# Structure Tables

The compound was crystallized from hot methanol by cooling. A colourless, plate-shaped crystal of cu\_BruecknerJK\_153F40\_0m was mounted on a MiTeGen micromount with perfluoroether oil. Data were collected from a shock-cooled single crystal at 102(2) K on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using a mirror optics as monochromator and a Bruker PHOTON III detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Cu*Kα* radiation (λ = 1.54178 Å). All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied.[1,2] The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares methods against *F*2 by SHELXL-2018/3.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic 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. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Crystallographic data for the structures reported here have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 1979688 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/​structures. This report and the CIF file were generated using FinalCif.[6]

## Table 1. Crystal data and structure refinement for cu\_BruecknerJK\_153F40\_0m

|  |  |
| --- | --- |
| CCDC number | 1979688 |
| Empirical formula | C38.50H40O12.50 |
| Formula weight | 702.70 |
| Temperature [K] | 102(2) |
| Crystal system | orthorhombic |
| Space group (number) | (18) |
| *a* [Å] | 19.678(3) |
| *b* [Å] | 37.0229(9) |
| *c* [Å] | 4.7720(4) |
| α [°] | 90 |
| β [°] | 90 |
| γ [°] | 90 |
| Volume [Å3] | 3476.6(7) |
| *Z* | 4 |
| *ρ*calc [gcm−3] | 1.343 |
| *μ* [mm−1] | 0.838 |
| *F*(000) | 1484 |
| Crystal size [mm3] | 0.220×0.100×0.040 |
| Crystal colour | colourless |
| Crystal shape | plate |
| Radiation | Cu*Kα* (λ=1.54178 Å) |
| 2θ range [°] | 4.77 to 156.95 (0.79 Å) |
| Index ranges | −24 ≤ h ≤ 24 −47 ≤ k ≤ 46 −5 ≤ l ≤ 5 |
| Reflections collected | 51638 |
| Independent reflections | 7338 *R*int = 0.0302 *R*sigma = 0.0149 |
| Completeness to  θ = 67.679° | 99.9 % |
| Data / Restraints / Parameters | 7338/5/479 |
| Absorption correction Tmin/Tmax (method) | 0.7697/0.9288 (multi-scan) |
| Goodness-of-fit on *F*2 | 1.198 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0364 w*R*2 = 0.0917 |
| Final *R* indexes  [all data] | *R*1 = 0.0368 w*R*2 = 0.0919 |
| Largest peak/hole [eÅ−3] | 0.26/−0.21 |
| Flack X parameter | 0.04(2) |

## Refinement details for cu\_BruecknerJK\_153F40\_0m

The methanol molecule is disordered around a special position and thus half occupied.

## Table 2. Atomic coordinates and *U*eq [Å2] for cu\_BruecknerJK\_153F40\_0m

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | ***U*eq** |
