Crystal structure of 6,6'-ditosyl- α - α' -trehalose-methanol-water (1/2/2), $C_{52}H_{68}O_{30}S_4 \cdot 2CH_3OH \cdot 2H_2O$

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Molecule A

Molecule B

Abstract

$C_{54}H_{80}O_{32}S_4$, monoclinic, $P12_11$ (No. 4), $a = 17.334(6)$ Å, $b = 7.814(6)$ Å, $c = 24.278(6)$ Å, $\beta = 99.82(2)^\circ$, $V = 3240.2$ Å³, $Z = 2$, $R_g(F) = 0.083$, $R_w(F^2) = 0.203$, $T = 293$ K.

Source of material

The title compound was obtained by a one-step synthesis [1]. In order to select the primary site, the most reactive, the reaction was carried out at low temperature, followed by an accurate purification by reverse-phase chromatography, thus obtaining the product in short time and in good yield. The compound was crystallised from methanol and water mixture and is characterized by two independent molecules (A and B) in the asymmetric unit.

Discussion

Hydrogen atoms of the solvent molecules are not refined.

The α, α' -trehalose is a peculiar disaccharide, in which two D-glucopyranosidic rings are linked by a bond between their anomeric carbon atoms, with a consequent non-reductive behaviour, while the molecule is symmetric. Owing to this peculiarity, this compound has attracted the interest of many researchers and many derivatives have been synthesized. One of the key intermediates in these syntheses is the 6,6'-ditosyl-trehalose, which was first synthesized and characterized in 1958 [2]. The two independent molecules are almost superimposable with angle between the planes of the two glucosidic rings of $46.5(4)^\circ$ and $53.5(5)^\circ$ for molecule A and B, respectively. The major difference between the two independent molecules is represented by one dihedral angles in one tosyl moiety ($C62A-O62A-S2A-C7A = 69(1)^\circ$ and $C63B-O63B-S1B-C4B = 177.1(8)^\circ$).

Table 1. Data collection and handling.

Crystal:	colorless needle, size 0.2 x 0.3 x 0.6 mm
Wavelength:	Cu $K\alpha$ radiation (1.54056 Å)
μ :	21.30 cm ⁻¹
Diffractometer, scan mode:	Nonius CAD4-Turbo, $\omega/2\theta$
$2\theta_{max}$:	140.22°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6654, 6654
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 3015
$N(param)_{refined}$:	830
Programs:	SDP [3], SIR92 [4], SHELXL-93 [5], PLATON [6]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1M1)	2a	0.961(1)	-0.877(2)	0.8661(8)	0.229
H(1M2)	2a	0.957(1)	-0.991(2)	0.8126(8)	0.229
H(1M3)	2a	0.888(1)	-0.997(2)	0.8467(8)	0.229
H(2A)	2a	0.940(1)	-0.591(2)	0.8453(6)	0.124
H(3A)	2a	0.8802(8)	-0.366(2)	0.7917(6)	0.104
H(5A)	2a	0.7633(9)	-0.713(2)	0.6882(6)	0.103
H(6A)	2a	0.8251(9)	-0.929(2)	0.7395(8)	0.127
H(61A)	2a	0.7085(7)	-0.296(1)	0.8037(5)	0.081
H(61B)	2a	0.6525(7)	-0.352(1)	0.7487(5)	0.081
H(51A)	2a	0.5939(7)	-0.128(1)	0.7919(4)	0.076
H(41A)	2a	0.6380(7)	-0.002(1)	0.6907(4)	0.068
H(41B)	2a	0.5749(4)	-0.2439(9)	0.6781(3)	0.101
H(31A)	2a	0.5086(7)	0.093(1)	0.7391(4)	0.078
H(31B)	2a	0.5264(5)	0.143(1)	0.6404(3)	0.117
H(21A)	2a	0.6414(7)	0.290(1)	0.7313(4)	0.069
H(21B)	2a	0.5379(5)	0.4448(9)	0.7327(3)	0.114

