Structure Tables

# Table 1. Crystal data and structure refinement for DK\_zucker2\_0m.cif

|  |  |
| --- | --- |
|  | **DK\_zucker2\_0m.cif** |
| Empirical formula | C12H22O11 |
| Formula weight | 342.29 |
| Temperature/K | 100(2) |
| Crystal system | monoclinic |
| Space group | *P*21 (4) |
| *a*/Å | 7.716(3) |
| *b*/Å | 8.664(2) |
| *c*/Å | 10.812(4) |
| α/° | 90 |
| β/° | 102.982(9) |
| γ/° | 90 |
| Volume/Å3 | 704.3(4) |
| *Z* | 2 |
| *ρ*calc g/cm3 | 1.614 |
| μ/mm-1 | 0.145 |
| *F*(000) | 364 |
| Crystal size/mm3 | ?×?×? |
| Crystal colour | ? |
| Crystal shape | ? |
| Radiation | Mo*Kα* (λ=0.71073) |
| 2ϴ range/° | 5.42 to 111.70 |
| Index ranges | -14 ≤ h ≤ 17 -20 ≤ k ≤ 20 -24 ≤ l ≤ 25 |
| Reflections collected | 118996 |
| Independent reflections | 18544 *R*int = 0.0326 *R*sigma = 0.0241 |
| Data / Restraints / Param. | 18544/1/224 |
| Goodness-of-fit on *F*2 | 1.080 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0226 w*R*2 = 0.0624 |
| Final *R* indexes  [all data] | *R*1 = 0.0234 w*R*2 = 0.0629 |
| Largest peak/hole /eÅ3 | 0.41/-0.24 |
| Flack x parameter | 0.06(6) |

## Table 2. Atomic coordinates (\*10^4) and equivalent isotropic displacement parameters (Å^2\*10^3) for DK\_zucker2\_0m.cif. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | *z* | ***U*eq** |
| O1 | 0.36906(4) | 0.53931(3) | 0.37832(2) | 0.00733(3) |
| C1 | 0.48619(4) | 0.57984(4) | 0.30013(3) | 0.00637(3) |
| H1 | 0.538448 | 0.683332 | 0.327374 | 0.008 |
| O2 | 0.39204(3) | 0.59003(3) | 0.17093(2) | 0.00638(3) |
| C2 | 0.63859(4) | 0.46254(4) | 0.31329(3) | 0.00709(4) |
| H2 | 0.710707 | 0.466096 | 0.402511 | 0.009 |
| O3 | 0.31892(3) | 0.84412(3) | 0.21218(2) | 0.00735(3) |
| C3 | 0.56603(5) | 0.29943(4) | 0.28574(3) | 0.00791(4) |
| H3 | 0.497597 | 0.292164 | 0.195672 | 0.009 |
| O4 | 0.28724(5) | 0.39273(4) | 0.58392(3) | 0.01166(4) |
| H4A | 0.2862(14) | 0.4848(18) | 0.6004(5) | 0.017 |
| C4 | 0.44351(5) | 0.26529(4) | 0.37537(3) | 0.00832(4) |
| H4 | 0.514346 | 0.266199 | 0.465003 | 0.010 |
| O5 | 0.35551(5) | 0.12166(4) | 0.34951(4) | 0.01418(5) |
| H5A | 0.4295(14) | 0.0531(13) | 0.3462(13) | 0.021 |
| C5 | 0.29556(4) | 0.38577(4) | 0.36007(3) | 0.00775(4) |
| H5 | 0.216926 | 0.377353 | 0.273178 | 0.009 |
| O6 | 0.70569(5) | 0.18758(4) | 0.30869(3) | 0.01250(4) |
| H6 | 0.7339(13) | 0.1650(13) | 0.2387(11) | 0.019 |
| C6 | 0.18421(5) | 0.36621(5) | 0.45909(3) | 0.01012(4) |
| H6A | 0.083329 | 0.439605 | 0.440932 | 0.012 |
| H6AB | 0.134865 | 0.260315 | 0.453677 | 0.012 |
| O7 | 0.75100(4) | 0.50226(3) | 0.22974(3) | 0.00917(3) |
| H7 | 0.8375(15) | 0.5579(15) | 0.2695(7) | 0.014 |
| C7 | 0.54677(4) | 0.80535(4) | 0.10149(3) | 0.00811(4) |
| H7A | 0.526957 | 0.905522 | 0.056467 | 0.010 |
| H7AB | 0.630439 | 0.822527 | 0.184252 | 0.010 |
| O8 | 0.62282(4) | 0.69831(4) | 0.02815(3) | 0.00969(3) |
| H8 | 0.6655(15) | 0.6208(15) | 0.0747(8) | 0.015 |
| C8 | 0.37051(4) | 0.74490(3) | 0.12359(3) | 0.00582(3) |
| C9 | 0.21451(4) | 0.74787(4) | 0.00598(3) | 0.00635(3) |
| H9 | 0.228268 | 0.842194 | -0.044253 | 0.008 |
| O9 | 0.20217(4) | 0.61994(3) | -0.07576(2) | 0.00862(3) |
| H9A | 0.1805(16) | 0.5415(12) | -0.0384(7) | 0.013 |
| C10 | 0.05440(4) | 0.77316(4) | 0.06461(3) | 0.00674(3) |
| H10 | 0.015998 | 0.672780 | 0.095482 | 0.008 |
| O10 | -0.09099(3) | 0.84376(4) | -0.02122(3) | 0.00951(3) |
| H10A | -0.1844(14) | 0.8010(12) | -0.0157(8) | 0.014 |
| C11 | 0.13039(4) | 0.87836(4) | 0.17722(3) | 0.00710(3) |
| H11 | 0.114319 | 0.988248 | 0.148660 | 0.009 |
| O11 | 0.04158(4) | 0.69896(4) | 0.32755(3) | 0.01075(4) |
| H11A | 0.1509(15) | 0.6602(7) | 0.3469(12) | 0.016 |
| C12 | 0.04882(5) | 0.85680(4) | 0.29116(3) | 0.00954(4) |
| H12A | 0.119321 | 0.915827 | 0.363650 | 0.011 |
| H12B | -0.073230 | 0.899676 | 0.271219 | 0.011 |

