Supplementary Material

Copper(II) Nanoballs as Monomers for Polyurethane Coatings: Synthesis, Urethane Derivatization and Kinetic Stability

Markus Tonigold, Julia Hitzbleck, Stefan Bahnmüller, Gerhard Langstein and Dirk Volkmer*

* To whom correspondence should be addressed:

Prof. D. Volkmer
Ulm University
Institute of Inorganic Chemistry 2, Materials and Catalysis
Albert-Einstein-Allee 11
D-89081 Ulm (Germany)
Fon: +49 (0)731-50-23921
Fax: +49 (0)731-50-23039
E-mail: dirk.volkmer@uni-ulm.de

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Details of SAXS measurements

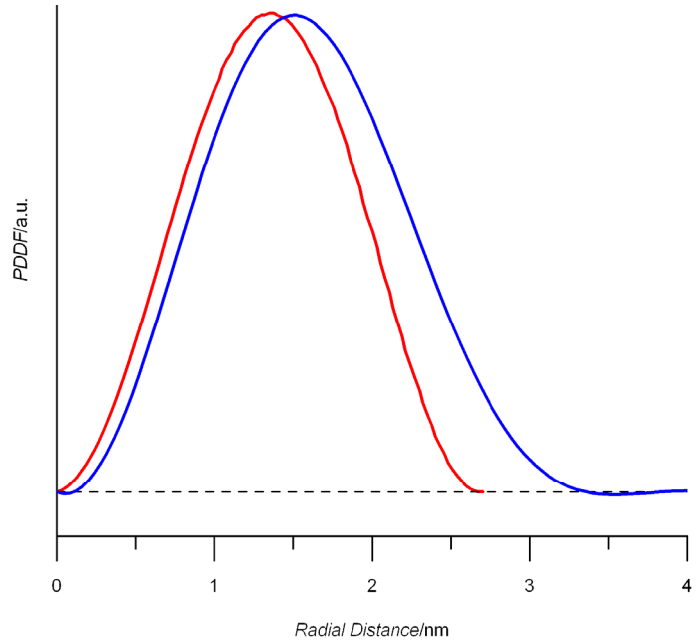

Figure S1. Pair-distance distribution functions (PDDF) for **2** (red) and **3** (blue).

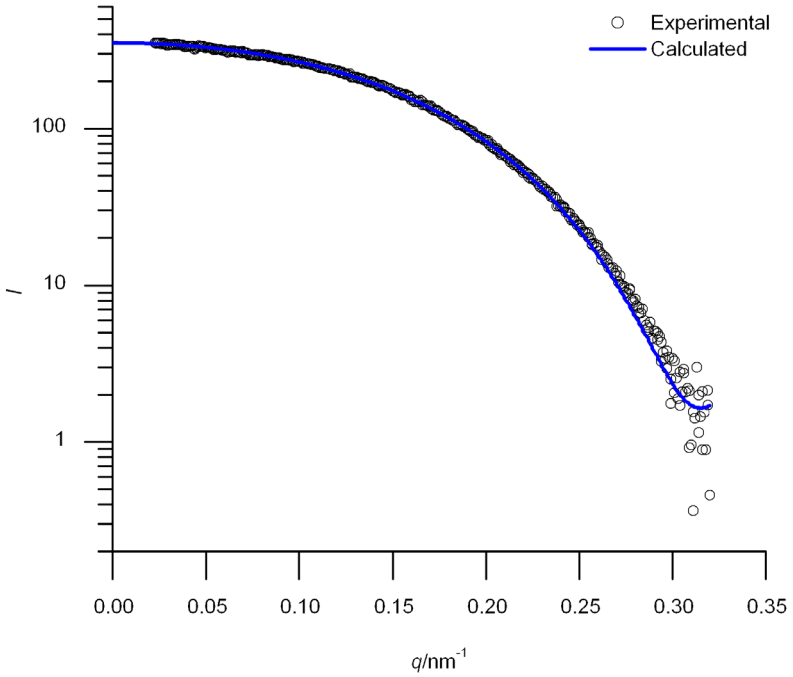

Figure S2. SAXS intensity (I) vs momentum transfer (q = 0.2 – 3.2 nm^{-1}) for a solution of **2** in DMF (110 g/L). The symbols and the solid line correspond to the experimental data points and the theoretical intensities, respectively. The theoretical intensities are calculated from the X-ray single-crystal structure using the program CRYSOL[1] (χ = 1.163).

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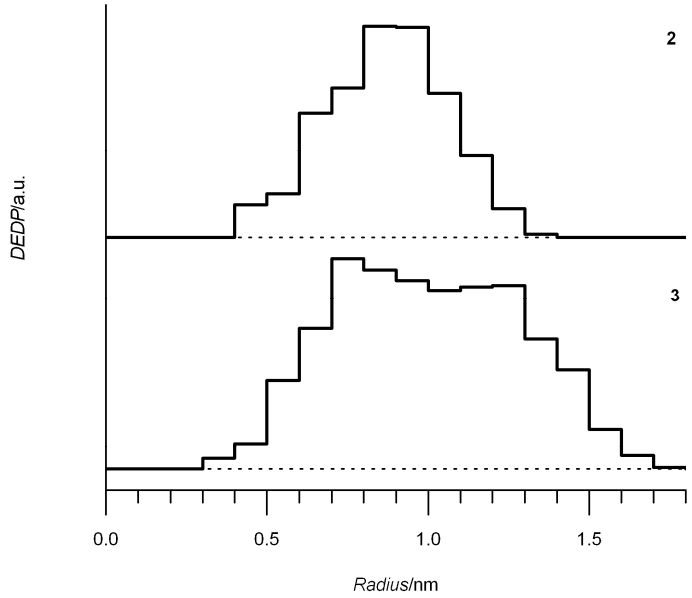

Figure S3. Difference electron-density profiles (DEDP) calculated from DAMMIN fits of **2** and **3**. The maximum around 0.8 to 1.0 nm is in good agreement with the distances of the copper ions from the centres (the distances of the interior and exterior copper ions from the centre of the Nanoballs are 0.8 and 1.1 nm, respectively). The radius of Nanoball **3** is extended by 0.4 nm when compared to Nanoball **2** (a value of 0.6 nm is expected from the crystal structure of the urethane[2]).

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Exemplary data analysis of kinetic measurements

The absorbances were processed as first order kinetics to obtain k_{obs} according to

$$\ln\left(\frac{A_\infty - A_t}{A_\infty - A_0}\right) = k_{obs} \cdot t$$

with

A_t Absorption after time t;

A_0 Absorption at $t = 0$;

A_∞ Absorption after complete dissociation.