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Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(11A)	2a	0.6859(7)	0.270(1)	0.8227(4)	0.073
H(12A)	2a	0.6631(9)	0.055(2)	0.9049(5)	0.101
H(22A)	2a	0.586(1)	0.097(2)	0.9710(6)	0.118
H(22B)	2a	0.4927(7)	-0.073(1)	0.9339(5)	0.175
H(32A)	2a	0.475(1)	0.263(2)	0.8879(6)	0.11
H(32B)	2a	0.4215(6)	0.133(1)	0.9511(4)	0.164
H(42A)	2a	0.566(1)	0.407(2)	0.9854(6)	0.113
H(42B)	2a	0.5078(6)	0.625(1)	0.9153(5)	0.174
H(52A)	2a	0.5931(9)	0.472(2)	0.8751(5)	0.094
H(62A)	2a	0.6266(8)	0.689(2)	0.9445(5)	0.096
H(62B)	2a	0.6830(8)	0.558(2)	0.9802(5)	0.096
H(8A)	2a	0.834(1)	0.367(2)	0.9148(7)	0.124
H(9A)	2a	0.891(1)	0.137(3)	0.9673(9)	0.144
H(91A)	2a	0.909(1)	0.400(3)	1.1052(7)	0.139
H(13A)	2a	0.855(1)	0.643(2)	1.0569(7)	0.127
H(2M1)	2a	0.945(1)	-0.003(3)	1.048(1)	0.263
H(2M2)	2a	0.905(1)	0.053(3)	1.098(1)	0.263
H(2M3)	2a	0.991(1)	0.112(3)	1.095(1)	0.263
H(1M4)	2a	0.070(1)	1.196(3)	0.6196(8)	0.212
H(1M5)	2a	0.031(1)	1.297(3)	0.5663(8)	0.212
H(1M6)	2a	0.121(1)	1.320(3)	0.5896(8)	0.212
H(2B)	2a	0.088(1)	0.901(2)	0.6023(7)	0.136
H(3B)	2a	0.118(1)	0.680(2)	0.5467(7)	0.141
H(5B)	2a	0.1408(9)	1.016(2)	0.4267(6)	0.107
H(6B)	2a	0.1070(7)	1.232(2)	0.4810(7)	0.106
H(63A)	2a	0.3106(7)	0.550(2)	0.4092(5)	0.081

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(63B)	2a	0.2399(7)	0.425(2)	0.4117(5)	0.081
H(53B)	2a	0.3580(6)	0.484(1)	0.5067(4)	0.067
H(43B)	2a	0.3478(7)	0.190(1)	0.4368(4)	0.069
H(43A)	2a	0.4770(5)	0.333(1)	0.4449(3)	0.101
H(33B)	2a	0.4572(7)	0.260(1)	0.5341(4)	0.074
H(33A)	2a	0.4658(5)	0.038(1)	0.4618(3)	0.118
H(23B)	2a	0.3356(7)	0.009(1)	0.5225(4)	0.073
H(23A)	2a	0.4360(5)	-0.0467(9)	0.5876(3)	0.106
H(13B)	2a	0.2671(6)	0.175(1)	0.5750(4)	0.066
H(14B)	2a	0.2547(7)	0.500(1)	0.5877(5)	0.08
H(24B)	2a	0.3023(7)	0.700(1)	0.6523(5)	0.078
H(24A)	2a	0.4108(5)	0.7682(9)	0.6213(3)	0.107
H(34B)	2a	0.4363(7)	0.502(1)	0.6936(5)	0.076
H(34A)	2a	0.4448(5)	0.782(1)	0.7058(3)	0.133
H(44B)	2a	0.3103(8)	0.544(1)	0.7507(5)	0.083
H(44A)	2a	0.4472(6)	0.446(1)	0.7845(3)	0.139
H(54B)	2a	0.3536(7)	0.252(1)	0.6932(5)	0.078
H(64A)	2a	0.2457(8)	0.105(2)	0.7140(5)	0.095
H(64B)	2a	0.3010(8)	0.151(2)	0.7704(5)	0.095
H(8B)	2a	0.019(1)	0.143(2)	0.7210(7)	0.118
H(9B)	2a	-0.035(1)	-0.099(2)	0.6764(6)	0.123
H(11B)	2a	0.1469(9)	-0.373(2)	0.7467(8)	0.133
H(12B)	2a	0.1982(9)	-0.135(2)	0.7984(7)	0.123
H(2M4)	2a	-0.037(1)	-0.377(2)	0.6541(8)	0.208
H(2M5)	2a	0.003(1)	-0.502(2)	0.7010(8)	0.208
H(2M6)	2a	0.045(1)	-0.454(2)	0.6511(8)	0.208

