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 CuK_α 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 sp^3 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	$C_{38.50}H_{40}O_{12.50}$
Formula weight	702.70
Temperature [K]	102(2)
Crystal system	orthorhombic
Space group (number)	$P2_12_12$ (18)
a [Å]	19.678(3)
b [Å]	37.0229(9)
c [Å]	4.7720(4)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	3476.6(7)
Z	4
ρ_{calc} [gcm^{-3}]	1.343
μ [mm^{-1}]	0.838
F(000)	1484
Crystal size [mm^3]	0.220×0.100×0.040
Crystal colour	colourless
Crystal shape	plate
Radiation	CuK_α (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 T_{min}/T_{max} (method)	0.7697/0.9288 (multi-scan)
Goodness-of-fit on F^2	1.198
Final R indexes [$I{\geq}2\sigma(I)$]	R_1 = 0.0364 wR$_2$ = 0.0917
Final R indexes [all data]	R_1 = 0.0368 wR$_2$ = 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 U_{ij} tensor.

Table 3. Bond lengths and angles for cu_BruecknerJK_153F40_0m

Atom–Atom	Length [Å]		
		C1–C2	1.527(3)
C1–O1	1.438(3)	C1–H1	1.0000
C1–C14	1.519(3)	O1–C13	1.436(3)

Atom–Atom	Distance [Å]	Atom–Atom	Distance [Å]
C2–O3	1.478(3)	C20–C33	1.520(3)
C2–C3	1.510(3)	C20–C21	1.528(3)
C2–H2	1.0000	C20–H20	1.0000
O2–C15	1.210(4)	C21–C22	1.502(3)
C3–C4	1.387(3)	C21–H21	1.0000
C3–C12	1.412(3)	C22–C23	1.384(3)
O3–C15	1.358(3)	C22–C31	1.417(3)
C4–O4	1.371(3)	C23–C24	1.428(3)
C4–C5	1.431(3)	C24–C29	1.431(3)
O4–C16	1.451(3)	C24–C25	1.447(3)
O5–C6	1.365(3)	C25–C26	1.377(3)
O5–C17	1.432(3)	C26–C27	1.422(3)
C5–C10	1.430(3)	C26–H26	0.9500
C5–C6	1.438(3)	C27–C28	1.367(3)
O6–C11	1.395(3)	C28–C29	1.422(3)
O6–C18	1.444(3)	C28–H28	0.9500
C6–C7	1.376(3)	C29–C30	1.424(3)
O7–C20	1.427(3)	C30–C31	1.378(3)
O7–C32	1.438(3)	C31–C32	1.518(3)
C7–C8	1.419(3)	C32–C38	1.536(3)
C7–H7	0.9500	C32–H32	1.0000
O8–C34	1.201(3)	C33–C34	1.505(3)
C8–C9	1.378(3)	C33–H33A	0.9900
C8–C27	1.490(3)	C33–H33B	0.9900
O9–C34	1.351(3)	C35–H35A	0.9800
O9–C21	1.476(3)	C35–H35B	0.9800
C9–C10	1.421(3)	C35–H35C	0.9800
C9–H9	0.9500	C36–H36A	0.9800
O10–C23	1.377(3)	C36–H36B	0.9800
O10–C35	1.443(3)	C36–H36C	0.9800
C10–C11	1.424(3)	C37–H37A	0.9800
O11–C25	1.359(3)	C37–H37B	0.9800
O11–C36	1.437(3)	C37–H37C	0.9800
C11–C12	1.370(3)	C38–H38A	0.9800
O12–C30	1.382(3)	C38–H38B	0.9800
O12–C37	1.437(3)	C38–H38C	0.9800
C12–C13	1.520(3)	O13–C39	1.423(11)
C13–C19	1.526(3)	O13–H13A	0.8400
C13–H13	1.0000	C39–H39A	0.9800
C14–C15	1.501(4)	C39–H39B	0.9800
C14–H14A	0.9900	C39–H39C	0.9800
C14–H14B	0.9900		
C16–H16A	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