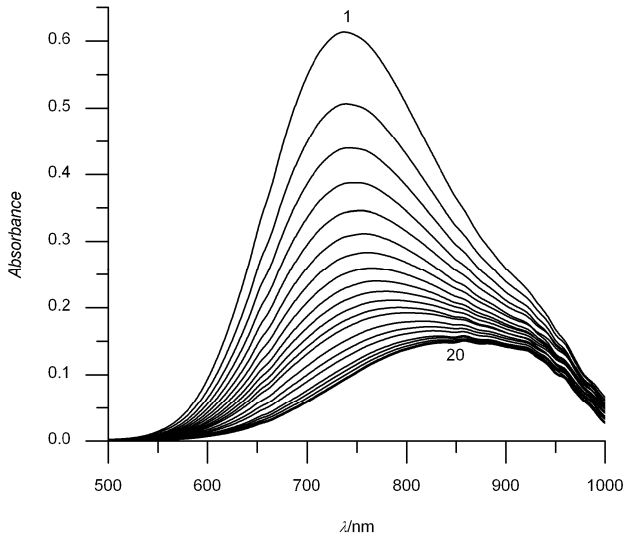

Figure S4. Time-resolved absorption spectra: dissociation kinetics of **2**. Solvent: DMSO; T = 25.0(2) °C; [**2**] = 15.4 x 10^{-5} M, [H_3PO_4] = 97.2 x 10^{-3} M, l = 1 cm. Spectrum 1 recorded before the addition of acid stock solution and spectra 2-20 recorded 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 16, 18, 20, 25, 30 and 80 min after the addition of acid stock solution.

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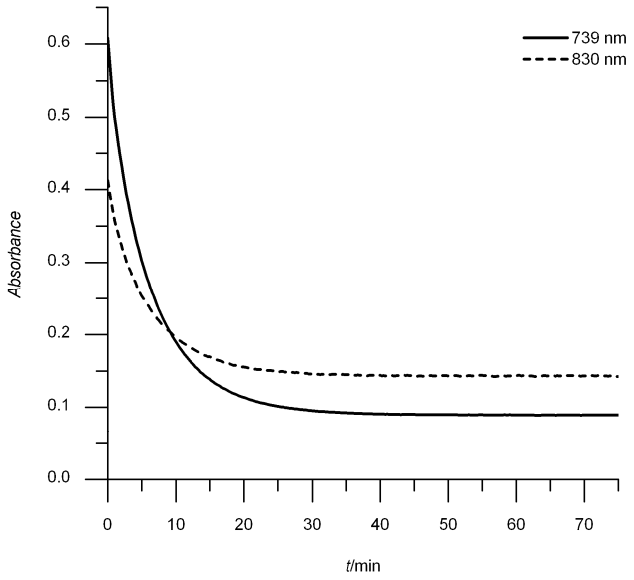

Figure S5. Dissociation kinetics of **2**. Solvent: DMSO; T = 25.0(2) °C; [**2**] = 15.4 x 10^{-5} M, [H_3PO_4] = 97.2 x 10^{-3} M, l = 1 cm.

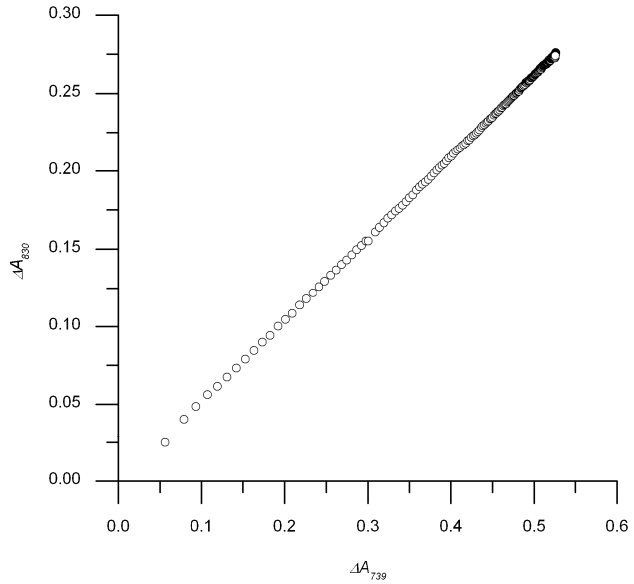

Figure S6. Change of absorbance $\Delta A_X = A_X(t) - A_X(t=0)$ over time for X_1 = 740 nm against X_2 = 830 nm. Due to the linear relationship, no intermediates are observed[3] during the acid assisted dissociation of **2** as well as **3** to copper(II).

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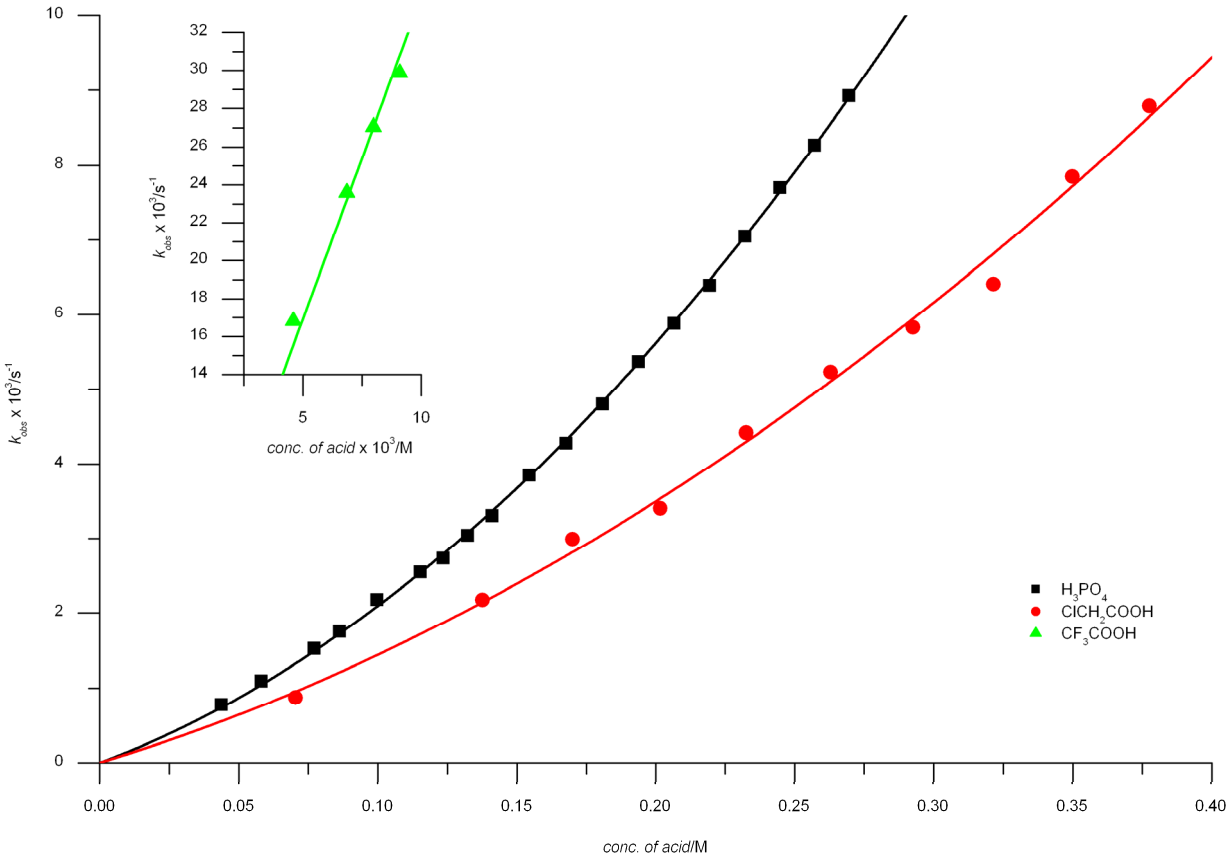

Figure S7. Pseudo-first-order rate constants k_{obs} of **2** for acids of different strengths. Solvent: DMSO, T = 25.0(2) °C; [**2**] = 15.4 x 10^{-5} M. Data shown for the dissociation with CF_3COOH (see insert) are less precise (due to the fast dissociation kinetics, low concentrations of CF_3COOH had to be chosen which no longer ensure pseudo-first order kinetics). The rate constants for dissociation with CF_3COOH are only shown to point out their order of magnitude.