| C1 | 0.00232(11) | 0.37061(7) | 0.3615(5) | 0.0240(5) |
| H1 | -0.004416 | 0.382450 | 0.547826 | 0.029 |
| O1 | 0.02619(8) | 0.39536(5) | 0.1512(4) | 0.0239(4) |
| C2 | 0.04929(11) | 0.33785(7) | 0.3773(5) | 0.0222(5) |
| H2 | 0.041865 | 0.324706 | 0.557764 | 0.027 |
| O2 | -0.06534(10) | 0.30877(7) | -0.1251(5) | 0.0444(5) |
| C3 | 0.12367(11) | 0.34684(6) | 0.3437(5) | 0.0188(4) |
| O3 | 0.02748(9) | 0.31504(5) | 0.1395(4) | 0.0280(4) |
| C4 | 0.17159(12) | 0.31982(6) | 0.3825(5) | 0.0191(4) |
| O4 | 0.14805(8) | 0.28609(4) | 0.4503(4) | 0.0215(3) |
| O5 | 0.27337(9) | 0.26484(4) | 0.3552(5) | 0.0296(4) |
| C5 | 0.24236(11) | 0.32684(6) | 0.3402(5) | 0.0191(4) |
| O6 | 0.23152(8) | 0.42552(4) | 0.1932(3) | 0.0192(3) |
| C6 | 0.29485(12) | 0.29983(6) | 0.3375(6) | 0.0235(5) |
| O7 | 0.73086(9) | 0.47914(4) | 0.6156(4) | 0.0278(4) |
| C7 | 0.36205(12) | 0.30935(6) | 0.3087(6) | 0.0246(5) |
| H7 | 0.395856 | 0.291035 | 0.307928 | 0.030 |
| O8 | 0.89175(9) | 0.42106(5) | 0.7874(4) | 0.0336(4) |
| C8 | 0.38186(12) | 0.34604(6) | 0.2800(6) | 0.0222(5) |
| O9 | 0.80099(8) | 0.40908(4) | 0.5219(4) | 0.0222(4) |
| C9 | 0.33258(11) | 0.37240(6) | 0.2656(5) | 0.0199(4) |
| H9 | 0.345488 | 0.396914 | 0.240601 | 0.024 |
| O10 | 0.71633(8) | 0.36267(4) | 0.1160(4) | 0.0267(4) |
| C10 | 0.26263(12) | 0.36330(6) | 0.2877(5) | 0.0195(4) |
| O11 | 0.61510(9) | 0.31944(5) | -0.0335(4) | 0.0284(4) |
| C11 | 0.21156(11) | 0.39014(6) | 0.2511(5) | 0.0180(4) |
| O12 | 0.52253(8) | 0.45508(4) | 0.5609(3) | 0.0189(3) |
| C12 | 0.14374(12) | 0.38230(6) | 0.2726(5) | 0.0194(4) |
| C13 | 0.09056(11) | 0.41131(6) | 0.2202(5) | 0.0202(5) |
| H13 | 0.105712 | 0.425160 | 0.051506 | 0.024 |
| C14 | -0.06280(13) | 0.35437(8) | 0.2459(6) | 0.0323(6) |
| H14A | -0.092167 | 0.345114 | 0.398248 | 0.039 |
| H14B | -0.088559 | 0.372267 | 0.134159 | 0.039 |
| C15 | -0.03688(13) | 0.32419(8) | 0.0651(6) | 0.0319(6) |
| C16 | 0.16202(14) | 0.27563(7) | 0.7376(6) | 0.0278(5) |
| H16A | 0.157773 | 0.249358 | 0.755926 | 0.042 |
| H16B | 0.129459 | 0.287461 | 0.862909 | 0.042 |
| H16C | 0.208276 | 0.282987 | 0.787893 | 0.042 |
| C17 | 0.32322(15) | 0.23737(6) | 0.3063(8) | 0.0377(7) |
| H17A | 0.300883 | 0.213739 | 0.298159 | 0.057 |
| H17B | 0.356507 | 0.237497 | 0.459030 | 0.057 |
| H17C | 0.346375 | 0.242092 | 0.128199 | 0.057 |
| C18 | 0.24752(12) | 0.43131(7) | -0.0987(5) | 0.0240(5) |
| H18A | 0.252400 | 0.457250 | -0.134199 | 0.036 |
| H18B | 0.210834 | 0.421604 | -0.215474 | 0.036 |
| H18C | 0.290174 | 0.418994 | -0.144651 | 0.036 |
| C19 | 0.08325(14) | 0.43854(7) | 0.4585(6) | 0.0286(5) |
