Supplementary material

For the paper entitled

A neutron diffraction study of xylitol:
Mean square internal vibrations for hydrogen atoms
derived from a rigid body description

Table 1: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the methyl α-D-lyxofuranoside neutron diffraction experiment [1]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1	63(11)	127	175	13.0	59	13.6	142	12.2	155
H2	67(10)	123	174	8.7	65	26.2	184	27.2	116
H3	48(12)	104	171	12.4	44	14.3	152	17.5	140
H4	50(9)	113	175	2.5	50	43.6	143	43.6	172
H5A	61(10)	134	202	13.0	52	7.3	141	12.7	255
H5B	63(12)	126	209	11.0	56	5.5	132	9.9	296
H15	24(10)	112	145	7.9	23	23.5	115	23.6	72
H13	29(9)	76	138	9.7	28	42.5	120	42.7	54
H12	42(10)	93	138	16.9	36	29.8	117	25.7	80
H6A	43(14)	130	251	4.1	42	3.0	332	3.5	162
H6B	36(20)	155	280	4.1	35	7.9	458	8.4	172
H6C	62(18)	159	268	17.7	51	3.6	334	17.5	165

Table 2: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the methyl β-D-arabinofuranoside neutron diffraction experiment [1]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1	45(13)	112	179	8.2	43	17.5	152	15.5	135
H2	66(14)	118	172	12.5	62	15.1	143	9.7	132
H3	92(14)	142	177	36.5	88	17.1	190	39.3	101
H4	75(12)	137	181	33.5	42	36.1	133	43.3	167
H5A	89(16)	150	207	13.4	83	23.5	129	26.8	208
H5B	63(15)	161	223	10.2	59	11.5	176	5.3	233
H15	68(16)	137	206	8.2	67	39.5	160	39.2	136
H13	49(23)	120	187	15.8	40	29.8	208	33.1	156
H12	67(23)	137	176	23.5	58	16.4	182	26.8	105
H6A	35(22)	147	258	17.6	23	15.7	328	23.6	143
H6B	48(15)	155	267	12.5	37	17.2	331	15.8	220
H6C	49(22)	160	274	8.2	42	17.5	375	15.9	149

Table 3: Analysis of residual root mean square displacements [10^{-4}Å^2] from tha TLS analysis of the maleate ion in sodium hydrogen maleate trihydrate neutron diffraction experiment [4]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system. The residual mean square displacements for the hydrogen atoms in the water molecules have been obtained by subtracting the corresponding water oxygen mean square displacements.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1	121(6)	217	241	34.3	129	40.6	113	38.1	99
H2	58(5)	150	291	7.9	57	11.6	159	13.7	129
H3	65(4)	171	296	16.2	59	18.1	153	17.6	128
H11	61(6)	193	294	8.5	58	29.3	190	28.9	218
H12	59(5)	218	310	3.6	58	11.8	231	12.3	218
H21	65(5)	202	272	7.0	63	10.9	184	8.4	161
H22	70(7)	190	275	8.2	68	10.4	190	12.5	164
H31	57(6)	179	283	5.1	56	13.0	227	12.4	179
H32	83(6)	219	274	9.0	81	20.0	174	21.4	160

Table 4: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the methylammonium hydrogen succinate (MAHS) neutron diffraction experiment [2]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1	204(47)	317	368	13.9	195	41.6	364	40.2	115
H2	63(13)	276	375	5.5	60	26.5	109	27.1	345
H3	59(12)	262	356	10.5	53	18.8	152	21.5	256
H6	50(15)	284	466	13.3	39	2.3	567	13.3	237
H7	32(21)	288	479	14.8	8	0.0	474	14.8	386
H4	20(6)	172	251	2.6	20	40.8	124	40.8	147
H5	51(10)	210	258	3.2	50	0.0	152	3.2	102
D8	5(8)	201	287	35.2	-4	35.2	23	0.6	0