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In-situ IR

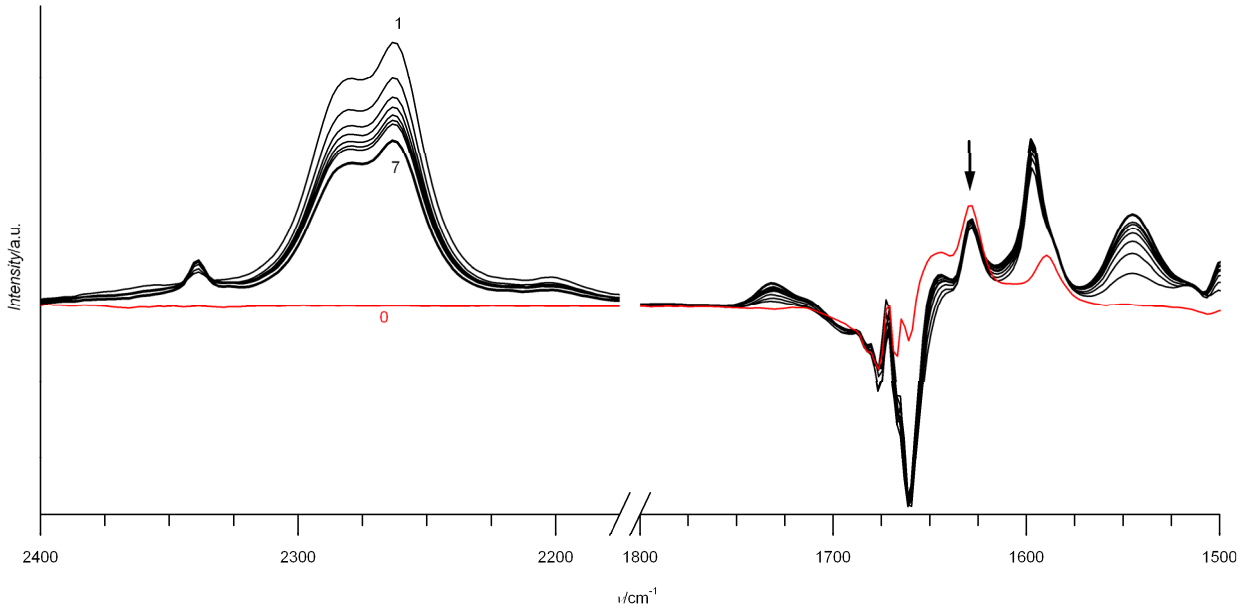

Figure S8. In-situ IR spectra in DMF for the reaction of **2** with excess phenylisocyanate. Spectra 0 corresponds to **2** in solution; Spectra 1-7 were recorded 2, 4, 6, 8, 10, 12 and 40 min after addition of phenylisocyanate. The position of the COO asymmetric stretching band at 1646 cm^{-1} (marked with arrow), typical for copper(II) paddle-wheel complexes,[4] shows no shift during the reaction, indicating the stability in solution during the conversion of **2** to **3**. The decreasing band at 2275 cm^{-1} is due to the NCO group of the phenylisocyanate, while the increasing bands at 1725 and 1545 cm^{-1} are due to the C=O and NH group of the forming urethane group, respectively.

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Analysis of conversion reactions

For the conversion of **2** to **3** in presence of methanol and water, simplifying the problem by treating methanol and water as one concurrent species ROH, the two equations for the concurrent reaction rates are:

$$\frac{\mathrm{d}[ROH]}{\mathrm{d}t} = k_{ROH} \cdot [ROH] \cdot [PhNCO] \tag{1}$$

$$\frac{\mathrm{d}[B]}{\mathrm{d}t} = k_{B} \cdot [B] \cdot [PhNCO] \tag{2}$$

with

[ROH]	concentration of water and methanol
[B]	concentration of hydroxy groups from Nanoball **2**
[PhNCO]	concentration of phenylisocyanate

Division of (1) by (2) followed by integration gives

$$\ln\left(\frac{[B]}{[B]_0}\right) = \frac{k_B}{k_{ROH}} \cdot \ln\left(\frac{[ROH]}{[ROH]_0}\right) \tag{3}$$

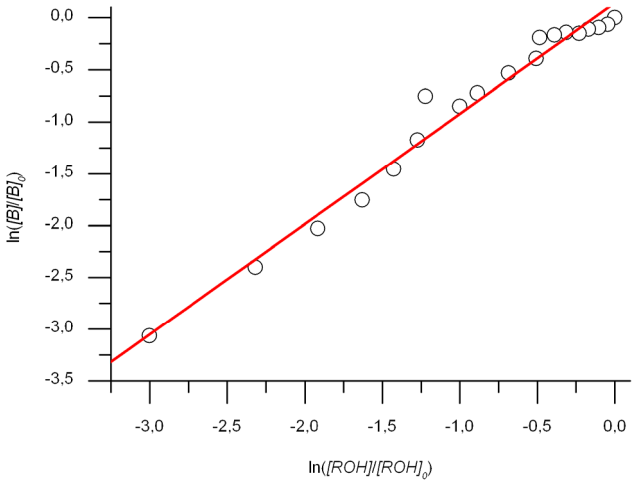

Figure S9. Double logarithmic plot of the relative concentrations of the Nanoball **2** ($[B]/[B]_0$) against the competing species ($[ROH]/[ROH]_0$).

Linear regression reveals k_B/k_{ROH} = 1.06(4). Both rate constants are nearly equal ($k_B \approx k_{ROH}$), revealing that the hydroxy groups of the Nanoball *[B]* react with phenylisocyanate as fast as the concurrent species *[ROH]*.

