

# SUPPLEMENTARY MATERIAL

## Reduced atomic coordinates for the stable anhydrous phase of $\alpha$ -lactose.

	First molecule			Second molecule		
	x	y	z	x	y	z
Ci1	0.4157 (11)	0.5519 (4)	0.824 (3)	0.4100 (11)	0.0719 (4)	0.593 (3)
Ci2	0.2271 (11)	0.5730 (4)	0.812 (3)	0.5985 (10)	0.1012 (4)	0.568 (3)
Ci3	0.2221 (11)	0.6383 (4)	0.662 (3)	0.6131 (11)	0.1781 (4)	0.593 (4)
Ci4	0.3910 (11)	0.6908 (6)	0.783 (2)	0.4474 (11)	0.2071 (7)	0.409 (2)
Ci5	0.5698 (11)	0.6604 (4)	0.844 (3)	0.2664 (11)	0.1668 (4)	0.410 (3)
Ci6	0.7358 (12)	0.7119 (6)	0.978 (5)	0.0976 (12)	0.1913 (7)	0.220 (4)
Oi1	0.4130 (16)	0.4922 (5)	0.970 (3)	0.3980	0.0007	0.589
Oi2	0.0724 (14)	0.5241 (6)	0.666 (3)	0.7538 (17)	0.0781 (7)	0.760 (3)
Oi3	0.0613 (15)	0.6709 (7)	0.624 (3)	0.7820 (13)	0.2143 (7)	0.579 (3)
Oi4	0.3914 (18)	0.7197 (7)	1.047 (2)	0.4561 (19)	0.2065 (7)	0.128 (2)
Oi5	0.5635 (16)	0.5998 (4)	0.985 (2)	0.2659 (18)	0.0943 (4)	0.380 (3)
Oi6	0.8926 (15)	0.6765 (7)	1.034 (4)	-0.0442 (16)	0.1411 (6)	0.260 (4)
Hi1	0.4309 (11)	0.5415 (4)	0.635 (3)	0.4024 (11)	0.0891 (4)	0.780 (3)
Hi2	0.2199 (11)	0.5838 (4)	1.005 (3)	0.6013 (10)	0.0863 (4)	0.375 (3)
Hi3	0.2241 (11)	0.6262 (4)	0.467 (3)	0.6107 (11)	0.1892 (4)	0.789 (4)
Hi4	0.3956 (11)	0.7285 (6)	0.657 (2)	0.4527 (11)	0.2549 (7)	0.484 (2)
Hi5	0.5836 (11)	0.6463 (4)	0.657 (3)	0.2560 (11)	0.1767 (4)	0.603 (3)
Hi6a	0.7220 (12)	0.7317 (6)	1.157 (5)	0.1038 (12)	0.1897 (7)	0.022 (4)
Hi6b	0.7460 (12)	0.7504 (6)	0.857 (5)	0.0824 (12)	0.2390 (7)	0.271 (4)
HOi2	-0.0047 (14)	0.5145 (6)	0.792 (3)	0.8236 (17)	0.0520 (7)	0.667 (3)
HOi3	-0.0053 (15)	0.6499 (7)	0.750 (3)	0.8468 (13)	0.1843 (7)	0.492 (3)
HOi4	0.2961 (18)	0.7501 (7)	1.012 (2)	0.5764 (19)	0.2071 (7)	0.093 (2)
HOi6	0.9615 (15)	0.6850 (7)	1.233 (4)	-0.1475 (16)	0.1401 (6)	0.105 (4)
Ci1'	0.7648 (14)	0.3448 (6)	1.126 (2)	0.0839 (12)	-0.1633 (5)	0.839 (2)
Ci2'	0.8531 (11)	0.4137 (4)	1.072 (4)	-0.0064 (11)	-0.1633 (5)	0.839 (2)
Ci3'	0.7280 (11)	0.4677 (4)	1.067 (4)	0.0817 (11)	-0.0496 (5)	0.603 (3)
Ci4'	0.5246 (11)	0.4421 (4)	0.936 (3)	0.2867 (11)	-0.0308 (5)	0.745 (3)
Ci5'	0.4530 (11)	0.3749 (4)	1.029 (3)	0.3736 (12)	-0.0956 (5)	0.820 (3)
Ci6'	0.2654 (15)	0.3496 (11)	0.832 (2)	0.5634 (16)	-0.0800 (6)	1.027 (4)
Oi1'	0.7952 (18)	0.3468 (8)	1.422 (2)	0.0630 (17)	-0.1952 (7)	0.569 (2)
Oi2'	1.0406 (12)	0.4232 (8)	1.241 (3)	-0.1978 (12)	-0.1115 (7)	0.631 (4)
Oi3'	0.8298 (18)	0.5264 (6)	0.993 (3)	-0.0018 (19)	0.0120 (6)	0.566 (3)
Oi5'	0.5724 (11)	0.3283 (6)	0.977 (3)	0.2783 (11)	-0.1420 (7)	0.961 (3)
Oi6'	0.2432 (20)	0.3357 (7)	0.537 (2)	0.6511 (18)	-0.1406 (5)	1.063 (4)