| H19A | 0.126943 | 0.450553 | 0.490553 | 0.043 |
| H19B | 0.069194 | 0.425955 | 0.629616 | 0.043 |
| H19C | 0.048924 | 0.456593 | 0.408303 | 0.043 |
| C20 | 0.77127(12) | 0.46820(7) | 0.3822(6) | 0.0275(5) |
| H20 | 0.764914 | 0.484217 | 0.215471 | 0.033 |
| C21 | 0.75888(11) | 0.42840(6) | 0.3143(5) | 0.0214(5) |
| H21 | 0.775876 | 0.423023 | 0.121291 | 0.026 |
| C22 | 0.68592(11) | 0.41693(6) | 0.3385(5) | 0.0192(4) |
| C23 | 0.66612(11) | 0.38373(6) | 0.2329(5) | 0.0203(5) |
| C24 | 0.59663(11) | 0.37266(6) | 0.2381(5) | 0.0193(4) |
| C25 | 0.56976(12) | 0.34054(6) | 0.1056(6) | 0.0223(5) |
| C26 | 0.50150(12) | 0.33263(6) | 0.1204(6) | 0.0238(5) |
| H26 | 0.484940 | 0.311299 | 0.033398 | 0.029 |
| C27 | 0.45523(11) | 0.35571(6) | 0.2630(5) | 0.0210(5) |
| C28 | 0.47865(11) | 0.38691(6) | 0.3818(5) | 0.0195(4) |
| H28 | 0.447679 | 0.402561 | 0.474499 | 0.023 |
| C29 | 0.54863(11) | 0.39632(6) | 0.3689(5) | 0.0172(4) |
| C30 | 0.57071(11) | 0.43045(6) | 0.4717(5) | 0.0178(4) |
| C31 | 0.63779(11) | 0.44097(6) | 0.4568(5) | 0.0179(4) |
| C32 | 0.65905(11) | 0.47805(6) | 0.5607(5) | 0.0212(5) |
| H32 | 0.635558 | 0.482025 | 0.743976 | 0.025 |
| C33 | 0.84430(13) | 0.46775(7) | 0.4856(8) | 0.0366(7) |
| H33A | 0.876675 | 0.470540 | 0.328242 | 0.044 |
| H33B | 0.852403 | 0.487182 | 0.624163 | 0.044 |
| C34 | 0.85057(11) | 0.43104(6) | 0.6186(5) | 0.0226(5) |
| C35 | 0.74027(13) | 0.33415(7) | 0.2969(7) | 0.0340(6) |
| H35A | 0.777024 | 0.320965 | 0.203420 | 0.051 |
| H35B | 0.702804 | 0.317537 | 0.337910 | 0.051 |
| H35C | 0.757238 | 0.344594 | 0.472124 | 0.051 |
| C36 | 0.58889(14) | 0.28982(7) | -0.1954(6) | 0.0308(6) |
| H36A | 0.626565 | 0.277149 | -0.286890 | 0.046 |
| H36B | 0.557544 | 0.299040 | -0.338024 | 0.046 |
| H36C | 0.564690 | 0.273068 | -0.071573 | 0.046 |
| C37 | 0.50029(14) | 0.45070(7) | 0.8456(6) | 0.0291(5) |
| H37A | 0.460892 | 0.466274 | 0.880081 | 0.044 |
| H37B | 0.537214 | 0.457407 | 0.973257 | 0.044 |
| H37C | 0.487593 | 0.425446 | 0.877807 | 0.044 |
| C38 | 0.63748(12) | 0.50904(6) | 0.3660(6) | 0.0242(5) |
| H38A | 0.587772 | 0.510127 | 0.356932 | 0.036 |
| H38B | 0.655813 | 0.504821 | 0.177915 | 0.036 |
| H38C | 0.655101 | 0.531940 | 0.439052 | 0.036 |
| O13 | 0.9588(2) | 0.48086(11) | 1.0443(9) | 0.0337(9) |
| H13A | 0.955437 | 0.460236 | 0.972254 | 0.051 |
| C39 | 1.0123(4) | 0.5002(5) | 0.9115(11) | 0.030(2) |
| H39A | 1.012625 | 0.525207 | 0.978836 | 0.045 |
| H39B | 1.005378 | 0.499988 | 0.708113 | 0.045 |
| H39C | 1.055913 | 0.488733 | 0.955932 | 0.045 |

*U*eq is defined as 1/3 of the trace of the orthogonalized *Uij* tensor.