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Crystallographic data of compound Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate (2)

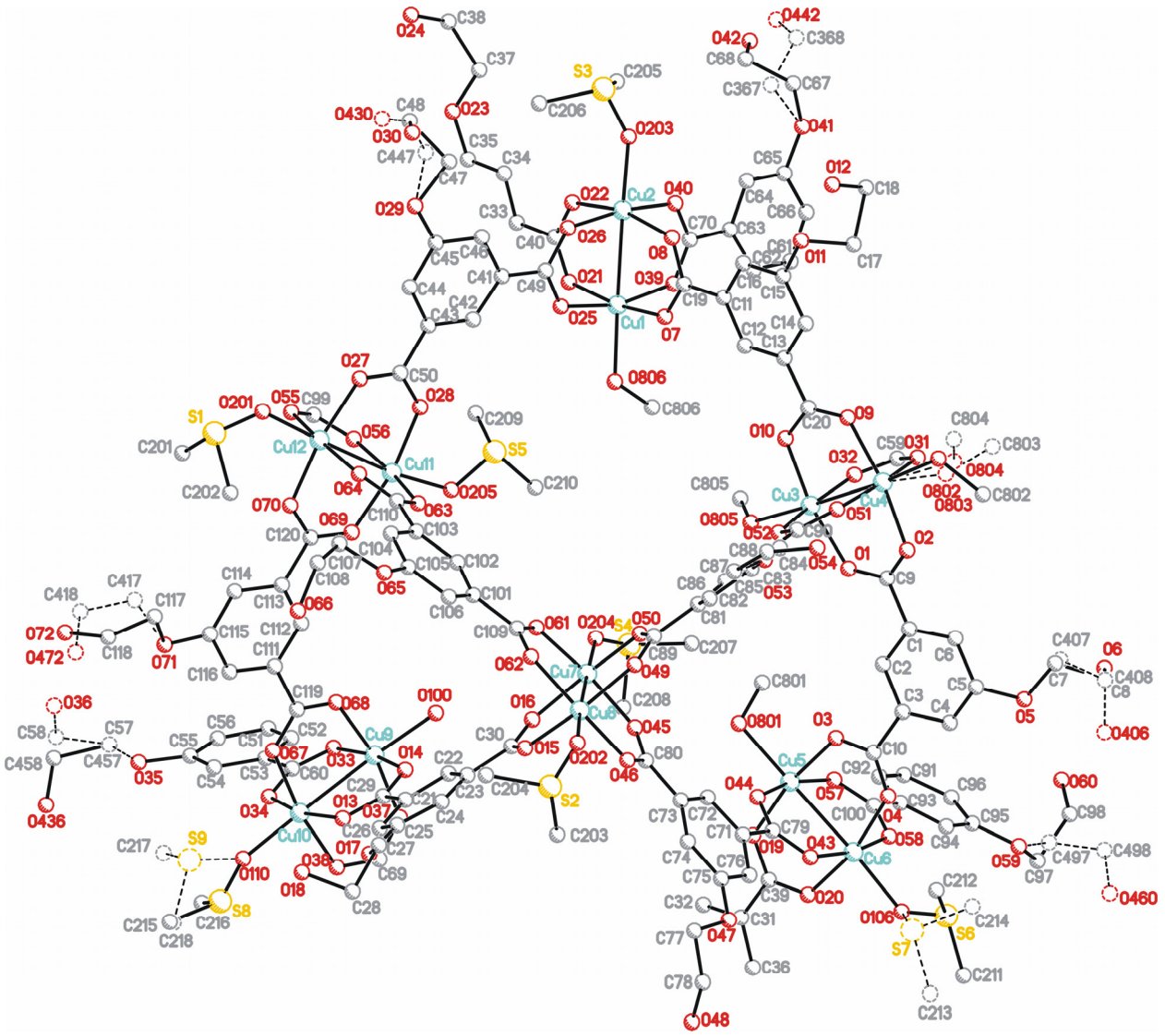

Figure S10. Atom numbering scheme for compound **2**. Hydrogen atoms and non-coordinated solvent molecules are omitted for clarity.

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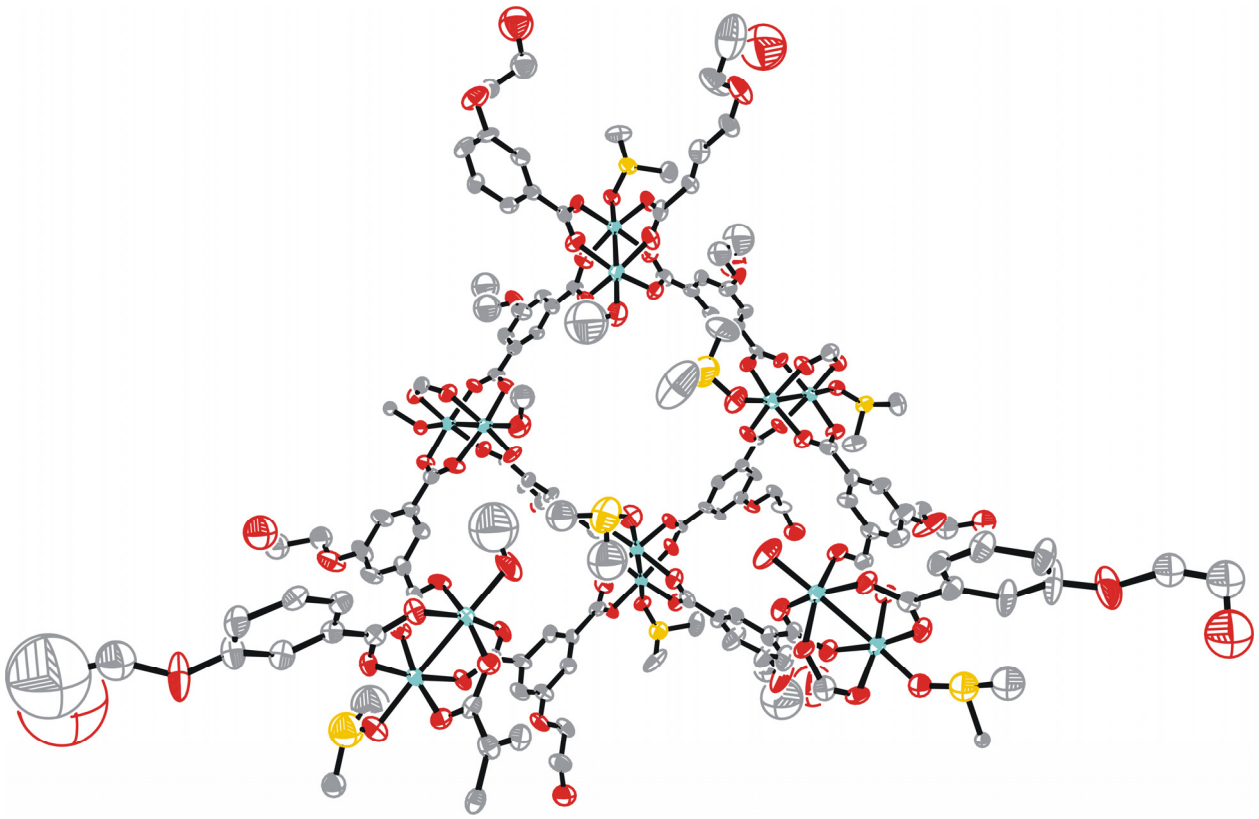

Figure S11. ORTEP representations of the asymmetric unit present in crystalline Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate **(2)**. All non-hydrogen atoms represented by thermal ellipsoids drawn are at the 40% probability level. All hydrogen atoms, minor disorder components and free solvent molecules are omitted for clarity.

