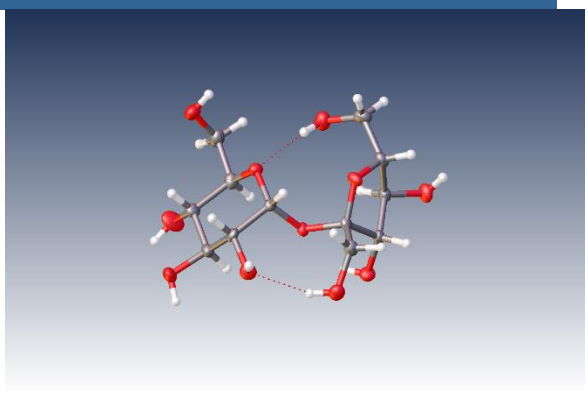
Sucrose

Crystal Submitted by:
John Doe
Crystal Submitted on:
2/1/2016
Data Collected on:
2/2/2016
Structure Solved by:
IMSERC



Experimental

Single crystals of $C_{12}H_{22}O_{11}$ [Sucrose] were supplied**.** A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Moly diffractometer. The crystal was kept at 100 K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the XL [3] refinement package using Least Squares minimization.

Crystal structure determination of Sucrose

Crystal Data for $C_{12}H_{22}O_{11}$ (M =342.29): monoclinic, space group $P2_1$ (no. 4), a = 7.7830(10) Å, b = 8.7364(12) Å, c = 10.9002(15) Å, β = 102.984(9)°, V = 722.21(17) Å^3, Z = 2, T = 100 K, μ(MoKα) = 0.141 mm^{-1}, D_{calc} = 1.574 g/mm^3, 6405 reflections measured (3.834 ≤ 2Θ ≤ 51.944), 2803 unique (R_{int} = 0.0609, R_{sigma} = 0.0549) which were used in all calculations. The final R_1 was 0.0511 (I > 2σ(I)) and wR_2 was 0.1137 (all data).

Refinement Details. No special refinement

Solvent Treatment Details. None

References

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Table 1. Crystal data and structure refinement for Sucrose

Identification code	Sucrose
Empirical formula	$C_{12}H_{22}O_{11}$
Formula weight	342.29
Temperature / K	100
Crystal system	Monoclinic
Space group	$P2_1$
a / Å, b / Å, c / Å	7.7830(10), 8.7364(12), 10.9002(15)
α/°, β/°, γ/°	90, 102.984(9), 90
Volume / $Å^3$	722.21(17)
Z	2
ρ_{calc} / mg mm^{-3}	1.574
μ / mm^{-1}	0.141
F(000)	364
Crystal size / mm^3	0.2 × 0.2 × 0.2
2Θ range for data collection	3.834 to 51.944°
Index ranges	$-9 \leq h \leq 9$, $-10 \leq k \leq 10$, $-13 \leq l \leq 13$
Reflections collected	6405
Independent reflections	2803[R(int) = 0.0609]
Data/restraints/parameters	2803/1/217
Goodness-of-fit on F^2	1.160
Final R indexes [I>2σ (I)]	R_1 = 0.0511, wR_2 = 0.1023
Final R indexes [all data]	R_1 = 0.0690, wR_2 = 0.1137
Largest diff. peak/hole / e $Å^{-3}$	0.324/-0.316

Table 2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Sucrose. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor

Atom	*x*	*y*	*z*	U(eq)
O1	-1317(4)	9354(4)	8772(3)	19.8(7)
O2	-2141(5)	7881(5)	10811(3)	33.6(9)
O3	-1451(6)	5202(4)	8484(4)	42.9(11)
O4	2024(5)	5867(5)	8089(4)	35.3(9)
O5	2477(5)	8977(4)	7292(3)	26.8(8)
O6	-1837(4)	12395(4)	7123(3)	19.9(7)
O7	-4609(5)	10954(5)	8267(4)	32.1(9)
O8	-5901(4)	12349(5)	4775(3)	27.9(8)
O9	-2950(5)	10160(4)	4255(3)	23.9(8)
O10	1212(5)	10989(4)	5296(3)	28.4(8)
O11	-1085(4)	9870(3)	6714(3)	16.5(7)
C1	-2057(6)	7821(6)	8594(4)	22.1(11)
C2	-3156(7)	7630(6)	9569(4)	28.6(12)
C3	-577(7)	6634(6)	8743(5)	22(1)
C4	645(7)	6979(5)	7858(4)	22.8(11)
C5	1345(6)	8590(6)	8127(4)	19.2(10)
C6	-140(6)	9755(5)	8002(4)	15.9(9)
C7	-1302(6)	11416(5)	6241(4)	16.7(10)
C8	433(6)	12031(6)	6033(4)	22.7(11)
C9	-2855(6)	11430(5)	5074(4)	17.5(10)
C10	-4446(6)	11670(6)	5652(4)	19.7(10)
C11	-3720(6)	12726(5)	6768(4)	21(1)
C12	-4533(7)	12522(6)	7887(5)	27.6(12)