## Table 3. Bond lengths and angles for cu\_BruecknerJK\_153F40\_0m

|  |  |
| --- | --- |
| **Atom–Atom** | **Length [Å]** |
| C1–O1 | 1.438(3) |
| C1–C14 | 1.519(3) |
| C1–C2 | 1.527(3) |
| C1–H1 | 1.0000 |
| O1–C13 | 1.436(3) |
| C2–O3 | 1.478(3) |
| C2–C3 | 1.510(3) |
| C2–H2 | 1.0000 |
| O2–C15 | 1.210(4) |
| C3–C4 | 1.387(3) |
| C3–C12 | 1.412(3) |
| O3–C15 | 1.358(3) |
| C4–O4 | 1.371(3) |
| C4–C5 | 1.431(3) |
| O4–C16 | 1.451(3) |
| O5–C6 | 1.365(3) |
| O5–C17 | 1.432(3) |
| C5–C10 | 1.430(3) |
| C5–C6 | 1.438(3) |
| O6–C11 | 1.395(3) |
| O6–C18 | 1.444(3) |
| C6–C7 | 1.376(3) |
| O7–C20 | 1.427(3) |
| O7–C32 | 1.438(3) |
| C7–C8 | 1.419(3) |
| C7–H7 | 0.9500 |
| O8–C34 | 1.201(3) |
| C8–C9 | 1.378(3) |
| C8–C27 | 1.490(3) |
| O9–C34 | 1.351(3) |
| O9–C21 | 1.476(3) |
| C9–C10 | 1.421(3) |
| C9–H9 | 0.9500 |
| O10–C23 | 1.377(3) |
| O10–C35 | 1.443(3) |
| C10–C11 | 1.424(3) |
| O11–C25 | 1.359(3) |
| O11–C36 | 1.437(3) |
| C11–C12 | 1.370(3) |
| O12–C30 | 1.382(3) |
| O12–C37 | 1.437(3) |
| C12–C13 | 1.520(3) |
| C13–C19 | 1.526(3) |
| C13–H13 | 1.0000 |
| C14–C15 | 1.501(4) |
| C14–H14A | 0.9900 |
| C14–H14B | 0.9900 |
| C16–H16A | 0.9800 |
| C16–H16B | 0.9800 |
| C16–H16C | 0.9800 |
| C17–H17A | 0.9800 |
| C17–H17B | 0.9800 |
| C17–H17C | 0.9800 |
| C18–H18A | 0.9800 |
| C18–H18B | 0.9800 |
| C18–H18C | 0.9800 |
| C19–H19A | 0.9800 |
| C19–H19B | 0.9800 |
| C19–H19C | 0.9800 |
| C20–C33 | 1.520(3) |
| C20–C21 | 1.528(3) |
| C20–H20 | 1.0000 |
| C21–C22 | 1.502(3) |
| C21–H21 | 1.0000 |
| C22–C23 | 1.384(3) |
| C22–C31 | 1.417(3) |
| C23–C24 | 1.428(3) |
| C24–C29 | 1.431(3) |
| C24–C25 | 1.447(3) |
| C25–C26 | 1.377(3) |
| C26–C27 | 1.422(3) |
| C26–H26 | 0.9500 |
| C27–C28 | 1.367(3) |
| C28–C29 | 1.422(3) |
| C28–H28 | 0.9500 |
| C29–C30 | 1.424(3) |
| C30–C31 | 1.378(3) |
| C31–C32 | 1.518(3) |
| C32–C38 | 1.536(3) |
| C32–H32 | 1.0000 |
| C33–C34 | 1.505(3) |
| C33–H33A | 0.9900 |
| C33–H33B | 0.9900 |
| C35–H35A | 0.9800 |
| C35–H35B | 0.9800 |
| C35–H35C | 0.9800 |
| C36–H36A | 0.9800 |
| C36–H36B | 0.9800 |
| C36–H36C | 0.9800 |
| C37–H37A | 0.9800 |
| C37–H37B | 0.9800 |
| C37–H37C | 0.9800 |
| C38–H38A | 0.9800 |
| C38–H38B | 0.9800 |
| C38–H38C | 0.9800 |