Table 1. Pairs of disordered groups and corresponding site occupancy factors.

Group	**(s.o.f.)**		**Group**	**(s.o.f.)**
C117/C118/O72	(0.53)	*and*	C417/C418/O472	(0.47)
C47	(0.72)	*and*	C447	(0.28)
O30	(0.78)	*and*	O430	(0.22)
C97/C98/O60	(0.42)	*and*	C497/C498/O460	(0.58)
C57/C58/O36	(0.34)	*and*	C457/C458/O436	(0.66)
C67/C68/O42	(0.65)	*and*	C367/C368/O442	(0.35)
C7/C8/O6	(0.64)	*and*	C407/C408/O406	(0.36)
C818/O818	(0.56)	*and*	C814/O814	(0.44)
S8/C215/C216	(0.49)	*and*	S9/C217/C218	(0.51)
S6/C211/C212	(0.67)	*and*	S7/C213/C214	(0.33)
C802/O802 (0.26)	*and*	C803/O803 (0.41)	*and*	C804/O804 (0.33)

Disordered groups were calculated with isotropic atoms.

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Table 2. Crystal data and structure refinement for Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate (**2**).

Empirical formula	$C_{343}H_{536}Cu_{24}O_{213}S_{36}$
M_r	10746.84
T/K	223(2)
λ/Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$ (No. 14)
a/Å	26.220(5)
b/Å	39.060(8)
c/Å	26.643(5)
β/°	95.64(3)
V/Å^3	27154(9)
Z	2
ρ_{calc}/Mg m^{-3}	1.314
μ (Mo Kα)/mm^{-1}	1.139
F(000)	11140
Crystal size/mm	0.53 x 0.38 x 0.31
Θ Range/°	1.73–24.09
Index ranges	–29≤h≤30, –43≤k≤44, –30≤l≤27
Reflections collected	85619
Independent reflections	39811 [R(int) = 0.1170]
Completeness to Θ = 24.09°	92.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	39811 / 301 / 2427
Goodness-of-Fit on F^2	0.853
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0993, wR_2 = 0.1891
R indices (all data)	R_1 = 0.2441, wR_2 = 0.3008
$\Delta\rho_{max, min}$/e Å^{-3}	1.995, –0.904

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Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	1784(1)	-1471(1)	6336(1)	44(1)
Cu(2)	2331(1)	-1995(1)	6730(1)	38(1)
Cu(3)	778(1)	-40(1)	8034(1)	37(1)
Cu(4)	987(1)	-52(1)	9025(1)	36(1)
Cu(5)	-967(1)	1438(1)	6718(1)	37(1)
Cu(6)	-1304(1)	1938(1)	7274(1)	33(1)
Cu(7)	1994(1)	1307(1)	6387(1)	36(1)
Cu(8)	2639(1)	1776(1)	6793(1)	33(1)
Cu(9)	1168(1)	1369(1)	3329(1)	36(1)
Cu(10)	1601(1)	1841(1)	2797(1)	36(1)
Cu(11)	2982(1)	-138(1)	4652(1)	38(1)
Cu(12)	3957(1)	-167(1)	4479(1)	34(1)
C(1)	-113(6)	731(4)	8644(6)	43(4)
C(2)	-301(5)	898(4)	8221(6)	42(4)
C(3)	-617(5)	1180(4)	8256(7)	47(4)
C(4)	-749(6)	1278(4)	8723(7)	59(5)
C(5)	-568(7)	1107(5)	9142(6)	77(6)
C(9)	254(6)	439(4)	8614(7)	42(4)
C(10)	-824(5)	1373(4)	7795(7)	43(4)
C(12)	1863(5)	-972(4)	7932(7)	43(4)
C(13)	1840(6)	-833(4)	8390(6)	45(4)
C(19)	2152(6)	-1423(4)	7381(7)	50(5)
C(20)	1497(6)	-543(4)	8466(8)	52(5)
C(21)	2020(6)	2015(4)	4345(6)	48(4)
C(22)	1984(5)	1864(4)	4808(6)	40(4)
C(24)	2603(10)	2260(5)	5193(8)	99(8)
C(25)	2660(8)	2391(5)	4720(8)	93(8)
C(26)	2345(7)	2301(5)	4293(7)	79(7)
C(29)	1750(6)	1876(5)	3880(6)	49(5)

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C(31)	-1665(5)	2160(4)	5731(6)	48(5)
C(32)	-1681(5)	2011(5)	5267(6)	51(5)
C(33)	1900(5)	-2182(4)	5171(6)	41(4)
C(35)	2076(7)	-2661(4)	4666(7)	70(6)
C(39)	-1452(5)	1987(5)	6185(7)	45(4)
C(40)	1931(5)	-2006(5)	5664(5)	44(4)
C(41)	3320(5)	-1354(4)	6066(6)	42(4)
C(42)	3288(6)	-1076(4)	5727(6)	48(4)
C(43)	3709(5)	-953(4)	5508(6)	36(4)
C(44)	4176(5)	-1118(4)	5601(6)	44(4)
C(45)	4211(6)	-1402(4)	5912(7)	60(5)
C(46)	3783(6)	-1518(4)	6143(6)	48(4)
C(49)	2866(6)	-1476(4)	6248(6)	50(5)
C(50)	3651(6)	-652(4)	5167(6)	41(4)
C(51)	246(6)	736(5)	1388(7)	60(5)
C(52)	452(6)	902(4)	1809(6)	48(4)
C(53)	824(6)	1138(4)	1786(6)	48(4)
C(54)	1014(7)	1204(5)	1322(7)	70(6)
C(55)	823(7)	1024(6)	898(6)	89(8)
C(56)	427(7)	799(5)	920(7)	69(6)
C(59)	186(6)	-467(4)	8596(7)	46(4)
C(60)	1031(5)	1318(4)	2264(7)	43(4)
C(61)	-111(5)	-2171(4)	6984(6)	43(4)
C(62)	328(5)	-2021(4)	6874(5)	39(4)
C(63)	796(6)	-2195(4)	6900(6)	45(4)
C(64)	794(5)	-2538(4)	7068(6)	50(5)
C(65)	353(6)	-2684(3)	7189(7)	59(5)
C(66)	-85(5)	-2503(4)	7159(7)	55(5)
C(69)	586(5)	1964(5)	3033(6)	48(5)
C(70)	1264(5)	-2028(4)	6770(6)	41(4)
C(71)	235(5)	2154(4)	7064(6)	43(4)
C(72)	637(5)	1959(4)	6913(5)	39(4)
C(73)	1131(5)	2103(4)	6956(6)	38(4)
C(74)	1202(5)	2442(4)	7124(6)	48(4)
C(75)	794(5)	2630(4)	7242(6)	49(5)
C(76)	305(5)	2482(4)	7215(7)	56(5)