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

C3–C2–H2	109.9	O2–C15–C14	128.7(3)
C1–C2–H2	109.9	O3–C15–C14	110.6(2)
C4–C3–C12	120.8(2)	O4–C16–H16A	109.5
C4–C3–C2	119.1(2)	O4–C16–H16B	109.5
C12–C3–C2	120.1(2)	H16A–C16–H16B	109.5
C15–O3–C2	109.2(2)	O4–C16–H16C	109.5
O4–C4–C3	117.3(2)	H16A–C16–H16C	109.5
O4–C4–C5	121.8(2)	H16B–C16–H16C	109.5
C3–C4–C5	120.8(2)	O5–C17–H17A	109.5
C4–O4–C16	113.73(18)	O5–C17–H17B	109.5
C6–O5–C17	116.85(19)	H17A–C17–H17B	109.5
C10–C5–C4	117.9(2)	O5–C17–H17C	109.5
C10–C5–C6	117.0(2)	H17A–C17–H17C	109.5
C4–C5–C6	125.0(2)	H17B–C17–H17C	109.5
C11–O6–C18	113.07(18)	O6–C18–H18A	109.5
O5–C6–C7	123.2(2)	O6–C18–H18B	109.5
O5–C6–C5	115.9(2)	H18A–C18–H18B	109.5
C7–C6–C5	120.9(2)	O6–C18–H18C	109.5
C20–O7–C32	113.43(19)	H18A–C18–H18C	109.5
C6–C7–C8	121.3(2)	H18B–C18–H18C	109.5
C6–C7–H7	119.4	C13–C19–H19A	109.5
C8–C7–H7	119.4	C13–C19–H19B	109.5
C9–C8–C7	119.3(2)	H19A–C19–H19B	109.5
C9–C8–C27	120.6(2)	C13–C19–H19C	109.5
C7–C8–C27	120.1(2)	H19A–C19–H19C	109.5
C34–O9–C21	110.05(17)	H19B–C19–H19C	109.5
C8–C9–C10	120.7(2)	O7–C20–C33	106.1(2)
C8–C9–H9	119.7	O7–C20–C21	110.49(19)
C10–C9–H9	119.7	C33–C20–C21	102.07(19)
C23–O10–C35	114.0(2)	O7–C20–H20	112.5
C9–C10–C11	120.6(2)	C33–C20–H20	112.5
C9–C10–C5	120.5(2)	C21–C20–H20	112.5
C11–C10–C5	118.9(2)	O9–C21–C22	110.36(18)
C25–O11–C36	117.75(19)	O9–C21–C20	103.62(18)
C12–C11–O6	119.2(2)	C22–C21–C20	114.1(2)
C12–C11–C10	122.0(2)	O9–C21–H21	109.5
O6–C11–C10	118.74(19)	C22–C21–H21	109.5
C30–O12–C37	115.20(18)	C20–C21–H21	109.5
C11–C12–C3	119.2(2)	C23–C22–C31	121.0(2)
C11–C12–C13	120.6(2)	C23–C22–C21	119.5(2)
C3–C12–C13	120.3(2)	C31–C22–C21	119.5(2)
O1–C13–C12	110.75(19)	O10–C23–C22	116.6(2)
O1–C13–C19	111.1(2)	O10–C23–C24	122.1(2)
C12–C13–C19	114.15(19)	C22–C23–C24	121.2(2)
O1–C13–H13	106.8	C23–C24–C29	117.6(2)
C12–C13–H13	106.8	C23–C24–C25	125.3(2)
C19–C13–H13	106.8	C29–C24–C25	116.9(2)
C15–C14–C1	102.5(2)	O11–C25–C26	122.9(2)
C15–C14–H14A	111.3	O11–C25–C24	116.5(2)
C1–C14–H14A	111.3	C26–C25–C24	120.6(2)
C15–C14–H14B	111.3	C25–C26–C27	121.4(2)
C1–C14–H14B	111.3	C25–C26–H26	119.3
H14A–C14–H14B	109.2	C27–C26–H26	119.3
O2–C15–O3	120.7(3)	C28–C27–C26	119.4(2)