Hi1'	0.8321 (14)	0.3090 (6)	1.072 (2)	0.0290 (12)	-0.1916 (5)	0.965 (2)
Hi2'	0.8580 (11)	0.4081 (4)	0.875 (3)	0.0024 (11)	-0.0735 (5)	0.955 (3)
Hi3'	0.7370 (11)	0.4775 (4)	1.269 (4)	0.0651 (11)	-0.0735 (5)	0.416 (3)
Hi4'	0.5045 (11)	0.4353 (4)	0.729 (3)	0.3039 (11)	-0.0019 (5)	0.921 (3)
Hi5'	0.4546 (11)	0.3787 (4)	1.230 (3)	0.3811 (12)	-0.1195 (5)	0.645 (3)
Hi6a'	0.1802 (15)	0.3816 (11)	0.860 (2)	0.5538 (16)	-0.0632 (6)	1.213 (4)
Hi6b'	0.2252 (15)	0.3050 (11)	0.898 (2)	0.6403 (16)	-0.0430 (6)	0.963 (4)
HOi1'	0.8259 (18)	0.3029 (8)	1.486 (2)	0.0066 (17)	-0.2410 (7)	0.583 (2)
HOi2'	1.0608 (12)	0.4668 (8)	1.353 (3)	-0.2040 (12)	-0.1174 (7)	0.433 (4)
HOi3'	0.7971 (18)	0.5680 (6)	1.068 (3)	0.0383 (19)	0.0384 (6)	0.424 (3)
HOi6'	0.2278 (20)	0.3781 (7)	0.446 (2)	0.7418 (18)	-0.1046 (5)	1.035 (4)

