JOC The Journal of Organic Chemistry

J. Org. Chem., 1997, 62(15), 5017-5022, DOI:10.1021/jo970615n

Table S1: Structure Determination Summary for $Cu_2C_{48}H_{62}O_{20}$ (X-ray analysis)

Crystal Data

Empirical Formula	$C_{48}\ H_{62}\ Cu_2\ O_{20}$
Color; Habit	green prisms
Crystal Size (mm)	0.8 x 0.6 x 0.4
Crystal System	Triclinic
Space Group	P1
Unit Cell Dimensions	a = 11.086(3) Å
	b = 11.244(3) Å
	c = 13.293(4) Å
	α = 111.59(2)°
	β = 101.71(2)°
	γ = 105.56(3)°
Volume	1397.6(7) $Å^3$
Z	1
Formula Weight	1086.1
Density(calc.)	1.290 g/cm^3
Absorption Coefficient	0.830 mm^{-1}
F(000)	568

Table S1 (continued): (b) Data Collection for $Cu_2C_{48}H_{62}O_{20}$

Diffractometer Used	Siemens P4
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	298
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 45.5°
Scan Type	ω
Scan Speed	Variable; 6.00 to 60.00°/min. in ω
Scan Range (ω)	2.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$-10 \le h \le 11$, $-10 \le k \le 10$ $-13 \le \ell \le 13$
Reflections Collected	3678
Independent Reflections	3672
Observed Reflections	3188 [$F > 4.0\sigma(F)$]

Table S1 (continued): (c) Solution and Refinement for $Cu_2C_{48}H_{62}O_{20}$

System Used	Siemens SHELXTL IRIS
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	Unit weights
Number of Parameters Refined	610
Final R Indices (obs. data)	R = 5.43 %, wR = 5.80 %
R Indices (all data)	R = 6.25 %, wR = 6.84 %
Goodness-of-Fit	1.16
Largest and Mean Δ/σ	1.114, 0.073
Data-to-Parameter Ratio	5.2:1
Largest Difference Peak	0.48 $eÅ^{-3}$
Largest Difference Hole	-0.71 $eÅ^{-3}$

Table S2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$) for $Cu_2C_{48}H_{62}O_{20}$