Table 3. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1MA)	2a	0.927(1)	-0.925(2)	0.8343(8)	0.18(2)	0.10(2)	0.20(2)	0.08(1)	0.08(2)	0.08(1)
C(1A)	2a	0.8869(9)	-0.783(2)	0.7991(7)	0.10(1)	0.055(9)	0.13(1)	-0.003(8)	0.017(9)	0.033(9)
C(2A)	2a	0.904(1)	-0.615(2)	0.8134(6)	0.14(1)	0.08(1)	0.078(9)	0.04(1)	-0.005(8)	0.013(8)
C(3A)	2a	0.8678(8)	-0.478(2)	0.7816(6)	0.11(1)	0.046(7)	0.097(9)	-0.013(7)	-0.010(8)	0.005(7)
C(4A)	2a	0.8119(8)	-0.517(2)	0.7335(6)	0.087(8)	0.039(6)	0.091(8)	0.004(6)	0.020(7)	-0.001(6)
C(5A)	2a	0.7990(9)	-0.687(2)	0.7202(6)	0.11(1)	0.033(7)	0.11(1)	0.003(7)	0.018(8)	-0.015(7)
C(6A)	2a	0.8352(9)	-0.816(2)	0.7510(8)	0.11(1)	0.048(9)	0.16(2)	0.016(8)	0.03(1)	-0.01(1)
S(1A)	2a	0.7664(2)	-0.3572(4)	0.6923(1)	0.102(2)	0.058(2)	0.078(2)	0.014(2)	0.020(2)	0.007(2)
O(7A)	2a	0.6958(6)	-0.428(1)	0.6604(4)	0.112(7)	0.092(7)	0.081(5)	0.011(6)	-0.004(5)	-0.013(5)
O(8A)	2a	0.8217(6)	-0.267(1)	0.6647(4)	0.138(8)	0.088(8)	0.128(8)	0.032(7)	0.070(7)	0.055(7)
O(61A)	2a	0.7440(5)	-0.2182(9)	0.7346(3)	0.095(6)	0.036(4)	0.093(6)	0.000(4)	0.033(5)	-0.007(4)
C(61A)	2a	0.6848(7)	-0.260(1)	0.7665(5)	0.099(8)	0.039(6)	0.068(7)	0.012(6)	0.027(6)	-0.001(5)
C(51A)	2a	0.6349(7)	-0.102(1)	0.7700(4)	0.111(9)	0.019(5)	0.056(6)	-0.015(5)	0.002(6)	-0.001(5)
O(51A)	2a	0.6854(5)	0.0290(9)	0.7983(3)	0.088(5)	0.034(4)	0.077(5)	0.001(4)	0.019(4)	0.001(4)
C(41A)	2a	0.5964(7)	-0.032(1)	0.7117(4)	0.083(7)	0.033(5)	0.052(5)	-0.014(5)	0.005(5)	0.006(4)
O(41A)	2a	0.5486(4)	-0.1586(9)	0.6815(3)	0.093(5)	0.034(4)	0.072(4)	-0.013(4)	0.007(4)	-0.010(4)
C(31A)	2a	0.5507(7)	0.125(1)	0.7188(4)	0.109(9)	0.025(5)	0.060(6)	-0.006(6)	0.011(6)	0.001(5)
O(31A)	2a	0.5153(5)	0.200(1)	0.6663(3)	0.115(6)	0.041(4)	0.070(5)	-0.015(5)	-0.007(4)	0.012(4)
C(21A)	2a	0.6020(7)	0.256(1)	0.7538(4)	0.085(7)	0.028(5)	0.058(6)	0.000(5)	0.008(5)	0.005(4)
O(21A)	2a	0.5618(5)	0.4096(9)	0.7627(3)	0.112(6)	0.026(4)	0.087(5)	0.009(4)	0.009(5)	-0.004(4)
C(11A)	2a	0.6467(7)	0.185(1)	0.8064(4)	0.085(7)	0.034(6)	0.066(6)	-0.004(5)	0.021(5)	-0.001(5)
O(4A)	2a	0.5927(5)	0.163(1)	0.8427(3)	0.104(5)	0.043(4)	0.059(4)	0.004(4)	0.017(4)	0.004(4)
