SUPPLEMENTARY MATERIAL

Reduced atomic coordinates for Γsorbitol.

	x	*y*	*z*
C11	0.3647 (1)	0.5124 (2)	0.6125 (10)
C12	0.4188 (1)	0.5035 (1)	0.4570 (7)
C13	0.4160 (1)	0.4403 (1)	0.2907 (6)
C14	0.4226 (1)	0.3800 (1)	0.4712 (7)
C15	0.4170 (2)	0.3159 (1)	0.3152 (7)
C16	0.4228 (2)	0.2534 (2)	0.4798 (10)
O11	0.3695 (1)	0.5698 (1)	0.7773 (7)
O12	0.4236 (2)	0.5581 (2)	0.2784 (7)
O13	0.4622 (1)	0.4428 (2)	0.1099 (8)
O14	0.4746 (1)	0.3794 (2)	0.6094 (8)
O15	0.3708 (1)	0.3170 (2)	0.1344 (7)
O16	0.3791 (1)	0.2556 (2)	0.6723 (7)
C21	0.1019 (1)	0.2208 (2)	0.3416 (9)
C22	0.0769 (1)	0.2790 (2)	0.1978 (7)
C23	0.1191 (1)	0.3147 (2)	0.0233 (7)
C24	0.1630 (1)	0.3494 (2)	0.1958 (7)
C25	0.2080 (1)	0.3795 (2)	0.0202 (7)
C26	0.2533 (2)	0.4122 (2)	0.1870 (10)
O21	0.0646 (1)	0.1935 (2)	0.5354 (7)
O22	0.0316 (1)	0.2572 (2)	0.0365 (7)
O23	0.0911 (1)	0.3611 (2)	-0.1472 (7)
O24	0.1395 (1)	0.4015 (1)	0.3502 (7)
O25	0.2329 (2)	0.3299 (2)	-0.1452 (8)
O26	0.2781 (2)	0.3662 (1)	0.3701 (8)
C31	0.4478 (2)	0.1069 (2)	0.9420 (12)
C32	0.4140 (1)	0.0520 (2)	0.8158 (7)
C33	0.3634 (1)	0.0765 (2)	0.6578 (7)
C34	0.3161 (1)	0.1047 (2)	0.8290 (7)
C35	0.2692 (1)	0.1322 (2)	0.6570 (7)
C36	0.2230 (1)	0.1562 (2)	0.8399 (9)
O31	0.4893 (1)	0.0791 (2)	1.1122 (8)
O32	0.4524 (1)	0.0260 (2)	0.6236 (7)
O33	0.3470 (2)	0.0292 (2)	0.4592 (7)
O34	0.2937 (1)	0.0507 (2)	0.9758 (9)
O35	0.2905 (1)	0.1845 (2)	0.5000 (9)
O36	0.2412 (2)	0.2022 (2)	1.0400 (8)

Bond lengths (Å) for Γsorbitol.

	Molecule 1	Molecule 2	Molecule 3
Ci1–Ci2	1.527 (5)	1.515 (5)	1.526 (5)
Ci2–Ci3	1.533 (4)	1.520 (4)	1.536 (4)
Ci3–Ci4	1.528 (4)	1.534 (4)	1.532 (4)
Ci4–Ci5	1.529 (4)	1.521 (4)	1.524 (4)
Ci5–Ci6	1.520 (5)	1.523 (5)	1.514 (5)
Ci1–Oi1	1.432 (5)	1.424 (5)	1.425 (6)
Ci2–Oi2	1.426 (4)	1.424 (4)	1.426 (4)
Ci3–Oi3	1.427 (5)	1.435 (5)	1.428 (5)
Ci4–Oi4	1.430 (4)	1.427 (4)	1.429 (5)
Ci5–Oi5	1.426 (5)	1.433 (5)	1.420 (5)
Ci6–Oi6	1.418 (6)	1.433 (5)	1.428 (6)
Ci1–Hi1A	0.998	0.993	0.999
Ci1–Hi1B	1.007	1.007	1.002
Ci2–Hi2	1.001	1.001	1.000
Ci3–Hi3	1.000	0.999	0.999
Ci4–Hi4	1.001	1.000	1.000
Ci5–Hi5	1.000	1.000	0.999
Ci6–Hi6A	0.998	0.999	1.001
Ci6–Hi6B	1.001	1.002	0.999
Oi1–HOi1	0.951	0.810	0.878
Oi2–HOi2	0.729	1.021	1.093
Oi3–HOi3	0.807	0.791	0.814
Oi4–HOi4	0.783	0.779	0.739
Oi5–HOi5	0.880	0.737	0.770
Oi6–HOi6	0.823	0.806	0.845

Bond angles (°) for Γsorbitol.