	x	y	z	U(eq)
Cu(1)	0	10000	0	44(1)
Cu(2)	2160(2)	9560(2)	807(1)	44(1)
O(16)	1229(6)	11151(6)	-463(6)	58(1)
O(15)	2989(6)	10604(6)	54(6)	56(1)
O(8)	975(6)	8554(6)	1438(5)	55(1)
O(7)	-851(7)	8791(6)	621(6)	61(1)
O(12)	1399(6)	7867(6)	-687(5)	52(1)
O(11)	-320(7)	8351(6)	-1406(5)	55(1)
O(3)	648(6)	11587(6)	1557(6)	60(1)
O(4)	2588(7)	11346(6)	2112(6)	66(1)
O(14)	4473(7)	12169(7)	-693(6)	87(1)
O(2)	3455(7)	13555(7)	4142(6)	111(1)
O(6)	-191(6)	7159(6)	2424(6)	73(1)
O(10)	827(6)	5694(6)	-2707(5)	59(1)
O(13)	6040(7)	12590(7)	-1491(7)	122(1)
O(1)	5118(8)	15520(8)	5516(8)	193(1)
O(5)	-296(7)	6605(7)	3880(6)	104(1)
O(9)	732(7)	3548(7)	-3669(6)	93(1)
O(1'')	-1743(7)	10334(7)	-685(6)	90(1)
O(1')	3844(6)	9116(7)	1426(6)	72(1)
C(40)	2394(7)	11142(7)	-436(7)	48(1)
C(10)	1821(8)	11987(7)	2258(6)	53(1)
C(20)	-192(8)	8385(7)	1222(7)	60(1)
C(30)	385(7)	7635(7)	-1425(7)	51(1)
C(31)	3059(7)	11802(7)	-1087(7)	55(1)
C(1)	2289(7)	13382(7)	3278(7)	58(1)
C(11)	-948(7)	7703(7)	1829(7)	57(1)
C(21)	-195(7)	6245(7)	-2499(7)	49(1)
C(36)	2637(8)	10926(8)	-2380(7)	76(1)
C(34)	3693(8)	11968(8)	-2534(7)	76(1)
C(35)	4902(8)	12272(8)	-1602(7)	89(1)
C(32)	2919(8)	13194(8)	-970(7)	89(1)
C(33)	3393(8)	13369(8)	-1929(7)	93(1)
C(39)	3903(8)	11700(8)	-3653(7)	128(1)
C(37)	1207(8)	10581(8)	-3031(7)	126(1)
C(38)	2877(8)	9587(8)	-2649(7)	110(1)
C(6)	2702(8)	14610(8)	3022(7)	76(1)
C(4)	3205(7)	15605(7)	4373(7)	73(1)
C(3)	1983(8)	15221(7)	4709(7)	77(1)
C(2)	1315(8)	13659(8)	3964(7)	85(1)
C(5)	4041(8)	15022(8)	4744(8)	130(1)
C(9)	3845(8)	17194(8)	4699(8)	115(1)
C(8)	3798(8)	14705(8)	2535(8)	121(1)
C(7)	1582(8)	14848(8)	2326(7)	91(1)
C(17)	-2148(8)	9441(8)	2527(7)	89(1)
C(16)	-1234(7)	8735(7)	2853(6)	55(1)
C(18)	65(8)	9935(8)	3787(7)	83(1)
C(15)	-723(8)	7078(8)	3270(7)	82(1)
C(19)	-2291(8)	7921(8)	4215(7)	82(1)
C(14)	-1833(8)	7595(8)	3161(7)	71(1)
C(13)	-2958(8)	6469(8)	2011(7)	87(1)
C(12)	-2281(8)	6589(8)	1134(7)	87(1)
C(28)	-624(8)	4805(7)	-1391(7)	80(1)
C(26)	-1235(7)	5078(7)	-2429(7)	60(1)

C(27)	-2509(8)	5280(8)	-2358(7)	94(1)
C(29)	-2158(8)	2431(8)	-4042(8)	103(1)
C(24)	-1339(7)	3924(7)	-3575(7)	67(1)
C(25)	124(7)	4276(7)	-3366(7)	64(1)
C(22)	-847(8)	6201(7)	-3633(7)	69(1)
C(23)	-1600(8)	4643(8)	-4401(7)	79(1)
C(3'')	-2708(8)	9651(8)	-2581(8)	161(1)
C(2'')	-1834(8)	10805(8)	-1550(8)	135(1)
C(2')	4046(8)	8787(8)	2442(8)	112(1)
C(3')	4436(8)	9952(8)	3460(8)	153(1)
C(100)	3530(8)	6761(8)	9325(8)	119(1)
C(101)	4718(8)	7717(8)	9143(8)	144(1)
O(102)	4658(8)	6956(8)	8221(8)	197(1)
C(200)	7509(9)	2965(8)	1541(8)	93(1)
C(201)	7287(9)	2169(8)	549(8)	90(1)
O(202)	6501(8)	1089(8)	500(8)	115(1)
O(302)	6528(8)	2607(8)	2168(8)	94(1)
C(301)	6730(8)	2019(8)	1434(8)	67(1)
C(300)	8279(9)	2424(8)	1335(8)	85(1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S3. Bond lengths (Å) for $Cu_2C_{48}H_{62}O_{20}$