C(12A)	2a	0.6247(9)	0.149(2)	0.9002(5)	0.14(1)	0.047(7)	0.059(6)	0.000(8)	0.003(7)	0.009(6)
C(22A)	2a	0.562(1)	0.106(2)	0.9315(6)	0.16(2)	0.043(8)	0.09(1)	-0.012(9)	0.03(1)	0.010(7)
O(22A)	2a	0.5274(7)	-0.053(1)	0.9156(5)	0.16(1)	0.060(7)	0.148(9)	-0.011(6)	0.059(8)	0.015(7)
C(32A)	2a	0.501(1)	0.252(2)	0.9268(6)	0.15(1)	0.039(7)	0.092(9)	0.010(8)	0.048(9)	0.017(7)
O(32A)	2a	0.4456(6)	0.221(1)	0.9612(4)	0.138(8)	0.081(7)	0.128(7)	0.000(7)	0.076(6)	0.023(7)
C(42A)	2a	0.546(1)	0.415(2)	0.9453(6)	0.14(1)	0.055(9)	0.09(1)	0.030(9)	0.039(9)	0.023(8)
O(42A)	2a	0.4920(6)	0.554(1)	0.9358(5)	0.127(9)	0.055(6)	0.18(1)	0.017(6)	0.052(8)	0.003(7)
C(52A)	2a	0.6122(9)	0.446(2)	0.9146(5)	0.12(1)	0.040(7)	0.072(8)	0.011(7)	0.019(7)	0.011(6)
O(52A)	2a	0.6630(5)	0.301(1)	0.9204(3)	0.104(6)	0.047(5)	0.069(5)	0.004(4)	0.004(4)	-0.008(4)
C(62A)	2a	0.6597(8)	0.590(2)	0.9425(5)	0.12(1)	0.049(8)	0.080(8)	-0.003(7)	0.022(7)	-0.006(6)
O(62A)	2a	0.7212(5)	0.632(1)	0.9101(3)	0.083(5)	0.061(5)	0.088(5)	-0.011(5)	0.019(4)	0.002(5)
S(2A)	2a	0.8021(3)	0.7034(5)	0.9411(2)	0.127(3)	0.048(2)	0.106(3)	-0.007(2)	0.011(2)	0.004(2)
O(9A)	2a	0.7884(7)	0.840(1)	0.9787(4)	0.17(1)	0.049(6)	0.121(8)	-0.009(6)	0.019(7)	-0.024(6)
O(10A)	2a	0.8461(7)	0.739(1)	0.8963(4)	0.18(1)	0.081(8)	0.109(7)	-0.021(8)	0.052(7)	0.032(6)
C(7A)	2a	0.8446(8)	0.531(2)	0.9792(6)	0.091(9)	0.047(7)	0.10(1)	-0.009(7)	0.021(7)	-0.007(7)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(8A)	2a	0.851(1)	0.379(2)	0.9530(7)	0.13(1)	0.06(1)	0.12(1)	-0.002(9)	0.03(1)	-0.01(1)
C(9A)	2a	0.885(1)	0.240(3)	0.9851(9)	0.11(1)	0.10(1)	0.16(2)	0.02(1)	0.04(1)	0.03(1)
C(10A)	2a	0.907(1)	0.252(3)	1.041(1)	0.14(2)	0.09(1)	0.14(2)	0.03(1)	-0.01(1)	0.02(1)
C(91A)	2a	0.896(1)	0.396(3)	1.0664(7)	0.14(1)	0.11(2)	0.09(1)	-0.00(1)	-0.00(1)	0.04(1)
C(13A)	2a	0.864(1)	0.543(2)	1.0379(7)	0.14(1)	0.08(1)	0.10(1)	0.00(1)	0.02(1)	0.01(1)
C(2MA)	2a	0.940(1)	0.088(3)	1.074(1)	0.14(2)	0.14(2)	0.24(2)	0.03(2)	0.03(2)	0.11(2)
C(1MB)	2a	0.078(1)	1.240(3)	0.5841(8)	0.11(1)	0.12(2)	0.19(2)	-0.02(1)	0.03(1)	-0.09(2)
C(1B)	2a	0.0968(8)	1.091(2)	0.5467(8)	0.076(8)	0.06(1)	0.15(2)	0.002(7)	0.025(9)	-0.03(1)
C(2B)	2a	0.098(1)	0.923(2)	0.5667(7)	0.17(2)	0.08(1)	0.10(1)	0.01(1)	0.05(1)	-0.02(1)
