# Structure Tables

**The following text is only a guideline:** The data for DK\_zucker2\_0m-finalcif.cif were collected from a shock-cooled single crystal at 100(2) K.The data were collected on a Bruker D8 VENTURE dual wavelength Mo/Cu with a microfocus sealed X-ray tube using mirror optics as monochromator. The diffractometer were equipped with an Oxford Cryostream 800 low temperature device and used Mo*Kα* radiation, λ = 0.71073 Å. All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied. The structure were solved by direct methods using SHELXT (G. Sheldrick) and refined by full-matrix least-squares methods against *F*2 by SHELXL-2018/3 (Sheldrick, 2018). All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their *U*iso values constrained to 1.5 times the *U*eq of their pivot atoms for terminal sp3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data (including structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre. CCDC ?????? contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data\_request/cif.

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

|  |  |
| --- | --- |
| CCDC number |  |
| Empirical formula | C12H22O11 |
| Formula weight | 342.29 |
| Temperature [K] | 100(2) |
| Crystal system | monoclinic |
| Space group (number) | *P*21 (4) |
| *a* [Å] | 7.716(3) |
| *b* [Å] | 8.664(2) |
| *c* [Å] | 10.812(4) |
| α [Å] | 90 |
| β [Å] | 102.982(9) |
| γ [Å] | 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] | 0.2×0.12×0.1 |
| Crystal colour | colourless |
| Crystal shape | block |
| 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 |
| Completeness to θ = 25.242° | 99.90 |
| Data / Restraints / Parameters | 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 and equivalent isotropic displacement parameters (Å2) for DK\_zucker2\_0m-finalcif.cif. Ueq is defined as 1/3 of the trace of the orthogonalized U*ij* 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 and angles for DK\_zucker2\_0m-finalcif.cif.

|  |  |
| --- | --- |
| **Atom - Atom** | **Length [Å]** |
| 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 |
|  |  |
| **Atom - Atom - Atom** | **Angle [°]** |
| 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-finalcif.cif.

|  |  |
| --- | --- |
| **Atom - Atom - Atom - Atom** | **Torsion Angle [°]** |
| 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 5. Hydrogen bonds for DK\_zucker2\_0m-finalcif.cif.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **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;