Cu(1)-Cu(2)	2.667	(2)	Cu(1)-O(16)	1.973	(8)
Cu(1)-O(7)	1.968	(8)	Cu(1)-O(11)	1.970	(6)
Cu(1)-O(3)	1.994	(6)	Cu(1)-O(1'')	2.152	(8)
Cu(2)-O(15)	1.971	(8)	Cu(2)-O(8)	2.014	(8)
Cu(2)-O(12)	1.989	(5)	Cu(2)-O(4)	1.964	(6)
Cu(2)-O(1')	2.143	(8)	O(16)-C(40)	1.287	(11)
O(15)-C(40)	1.247	(13)	O(8)-C(20)	1.212	(11)
O(7)-C(20)	1.262	(13)	O(12)-C(30)	1.225	(10)
O(11)-C(30)	1.261	(12)	O(3)-C(10)	1.284	(10)
O(4)-C(10)	1.254	(12)	O(14)-C(31)	1.436	(11)
O(14)-C(35)	1.416	(13)	O(2)-C(1)	1.458	(11)
O(2)-C(5)	1.424	(10)	O(6)-C(11)	1.438	(13)
O(6)-C(15)	1.391	(13)	O(10)-C(21)	1.457	(12)
O(10)-C(25)	1.395	(8)	O(13)-C(35)	1.176	(12)
O(1)-C(5)	1.230	(11)	O(5)-C(15)	1.209	(14)
O(9)-C(25)	1.204	(12)	O(1'')-C(2'')	1.430	(15)
O(1')-C(2')	1.517	(14)	C(40)-C(31)	1.510	(14)
C(10)-C(1)	1.510	(9)	C(20)-C(11)	1.525	(14)
C(30)-C(21)	1.530	(9)	C(31)-C(36)	1.524	(11)
C(31)-C(32)	1.568	(13)	C(1)-C(6)	1.517	(13)
C(1)-C(2)	1.570	(13)	C(11)-C(16)	1.585	(12)
C(11)-C(12)	1.485	(9)	C(21)-C(26)	1.543	(12)
C(21)-C(22)	1.510	(13)	C(36)-C(34)	1.524	(12)
C(36)-C(37)	1.510	(12)	C(36)-C(38)	1.524	(13)
C(34)-C(35)	1.488	(12)	C(34)-C(33)	1.643	(12)
C(34)-C(39)	1.485	(14)	C(32)-C(33)	1.531	(15)
C(6)-C(4)	1.603	(11)	C(6)-C(8)	1.486	(14)
C(6)-C(7)	1.537	(13)	C(4)-C(3)	1.515	(13)
C(4)-C(5)	1.381	(14)	C(4)-C(9)	1.584	(12)
C(3)-C(2)	1.529	(10)	C(17)-C(16)	1.534	(13)
C(16)-C(18)	1.561	(8)	C(16)-C(14)	1.514	(13)
C(15)-C(14)	1.498	(13)	C(19)-C(14)	1.538	(13)
C(14)-C(13)	1.566	(9)	C(13)-C(12)	1.535	(14)
C(28)-C(26)	1.582	(14)	C(26)-C(27)	1.506	(13)
C(26)-C(24)	1.553	(11)	C(29)-C(24)	1.489	(10)
C(24)-C(25)	1.502	(11)	C(24)-C(23)	1.611	(14)
C(22)-C(23)	1.536	(9)	C(3'')-C(2'')	1.406	(9)
C(2')-C(3')	1.375	(11)	C(100)-C(101)	1.584	(14)
C(101)-O(102)	1.185	(13)	C(200)-C(201)	1.218	(13)
C(200)-O(202)	1.890	(10)	C(200)-O(302)	1.555	(16)
C(200)-C(301)	1.115	(13)	C(200)-C(300)	1.194	(15)
C(201)-O(202)	1.261	(13)	C(201)-C(301)	1.476	(16)
C(201)-C(300)	1.237	(13)	O(202)-C(301)	1.214	(12)
O(202)-C(300)	1.915	(10)	O(302)-C(301)	1.065	(14)
C(301)-C(300)	1.700	(14)			