| O13–C39 | 1.423(11) |
| O13–H13A | 0.8400 |
| C39–H39A | 0.9800 |
| C39–H39B | 0.9800 |
| C39–H39C | 0.9800 |
|  |  |
| **Atom–Atom–Atom** | **Angle [°]** |
| O1–C1–C14 | 105.9(2) |
| O1–C1–C2 | 110.05(19) |
| C14–C1–C2 | 102.4(2) |
| O1–C1–H1 | 112.6 |
| C14–C1–H1 | 112.6 |
| C2–C1–H1 | 112.6 |
| C13–O1–C1 | 112.98(18) |
| O3–C2–C3 | 109.02(19) |
| O3–C2–C1 | 103.91(19) |
| C3–C2–C1 | 114.0(2) |
| O3–C2–H2 | 109.9 |
| C3–C2–H2 | 109.9 |
| C1–C2–H2 | 109.9 |
| C4–C3–C12 | 120.8(2) |
| C4–C3–C2 | 119.1(2) |
| C12–C3–C2 | 120.1(2) |
| C15–O3–C2 | 109.2(2) |
| O4–C4–C3 | 117.3(2) |
| O4–C4–C5 | 121.8(2) |
| C3–C4–C5 | 120.8(2) |
| C4–O4–C16 | 113.73(18) |
| C6–O5–C17 | 116.85(19) |
| C10–C5–C4 | 117.9(2) |
| C10–C5–C6 | 117.0(2) |
| C4–C5–C6 | 125.0(2) |
| C11–O6–C18 | 113.07(18) |
| O5–C6–C7 | 123.2(2) |
| O5–C6–C5 | 115.9(2) |
| C7–C6–C5 | 120.9(2) |
| C20–O7–C32 | 113.43(19) |
| C6–C7–C8 | 121.3(2) |
| C6–C7–H7 | 119.4 |
| C8–C7–H7 | 119.4 |
| C9–C8–C7 | 119.3(2) |
| C9–C8–C27 | 120.6(2) |
| C7–C8–C27 | 120.1(2) |
| C34–O9–C21 | 110.05(17) |
| C8–C9–C10 | 120.7(2) |
| C8–C9–H9 | 119.7 |
| C10–C9–H9 | 119.7 |
| C23–O10–C35 | 114.0(2) |
| C9–C10–C11 | 120.6(2) |
| C9–C10–C5 | 120.5(2) |
| C11–C10–C5 | 118.9(2) |
| C25–O11–C36 | 117.75(19) |
| C12–C11–O6 | 119.2(2) |
| C12–C11–C10 | 122.0(2) |
| O6–C11–C10 | 118.74(19) |
| C30–O12–C37 | 115.20(18) |
| C11–C12–C3 | 119.2(2) |
| C11–C12–C13 | 120.6(2) |
| C3–C12–C13 | 120.3(2) |
| O1–C13–C12 | 110.75(19) |
| O1–C13–C19 | 111.1(2) |
| C12–C13–C19 | 114.15(19) |
| O1–C13–H13 | 106.8 |
| C12–C13–H13 | 106.8 |
| C19–C13–H13 | 106.8 |
| C15–C14–C1 | 102.5(2) |
| C15–C14–H14A | 111.3 |
| C1–C14–H14A | 111.3 |
| C15–C14–H14B | 111.3 |
| C1–C14–H14B | 111.3 |
| H14A–C14–H14B | 109.2 |
| O2–C15–O3 | 120.7(3) |
| O2–C15–C14 | 128.7(3) |
| O3–C15–C14 | 110.6(2) |
| O4–C16–H16A | 109.5 |
| O4–C16–H16B | 109.5 |
| H16A–C16–H16B | 109.5 |
| O4–C16–H16C | 109.5 |
| H16A–C16–H16C | 109.5 |
| H16B–C16–H16C | 109.5 |
| O5–C17–H17A | 109.5 |
| O5–C17–H17B | 109.5 |
| H17A–C17–H17B | 109.5 |
| O5–C17–H17C | 109.5 |
| H17A–C17–H17C | 109.5 |
| H17B–C17–H17C | 109.5 |
| O6–C18–H18A | 109.5 |
| O6–C18–H18B | 109.5 |
| H18A–C18–H18B | 109.5 |
| O6–C18–H18C | 109.5 |