Table 3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Sucrose. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	23.6(18)	17.6(18)	20.0(16)	-0.3(14)	9.0(14)	-1.1(14)
O2	47(2)	32(2)	24.7(17)	4.7(16)	14.2(17)	7.0(19)
O3	49(3)	18(2)	66(3)	-9(2)	24(2)	-9.9(19)
O4	49(2)	27(2)	36(2)	10.3(18)	20.6(19)	19.5(18)
O5	21.8(19)	29(2)	30(2)	0.1(16)	8.5(15)	-1.2(15)
O6	13.8(16)	20.6(17)	23.4(16)	-5.3(14)	0.2(13)	2.3(14)
O7	26(2)	33(2)	37(2)	8.5(18)	8.3(17)	1.9(17)
O8	19.6(18)	28.7(19)	31.9(19)	4.7(17)	-1.8(15)	3.6(16)
O9	29.3(19)	20.3(18)	21.6(17)	-4.7(15)	4.5(15)	-2.0(16)
O10	24.6(19)	34(2)	29.8(19)	5.6(17)	12.0(15)	2.4(16)
O11	17.3(16)	12.2(16)	19.2(15)	0.3(13)	2.3(13)	-1.2(13)
C1	22(3)	19(3)	24(2)	1(2)	2(2)	-3(2)
C2	28(3)	29(3)	30(3)	8(2)	9(2)	0(2)
C3	28(3)	16(2)	24(2)	-2.4(19)	8(2)	-3(2)
C4	30(3)	19(3)	19(2)	0.6(19)	5(2)	7(2)
C5	20(3)	24(3)	13(2)	3.2(19)	2.2(19)	1(2)
C6	18(2)	15(2)	14(2)	-0.6(18)	3.0(17)	-2.1(18)
C7	18(2)	11(2)	21(2)	-0.1(18)	3.6(18)	0.0(18)
C8	20(3)	21(3)	28(3)	2(2)	7(2)	-1.3(19)
C9	17(2)	16(2)	20(2)	3.9(18)	5.0(18)	0.6(18)
C10	17(2)	18(2)	24(2)	3.7(19)	2.9(19)	1(2)
C11	19(2)	15(3)	30(2)	1(2)	7(2)	3.6(19)
C12	23(3)	32(3)	30(3)	-6(2)	10(2)	3(2)

Table 4. Bond Lengths for Sucrose

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.454(6)	O11	C6	1.435(5)
O1	C6	1.418(5)	O11	C7	1.443(5)
O2	C2	1.423(6)	C1	C2	1.515(7)
O3	C3	1.422(6)	C1	C3	1.531(7)
O4	C4	1.428(6)	C3	C4	1.529(7)
O5	C5	1.442(6)	C4	C5	1.514(7)
O6	C7	1.416(5)	C5	C6	1.523(6)
O6	C11	1.458(5)	C7	C8	1.517(6)
O7	C12	1.436(7)	C7	C9	1.546(6)
O8	C10	1.435(5)	C9	C10	1.525(7)
O9	C9	1.415(5)	C10	C11	1.531(7)
O10	C8	1.436(6)	C11	C12	1.505(7)

Table 5 Bond Angles for Sucrose

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	O1	C1	116.0(3)	O11	C6	C5	110.2(3)
C7	O6	C11	111.8(3)	O6	C7	O11	110.6(3)
C6	O11	C7	114.1(3)	O6	C7	C8	107.2(4)
O1	C1	C2	106.1(4)	O6	C7	C9	105.0(3)
O1	C1	C3	110.1(4)	O11	C7	C8	110.4(4)
C2	C1	C3	112.4(4)	O11	C7	C9	108.0(3)
O2	C2	C1	111.7(4)	C8	C7	C9	115.6(4)
O3	C3	C1	105.0(4)	O10	C8	C7	111.2(4)
O3	C3	C4	112.7(4)	O9	C9	C7	115.7(4)
C4	C3	C1	111.1(4)	O9	C9	C10	115.8(4)
O4	C4	C3	107.7(4)	C10	C9	C7	102.6(4)
O4	C4	C5	112.0(4)	O8	C10	C9	112.0(4)
C5	C4	C3	108.0(4)	O8	C10	C11	112.1(4)
O5	C5	C4	109.9(4)	C9	C10	C11	102.8(4)
O5	C5	C6	110.2(4)	O6	C11	C10	105.1(4)
C4	C5	C6	111.8(4)	O6	C11	C12	110.0(4)
O1	C6	O11	109.8(3)	C12	C11	C10	115.2(4)
O1	C6	C5	111.1(3)	O7	C12	C11	113.6(4)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Sucrose

Atom	*x*	*y*	*z*	U(eq)
H2	-2270	8768	11020	50
H3	-734	4541	8409	64
H4	2345	5697	7436	53
H5	3240	9577	7645	40
H7	-3606	10613	8490	48
H8	-5959	13262	4935	42
H9	-3057	9372	4639	36
H10	1644	10262	5734	43
H1	-2820	7737	7750	33
H2A	-4131	8349	9393	43
H2B	-3644	6604	9510	43
H3A	109	6642	9615	33
H4A	-16	6906	6982	34
H5A	2048	8624	8994	29
H6	376	10757	8273	24
H8A	233	13010	5605	34
H8B	1240	12193	6841	34
H9A	-2731	12350	4586	26
H10A	-4808	10692	5954	29
H11	-3881	13791	6483	31
H12A	-3855	13104	8588	41
H12B	-5719	12937	7685	41