Table S4. Bond angles (°) for $Cu_2C_{48}H_{62}O_{20}$

Cu(2)-Cu(1)-O(16)	82.5(2)	Cu(2)-Cu(1)-O(7)	84.1(2)
O(16)-Cu(1)-O(7)	166.5(3)	Cu(2)-Cu(1)-O(11)	83.6(2)
O(16)-Cu(1)-O(11)	89.8(3)	O(7)-Cu(1)-O(11)	89.4(3)
Cu(2)-Cu(1)-O(3)	84.4(2)	O(16)-Cu(1)-O(3)	89.3(3)
O(7)-Cu(1)-O(3)	88.7(3)	O(11)-Cu(1)-O(3)	168.0(3)
Cu(2)-Cu(1)-O(1'')	178.9(2)	O(16)-Cu(1)-O(1'')	97.1(3)
O(7)-Cu(1)-O(1'')	96.4(3)	O(11)-Cu(1)-O(1'')	95.4(3)
O(3)-Cu(1)-O(1'')	96.6(3)	Cu(1)-Cu(2)-O(15)	85.1(2)
Cu(1)-Cu(2)-O(8)	83.0(2)	O(15)-Cu(2)-O(8)	168.1(3)
Cu(1)-Cu(2)-O(12)	83.9(2)	O(15)-Cu(2)-O(12)	89.0(3)
O(8)-Cu(2)-O(12)	89.4(3)	Cu(1)-Cu(2)-O(4)	82.9(2)
O(15)-Cu(2)-O(4)	87.4(3)	O(8)-Cu(2)-O(4)	91.5(3)
O(12)-Cu(2)-O(4)	166.6(3)	Cu(1)-Cu(2)-O(1')	177.6(2)
O(15)-Cu(2)-O(1')	96.4(3)	O(8)-Cu(2)-O(1')	95.4(3)
O(12)-Cu(2)-O(1')	94.2(3)	O(4)-Cu(2)-O(1')	99.0(3)
Cu(1)-O(16)-C(40)	123.8(7)	Cu(2)-O(15)-C(40)	122.1(6)
Cu(2)-O(8)-C(20)	122.1(7)	Cu(1)-O(7)-C(20)	121.9(6)
Cu(2)-O(12)-C(30)	121.2(6)	Cu(1)-O(11)-C(30)	121.5(5)
Cu(1)-O(3)-C(10)	121.0(6)	Cu(2)-O(4)-C(10)	125.3(5)
C(31)-O(14)-C(35)	105.8(7)	C(1)-O(2)-C(5)	99.9(7)
C(11)-O(6)-C(15)	106.2(7)	C(21)-O(10)-C(25)	104.2(6)
Cu(1)-O(1'')-C(2'')	121.2(6)	Cu(2)-O(1')-C(2')	122.4(6)
O(16)-C(40)-O(15)	125.3(9)	O(16)-C(40)-C(31)	116.5(8)
O(15)-C(40)-C(31)	118.2(8)	O(3)-C(10)-O(4)	124.8(6)
O(3)-C(10)-C(1)	114.8(8)	O(4)-C(10)-C(1)	120.2(6)
O(8)-C(20)-O(7)	128.3(10)	O(8)-C(20)-C(11)	116.7(9)
O(7)-C(20)-C(11)	114.8(8)	O(12)-C(30)-O(11)	129.1(7)