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C(77)	1296(5)	3144(3)	7332(7)	57(5)
C(79)	-285(5)	1995(5)	7033(6)	43(4)
C(80)	1561(5)	1893(4)	6822(6)	41(4)
C(81)	2372(6)	1057(4)	7928(6)	44(4)
C(82)	2017(5)	802(4)	7979(6)	44(4)
C(83)	2004(6)	643(4)	8423(6)	46(4)
C(84)	2338(6)	732(5)	8829(6)	60(5)
C(85)	2699(7)	967(5)	8774(7)	69(6)
C(86)	2728(6)	1145(4)	8312(6)	51(4)
C(89)	2380(5)	1239(4)	7429(8)	55(5)
C(90)	1593(6)	383(4)	8476(7)	43(4)
C(91)	-3112(6)	856(4)	6510(6)	43(4)
C(92)	-2635(5)	984(4)	6565(6)	43(4)
C(93)	-2518(5)	1248(4)	6920(6)	43(4)
C(94)	-2897(6)	1362(4)	7200(6)	54(5)
C(96)	-3493(6)	962(4)	6805(7)	57(5)
C(99)	3249(6)	-586(4)	3875(6)	48(5)
C(100)	-2004(6)	1395(4)	6971(6)	40(4)
C(101)	3506(5)	1051(4)	6081(6)	38(4)
C(102)	3405(5)	751(4)	5793(6)	38(4)
C(103)	3791(5)	595(4)	5568(6)	35(4)
C(105)	4364(5)	1030(4)	5915(6)	39(4)
C(106)	3982(5)	1184(4)	6136(6)	41(4)
C(107)	5252(5)	1048(4)	5724(7)	55(5)
C(108)	5692(6)	1296(4)	5801(8)	76(7)
C(109)	3064(6)	1221(4)	6300(6)	39(4)
C(110)	3665(6)	299(3)	5230(6)	34(4)
C(111)	2704(5)	1066(4)	3199(6)	43(4)
C(112)	2751(5)	795(4)	3512(6)	40(4)
C(113)	3216(6)	634(4)	3604(6)	45(4)
C(114)	3636(6)	750(4)	3355(7)	59(5)
C(115)	3571(5)	1021(6)	3039(8)	84(7)
C(116)	3103(6)	1177(5)	2965(7)	59(5)
C(119)	2204(6)	1258(4)	3128(6)	42(4)
C(120)	3294(6)	341(4)	3956(6)	44(4)
C(201)	4711(6)	-14(5)	3409(5)	80(6)

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C(202)	4950(6)	425(3)	4173(7)	77(7)
C(203)	2721(7)	2699(5)	6668(7)	108(9)
C(204)	3565(7)	2434(6)	6403(6)	102(8)
C(205)	2407(6)	-2938(4)	6623(7)	87(7)
C(206)	3225(6)	-2620(5)	6313(7)	86(7)
C(36)	-1865(6)	2488(4)	5757(6)	48(4)
C(104)	4271(5)	731(4)	5621(6)	45(4)
O(1)	300(4)	329(3)	8173(4)	52(3)
O(2)	494(4)	329(2)	9001(4)	44(3)
O(3)	-760(4)	1236(3)	7381(4)	48(3)
O(4)	-1028(4)	1655(3)	7851(4)	51(3)
O(5)	-760(7)	1199(4)	9579(5)	114(6)
O(7)	1919(4)	-1278(3)	7008(4)	53(3)
O(8)	2367(4)	-1715(3)	7359(4)	58(3)
O(9)	1437(4)	-435(3)	8892(4)	47(3)
O(10)	1284(4)	-414(3)	8060(4)	53(3)
O(13)	1832(4)	2013(3)	3475(4)	53(3)
O(14)	1468(4)	1616(3)	3920(4)	51(3)
O(15)	2530(4)	1949(3)	6096(4)	52(3)
O(16)	1975(4)	1569(3)	5755(4)	49(3)
O(17)	2969(7)	2670(4)	4635(5)	137(8)
O(19)	-1220(4)	1707(3)	6132(4)	50(3)
O(20)	-1519(4)	2126(3)	6606(4)	48(3)
O(21)	1720(4)	-1728(3)	5704(4)	57(3)
O(22)	2189(4)	-2164(3)	6027(4)	52(3)
O(23)	2251(6)	-2986(4)	4580(5)	100(5)
O(25)	2462(4)	-1318(3)	6159(4)	54(3)
O(26)	2915(4)	-1752(3)	6514(4)	55(3)
O(27)	4027(4)	-548(2)	4959(4)	43(3)
O(28)	3214(4)	-518(2)	5106(4)	46(3)
O(29)	4684(4)	-1549(3)	5976(5)	79(4)
O(31)	408(4)	-376(3)	8999(4)	49(3)
O(32)	263(4)	-377(3)	8164(4)	48(3)
O(33)	942(4)	1187(3)	2673(4)	48(3)
O(34)	1307(4)	1586(3)	2209(4)	48(3)
O(35)	1083(6)	1079(4)	476(5)	110(5)

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O(37)	590(3)	1684(3)	3253(4)	46(3)
O(38)	958(3)	2089(2)	2813(4)	46(3)
O(39)	1216(3)	-1739(3)	6573(4)	54(3)
O(40)	1677(3)	-2184(3)	6876(4)	44(3)
O(41)	326(4)	-3023(3)	7345(6)	91(5)
O(43)	-623(3)	2135(3)	7255(4)	44(3)
O(44)	-339(3)	1710(3)	6797(4)	45(3)
O(45)	1465(3)	1601(3)	6606(4)	48(3)
O(46)	2011(3)	2009(2)	6934(4)	41(3)
O(47)	835(3)	2959(3)	7393(5)	60(3)
O(49)	2645(3)	1511(3)	7413(4)	42(3)
O(50)	2105(4)	1117(2)	7060(4)	44(3)
O(51)	1540(4)	266(3)	8896(4)	48(3)
O(52)	1330(4)	298(3)	8076(4)	54(3)
O(53)	3063(5)	1031(4)	9185(5)	97(5)
O(55)	3706(3)	-490(3)	3943(4)	47(3)
O(56)	2886(4)	-469(3)	4107(4)	53(3)
O(57)	-1664(4)	1259(3)	6730(4)	51(3)
O(58)	-1934(3)	1667(3)	7228(4)	43(3)
O(59)	-3713(4)	1345(4)	7481(6)	103(6)
O(61)	2626(3)	1099(2)	6212(4)	42(3)
O(62)	3180(3)	1483(3)	6567(4)	46(3)
O(63)	3220(3)	204(2)	5159(4)	43(3)
O(64)	4043(3)	168(2)	5031(4)	42(3)
O(65)	4835(4)	1187(3)	5972(5)	60(3)
O(66)	5576(5)	1594(3)	5516(6)	101(5)
O(67)	2185(3)	1526(3)	2861(4)	50(3)
O(68)	1838(3)	1139(3)	3322(4)	44(3)
O(69)	2911(3)	235(3)	4164(4)	46(3)
O(70)	3744(3)	215(2)	4023(4)	45(3)
O(71)	3953(4)	1158(4)	2786(7)	134(8)
O(806)	1353(5)	-1039(3)	6050(5)	91(5)
C(806)	794(11)	-952(13)	6123(18)	290(20)
O(805)	628(5)	-37(3)	7225(4)	79(4)
O(100)	763(4)	1004(3)	3724(5)	90(5)
O(201)	4726(3)	-208(2)	4347(4)	42(3)

