SUPPLEMENTARY MATERIAL

^{13}C chemical shifts in saccharides in the solid state: a density functional theory study

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TABLE S1 Calculated chemical shifts for monosaccharides, using a reference value of 168.1 ppm.

name/site (ppm)	C_1	C_2	C_3	C_4	C_5	C_6
Fructose	104.91	67.69	68.43	72.17	65.67	64.56
α-Glucose	96.38	69.41	71.63	72.9	71.52	63.54
α-Glucose monohydrate	96.37	69.99	72.19	69.66	72.12	59.88
β-Glucose	98.93	76.39	74.54	70.25	74.55	61.39
α-galactose	95.42	70.64	70.05	70.97	69.05	57.47
β-galactose	102.02	69.99	74.68	68.59	74.37	60.17

TABLE S2 Calculated chemical shifts for monosaccharides using a reference value of 156 ppm.

name/site (ppm)	C_1	C_2	C_3	C_4	C_5	C_6
Fructose	92.81	55.59	56.33	60.07	53.57	52.46
α-D-Glucose	84.28	57.31	59.53	60.80	59.42	51.44
α-D-Glucose monohydrate	85.84.27	57.89	60.09	57.56	60.02	47.78
β-D-Glucose	86.83	64.29	62.44	58.15	62.45	49.29
α-D-galactose	83.32	58.54	57.95	58.87	56.95	45.37
β-D-galactose	89.92	57.89	62.58	56.49	62.27	48.07

TABLE S3 Calculated chemical shifts for monosaccharides, using the linear regression technique.

name/site (ppm)	C_1	C_2	C_3	C_4	C_5	C_6
Fructose	100.77	67.84	68.49	71.80	66.05	65.07
α-Glucose	93.22	69.36	71.32	72.45	71.23	64.17
α-Glucose monohydrate	93.21	69.87	71.82	69.58	71.76	60.93
β-Glucose	95.48	75.53	73.90	70.10	73.91	62.26
α-galactose	92.37	70.45	69.93	70.74	69.04	58.79
β-galactose	98.21	69.87	74.02	68.63	73.75	61.18