873	2989	2943	2939	2885	2893	2931	2974	2848	2926	-	-	-	-	-	-	-	-	+	-	-	-				
1728												-	-	-	-	-	-	-	-	+	-	-	-				
1714													+	-	+	+	+	+	+	+	+	+	+				
1705														-	-	+	-	-	+	+	-	-	-				
1699															+	+	+	+	+	+	+	+	+				
1693																+	+	-	+	+	-	+					
1687																	-	-	+	+	-	-					
1684												1699	1693	1714	1684	1705	1687	1728	-	+	+	-	+				
1655																				+	+	+	+				
1643																					-	-	-				
1639																						-	-				
1622																							+				
1605																							1655	1622	1605	1639	1643
	2968	2873	1655	1622	1699	1693	1714	2989	1684	1605	1705	1687	1639	2943	2939	2885	2893	1728	2931	2974	2848	1643	2926				

Figure S2. Operation details of the sequence order determination in PNIPAM-co-AA hydrogel based on calculated results of 2D spectra during cooling.