O(12)-C(30)-C(21)	117.3(8)	O(11)-C(30)-C(21)	113.5(6)
O(14)-C(31)-C(40)	111.7(8)	O(14)-C(31)-C(36)	103.9(7)
C(40)-C(31)-C(36)	116.6(6)	O(14)-C(31)-C(32)	103.2(6)
C(40)-C(31)-C(32)	116.0(7)	C(36)-C(31)-C(32)	103.9(8)
O(2)-C(1)-C(10)	109.2(7)	O(2)-C(1)-C(6)	106.0(6)
C(10)-C(1)-C(6)	115.2(8)	O(2)-C(1)-C(2)	103.2(7)
C(10)-C(1)-C(2)	117.5(6)	C(6)-C(1)-C(2)	104.5(7)
O(6)-C(11)-C(20)	112.6(7)	O(6)-C(11)-C(16)	100.7(7)
C(20)-C(11)-C(16)	114.3(6)	O(6)-C(11)-C(12)	106.7(7)
C(20)-C(11)-C(12)	118.0(7)	C(16)-C(11)-C(12)	102.7(7)
O(10)-C(21)-C(30)	111.3(6)	O(10)-C(21)-C(26)	103.1(7)
C(30)-C(21)-C(26)	114.8(7)	O(10)-C(21)-C(22)	103.7(7)
C(30)-C(21)-C(22)	118.0(7)	C(26)-C(21)-C(22)	104.3(5)
C(31)-C(36)-C(34)	94.0(5)	C(31)-C(36)-C(37)	114.4(8)
C(34)-C(36)-C(37)	116.6(8)	C(31)-C(36)-C(38)	111.0(8)
C(34)-C(36)-C(38)	111.5(8)	C(37)-C(36)-C(38)	108.7(6)
C(36)-C(34)-C(35)	101.2(8)	C(36)-C(34)-C(33)	100.7(7)
C(35)-C(34)-C(33)	99.5(5)	C(36)-C(34)-C(39)	122.8(5)
C(35)-C(34)-C(39)	113.4(8)	C(33)-C(34)-C(39)	115.7(8)
O(14)-C(35)-O(13)	119.7(9)	O(14)-C(35)-C(34)	106.4(7)
O(13)-C(35)-C(34)	133.8(10)	C(31)-C(32)-C(33)	101.6(7)
C(34)-C(33)-C(32)	103.4(7)	C(1)-C(6)-C(4)	88.7(7)
C(1)-C(6)-C(8)	114.9(8)	C(4)-C(6)-C(8)	112.8(6)
C(1)-C(6)-C(7)	116.6(6)	C(4)-C(6)-C(7)	113.0(7)
C(8)-C(6)-C(7)	109.6(8)	C(6)-C(4)-C(3)	103.8(5)
C(6)-C(4)-C(5)	98.4(7)	C(3)-C(4)-C(5)	108.0(9)
C(6)-C(4)-C(9)	113.8(8)	C(3)-C(4)-C(9)	114.0(7)
C(5)-C(4)-C(9)	116.9(6)	C(4)-C(3)-C(2)	103.0(7)
C(1)-C(2)-C(3)	101.4(6)	O(2)-C(5)-O(1)	116.3(10)