## Table 3. Bond lengths [Å] and angles [°] for DK\_zucker2\_0m.cif.

|  |  |
| --- | --- |
| O1 - C1 | 1.4136(5) |
| O1 - C5 | 1.4421(5) |
| C1 - O2 | 1.4251(6) |
| C1 - C2 | 1.5364(6) |
| C1 - H1 | 1.0000 |
| O2 - C8 | 1.4324(5) |
| C2 - O7 | 1.4278(5) |
| C2 - C3 | 1.5245(6) |
| C2 - H2 | 1.0000 |
| O3 - C8 | 1.4093(5) |
| O3 - C11 | 1.4491(6) |
| C3 - O6 | 1.4289(6) |
| C3 - C4 | 1.5271(6) |
| C3 - H3 | 1.0000 |
| O4 - C6 | 1.4228(6) |
| O4 - H4A | 0.817(16) |
| C4 - O5 | 1.4150(6) |
| C4 - C5 | 1.5281(6) |
| C4 - H4 | 1.0000 |
| O5 - H5A | 0.830(15) |
| C5 - C6 | 1.5252(6) |
| C5 - H5 | 1.0000 |
| O6 - H6 | 0.855(13) |
| C6 - H6A | 0.9900 |
| C6 - H6AB | 0.9900 |
| O7 - H7 | 0.856(13) |
| C7 - O8 | 1.4290(5) |
| C7 - C8 | 1.5254(6) |
| C7 - H7A | 0.9900 |
| C7 - H7AB | 0.9900 |
| O8 - H8 | 0.859(14) |
| C8 - C9 | 1.5423(6) |
| C9 - O9 | 1.4074(5) |
| C9 - C10 | 1.5257(6) |
| C9 - H9 | 1.0000 |
| O9 - H9A | 0.827(13) |
| C10 - O10 | 1.4234(5) |
| C10 - C11 | 1.5284(6) |
| C10 - H10 | 1.0000 |
| O10 - H10A | 0.825(12) |
| C11 - C12 | 1.5155(6) |
| C11 - H11 | 1.0000 |
| O11 - C12 | 1.4276(6) |
| O11 - H11A | 0.889(12) |
| C12 - H12A | 0.9900 |
| C12 - H12B | 0.9900 |
|  |  |
| C1 - O1 - C5 | 115.59(3) |
| O1 - C1 - O2 | 110.36(3) |
| O1 - C1 - C2 | 111.05(3) |
| O2 - C1 - C2 | 110.05(3) |
| O1 - C1 - H1 | 108.4 |
| O2 - C1 - H1 | 108.4 |
| C2 - C1 - H1 | 108.4 |
| C1 - O2 - C8 | 113.64(2) |
| O7 - C2 - C3 | 110.39(3) |
| O7 - C2 - C1 | 110.06(3) |
| C3 - C2 - C1 | 110.80(3) |
| O7 - C2 - H2 | 108.5 |
| C3 - C2 - H2 | 108.5 |
| C1 - C2 - H2 | 108.5 |
| C8 - O3 - C11 | 111.58(3) |
| O6 - C3 - C2 | 111.42(4) |
| O6 - C3 - C4 | 107.98(3) |
| C2 - C3 - C4 | 107.94(3) |
| O6 - C3 - H3 | 109.8 |
| C2 - C3 - H3 | 109.8 |