Table 5: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the D-glucitol neutron diffraction experiment [6]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1A	77(102)	295	415	28.8	1	12.8	235	30.7	328
H1B	-12(90)	220	396	20.3	-44	21.6	191	13.7	516
H2	131(79)	275	344	36.2	74	40.5	113	36.3	305
H3	100(75)	272	341	41.9	-22	42.2	259	24.9	168
H4	75(70)	205	334	29.3	22	33.1	196	38.2	305
H5	73(70)	254	359	38.7	16	39.1	85	45.8	281
H6A	122(76)	377	450	43.6	24	46.8	153	29.8	365
H6B	81(96)	363	450	44.7	-142	41.9	481	48.6	481
H11	19(90)	335	432	31.7	-81	28.9	226	28.5	314
H12	15(80)	275	408	25.4	-18	1.4	392	25.4	163
H13	142(73)	349	379	44.9	117	43.9	-109	47.9	-109
H14	111(88)	349	364	49.4	167	30.3	223	41.3	167
H15	61(87)	391	425	31.5	30	46.8	244	45.5	115
H16	98(92)	397	368	33.3	58	47.6	-206	42.5	-206

Table 6: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the potassium-D-gluconate A-form [5]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H2	32(23)	233	363	5.1	31	24.7	141	24.8	187
H3	53(24)	235	327	34.0	12	35.3	138	18.2	257
H4	23(27)	232	369	19.6	4	21.2	163	8.9	306
H5	5(27)	257	381	18.1	-23	41.1	110	39.6	346
H6A	145(36)	577	536	31.0	9	12.4	183	28.5	575
H6B	99(42)	361	571	17.3	74	16.0	147	13.6	812
H12	30(29)	369	437	13.5	22	18.0	310	22.0	137
H13	6(22)	232	331	11.3	2	31.5	67	32.8	136
H14	91(29)	297	389	13.6	90	25.9	206	25.8	64
H15	-0(25)	306	408	17.5	-29	46.1	293	42.2	191
H16	121(33)	483	480	48.8	136	29.5	-200	38.1	285

Table 7: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the potassium-D-gluconate B-form [5]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H2	24(19)	165	266	10.4	16	10.0	137	12.0	298
H3	58(14)	241	291	10.3	54	14.2	143	13.0	241
H4	40(16)	202	269	20.5	25	20.4	129	24.0	162
H5	74(21)	235	323	13.2	67	17.0	204	11.6	285
H6A	159(30)	316	385	33.7	71	24.3	157	29.0	435
H6B	31(22)	242	423	9.3	12	1.5	225	9.2	724
H12	74(19)	251	331	41.8	128	13.0	305	43.7	-6
H13	29(5)	219	344	12.3	21	18.0	193	21.3	211
H14	49(21)	278	315	20.3	33	14.5	192	16.2	148
H15	151(22)	351	335	43.9	186	46.2	186	43.1	23
H16	44(20)	272	338	9.3	41	24.4	76	24.1	205

Table 8: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the α-L-Xylopyranose neutron diffraction experiment [3]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1	60(8)	159	266	34.2	35	32.6	108	13.5	177
H2	49(8)	161	245	20.0	35	13.2	199	15.9	126
H3	44(8)	167	231	9.8	40	33.4	164	34.7	148
H4	35(8)	154	254	4.9	34	10.7	116	11.6	180
H5	66(9)	273	297	17.9	51	9.9	132	18.1	232
H6	68(10)	174	321	24.4	52	33.0	107	26.2	210
H7	26(7)	134	218	16.2	29	15.2	-106	18.1	58
H8	15(7)	145	190	33.8	44	30.0	-110	26.4	99
H9	22(6)	130	218	17.8	19	9.9	-75	19.0	71
H10	31(7)	161	210	26.8	41	26.3	-95	27.8	126

Table 9: Analysis of residual root mean square displacements [10^{-4}Å^2] from the TLS analysis of the β-L-arabinopyranose neutron diffraction experiment [3]. The total and residual MSDs in the X-H direction and the U_{iso} calculated as suggested by Stewart [7] are listed in the section to the left. The eigenvalues of the residual MSD matrix are listed with the angle between the corresponding eigenvector and the closest axis in the local atomic coordinate system.

