Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Discrimination between Coupling Networks of Glucopyranosides Varying at a Single Stereocenter Using Two-Dimensional Vibrational Correlation Spectroscopy

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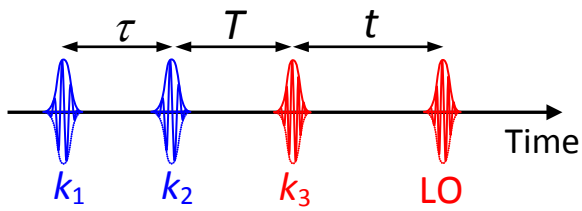

Fig. S1. Experimental pulse sequence and the time-delay notation.

Table S1. Scaling factors of the frequencies of the computed transitions used to match the computed and experimental spectra of both anomers.

Mode #	α anomer	β anomer
50-69	0.963	0.986
70-80	1.012	1.012
81-105	0.979	0.979
106-109	0.9582	0.9582

Table S2. Widths of computed transitions used to match the computed and experimental spectra of both anomers.

Mode #	Width / cm^{-1}	Mode #	Width / cm^{-1}	Mode #	Width / cm^{-1}
56	10	75	12	93	16
57	12	76	17	94	14
58	13	77	17	95	12
59	12	78	19	96	12
60	12	79	16	97	12
61	12	80	12	98	12
62	12	81	12	99	12
63	12	82	30	100	12
64	12	83	30	101	12
65	12	84	30	102	12
66	12	85	30	103	12
67	12	86	30	104	12
68	12	87	30	105	12
69	10	88	30	106	30
70	17	89	10	107	30
71	17	90	10	108	20
72	12	91	14	109	21
73	15.5	92	16		
74	16.5	93	16		