C(3B)	2a	0.116(1)	0.792(2)	0.5334(7)	0.18(2)	0.07(1)	0.12(1)	0.04(1)	0.06(1)	0.02(1)
C(4B)	2a	0.1302(7)	0.824(2)	0.4807(6)	0.083(8)	0.047(7)	0.099(9)	0.023(6)	0.031(7)	0.011(7)
C(5B)	2a	0.1289(9)	0.992(2)	0.4618(6)	0.13(1)	0.043(8)	0.10(1)	0.008(8)	0.047(9)	0.015(7)
C(6B)	2a	0.1104(7)	1.121(2)	0.4947(7)	0.086(9)	0.055(9)	0.12(1)	-0.009(7)	0.018(8)	0.009(9)
S(1B)	2a	0.1464(2)	0.6587(4)	0.4374(2)	0.094(2)	0.057(2)	0.102(2)	0.018(2)	0.018(2)	0.004(2)
O(7B)	2a	0.1085(7)	0.507(1)	0.4518(6)	0.116(8)	0.046(6)	0.23(1)	-0.023(6)	0.050(9)	-0.004(8)
O(8B)	2a	0.1347(6)	0.713(2)	0.3812(4)	0.131(8)	0.117(9)	0.084(6)	0.045(7)	0.014(5)	0.019(6)
O(63B)	2a	0.2364(4)	0.638(1)	0.4577(3)	0.083(5)	0.039(4)	0.103(5)	0.026(4)	0.022(4)	-0.005(4)
C(63B)	2a	0.2774(7)	0.502(2)	0.4336(5)	0.088(8)	0.043(7)	0.074(7)	0.018(6)	0.017(6)	0.000(6)
C(53B)	2a	0.3267(6)	0.403(1)	0.4811(4)	0.084(7)	0.025(5)	0.060(6)	0.001(5)	0.017(5)	0.008(5)
O(53B)	2a	0.2711(4)	0.317(1)	0.5097(3)	0.079(4)	0.046(4)	0.064(4)	-0.007(4)	0.012(3)	0.008(4)
C(43B)	2a	0.3800(7)	0.272(1)	0.4610(4)	0.090(7)	0.018(5)	0.066(6)	0.010(5)	0.015(5)	0.000(5)
O(43B)	2a	0.4317(5)	0.352(1)	0.4300(3)	0.091(5)	0.052(5)	0.061(4)	0.005(4)	0.018(4)	0.011(4)
C(33B)	2a	0.4235(7)	0.179(1)	0.5105(4)	0.088(7)	0.025(5)	0.071(6)	0.008(5)	0.013(5)	-0.001(5)
O(33B)	2a	0.4703(5)	0.044(1)	0.4959(3)	0.122(7)	0.048(5)	0.068(4)	0.037(5)	0.022(5)	0.000(4)
C(23B)	2a	0.3649(7)	0.100(1)	0.5450(4)	0.096(8)	0.019(5)	0.063(6)	-0.007(5)	-0.001(5)	0.002(4)
O(23B)	2a	0.4049(5)	0.0251(9)	0.5951(3)	0.123(7)	0.026(4)	0.063(4)	-0.004(4)	0.014(4)	0.002(3)
C(13B)	2a	0.3074(6)	0.232(1)	0.5579(4)	0.084(7)	0.015(5)	0.063(6)	-0.002(5)	0.005(5)	-0.001(4)
O(4B)	2a	0.3493(4)	0.3494(8)	0.5978(3)	0.075(4)	0.027(4)	0.074(4)	-0.002(3)	0.023(4)	-0.003(3)
C(14B)	2a	0.2945(7)	0.461(1)	0.6188(5)	0.108(9)	0.030(5)	0.076(7)	0.004(6)	0.056(7)	0.008(5)
C(24B)	2a	0.3402(7)	0.613(1)	0.6452(5)	0.103(8)	0.019(5)	0.075(7)	-0.002(5)	0.022(6)	-0.001(5)
O(24B)	2a	0.3861(5)	0.6857(9)	0.6067(3)	0.124(6)	0.029(4)	0.066(4)	-0.011(4)	0.028(4)	0.010(3)
C(34B)	2a	0.3919(7)	0.570(1)	0.7012(5)	0.095(8)	0.026(5)	0.070(7)	0.002(5)	0.018(6)	-0.002(5)