O(2)-C(5)-C(4)	110.9(6)	O(1)-C(5)-C(4)	132.6(8)
C(11)-C(16)-C(17)	116.3(7)	C(11)-C(16)-C(18)	112.4(7)
C(17)-C(16)-C(18)	105.3(6)	C(11)-C(16)-C(14)	91.3(6)
C(17)-C(16)-C(14)	116.3(7)	C(18)-C(16)-C(14)	115.3(7)
O(6)-C(15)-O(5)	120.1(9)	O(6)-C(15)-C(14)	106.4(8)
O(5)-C(15)-C(14)	133.4(10)	C(16)-C(14)-C(15)	99.6(7)
C(16)-C(14)-C(19)	120.1(7)	C(15)-C(14)-C(19)	112.7(8)
C(16)-C(14)-C(13)	103.1(7)	C(15)-C(14)-C(13)	105.8(6)
C(19)-C(14)-C(13)	113.7(7)	C(14)-C(13)-C(12)	100.7(6)
C(11)-C(12)-C(13)	105.2(6)	C(21)-C(26)-C(28)	111.1(6)
C(21)-C(26)-C(27)	115.5(8)	C(28)-C(26)-C(27)	109.0(8)
C(21)-C(26)-C(24)	94.9(7)	C(28)-C(26)-C(24)	109.7(7)
C(27)-C(26)-C(24)	116.0(6)	C(26)-C(24)-C(29)	125.1(8)
C(26)-C(24)-C(25)	97.8(5)	C(29)-C(24)-C(25)	115.6(8)
C(26)-C(24)-C(23)	99.1(7)	C(29)-C(24)-C(23)	116.8(6)
C(25)-C(24)-C(23)	97.6(7)	O(10)-C(25)-O(9)	118.6(7)
O(10)-C(25)-C(24)	110.7(7)	O(9)-C(25)-C(24)	130.7(6)
C(21)-C(22)-C(23)	102.1(7)	C(24)-C(23)-C(22)	105.4(6)
O(1'')-C(2'')-C(3'')	105.9(8)	O(1')-C(2')-C(3')	111.3(8)
C(100)-C(101)-O(102)	100.6(7)	C(201)-C(200)-O(202)	41.1(6)
C(201)-C(200)-O(302)	119.4(7)	O(202)-C(200)-O(302)	80.2(6)
C(201)-C(200)-C(301)	78.4(8)	O(202)-C(200)-C(301)	37.5(7)
O(302)-C(200)-C(301)	43.2(7)	C(201)-C(200)-C(300)	61.7(8)
O(202)-C(200)-C(300)	72.8(6)	O(302)-C(200)-C(300)	124.6(11)
C(301)-C(200)-C(300)	94.7(10)	C(200)-C(201)-O(202)	99.4(11)
C(200)-C(201)-C(301)	47.7(7)	O(202)-C(201)-C(301)	51.9(7)
C(200)-C(201)-C(300)	58.2(8)	O(202)-C(201)-C(300)	100.1(11)
C(301)-C(201)-C(300)	77.0(9)	C(200)-O(202)-C(201)	39.5(6)
C(200)-O(202)-C(301)	34.0(6)	C(201)-O(202)-C(301)	73.2(8)
C(200)-O(202)-C(300)	36.6(5)	C(201)-O(202)-C(300)	39.5(6)
C(301)-O(202)-C(300)	61.0(6)	C(200)-O(302)-C(301)	45.8(7)
C(200)-C(301)-C(201)	53.9(8)	C(200)-C(301)-O(202)	108.4(12)
C(201)-C(301)-O(202)	54.8(7)	C(200)-C(301)-O(302)	91.0(9)
C(201)-C(301)-O(302)	141.1(11)	O(202)-C(301)-O(302)	157.4(10)
C(200)-C(301)-C(300)	44.4(7)	C(201)-C(301)-C(300)	45.1(6)
O(202)-C(301)-C(300)	80.3(8)	O(302)-C(301)-C(300)	122.3(7)
C(200)-C(300)-C(201)	60.1(8)	C(200)-C(300)-O(202)	70.6(6)
C(201)-C(300)-O(202)	40.4(6)	C(200)-C(300)-C(301)	40.8(6)
C(201)-C(300)-C(301)	57.8(7)	O(202)-C(300)-C(301)	38.7(4)