				Eigenvalues of the residual MSD matrix					
	$\langle u^2 \rangle$ in X-H direction			bond-direction		out-of-plane		in-plane	
atom	residual	total	U_{iso}	angle	value	angle	value	angle	value
H1	51	140	228	6.0	50	6.8	122	5.4	153
H2	64	152	214	8.3	63	4.1	152	9.2	116
H3	50	138	210	3.2	50	2.6	136	3.9	143
H4	52	141	265	1.6	52	24.7	107	24.7	165
H5	59	153	283	4.9	59	4.9	122	5.0	146
H6	44	215	262	5.2	43	6.5	142	5.8	181
H7	35	109	192	34.1	25	53.1	43	44.2	66
H8	24	129	183	52.6	-17	36.8	66	37.1	33
H9	39	148	201	9.8	38	7.1	-17	11.8	75
H10	31	154	266	40.3	-21	50.1	-21	42.6	159

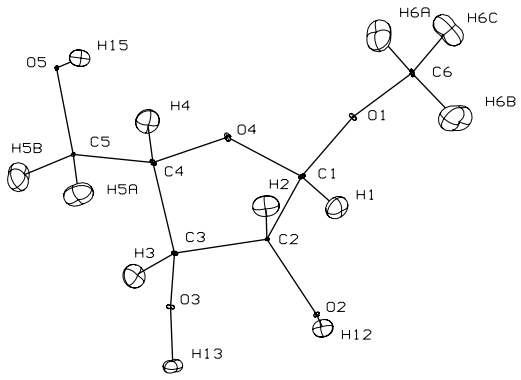


Figure 1: PEANUT plot of the methyl-α-D lyxofuranoside neutron experiment TLS refinement difference RMSD surface ($U_{obs} - U_{calc}$) (scale: 1.54).

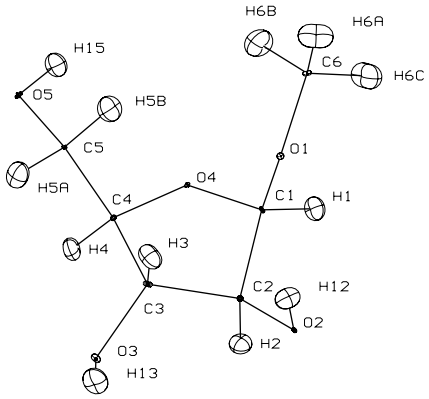


Figure 2: PEANUT plot of the methyl-β-D arabinofuranoside neutron experiment TLS refinement difference RMSD surface ($U_{obs} - U_{calc}$) (scale: 1.54).

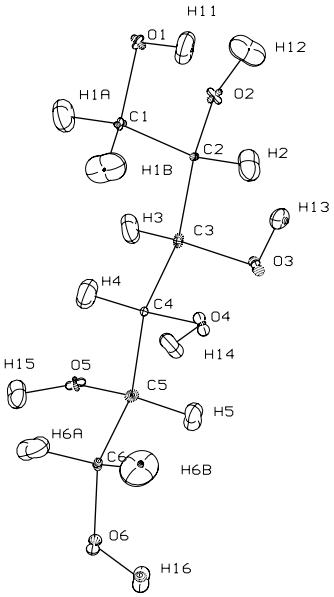


Figure 3: PEANUT plot of the D-glucitol neutron experiment TLS refinement difference RMSD surface ($U_{obs} - U_{calc}$) (scale: 1.54).

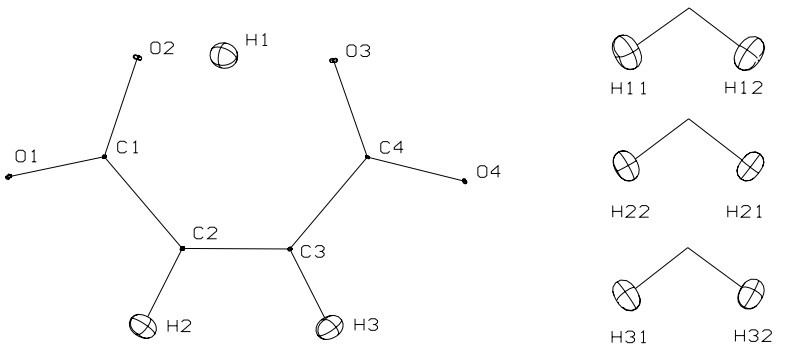


Figure 4: PEANUT plot of sodium hydrogenmaleate trihydrate difference RMSD surfaces (scale: 1.54). The residual mean square displacements for the water hydrogen atoms have been obtained by subtraction of the corresponding oxygen mean square displacements.