| H18A–C18–H18C | 109.5 |
| H18B–C18–H18C | 109.5 |
| C13–C19–H19A | 109.5 |
| C13–C19–H19B | 109.5 |
| H19A–C19–H19B | 109.5 |
| C13–C19–H19C | 109.5 |
| H19A–C19–H19C | 109.5 |
| H19B–C19–H19C | 109.5 |
| O7–C20–C33 | 106.1(2) |
| O7–C20–C21 | 110.49(19) |
| C33–C20–C21 | 102.07(19) |
| O7–C20–H20 | 112.5 |
| C33–C20–H20 | 112.5 |
| C21–C20–H20 | 112.5 |
| O9–C21–C22 | 110.36(18) |
| O9–C21–C20 | 103.62(18) |
| C22–C21–C20 | 114.1(2) |
| O9–C21–H21 | 109.5 |
| C22–C21–H21 | 109.5 |
| C20–C21–H21 | 109.5 |
| C23–C22–C31 | 121.0(2) |
| C23–C22–C21 | 119.5(2) |
| C31–C22–C21 | 119.5(2) |
| O10–C23–C22 | 116.6(2) |
| O10–C23–C24 | 122.1(2) |
| C22–C23–C24 | 121.2(2) |
| C23–C24–C29 | 117.6(2) |
| C23–C24–C25 | 125.3(2) |
| C29–C24–C25 | 116.9(2) |
| O11–C25–C26 | 122.9(2) |
| O11–C25–C24 | 116.5(2) |
| C26–C25–C24 | 120.6(2) |
| C25–C26–C27 | 121.4(2) |
| C25–C26–H26 | 119.3 |
| C27–C26–H26 | 119.3 |
| C28–C27–C26 | 119.4(2) |
| C28–C27–C8 | 120.5(2) |
| C26–C27–C8 | 120.1(2) |
| C27–C28–C29 | 121.0(2) |
| C27–C28–H28 | 119.5 |
| C29–C28–H28 | 119.5 |
| C28–C29–C30 | 119.9(2) |
| C28–C29–C24 | 120.5(2) |
| C30–C29–C24 | 119.48(19) |
| C31–C30–O12 | 119.1(2) |
| C31–C30–C29 | 121.7(2) |
| O12–C30–C29 | 118.83(19) |
| C30–C31–C22 | 118.9(2) |
| C30–C31–C32 | 120.2(2) |
| C22–C31–C32 | 120.9(2) |
| O7–C32–C31 | 110.83(18) |
| O7–C32–C38 | 111.15(19) |
| C31–C32–C38 | 113.68(19) |
| O7–C32–H32 | 106.9 |
| C31–C32–H32 | 106.9 |
| C38–C32–H32 | 106.9 |
| C34–C33–C20 | 102.96(19) |
| C34–C33–H33A | 111.2 |
| C20–C33–H33A | 111.2 |
| C34–C33–H33B | 111.2 |
| C20–C33–H33B | 111.2 |
| H33A–C33–H33B | 109.1 |
| O8–C34–O9 | 122.1(2) |
| O8–C34–C33 | 128.0(2) |
| O9–C34–C33 | 109.9(2) |
| O10–C35–H35A | 109.5 |
| O10–C35–H35B | 109.5 |
| H35A–C35–H35B | 109.5 |
| O10–C35–H35C | 109.5 |
| H35A–C35–H35C | 109.5 |
| H35B–C35–H35C | 109.5 |
| O11–C36–H36A | 109.5 |
| O11–C36–H36B | 109.5 |
| H36A–C36–H36B | 109.5 |
| O11–C36–H36C | 109.5 |
| H36A–C36–H36C | 109.5 |
| H36B–C36–H36C | 109.5 |
| O12–C37–H37A | 109.5 |
| O12–C37–H37B | 109.5 |
| H37A–C37–H37B | 109.5 |
| O12–C37–H37C | 109.5 |
| H37A–C37–H37C | 109.5 |
| H37B–C37–H37C | 109.5 |
| C32–C38–H38A | 109.5 |
| C32–C38–H38B | 109.5 |