Table S5. Anisotropic displacement coefficients for $Cu_2C_{48}H_{62}O_{20}$ ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	50(1)	51(1)	38(1)	24(1)	17(1)	22(1)
Cu(2)	53(1)	48(1)	37(1)	22(1)	18(1)	21(1)
O(16)	68(1)	70(1)	68(1)	38(1)	35(1)	48(1)
O(15)	52(1)	66(1)	58(1)	16(1)	21(1)	39(1)
O(8)	63(1)	68(1)	55(1)	30(1)	35(1)	37(1)
O(7)	60(1)	83(1)	56(1)	29(1)	18(1)	46(1)
O(12)	63(1)	51(1)	44(1)	24(1)	28(1)	17(1)
O(11)	80(1)	53(1)	34(1)	32(1)	17(1)	20(1)
O(3)	62(1)	63(1)	43(1)	29(1)	16(1)	10(1)
O(4)	77(1)	68(1)	50(1)	42(1)	11(1)	17(1)
O(14)	76(1)	113(1)	102(1)	29(1)	26(1)	84(1)
O(2)	107(1)	86(1)	99(1)	65(1)	-5(1)	1(1)
O(6)	81(1)	102(1)	84(1)	50(1)	51(1)	67(1)
O(10)	63(1)	58(1)	45(1)	26(1)	20(1)	10(1)
O(13)	80(1)	154(1)	160(1)	29(1)	46(1)	106(1)
O(1)	152(1)	166(1)	179(1)	90(1)	5(1)	-1(1)
O(5)	128(1)	150(1)	104(1)	75(1)	62(1)	99(1)
O(9)	102(1)	101(1)	80(1)	65(1)	33(1)	25(1)
O(1'')	90(1)	138(1)	76(1)	72(1)	24(1)	65(1)
O(1')	61(1)	108(1)	70(1)	47(1)	26(1)	50(1)
C(40)	48(1)	39(1)	48(1)	17(1)	8(1)	12(1)
C(10)	65(1)	52(1)	33(1)	14(1)	12(1)	19(1)
C(20)	71(1)	63(1)	51(1)	18(1)	40(1)	26(1)
C(30)	65(1)	57(1)	50(1)	32(1)	34(1)	30(1)
C(31)	50(1)	63(1)	66(1)	17(1)	19(1)	47(1)
C(1)	55(1)	63(1)	52(1)	28(1)	17(1)	17(1)
C(11)	54(1)	60(1)	62(1)	23(1)	30(1)	28(1)
C(21)	63(1)	47(1)	46(1)	31(1)	16(1)	24(1)
C(36)	62(1)	88(1)	58(1)	1(1)	22(1)	30(1)
C(34)	73(1)	99(1)	63(1)	9(1)	32(1)	58(1)
C(35)	79(1)	97(1)	113(1)	22(1)	37(1)	75(1)
C(32)	95(1)	80(1)	103(1)	35(1)	40(1)	46(1)
C(33)	87(1)	102(1)	107(1)	29(1)	32(1)	68(1)
C(39)	123(1)	146(1)	102(1)	7(1)	49(1)	67(1)
C(37)	107(1)	143(1)	98(1)	-12(1)	31(1)	66(1)
C(38)	110(1)	107(1)	97(1)	19(1)	64(1)	28(1)
C(6)	61(1)	66(1)	61(1)	5(1)	26(1)	-3(1)
C(4)	60(1)	65(1)	71(1)	28(1)	20(1)	3(1)
C(3)	88(1)	70(1)	65(1)	42(1)	31(1)	10(1)
C(2)	99(1)	88(1)	77(1)	41(1)	43(1)	34(1)
C(5)	98(1)	125(1)	116(1)	48(1)	27(1)	3(1)
C(9)	97(1)	91(1)	108(1)	14(1)	34(1)	10(1)
C(8)	112(1)	100(1)	120(1)	19(1)	64(1)	19(1)
C(7)	113(1)	83(1)	83(1)	39(1)	30(1)	41(1)
C(17)	94(1)	103(1)	102(1)	57(1)	57(1)	54(1)
C(16)	65(1)	63(1)	42(1)	27(1)	28(1)	23(1)
C(18)	88(1)	94(1)	61(1)	21(1)	38(1)	31(1)
C(15)	100(1)	94(1)	88(1)	50(1)	53(1)	57(1)
C(19)	81(1)	115(1)	68(1)	33(1)	43(1)	52(1)
C(14)	69(1)	86(1)	64(1)	29(1)	30(1)	37(1)
C(13)	89(1)	95(1)	86(1)	23(1)	46(1)	49(1)
C(12)	91(1)	84(1)	74(1)	12(1)	32(1)	36(1)
C(28)	105(1)	67(1)	65(1)	14(1)	26(1)	41(1)
C(26)	57(1)	61(1)	56(1)	11(1)	23(1)	27(1)