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O(202)	3119(4)	2167(2)	7136(4)	49(3)
O(203)	2779(3)	-2393(2)	7075(4)	45(3)
O(204)	1507(3)	904(3)	6115(5)	73(4)
S(1)	5051(1)	-7(1)	4021(2)	56(1)
S(2)	3273(2)	2507(1)	6951(2)	72(2)
S(3)	2962(2)	-2725(1)	6875(2)	56(1)
S(16)	3499(3)	-4380(2)	10173(3)	117(2)
O(216)	3919(7)	-4125(6)	10274(9)	213(12)
C(231)	2916(7)	-4185(8)	10097(12)	240(20)
C(232)	3472(11)	-4578(6)	10763(8)	171(15)
S(17)	-1846(2)	-2969(2)	9494(3)	106(2)
C(233)	-1609(9)	-2937(6)	10122(6)	125(10)
O(217)	-1391(6)	-2976(5)	9197(6)	134(7)
C(234)	-2062(10)	-3394(6)	9478(10)	154(12)
S(18)	1066(5)	-5596(3)	8227(4)	177(4)
C(236)	1398(9)	-5270(6)	8599(9)	133(11)
C(235)	1516(10)	-5635(9)	7789(10)	196(15)
O(218)	605(7)	-5430(8)	7988(11)	267(17)
S(19)	1438(5)	-4418(4)	7608(6)	243(6)
C(237)	832(9)	-4502(8)	7870(10)	170(13)
C(238)	1728(13)	-4807(9)	7670(15)	280(20)
O(106)	-1625(4)	2339(3)	7652(4)	62(4)
O(48)	895(5)	3667(3)	7066(6)	102(5)
C(78)	1232(7)	3515(4)	7414(9)	82(7)
S(4)	966(3)	820(3)	6117(4)	163(4)
O(11)	2711(6)	-1414(4)	9138(6)	111(6)
C(14)	2111(6)	-980(5)	8812(7)	62(5)
C(15)	2431(7)	-1264(5)	8746(7)	68(6)
C(16)	2451(6)	-1405(4)	8277(7)	54(5)
C(805)	384(7)	-309(5)	6910(8)	88(6)
C(207)	812(9)	834(8)	6742(8)	162(12)
C(30)	2255(6)	1829(4)	5729(6)	47(4)
C(23)	2268(6)	1991(4)	5234(6)	49(4)
C(11)	2172(6)	-1262(4)	7871(7)	54(5)
C(208)	597(11)	1166(9)	5845(12)	236(19)
S(10)	2884(8)	-5212(5)	8365(8)	344(10)

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C(219)	3090(9)	-4814(6)	8077(10)	134(10)
O(210)	3404(13)	-5351(8)	8590(14)	350(20)
C(220)	2720(20)	-4950(13)	8897(15)	450(40)
S(13)	724(6)	-1783(4)	8194(6)	278(7)
O(213)	1036(7)	-1590(5)	8644(8)	163(8)
C(225)	644(15)	-1408(10)	7817(12)	290(20)
C(226)	129(10)	-1755(13)	8489(16)	340(30)
C(27)	3356(10)	2753(8)	5063(10)	157(12)
C(48)	5200(14)	-2058(12)	6196(19)	270(20)
C(47)	4692(11)	-1861(10)	6300(20)	143(18)
C(447)	4640(30)	-1961(12)	5980(60)	150(30)
O(30)	5562(11)	-1828(10)	6520(20)	215(16)
O(430)	5603(19)	-1953(16)	6210(30)	70(30)
C(18)	2857(13)	-1666(9)	9967(15)	216(17)
C(17)	2555(11)	-1368(10)	9649(9)	204(16)
O(12)	3390(11)	-1565(9)	9939(13)	303(16)
C(7)	-596(10)	1022(9)	10041(9)	93(12)
C(8)	-1117(13)	1040(10)	10279(14)	118(15)
O(6)	-1493(11)	835(10)	9978(14)	191(17)
C(407)	-750(30)	964(10)	9996(11)	75(14)
C(408)	-760(30)	1155(13)	10493(16)	120(30)
O(406)	-933(14)	1494(10)	10452(15)	108(17)
O(219)	1178(14)	-4434(12)	7037(10)	400(20)
C(38)	2505(14)	-3556(8)	4810(12)	215(18)
C(37)	2452(13)	-3179(6)	5034(9)	162(15)
C(67)	761(9)	-3218(6)	7507(11)	59(8)
C(68)	974(13)	-3396(10)	7074(13)	113(15)
O(42)	617(14)	-3637(10)	6840(14)	173(15)
C(367)	812(13)	-3217(8)	7290(20)	54(12)
C(368)	710(30)	-3576(12)	7470(20)	110(30)
O(442)	500(20)	-3784(13)	7080(30)	170(30)
C(457)	921(11)	900(8)	16(8)	76(9)
C(458)	1271(15)	991(9)	-389(14)	105(12)
O(436)	1344(11)	1349(8)	-419(12)	177(15)
C(57)	1080(20)	782(13)	130(18)	83(16)
C(58)	1470(20)	869(19)	-240(20)	87(16)

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O(36)	1974(18)	822(17)	-20(30)	180(30)
O(18)	3918(16)	3021(12)	4575(17)	400(30)
C(28)	3540(20)	3109(10)	4930(20)	400(40)
C(95)	-3375(5)	1223(5)	7161(7)	64(5)
S(6)	-1660(6)	2419(4)	8167(6)	165(6)
C(211)	-1830(10)	2850(6)	8241(11)	76(9)
C(212)	-1078(14)	2410(12)	8504(15)	230(30)
S(7)	-1350(5)	2585(3)	7988(5)	47(5)
C(213)	-1470(50)	2977(9)	7660(40)	300(80)
C(214)	-1740(40)	2660(30)	8480(30)	500(200)
C(117)	4478(8)	1097(10)	3026(12)	77(12)
C(118)	4883(15)	1314(11)	2779(13)	107(16)
O(72)	4864(12)	1225(10)	2254(11)	110(11)
C(417)	4383(9)	921(7)	2713(13)	55(11)
C(418)	4684(15)	1032(9)	2290(13)	76(14)
O(472)	4866(9)	1382(6)	2389(11)	62(9)
S(12)	859(6)	1526(4)	-1542(6)	303(10)
O(212)	1398(7)	1562(5)	-1330(7)	157(8)
C(223)	846(12)	1297(8)	-2074(11)	210(18)
C(224)	536(11)	1891(6)	-1702(10)	172(15)
S(8)	1800(5)	2448(4)	2049(5)	110(6)
C(216)	1270(20)	2391(15)	1670(20)	230(40)
C(215)	1900(40)	2864(7)	2140(30)	380(70)
S(9)	2262(5)	2256(3)	2000(5)	107(6)
C(217)	1955(17)	2078(9)	1478(10)	130(19)
C(218)	2281(9)	2683(5)	1813(9)	29(7)
O(110)	1963(4)	2224(3)	2422(4)	66(3)
C(6)	-239(7)	821(5)	9107(7)	68(6)
C(801)	-897(18)	687(9)	6250(20)	300(20)
O(801)	-651(6)	1040(4)	6306(6)	122(6)
C(34)	2100(6)	-2502(5)	5127(7)	64(6)
C(87)	3499(12)	1227(12)	9025(13)	280(20)
C(88)	3880(30)	1100(30)	9480(19)	630(60)
O(54)	3688(15)	1241(11)	9929(13)	350(20)
C(497)	-4153(14)	1144(12)	7585(19)	118(17)
C(498)	-4520(40)	1200(40)	7990(40)	530(90)