## Bond lengths (Å) of the stable anhydrous phase of $\alpha$ -lactose.

	1 <sup>st</sup> molec.	2 <sup>nd</sup> molec.		1 <sup>st</sup> molec.	2 <sup>nd</sup> molec.
Ci1–Ci2	1.538 (13)	1.527 (14)	Oi1–Ci4'	1.426 (15)	1.414 (12)
Ci1–Oi1	1.416 (15)	1.406 (9)	Ci1'–Ci2'	1.517 (15)	1.540 (15)
Ci1–Oi5	1.415 (12)	1.430 (16)	Ci1'–Oi1'	1.424 (13)	1.424 (15)
Ci1–Hi1	1.000	1.000	Ci1'–Oi5'	1.442 (12)	1.442 (12)
Ci2–Ci3	1.516 (15)	1.515 (12)	Ci1'–Hi1'	1.000	1.000
Ci2–Oi2	1.434 (13)	1.439 (16)	Ci2'–Ci3'	1.521 (13)	1.525 (18)
Ci2–Hi2	1.000	1.000	Ci2'–Oi2'	1.430 (12)	1.424 (12)
Ci3–Ci4	1.518 (12)	1.533 (14)	Ci2'–Hi2'	1.000	1.000
Ci3–Oi3	1.430 (15)	1.420 (15)	Ci3'–Ci4'	1.523 (11)	1.522 (11)
Ci3–Hi3	1.000	1.000	Ci3'–Oi3'	1.438 (18)	1.444 (16)
Ci4–Ci5	1.521 (13)	1.512 (13)	Ci3'–Hi3'	1.000	1.000
Ci4–Oi4	1.415 (16)	1.420 (14)	Ci4'–Ci5'	1.517 (14)	1.532 (14)
Ci4–Hi4	1.001	1.000	Ci4'–Hi4'	1.000	1.000
Ci5–Ci6	1.503 (12)	1.520 (15)	Ci5'–Ci6'	1.509 (13)	1.515 (15)
Ci5–Oi5	1.419 (15)	1.441 (12)	Ci5'–Oi5'	1.444 (15)	1.426 (17)
Ci5–Hi5	1.000	1.000	Ci5'–Hi5'	1.000	1.000
Ci6–Oi6	1.431 (17)	1.442 (18)	Ci6'–Oi6'	1.441 (14)	1.443 (17)
Ci6–Hi6a	1.001	1.000	Ci6'–Hi6a'	0.999	1.000
Ci6–Hi6b	1.000	1.000	Ci6'–Hi6b'	1.001	1.000
Oi2–HOi2	0.985	0.980	Oi1'–HOi1'	0.974	0.972
Oi3–HOi3	0.986	0.982	Oi2'–HOi2'	0.985	0.979
Oi4–HOi4	0.986	0.982	Oi3'–HOi3'	0.984	0.987
Oi6–HOi6	0.986	0.938	Oi6'–HOi6'	0.975	0.976

## Bond angles (°) of the stable anhydrous phase of $\alpha$ -lactose.

	1 <sup>st</sup> molecule	2 <sup>nd</sup> molecule
Ci2–Ci1–Oi1	101.7(8)	108.9 (7)
Ci2–Ci1–Oi5	112.6 (9)	111.1 (9)
Oi1–Ci1–Ci5	107.7 (8)	112.9 (7)
Ci2–Ci1–Hi1	113.1	107.3
Oi1–Ci1–Hi1	110.5	107.9
Oi5–Ci1–Hi1	110.7	108.6
Ci1–Ci2–Ci3	104.7 (7)	107.8 (7)
Ci1–Ci2–Oi2	114.8 (9)	115.8 (9)
Ci3–Ci2–Oi2	109.8 (8)	111.2 (9)
Ci1–Ci2–Hi2	110.0	106.6
Ci3–Ci2–Hi2	108.0	108.7

Oi2–Ci2–Hi2	109.3	106.3
Ci2–Ci3–Ci4	113.7 (8)	114.8 (8)
Ci2–Ci3–Oi3	117.4 (9)	115.8 (9)
Ci4–Ci3–Oi3	109.0 (9)	111.7 (9)
Ci2–Ci3–Hi3	106.9	104.3
Ci4–Ci3–Hi3	104.8	104.4
Oi3–Ci3–Hi3	103.7	104.1
Ci3–Ci4–Ci5	113.1 (8)	112.4 (8)
Ci3–Ci4–Oi4	110.9 (10)	109.8 (9)
Ci5–Ci4–Oi4	104.1 (9)	108.2 (9)
Ci3–Ci4–Hi4	111.3	107.7
Ci5–Ci4–Hi4	109.3	108.9
Oi4–Ci4–Hi4	107.9	109.9
Ci4–Ci5–Ci6	112.8 (8)	114.6 (8)
Ci4–Ci5–Oi5	112.8 (9)	112.8 (9)
Ci6–Ci5–Oi5	113.9 (8)	113.8 (9)
Ci4–Ci5–Hi5	105.9	104.7
Ci6–Ci5–Hi5	105.1	103.7
Oi5–Ci5–Hi5	105.4	106.0
Ci5–Ci6–Oi6	107.1 (10)	99.9 (9)
Ci5–Ci6–Hi6a	108.5	110.1
Ci5–Ci6–Hi6b	111.5	114.1
Oi6–Ci6–Hi6a	110.4	112.5
Oi6–Ci6–Hi6b	112.4	113.3
Hi6a–Ci6–Hi6b	107.0	107.0
Ci1–Oi1–Ci4'	119.8 (8)	115.2 (6)
Ci2–Oi2–HOi2	107.8	113.2
Ci3–Oi3–HOi3	105.9	109.7
Ci4–Oi4–HOi4	107.2	118.7
Ci1–Oi5–Ci5	109.1 (8)	112.0 (8)
Ci6–Oi6–HOi6	109.0	107.2
Ci2'–Ci1'–Oi1'	105.0 (10)	103.6 (9)
Ci2'–Ci1'–Oi5'	114.3 (9)	107.1 (8)
Oi1'–Ci1'–Oi5'	111.9 (9)	106.3 (9)
Ci2'–Ci1'–Hi1'	108.5	111.9
Oi1'–Ci1'–Hi1'	108.4	115.2
Oi5'–Ci1'–Hi1'	108.5	112.1
Ci1'–Ci2'–Ci3'	111.5 (8)	114.8 (9)
Ci1'–Ci2'–Oi2'	107.4 (9)	113.7 (9)
Ci3'–Ci2'–Oi2'	122.2 (9)	107.1 (9)
Ci1'–Ci2'–Hi2'	104.4	107.7
Ci3'–Ci2'–Hi2'	104.3	107.9
Oi2'–Ci2'–Hi2'	105.3	105.2

