Structure Tables

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

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| --- | --- |
|  | **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* | 42 |
| *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. | 18544/1/227 |
| Goodness-of-fit on *F*2 | 1.279 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0226 w*R*2 = 0.0603 |
| Final *R* indexes  [all data] | *R*1 = 0.0234 w*R*2 = 0.0606 |
| Largest peak/hole /eÅ3 | 0.41/-0.23 |
| 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** |
| O001 | 0.36906(4) | 0.53931(3) | 0.37833(2) | 0.00734(3) |
| O002 | 0.39202(3) | 0.59002(3) | 0.17092(2) | 0.00639(3) |
| O003 | 0.31893(3) | 0.84412(3) | 0.21219(2) | 0.00736(3) |
| O004 | 0.62280(4) | 0.69831(4) | 0.02814(3) | 0.00971(4) |
| H004 | 0.6644(15) | 0.6209(14) | 0.0742(7) | 0.015 |
| O005 | 0.75100(4) | 0.50226(4) | 0.22972(3) | 0.00917(3) |
| H005 | 0.8365(15) | 0.5577(15) | 0.2691(6) | 0.014 |
| O006 | -0.09098(4) | 0.84377(4) | -0.02123(3) | 0.00953(3) |
| H006 | -0.1844(13) | 0.8017(12) | -0.0151(8) | 0.014 |
| O007 | 0.20218(4) | 0.61994(3) | -0.07577(3) | 0.00862(3) |
| H007 | 0.1802(15) | 0.5420(12) | -0.0388(7) | 0.013 |
| O008 | 0.04157(4) | 0.69894(4) | 0.32755(3) | 0.01076(4) |
| H008 | 0.1499(14) | 0.6605(6) | 0.3467(12) | 0.016 |
| O009 | 0.70569(5) | 0.18757(4) | 0.30871(3) | 0.01252(4) |
| H009 | 0.7346(13) | 0.1662(12) | 0.2398(11) | 0.019 |
| O00A | 0.35551(5) | 0.12166(4) | 0.34952(4) | 0.01419(5) |
| H0A | 0.4294(13) | 0.0533(12) | 0.3462(12) | 0.021 |
| O00B | 0.28726(5) | 0.39272(4) | 0.58393(3) | 0.01167(4) |
| H00O | 0.2854(13) | 0.4842(17) | 0.6006(5) | 0.018 |
| C00C | 0.48621(4) | 0.57984(4) | 0.30012(3) | 0.00638(3) |
| H00C | 0.5298(13) | 0.6762(14) | 0.3282(10) | 0.008 |
| C00D | 0.37052(4) | 0.74491(4) | 0.12358(3) | 0.00582(3) |
| C00E | 0.56603(5) | 0.29944(4) | 0.28574(3) | 0.00792(4) |
| H00E | 0.497599 | 0.292169 | 0.195674 | 0.010 |
| C00F | 0.54676(4) | 0.80535(4) | 0.10150(3) | 0.00811(4) |
| H00A | 0.526956 | 0.905538 | 0.056500 | 0.010 |
| H00B | 0.630429 | 0.822505 | 0.184271 | 0.010 |
| C00G | 0.05440(4) | 0.77316(4) | 0.06462(3) | 0.00674(3) |
| H00G | 0.015994 | 0.672778 | 0.095485 | 0.008 |
| C00H | 0.63858(4) | 0.46254(4) | 0.31329(3) | 0.00710(4) |
| H00H | 0.710694 | 0.466104 | 0.402513 | 0.009 |
| C00I | 0.44351(5) | 0.26530(4) | 0.37537(3) | 0.00832(4) |
| H00I | 0.514349 | 0.266214 | 0.465006 | 0.010 |
| C00J | 0.21450(4) | 0.74788(4) | 0.00598(3) | 0.00634(3) |
| H00J | 0.228254 | 0.842213 | -0.044248 | 0.008 |
| C00K | 0.13039(4) | 0.87835(4) | 0.17722(3) | 0.00711(4) |
| H00K | 0.114317 | 0.988240 | 0.148655 | 0.009 |
| C00L | 0.18420(5) | 0.36621(5) | 0.45908(4) | 0.01013(4) |
| H00D | 0.083328 | 0.439613 | 0.440935 | 0.012 |
| H00F | 0.134843 | 0.260317 | 0.453667 | 0.012 |
| C00M | 0.29555(4) | 0.38576(4) | 0.36007(3) | 0.00776(4) |
| H00M | 0.216915 | 0.377350 | 0.273173 | 0.009 |
| C00N | 0.04883(5) | 0.85681(4) | 0.29117(3) | 0.00955(4) |
| H00L | 0.119343 | 0.915829 | 0.363653 | 0.011 |
| H00N | -0.073217 | 0.899698 | 0.271231 | 0.011 |