| H38A–C38–H38B | 109.5 |
| C32–C38–H38C | 109.5 |
| H38A–C38–H38C | 109.5 |
| H38B–C38–H38C | 109.5 |
| C39–O13–H13A | 109.5 |
| O13–C39–H39A | 109.5 |
| O13–C39–H39B | 109.5 |
| H39A–C39–H39B | 109.5 |
| O13–C39–H39C | 109.5 |
| H39A–C39–H39C | 109.5 |
| H39B–C39–H39C | 109.5 |

## Table 4. Torsion angles for cu\_BruecknerJK\_153F40\_0m

|  |  |
| --- | --- |
| **Atom–Atom–Atom–Atom** | **Torsion Angle [°]** |
| C14–C1–O1–C13 | −175.9(2) |
| C2–C1–O1–C13 | −66.0(3) |
| O1–C1–C2–O3 | −80.0(2) |
| C14–C1–C2–O3 | 32.3(2) |
| O1–C1–C2–C3 | 38.6(3) |
| C14–C1–C2–C3 | 150.9(2) |
| O3–C2–C3–C4 | −70.9(3) |
| C1–C2–C3–C4 | 173.5(2) |
| O3–C2–C3–C12 | 108.9(2) |
| C1–C2–C3–C12 | −6.7(3) |
| C3–C2–O3–C15 | −143.1(2) |
| C1–C2–O3–C15 | −21.2(2) |
| C12–C3–C4–O4 | −179.8(2) |
| C2–C3–C4–O4 | −0.1(3) |
| C12–C3–C4–C5 | −2.6(4) |
| C2–C3–C4–C5 | 177.2(2) |
| C3–C4–O4–C16 | −108.9(2) |
| C5–C4–O4–C16 | 73.9(3) |
| O4–C4–C5–C10 | −176.1(2) |
| C3–C4–C5–C10 | 6.8(3) |
| O4–C4–C5–C6 | 6.0(4) |
| C3–C4–C5–C6 | −171.1(2) |
| C17–O5–C6–C7 | −7.9(4) |
| C17–O5–C6–C5 | 169.9(3) |
| C10–C5–C6–O5 | −172.6(2) |
| C4–C5–C6–O5 | 5.3(4) |
| C10–C5–C6–C7 | 5.2(4) |
| C4–C5–C6–C7 | −176.8(3) |
| O5–C6–C7–C8 | 177.5(3) |
| C5–C6–C7–C8 | −0.2(4) |
| C6–C7–C8–C9 | −3.6(4) |
| C6–C7–C8–C27 | 177.1(3) |
| C7–C8–C9–C10 | 1.9(4) |
| C27–C8–C9–C10 | −178.7(2) |
| C8–C9–C10–C11 | −175.1(2) |
| C8–C9–C10–C5 | 3.3(4) |
| C4–C5–C10–C9 | 175.1(2) |
| C6–C5–C10–C9 | −6.8(3) |
| C4–C5–C10–C11 | −6.4(3) |
| C6–C5–C10–C11 | 171.7(2) |
| C18–O6–C11–C12 | −98.9(2) |
| C18–O6–C11–C10 | 81.4(3) |
| C9–C10–C11–C12 | −179.6(2) |
| C5–C10–C11–C12 | 1.9(4) |
| C9–C10–C11–O6 | 0.0(3) |
| C5–C10–C11–O6 | −178.5(2) |
| O6–C11–C12–C3 | −177.2(2) |
| C10–C11–C12–C3 | 2.5(4) |
| O6–C11–C12–C13 | 2.9(3) |
| C10–C11–C12–C13 | −177.4(2) |
| C4–C3–C12–C11 | −2.2(3) |
| C2–C3–C12–C11 | 178.1(2) |
| C4–C3–C12–C13 | 177.8(2) |
| C2–C3–C12–C13 | −2.0(3) |
| C1–O1–C13–C12 | 56.3(2) |
| C1–O1–C13–C19 | −71.7(2) |
| C11–C12–C13–O1 | 158.6(2) |
| C3–C12–C13–O1 | −21.3(3) |
| C11–C12–C13–C19 | −75.2(3) |
| C3–C12–C13–C19 | 104.9(3) |
| O1–C1–C14–C15 | 84.1(2) |
| C2–C1–C14–C15 | −31.2(3) |
| C2–O3–C15–O2 | −179.6(2) |
| C2–O3–C15–C14 | 0.8(3) |