Ci2'–Ci3'–Ci4'	114.1 (8)	110.8 (8)
Ci2'–Ci3'–Oi3'	102.5 (8)	111.6 (9)
Ci4'–Ci3'–Oi3'	126.0 (9)	108.7 (9)
Ci2'–Ci3'–Hi3'	103.8	107.7
Ci4'–Ci3'–Hi3'	103.2	108.4
Oi3'–Ci3'–Hi3'	105.0	109.5
Oi1–Ci4'–Ci3'	111.4 (9)	118.4 (7)
Oi1–Ci4'–Ci5'	109.6 (7)	101.6 (8)
Ci3'–Ci4'–Ci5'	116.1 (7)	109.5 (8)
Oi1–Ci4'–Hi4'	105.3	109.4
Ci3'–Ci4'–Hi4'	107.0	108.7
Ci5'–Ci4'–Hi4'	106.7	108.8
Ci4'–Ci5'–Ci6'	108.5 (9)	111.7 (9)
Ci4'–Ci5'–Oi5'	104.4 (8)	114.7 (9)
Ci6'–Ci5'–Oi5'	105.6 (9)	102.8 (9)
Ci4'–Ci5'–Hi5'	111.8	108.8
Ci6'–Ci5'–Hi5'	113.5	109.9
Oi5'–Ci5'–Hi5'	112.4	108.8
Ci5'–Ci6'–Oi6'	120.2 (9)	110.1 (11)
Ci5'–Ci6'–Hi6a'	107.4	110.0
Ci5'–Ci6'–Hi6b'	105.5	110.7
Oi6'–Ci6'–Hi6a'	110.6	108.4
Oi6'–Ci6'–Hi6b'	105.2	110.5
Hi6a'–Ci6'–Hi6b'	107.0	107.0
Ci1'–Oi1'–HOi1'	108.5	102.5
Ci2'–Oi2'–HOi2'	106.7	104.6
Ci3'–Oi3'–HOi3'	109.5	110.3
Ci1'–Oi5'–Ci5'	116.3 (9)	119.0 (9)
Ci6'–Oi6'–HOi6'	108.1	73.7