Atom–Atom–Atom	Angle	Atom–Atom–Atom	Angle
C28–C27–C8	120.5(2)	O10–C35–H35B	109.5
C26–C27–C8	120.1(2)	H35A–C35–H35B	109.5
C27–C28–C29	121.0(2)	O10–C35–H35C	109.5
C27–C28–H28	119.5	H35A–C35–H35C	109.5
C29–C28–H28	119.5	H35B–C35–H35C	109.5
C28–C29–C30	119.9(2)	O11–C36–H36A	109.5
C28–C29–C24	120.5(2)	O11–C36–H36B	109.5
C30–C29–C24	119.48(19)	H36A–C36–H36B	109.5
C31–C30–O12	119.1(2)	O11–C36–H36C	109.5
C31–C30–C29	121.7(2)	H36A–C36–H36C	109.5
O12–C30–C29	118.83(19)	H36B–C36–H36C	109.5
C30–C31–C22	118.9(2)	O12–C37–H37A	109.5
C30–C31–C32	120.2(2)	O12–C37–H37B	109.5
C22–C31–C32	120.9(2)	H37A–C37–H37B	109.5
O7–C32–C31	110.83(18)	O12–C37–H37C	109.5
O7–C32–C38	111.15(19)	H37A–C37–H37C	109.5
C31–C32–C38	113.68(19)	H37B–C37–H37C	109.5
O7–C32–H32	106.9	C32–C38–H38A	109.5
C31–C32–H32	106.9	C32–C38–H38B	109.5
C38–C32–H32	106.9	H38A–C38–H38B	109.5
C34–C33–C20	102.96(19)	C32–C38–H38C	109.5
C34–C33–H33A	111.2	H38A–C38–H38C	109.5
C20–C33–H33A	111.2	H38B–C38–H38C	109.5
C34–C33–H33B	111.2	C39–O13–H13A	109.5
C20–C33–H33B	111.2	O13–C39–H39A	109.5
H33A–C33–H33B	109.1	O13–C39–H39B	109.5
O8–C34–O9	122.1(2)	H39A–C39–H39B	109.5
O8–C34–C33	128.0(2)	O13–C39–H39C	109.5
O9–C34–C33	109.9(2)	H39A–C39–H39C	109.5
O10–C35–H35A	109.5	H39B–C39–H39C	109.5

Table 4. Torsion angles for cu_BruecknerJK_153F40_0m

Atom–Atom–Atom–Atom	Torsion Angle [°]	Atom–Atom–Atom–Atom	Torsion Angle [°]
C14–C1–O1–C13	−175.9(2)	O4–C4–C5–C6	6.0(4)
C2–C1–O1–C13	−66.0(3)	C3–C4–C5–C6	−171.1(2)
O1–C1–C2–O3	−80.0(2)	C17–O5–C6–C7	−7.9(4)
C14–C1–C2–O3	32.3(2)	C17–O5–C6–C5	169.9(3)
O1–C1–C2–C3	38.6(3)	C10–C5–C6–O5	−172.6(2)
C14–C1–C2–C3	150.9(2)	C4–C5–C6–O5	5.3(4)
O3–C2–C3–C4	−70.9(3)	C10–C5–C6–C7	5.2(4)
C1–C2–C3–C4	173.5(2)	C4–C5–C6–C7	−176.8(3)
O3–C2–C3–C12	108.9(2)	O5–C6–C7–C8	177.5(3)
C1–C2–C3–C12	−6.7(3)	C5–C6–C7–C8	−0.2(4)
C3–C2–O3–C15	−143.1(2)	C6–C7–C8–C9	−3.6(4)
C1–C2–O3–C15	−21.2(2)	C6–C7–C8–C27	177.1(3)
C12–C3–C4–O4	−179.8(2)	C7–C8–C9–C10	1.9(4)
C2–C3–C4–O4	−0.1(3)	C27–C8–C9–C10	−178.7(2)
C12–C3–C4–C5	−2.6(4)	C8–C9–C10–C11	−175.1(2)
C2–C3–C4–C5	177.2(2)	C8–C9–C10–C5	3.3(4)
C3–C4–O4–C16	−108.9(2)	C4–C5–C10–C9	175.1(2)
C5–C4–O4–C16	73.9(3)	C6–C5–C10–C9	−6.8(3)
O4–C4–C5–C10	−176.1(2)	C4–C5–C10–C11	−6.4(3)
C3–C4–C5–C10	6.8(3)	C6–C5–C10–C11	171.7(2)
		C18–O6–C11–C12	−98.9(2)