	Molecule 1	Molecule 2	Molecule 3
Ci2–Ci1–Oi1	107.9 (3)	111.4 (4)	108.6 (4)
Ci2–Ci1–Hi1A	110.2	109.6	109.8
Ci2–Ci1–Hi1B	109.6	108.8	109.7
Oi1–Ci1–Hi1A	110.6	109.6	110.0
Oi1–Ci1–Hi1B	109.8	108.6	109.8

Hi1A–Ci1–Hi1B	108.8	108.9	109.0
Ci1–Ci2–Ci3	109.0 (3)	111.8 (3)	112.9 (3)
Ci1–Ci2–Oi2	106.2 (3)	108.4 (3)	100.8 (3)
Ci1–Ci2–Hi2	110.5	108.5	111.3
Ci3–Ci2–Oi2	110.5 (2)	111.4 (2)	108.6 (2)
Ci3–Ci2–Hi2	110.2	108.4	111.3
Oi2–Ci2–Hi2	110.3	108.4	111.3
Ci2–Ci3–Ci4	112.3 (2)	112.8 (2)	116.9 (2)
Ci2–Ci3–Oi3	105.1 (3)	109.0 (3)	109.7 (3)
Ci2–Ci3–Hi3	110.5	108.4	104.7
Ci4–Ci3–Oi3	107.5 (3)	109.7 (3)	114.7 (3)
Ci4–Ci3–Hi3	110.6	108.4	104.6
Oi3–Ci3–Hi3	110.6	108.4	104.8
Ci3–Ci4–Ci5	113.9 (2)	112.5 (2)	113.8 (2)
Ci3–Ci4–Oi4	111.7 (3)	111.1 (3)	105.3 (3)
Ci3–Ci4–Hi4	107.7	109.0	110.6
Ci5–Ci4–Oi4	107.7 (3)	106.1 (3)	106.0 (3)
Ci5–Ci4–Hi4	107.8	109.0	110.4
Oi4–Ci4–Hi4	107.8	109.0	110.4
Ci4–Ci5–Ci6	117.3 (2)	113.6 (3)	110.7 (2)
Ci4–Ci5–Oi5	111.2 (3)	109.2 (3)	107.6 (3)
Ci4–Ci5–Hi5	104.1	108.7	109.5
Ci6–Ci5–Oi5	114.4 (3)	108.0 (3)	109.8 (3)
Ci6–Ci5–Hi5	104.0	108.6	109.6
Oi5–Ci5–Hi5	103.9	108.5	109.6
Ci5–Ci6–Oi6	104.6 (3)	110.1 (4)	112.9 (4)
Ci5–Ci6–Hi6A	110.9	109.5	108.7
Ci5–Ci6–Hi6B	110.7	109.4	108.7
Oi6–Ci6–Hi6A	110.8	109.6	108.7
Oi6–Ci6–Hi6B	110.7	109.3	108.8
Hi6A–Ci6–Hi6B	109.1	108.8	109.0
Ci1–Oi1–HOi1	99.4	118.4	116.8
Ci2–Oi2–HOi2	100.7	107.0	115.4
Ci3–Oi3–HOi3	115.8	100.8	111.1
Ci4–Oi4–HOi4	108.5	140.8	102.7
Ci5–Oi5–HOi5	118.1	102.5	109.9
Ci6–Oi6–HOi6	114.6	104.9	104.5

Calculated torsion angles (°) for Γsorbitol.

	Molecule 1	Molecule 2	Molecule 3
Ci1-Ci2-Ci3-Ci4	-75.4 (3)	-69.0 (3)	-70.6 (4)
Ci2-Ci3-Ci4-Ci5	176.9 (3)	174.5 (2)	176.1 (3)
Ci3-Ci4-Ci5-Ci6	-179.8 (3)	-177.9 (3)	177.4 (3)
Oi1-Ci1-Ci2-Ci3	176.9 (3)	171.3 (3)	172.6 (3)
Oi2-Ci2-Ci3-Ci4	168.3 (3)	169.6 (3)	178.4 (3)
Oi3-Ci3-Ci4-Ci5	-68.0 (3)	-63.8 (3)	-53.4 (4)
Ci1-Ci2-Ci3-Oi3	168.0 (3)	169.0 (3)	156.6 (3)
Oi4-Ci4-Ci5-Ci6	55.6 (4)	60.4 (4)	62.1 (4)
Ci2-Ci3-Ci4-Oi4	-60.8 (3)	-66.7 (3)	-68.3 (3)
Ci3-Ci4-Ci5-Oi5	-45.4 (4)	-57.3 (3)	-62.6 (3)
Ci4-Ci5-Ci6-Oi6	62.0 (4)	58.3 (4)	54.7 (4)
Oi1-Ci1-Ci2-Oi2	-64.0 (4)	-65.5 (4)	-71.7 (4)
Oi2-Ci2-Ci3-Oi3	51.7 (3)	47.6 (4)	45.6 (4)
Oi3-Ci3-Ci4-Oi4	54.4 (3)	55.0 (3)	62.3 (4)
Oi4-Ci4-Ci5-Oi5	-170.0 (3)	-179.0 (3)	-177.8 (3)
Oi5-Ci5-Ci6-Oi6	-71.0 (4)	-63.0 (4)	-64.0 (4)