| C1–C14–C15–O2 | −159.6(3) |
| C1–C14–C15–O3 | 19.9(3) |
| C32–O7–C20–C33 | −174.99(18) |
| C32–O7–C20–C21 | −65.1(2) |
| C34–O9–C21–C22 | −144.3(2) |
| C34–O9–C21–C20 | −21.7(2) |
| O7–C20–C21–O9 | −80.1(2) |
| C33–C20–C21–O9 | 32.3(3) |
| O7–C20–C21–C22 | 39.9(3) |
| C33–C20–C21–C22 | 152.4(2) |
| O9–C21–C22–C23 | −75.8(3) |
| C20–C21–C22–C23 | 167.9(2) |
| O9–C21–C22–C31 | 107.2(2) |
| C20–C21–C22–C31 | −9.1(3) |
| C35–O10–C23–C22 | 101.2(2) |
| C35–O10–C23–C24 | −80.8(3) |
| C31–C22–C23–O10 | 178.4(2) |
| C21–C22–C23–O10 | 1.5(3) |
| C31–C22–C23–C24 | 0.4(4) |
| C21–C22–C23–C24 | −176.6(2) |
| O10–C23–C24–C29 | 179.0(2) |
| C22–C23–C24–C29 | −3.1(3) |
| O10–C23–C24–C25 | −5.3(4) |
| C22–C23–C24–C25 | 172.6(2) |
| C36–O11–C25–C26 | 6.6(4) |
| C36–O11–C25–C24 | −172.6(2) |
| C23–C24–C25–O11 | 0.2(4) |
| C29–C24–C25–O11 | 175.9(2) |
| C23–C24–C25–C26 | −179.1(2) |
| C29–C24–C25–C26 | −3.4(3) |
| O11–C25–C26–C27 | −178.7(2) |
| C24–C25–C26–C27 | 0.5(4) |
| C25–C26–C27–C28 | 1.8(4) |
| C25–C26–C27–C8 | −178.8(2) |
| C9–C8–C27–C28 | 36.1(4) |
| C7–C8–C27–C28 | −144.5(3) |
| C9–C8–C27–C26 | −143.3(3) |
| C7–C8–C27–C26 | 36.1(4) |
| C26–C27–C28–C29 | −1.0(4) |
| C8–C27–C28–C29 | 179.5(2) |
| C27–C28–C29–C30 | 174.3(2) |
| C27–C28–C29–C24 | −1.9(4) |
| C23–C24–C29–C28 | −179.9(2) |
| C25–C24–C29–C28 | 4.1(3) |
| C23–C24–C29–C30 | 3.9(3) |
| C25–C24–C29–C30 | −172.2(2) |
| C37–O12–C30–C31 | −102.1(2) |
| C37–O12–C30–C29 | 84.8(3) |
| C28–C29–C30–C31 | −178.4(2) |
| C24–C29–C30–C31 | −2.1(3) |
| C28–C29–C30–O12 | −5.4(3) |
| C24–C29–C30–O12 | 170.9(2) |
| O12–C30–C31–C22 | −173.6(2) |
| C29–C30–C31–C22 | −0.6(3) |
| O12–C30–C31–C32 | 5.2(3) |
| C29–C30–C31–C32 | 178.2(2) |
| C23–C22–C31–C30 | 1.5(3) |
| C21–C22–C31–C30 | 178.5(2) |
| C23–C22–C31–C32 | −177.3(2) |
| C21–C22–C31–C32 | −0.3(3) |
| C20–O7–C32–C31 | 54.4(3) |
| C20–O7–C32–C38 | −73.0(2) |
| C30–C31–C32–O7 | 160.4(2) |
| C22–C31–C32–O7 | −20.8(3) |
| C30–C31–C32–C38 | −73.5(3) |
| C22–C31–C32–C38 | 105.2(2) |
| O7–C20–C33–C34 | 84.5(3) |
| C21–C20–C33–C34 | −31.2(3) |
| C21–O9–C34–O8 | −179.1(2) |
| C21–O9–C34–C33 | 1.4(3) |
| C20–C33–C34–O8 | −160.0(3) |
| C20–C33–C34–O9 | 19.6(3) |

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