O(34B)	2a	0.4221(5)	0.728(1)	0.7273(3)	0.137(7)	0.058(6)	0.077(5)	-0.030(6)	0.031(5)	-0.014(5)
C(44B)	2a	0.3508(8)	0.472(1)	0.7388(5)	0.109(9)	0.032(6)	0.066(7)	-0.006(6)	0.010(6)	0.005(5)
O(44B)	2a	0.4026(6)	0.414(1)	0.7863(3)	0.115(7)	0.085(7)	0.078(6)	-0.016(6)	0.018(5)	0.004(5)
C(54B)	2a	0.3127(7)	0.319(1)	0.7069(5)	0.084(7)	0.040(6)	0.079(7)	0.002(5)	0.035(6)	0.006(6)
O(54B)	2a	0.2572(5)	0.375(1)	0.6593(3)	0.087(5)	0.047(5)	0.072(4)	-0.004(4)	0.027(4)	-0.005(4)
C(64B)	2a	0.2670(8)	0.198(2)	0.7381(5)	0.104(9)	0.048(7)	0.098(8)	0.006(7)	0.051(7)	0.002(7)
O(64B)	2a	0.2030(6)	0.297(1)	0.7562(4)	0.135(8)	0.043(5)	0.109(6)	0.002(5)	0.059(6)	0.021(5)
S(2B)	2a	0.1580(3)	0.2074(5)	0.7996(2)	0.149(4)	0.060(2)	0.115(3)	-0.023(3)	0.064(3)	-0.013(2)
O(9B)	2a	0.0999(8)	0.327(2)	0.8080(5)	0.19(1)	0.085(8)	0.19(1)	-0.040(8)	0.13(1)	-0.052(9)
O(10B)	2a	0.2154(7)	0.152(2)	0.8457(4)	0.104(8)	0.064(8)	0.054(6)	-0.012(7)	0.014(6)	0.007(6)
C(7B)	2a	0.1117(8)	0.029(2)	0.7648(6)	0.088(9)	0.043(7)	0.11(1)	-0.003(7)	0.032(8)	0.009(7)
C(8B)	2a	0.044(1)	0.038(2)	0.7280(7)	0.10(1)	0.07(1)	0.13(1)	-0.015(9)	0.03(1)	0.00(1)
C(9B)	2a	0.012(1)	-0.106(2)	0.7006(6)	0.12(1)	0.09(1)	0.10(1)	-0.02(1)	0.016(9)	-0.02(1)
C(10B)	2a	0.050(1)	-0.262(2)	0.7085(8)	0.12(1)	0.06(1)	0.15(2)	-0.004(9)	0.05(1)	0.00(1)
C(11B)	2a	0.1194(9)	-0.270(2)	0.7429(8)	0.084(9)	0.06(1)	0.18(2)	-0.007(8)	0.00(1)	0.01(1)
C(12B)	2a	0.1515(9)	-0.126(2)	0.7733(7)	0.090(9)	0.07(1)	0.14(1)	-0.006(8)	-0.005(9)	0.01(1)
C(2MB)	2a	0.012(1)	-0.413(2)	0.6757(8)	0.15(2)	0.07(1)	0.20(2)	-0.03(1)	0.03(1)	-0.06(1)
Ow(1)	2a	0.5296(5)	0.501(1)	0.6152(3)	0.119(6)	0.041(5)	0.068(5)	-0.015(4)	0.018(4)	0.000(4)
Ow(2)	2a	0.339(2)	0.000(5)	0.911(1)	0.25(2)	0.42(5)	0.30(3)	0.06(3)	0.03(2)	0.06(3)
Om(1)	2a	0.396(1)	-0.090(3)	0.8190(8)	0.23(2)	0.19(2)	0.20(2)	0.03(2)	0.01(1)	-0.05(2)
Cm(1)	2a	0.453(2)	-0.223(4)	0.846(2)	0.56(9)	0.11(3)	0.59(9)	-0.02(4)	0.21(8)	0.05(4)
Om(2)	2a	0.666(2)	0.053(6)	1.1205(8)	0.40(4)	0.57(7)	0.14(1)	-0.12(5)	-0.04(2)	0.06(3)
Cm(2)	2a	0.713(2)	0.040(8)	1.072(2)	0.21(3)	0.46(8)	0.29(4)	0.08(4)	0.08(3)	0.07(5)

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