| C4 - C3 - H3 | 109.8 |
| C6 - O4 - H4A | 109.5 |
| O5 - C4 - C3 | 112.52(3) |
| O5 - C4 - C5 | 105.41(4) |
| C3 - C4 - C5 | 110.67(3) |
| O5 - C4 - H4 | 109.4 |
| C3 - C4 - H4 | 109.4 |
| C5 - C4 - H4 | 109.4 |
| C4 - O5 - H5A | 109.5 |
| O1 - C5 - C6 | 105.82(3) |
| O1 - C5 - C4 | 110.73(3) |
| C6 - C5 - C4 | 111.91(3) |
| O1 - C5 - H5 | 109.4 |
| C6 - C5 - H5 | 109.4 |
| C4 - C5 - H5 | 109.4 |
| C3 - O6 - H6 | 109.5 |
| O4 - C6 - C5 | 111.41(4) |
| O4 - C6 - H6A | 109.3 |
| C5 - C6 - H6A | 109.3 |
| O4 - C6 - H6AB | 109.3 |
| C5 - C6 - H6AB | 109.3 |
| H6A - C6 - H6AB | 108.0 |
| C2 - O7 - H7 | 109.5 |
| O8 - C7 - C8 | 110.84(3) |
| O8 - C7 - H7A | 109.5 |
| C8 - C7 - H7A | 109.5 |
| O8 - C7 - H7AB | 109.5 |
| C8 - C7 - H7AB | 109.5 |
| H7A - C7 - H7AB | 108.1 |
| C7 - O8 - H8 | 109.5 |
| O3 - C8 - O2 | 110.87(3) |
| O3 - C8 - C7 | 107.15(3) |
| O2 - C8 - C7 | 109.98(3) |
| O3 - C8 - C9 | 105.24(3) |
| O2 - C8 - C9 | 108.46(2) |
| C7 - C8 - C9 | 115.04(3) |
| O9 - C9 - C10 | 115.29(3) |
| O9 - C9 - C8 | 115.77(3) |
| C10 - C9 - C8 | 102.40(4) |
| O9 - C9 - H9 | 107.6 |
| C10 - C9 - H9 | 107.6 |
| C8 - C9 - H9 | 107.6 |
| C9 - O9 - H9A | 109.5 |
| O10 - C10 - C9 | 112.58(4) |
| O10 - C10 - C11 | 111.61(3) |
| C9 - C10 - C11 | 102.42(3) |
| O10 - C10 - H10 | 110.0 |
| C9 - C10 - H10 | 110.0 |
| C11 - C10 - H10 | 110.0 |
| C10 - O10 - H10A | 109.5 |
| O3 - C11 - C12 | 109.79(3) |
| O3 - C11 - C10 | 105.59(3) |
| C12 - C11 - C10 | 114.77(3) |
| O3 - C11 - H11 | 108.8 |
| C12 - C11 - H11 | 108.8 |
| C10 - C11 - H11 | 108.8 |
| C12 - O11 - H11A | 109.5 |
| O11 - C12 - C11 | 113.03(3) |
| O11 - C12 - H12A | 109.0 |
| C11 - C12 - H12A | 109.0 |
| O11 - C12 - H12B | 109.0 |
| C11 - C12 - H12B | 109.0 |
| H12A - C12 - H12B | 107.8 |