C18–O6–C11–C10	81.4(3)	C36–O11–C25–C24	−172.6(2)
C9–C10–C11–C12	−179.6(2)	C23–C24–C25–O11	0.2(4)
C5–C10–C11–C12	1.9(4)	C29–C24–C25–O11	175.9(2)
C9–C10–C11–O6	0.0(3)	C23–C24–C25–C26	−179.1(2)
C5–C10–C11–O6	−178.5(2)	C29–C24–C25–C26	−3.4(3)
O6–C11–C12–C3	−177.2(2)	O11–C25–C26–C27	−178.7(2)
C10–C11–C12–C3	2.5(4)	C24–C25–C26–C27	0.5(4)
O6–C11–C12–C13	2.9(3)	C25–C26–C27–C28	1.8(4)
C10–C11–C12–C13	−177.4(2)	C25–C26–C27–C8	−178.8(2)
C4–C3–C12–C11	−2.2(3)	C9–C8–C27–C28	36.1(4)
C2–C3–C12–C11	178.1(2)	C7–C8–C27–C28	−144.5(3)
C4–C3–C12–C13	177.8(2)	C9–C8–C27–C26	−143.3(3)
C2–C3–C12–C13	−2.0(3)	C7–C8–C27–C26	36.1(4)
C1–O1–C13–C12	56.3(2)	C26–C27–C28–C29	−1.0(4)
C1–O1–C13–C19	−71.7(2)	C8–C27–C28–C29	179.5(2)
C11–C12–C13–O1	158.6(2)	C27–C28–C29–C30	174.3(2)
C3–C12–C13–O1	−21.3(3)	C27–C28–C29–C24	−1.9(4)
C11–C12–C13–C19	−75.2(3)	C23–C24–C29–C28	−179.9(2)
C3–C12–C13–C19	104.9(3)	C25–C24–C29–C28	4.1(3)
O1–C1–C14–C15	84.1(2)	C23–C24–C29–C30	3.9(3)
C2–C1–C14–C15	−31.2(3)	C25–C24–C29–C30	−172.2(2)
C2–O3–C15–O2	−179.6(2)	C37–O12–C30–C31	−102.1(2)
C2–O3–C15–C14	0.8(3)	C37–O12–C30–C29	84.8(3)
C1–C14–C15–O2	−159.6(3)	C28–C29–C30–C31	−178.4(2)
C1–C14–C15–O3	19.9(3)	C24–C29–C30–C31	−2.1(3)
C32–O7–C20–C33	−174.99(18)	C28–C29–C30–O12	−5.4(3)
C32–O7–C20–C21	−65.1(2)	C24–C29–C30–O12	170.9(2)
C34–O9–C21–C22	−144.3(2)	O12–C30–C31–C22	−173.6(2)
C34–O9–C21–C20	−21.7(2)	C29–C30–C31–C22	−0.6(3)
O7–C20–C21–O9	−80.1(2)	O12–C30–C31–C32	5.2(3)
C33–C20–C21–O9	32.3(3)	C29–C30–C31–C32	178.2(2)
O7–C20–C21–C22	39.9(3)	C23–C22–C31–C30	1.5(3)
C33–C20–C21–C22	152.4(2)	C21–C22–C31–C30	178.5(2)
O9–C21–C22–C23	−75.8(3)	C23–C22–C31–C32	−177.3(2)
C20–C21–C22–C23	167.9(2)	C21–C22–C31–C32	−0.3(3)
O9–C21–C22–C31	107.2(2)	C20–O7–C32–C31	54.4(3)
C20–C21–C22–C31	−9.1(3)	C20–O7–C32–C38	−73.0(2)
C35–O10–C23–C22	101.2(2)	C30–C31–C32–O7	160.4(2)
C35–O10–C23–C24	−80.8(3)	C22–C31–C32–O7	−20.8(3)
C31–C22–C23–O10	178.4(2)	C30–C31–C32–C38	−73.5(3)
C21–C22–C23–O10	1.5(3)	C22–C31–C32–C38	105.2(2)
C31–C22–C23–C24	0.4(4)	O7–C20–C33–C34	84.5(3)
C21–C22–C23–C24	−176.6(2)	C21–C20–C33–C34	−31.2(3)
O10–C23–C24–C29	179.0(2)	C21–O9–C34–O8	−179.1(2)
C22–C23–C24–C29	−3.1(3)	C21–O9–C34–C33	1.4(3)
O10–C23–C24–C25	−5.3(4)	C20–C33–C34–O8	−160.0(3)
C22–C23–C24–C25	172.6(2)	C20–C33–C34–O9	19.6(3)
C36–O11–C25–C26	6.6(4)		

Bibliography

[1] Bruker, *SAINT*, *V8.40A*, Bruker AXS Inc., Madison, Wisconsin, USA.

[2] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst.* **2015**, *48*, 3–10, doi:10.1107/S1600576714022985.

[3] G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3–8, doi:10.1107/S2053273314026370.

[4] G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3–8, doi:10.1107/S2053229614024218.

[5] C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, *Acta Cryst.* **2016**, *B72*, 171–179, doi:10.1107/S2052520616003954.

[6] D. Kratzert, *FinalCif*, *V141*, https://dkratzert.de/finalcif.html.