# Torsion angles ( $^{\circ}$ ) of the stable anhydrous phase of $\alpha$ -lactose after Rietveld refinements.

	1 <sup>st</sup> molecule	2 <sup>nd</sup> molecule
Oi1–Ci1–Ci2–Ci3	178.5 (9)	-176.1 (8)
Oi1–Ci1–Ci2–Oi2	-61.0 (12)	-50.8 (13)
Oi5–Ci1–Ci2–Ci3	63.5 (11)	59.0 (12)
Oi5–Ci1–Ci2–Oi2	-176.0 (10)	-175.7 (11)
Ci2–Ci1–Oi1–Ci4'	155.6 (11)	148.8 (8)
Oi5–Ci1–Oi1–Ci4'	-85.9 (13)	-87.3 (10)
Ci2–Ci1–Oi5–Ci5	-68.6 (12)	-65.1 (13)
Oi1–Ci1–Oi5–Ci5	-179.9 (10)	172.3 (9)
Ci1–Ci2–Ci3–Ci4	-50.1 (12)	-48.3 (13)
Ci1–Ci2–Ci3–Oi3	-179.0 (10)	179.0 (10)
Oi2–Ci2–Ci3–Ci4	-173.9 (10)	-176.3 (10)
Oi2–Ci2–Ci3–Oi3	57.2 (14)	51.0 (15)
Ci2–Ci3–Ci4–Ci5	44.4 (13)	42.6 (13)
Ci2–Ci3–Ci4–Oi4	-72.0 (12)	-77.8 (13)
Oi3–Ci3–Ci4–Ci5	177.4 (10)	177.1 (10)
Oi3–Ci3–Ci4–Oi4	61.0 (13)	56.7 (14)
Ci3–Ci4–Ci5–Ci6	-176.8 (10)	-177.2 (10)
Ci3–Ci4–Ci5–Oi5	-46.0 (13)	-44.8 (13)
Oi4–Ci4–Ci5–Ci6	-56.5 (13)	-55.9 (13)
Oi4–Ci4–Ci5–Oi5	74.3 (12)	76.5 (13)
Ci4–Ci5–Ci6–Oi6	177.8 (11)	177.1 (11)
Oi5–Ci5–Ci6–Oi6	47.6 (15)	45.3 (14)
Ci4–Ci5–Oi5–Ci1	57.1 (12)	57.1 (13)
Ci6–Ci5–Oi5–Ci1	-172.7 (10)	-170.2 (11)
Ci1–Oi1–Ci4’–Ci3’	69.1 (14)	87.0 (10)
Ci1–Oi1–Ci4’–Ci5’	-160.9 (10)	-153.0 (8)
Oi1’–Ci1’–Ci2’–Ci3’	-81.1 (12)	-60.4 (12)
Oi1’–Ci1’–Ci2’–Oi2’	55.3 (12)	63.3 (12)
Oi5’–Ci1’–Ci2’–Ci3’	42.0 (14)	51.6 (12)
Oi5’–Ci1’–Ci2’–Oi2’	178.4 (10)	175.4 (10)
Ci2’–Ci1’–Oi5’–Ci5’	-58.6 (14)	-50.6 (13)
Oi1’–Ci1’–Oi5’–Ci5’	60.6 (14)	59.6 (13)
Ci1’–Ci2’–Ci3’–Ci4’	-36.4 (14)	-54.7 (12)
Ci1’–Ci2’–Ci3’–Oi3’	-175.8 (10)	-176.0 (10)
Oi2’–Ci2’–Ci3’–Ci4’	-165.4 (11)	178.2 (10)
Oi2’–Ci2’–Ci3’–Oi3’	55.2 (15)	56.8 (13)
Ci2’–Ci3’–Ci4’–Oi1	172.2 (10)	165.5 (9)
Ci2’–Ci3’–Ci4’–Ci5’	45.8 (14)	49.7 (12)

Oi3'-Ci3'-Ci4'-Oi1	-59.7 (17)	-71.5 (12)
Oi3'-Ci3'-Ci4'-Ci5'	173.9 (12)	172.8 (10)
Oi1-Ci4'-Ci5'-Ci6'	66.1 (12)	69.1 (11)
Oi1-Ci4'-Ci5'-Oi5'	178.3 (10)	-174.5 (9)
Ci3'-Ci4'-Ci5'-Ci6'	-166.6 (11)	-164.9 (10)
Ci3'-Ci4'-Ci5'-Oi5'	-54.4 (13)	-48.5 (13)
Ci4'-Ci5'-Ci6'-Oi6'	60.4 (15)	-171.9 (11)
Oi5'-Ci5'-Ci6'-Oi6'	-51.0 (15)	64.6 (13)
Ci4'-Ci5'-Oi5'-Ci1'	61.1 (12)	52.1 (14)
Ci6'-Ci5'-Oi5'-Ci1'	175.4 (10)	173.5 (10)

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