## Table 4. Torsion angles [°] for DK\_zucker2\_0m.cif.

|  |  |
| --- | --- |
| C5 - O1 - C1 - O2 | 67.36(3) |
| C5 - O1 - C1 - C2 | -54.96(4) |
| O1 - C1 - O2 - C8 | 108.22(3) |
| C2 - C1 - O2 - C8 | -128.88(3) |
| O1 - C1 - C2 - O7 | 177.65(3) |
| O2 - C1 - C2 - O7 | 55.15(4) |
| O1 - C1 - C2 - C3 | 55.27(4) |
| O2 - C1 - C2 - C3 | -67.24(3) |
| O7 - C2 - C3 - O6 | 63.05(4) |
| C1 - C2 - C3 - O6 | -174.76(3) |
| O7 - C2 - C3 - C4 | -178.56(3) |
| C1 - C2 - C3 - C4 | -56.37(4) |
| O6 - C3 - C4 - O5 | -65.05(4) |
| C2 - C3 - C4 - O5 | 174.38(3) |
| O6 - C3 - C4 - C5 | 177.32(3) |
| C2 - C3 - C4 - C5 | 56.75(4) |
| C1 - O1 - C5 - C6 | 176.70(3) |
| C1 - O1 - C5 - C4 | 55.24(4) |
| O5 - C4 - C5 - O1 | -177.27(3) |
| C3 - C4 - C5 - O1 | -55.37(4) |
| O5 - C4 - C5 - C6 | 64.92(4) |
| C3 - C4 - C5 - C6 | -173.17(3) |
| O1 - C5 - C6 - O4 | -56.30(4) |
| C4 - C5 - C6 - O4 | 64.40(4) |
| C11 - O3 - C8 - O2 | -102.15(3) |
| C11 - O3 - C8 - C7 | 137.82(3) |
| C11 - O3 - C8 - C9 | 14.92(3) |
| C1 - O2 - C8 - O3 | -44.39(4) |
| C1 - O2 - C8 - C7 | 73.93(4) |
| C1 - O2 - C8 - C9 | -159.47(2) |
| O8 - C7 - C8 - O3 | 170.96(3) |
| O8 - C7 - C8 - O2 | 50.36(4) |
| O8 - C7 - C8 - C9 | -72.43(4) |
| O3 - C8 - C9 - O9 | -157.59(3) |
| O2 - C8 - C9 - O9 | -38.89(4) |
| C7 - C8 - C9 - O9 | 84.72(4) |
| O3 - C8 - C9 - C10 | -31.31(3) |
| O2 - C8 - C9 - C10 | 87.39(3) |
| C7 - C8 - C9 - C10 | -149.00(3) |
| O9 - C9 - C10 - O10 | -78.45(4) |
| C8 - C9 - C10 - O10 | 154.96(3) |
| O9 - C9 - C10 - C11 | 161.56(3) |
| C8 - C9 - C10 - C11 | 34.96(3) |
| C8 - O3 - C11 - C12 | 131.96(3) |
| C8 - O3 - C11 - C10 | 7.72(3) |
| O10 - C10 - C11 - O3 | -147.71(3) |
| C9 - C10 - C11 - O3 | -27.03(3) |
| O10 - C10 - C11 - C12 | 91.23(4) |
| C9 - C10 - C11 - C12 | -148.09(3) |
| O3 - C11 - C12 - O11 | -69.64(4) |
| C10 - C11 - C12 - O11 | 49.08(4) |

## Table 7. Hydrogen bonds for DK\_zucker2\_0m.cif [Å and °].

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **D-H...A** | **d(D-H)** | **d(H...A)** | **d(D...A)** | **<(DHA)** |
| C1 - H1 ... O4#1 | 1.00 | 2.33 | 3.3154(8) | 167.3 |
| C3 - H3 ... O8#2 | 1.00 | 2.52 | 3.4909(11) | 162.6 |
| O4 - H4A ... O6#1 | 0.82 | 2.01 | 2.8015(8) | 163.7 |
| O11 - H11A ... O1 | 0.89 | 1.95 | 2.8242(9) | 169.4 |

Symmetry transformations used to generate equivalent atoms: #1: 1-X, 0.5+Y, 1-Z; #2: 1-X, -0.5+Y, -Z;