Figure 5: PEANUT plot of the Potassium D-gluconate (A- and B-forms) neutron experiment TLS refinement difference RMSD surface ($U_{obs} - U_{calc}$) (scale: 1.54). Only the gluconate molecule is shown.

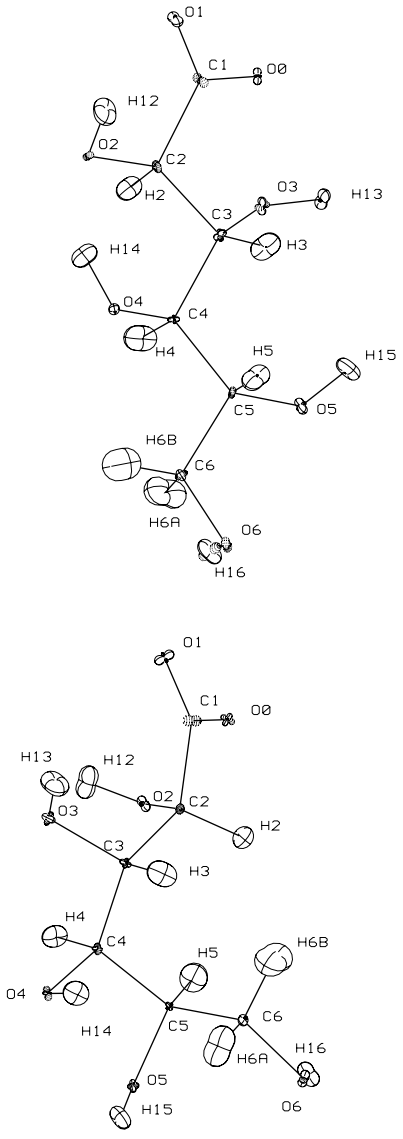
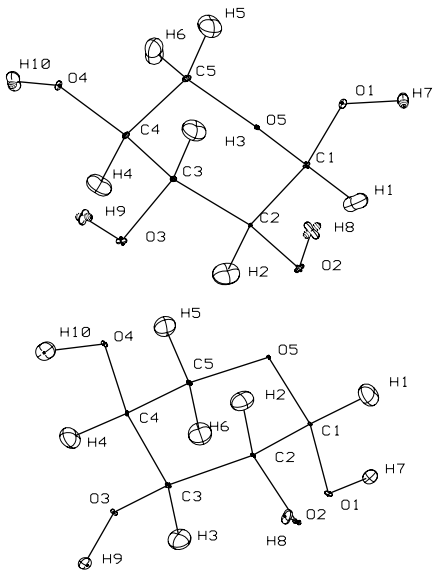


Figure 6: PEANUT plots of the α-L-xylopyranose and β-L-arabinopyranose neutron experiment TLS refinements. Difference RMSD surfaces ($U_{obs} - U_{calc}$) (scale: 1.54).



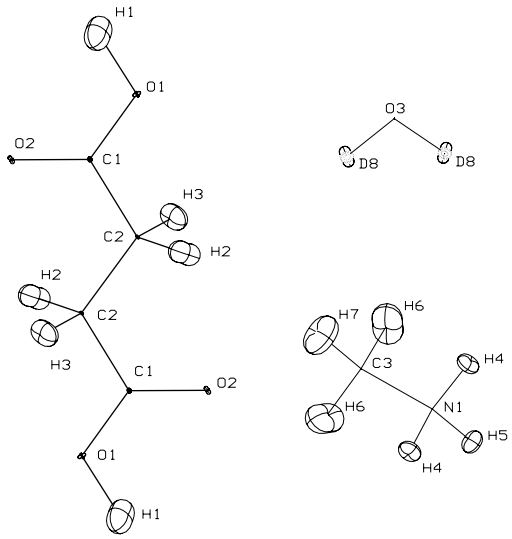


Figure 7: PEANUT plot of methylammonium hydrogen succinate neutron experiment TLS refinement. Difference RMSD surfaces ($U_{obs} - U_{calc}$) (scale: 1.54).

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