# Structure Tables

**The following text is only a suggestion:** [No crystallization method was given]. The data for cu\_BruecknerJK\_153F40\_0m were collected from a shock-cooled single crystal at 102(2) K on a [No measurement device type given] [No measurement device given] with a [No radiation source given] using [No monochromator type given] as monochromator and a [No detector type given] detector. The diffractometer was equipped with a 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 were 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. 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. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Crystallographic data for the structures reported in this paper 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 |
| 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) |

## 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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