C(27)	77(1)	97(1)	94(1)	32(1)	46(1)	20(1)
C(29)	89(1)	64(1)	100(1)	11(1)	23(1)	-2(1)
C(24)	76(1)	48(1)	65(1)	29(1)	28(1)	6(1)
C(25)	84(1)	67(1)	51(1)	52(1)	31(1)	18(1)
C(22)	80(1)	79(1)	44(1)	31(1)	15(1)	27(1)
C(23)	78(1)	94(1)	50(1)	36(1)	18(1)	17(1)
C(3'')	150(1)	160(1)	131(1)	42(1)	31(1)	42(1)
C(2'')	119(1)	131(1)	137(1)	51(1)	15(1)	53(1)
C(2')	104(1)	118(1)	120(1)	57(1)	20(1)	57(1)
C(3')	139(1)	152(1)	131(1)	52(1)	16(1)	42(1)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table S6. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients for $Cu_2C_{48}H_{62}O_{20}$ ($Å^2x10^3$)

	x	y	z	U
H(1)	4102	10927	-3939	140
H(2)	3092	11591	-4216	140
H(3)	4605	12502	-3602	140
H(4)	1006	11375	-2948	134
H(5)	1076	10101	-3904	134
H(6)	568	9946	-2931	134
H(7)	2416	9059	-2326	119
H(8)	2681	9073	-3430	119
H(9)	3847	9839	-2259	119
H(10)	4196	17766	5496	116
H(11)	4521	17377	4357	116
H(12)	3141	17460	4365	116
H(13)	4466	14463	2902	131
H(14)	3402	13931	1706	131
H(15)	4143	15514	2497	131
H(16)	-2292	9999	3227	118
H(17)	-1710	10067	2267	118
H(18)	-2960	8794	1982	118
H(19)	702	9557	4035	97
H(20)	463	10521	3488	97
H(21)	-122	10450	4446	97
H(22)	-1550	8663	4931	100
H(23)	-2978	8297	4144	100
H(24)	-2594	7154	4360	100
H(25)	-1250	4015	-1387	96
H(26)	184	4700	-1369	96
H(27)	-476	5605	-660	96
H(28)	-2383	6017	-1658	108
H(29)	-2951	5376	-2995	108
H(30)	-3157	4427	-2386	108
H(31)	-3102	2330	-4189	102
H(32)	-2122	1932	-4818	102
H(33)	-1927	2046	-3586	102
H(34)	-3474	9327	-2555	167
H(35)	-2716	9971	-3212	167
H(36)	-2213	9048	-2740	167
H(37)	4637	9797	4063	162
H(38)	5368	10583	3475	162
H(39)	3929	10484	3441	162
H(43)	2114	13280	-943	109
H(44)	3604	13960	-159	109
H(45)	4191	14199	-1651	108
H(46)	2712	13410	-2462	119
H(47)	2219	15488	5547	93
H(48)	1428	15724	4573	93
H(49)	411	13373	3457	106
H(50)	1226	13137	4418	102
H(51)	-1413	6754	-3546	81
H(52)	-180	6655	-3911	81
H(53)	-1306	4294	-5045	91
H(54)	-2555	4401	-4711	100
H(55)	-3163	5550	2011	104
H(56)	-3762	6630	1931	104
H(57)	-2834	6775	558	96

H(58)	-2241	5688	634	167
H(59)	-2169	11619	-1325	146
H(60)	-907	11347	-1515	146
H(61)	3216	8316	2455	135
H(62)	4655	8422	2483	131
H(63)	2000	15763	2332	110
H(64)	1258	14178	1554	110
H(65)	936	14898	2660	110