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O(460)	-4330(50)	1450(40)	8340(40)	690(90)
C(97)	-4261(8)	1271(10)	7365(17)	64(15)
C(98)	-4410(40)	972(15)	7690(30)	220(50)
O(60)	-4340(20)	652(12)	7440(30)	230(40)
C(239)	-786(11)	-2266(8)	10488(11)	162(12)
S(20)	-404(13)	-2103(10)	10077(13)	650(30)
C(240)	-904(16)	-1980(12)	9606(13)	290(20)
O(220)	-210(20)	-1755(15)	10260(20)	730(70)
O(803)	1110(30)	-6(15)	9815(18)	39(11)
C(803)	825(18)	-235(14)	10150(20)	39(17)
O(802)	1191(15)	-106(10)	9814(12)	44(9)
C(802)	896(17)	119(13)	10170(17)	87(18)
O(804)	999(15)	-78(16)	9849(9)	52(10)
C(804)	1479(13)	-113(10)	10188(16)	33(13)
O(811)	-220(18)	305(14)	5397(19)	240(20)
C(811)	108(13)	149(9)	5037(14)	60(10)
O(812)	670(30)	2365(16)	5540(30)	550(40)
C(812)	900(20)	2706(15)	5600(20)	330(30)
O(807)	-480(40)	1470(30)	5140(40)	730(70)
C(807)	-10(40)	1640(30)	5440(40)	670(90)
O(815)	195(8)	-1237(6)	5371(10)	188(9)
C(815)	237(11)	-1549(7)	5679(11)	148(11)
O(816)	2085(19)	-5229(15)	6530(20)	470(30)
C(816)	1628(16)	-5340(12)	6143(17)	260(20)
O(814)	4143(15)	1946(11)	1454(17)	119(15)
C(814)	4647(15)	1827(13)	1423(19)	100(20)
O(818)	3989(17)	1726(14)	1288(18)	190(20)
C(818)	3910(30)	1852(19)	1800(20)	210(30)
O(810)	1169(16)	3013(12)	3844(16)	350(20)
C(810)	1580(20)	2960(16)	3510(20)	350(30)
O(819)	1280(50)	-330(40)	3120(70)	1130(100)
C(819)	810(50)	-120(30)	2960(50)	760(80)
S(15)	289(17)	-2724(14)	8994(15)	920(40)
O(215)	500(40)	-3090(20)	8990(20)	1340(90)
C(229)	96(10)	-2689(8)	9606(10)	153(11)
C(230)	-210(19)	-2715(15)	8548(13)	330(30)

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S(14)	-2137(11)	1166(8)	8727(13)	491(16)
O(214)	-2080(30)	1143(16)	9290(16)	640(60)
C(227)	-2250(20)	1616(10)	8590(20)	370(30)
C(228)	-2770(20)	1034(18)	8550(30)	610(60)
O(813)	4158(12)	2203(9)	9394(12)	257(13)
C(813)	4610(20)	2017(17)	9340(30)	410(40)
C(808)	2450(20)	927(16)	1490(20)	370(40)
O(808)	2840(20)	1191(15)	1560(20)	450(30)
C(809)	2860(30)	-200(20)	2400(40)	550(70)
O(809)	3340(20)	-1(14)	2450(20)	430(30)
O(817)	4650(20)	295(8)	1920(20)	530(40)
C(817)	4639(5)	-81(4)	1976(6)	390(40)
S(11)	1230(5)	-3419(4)	10314(6)	367(11)
O(211)	1247(5)	-3127(4)	10677(6)	216(11)
C(221)	1802(5)	-3644(4)	10426(6)	189(14)
C(222)	821(8)	-3726(6)	10568(11)	165(12)
S(5)	2030(3)	-460(3)	5161(5)	182(4)
C(209)	1892(16)	-835(6)	4782(12)	250(20)
C(210)	1402(8)	-353(9)	5193(15)	290(30)
O(205)	2214(4)	-177(3)	4802(5)	86(4)
O(24)	2968(14)	-3523(11)	4569(16)	370(20)

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Table 4. Bond lengths [Å] and angles [°] for Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate (**2**).

Cu(1)-O(7)	1.942(11)
Cu(1)-O(21)	1.954(11)
Cu(1)-O(39)	1.974(10)
Cu(1)-O(25)	1.976(10)
Cu(1)-O(806)	2.130(11)
Cu(1)-Cu(2)	2.655(2)
Cu(2)-O(26)	1.936(11)
Cu(2)-O(40)	1.941(9)
Cu(2)-O(22)	1.987(10)
Cu(2)-O(8)	1.992(11)
Cu(2)-O(203)	2.104(8)
Cu(3)-O(32)	1.943(10)
Cu(3)-O(52)	1.954(10)
Cu(3)-O(1)	1.969(11)
Cu(3)-O(10)	1.971(10)
Cu(3)-O(805)	2.153(10)
Cu(3)-Cu(4)	2.642(2)
Cu(4)-O(9)	1.959(10)
Cu(4)-O(51)	1.967(10)
Cu(4)-O(2)	1.971(10)
Cu(4)-O(31)	1.971(10)
Cu(4)-O(803)	2.11(5)
Cu(4)-O(802)	2.13(3)
Cu(4)-O(804)	2.20(3)
Cu(5)-O(19)	1.945(10)
Cu(5)-O(44)	1.953(9)
Cu(5)-O(57)	1.959(10)
Cu(5)-O(3)	1.960(10)
Cu(5)-O(801)	2.120(13)
Cu(5)-Cu(6)	2.652(3)
Cu(6)-O(43)	1.948(9)
Cu(6)-O(20)	1.955(10)
Cu(6)-O(58)	1.957(9)

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Cu(6)-O(4)	1.971(10)
Cu(6)-O(106)	2.087(10)
Cu(7)-O(45)	1.934(10)
Cu(7)-O(50)	1.935(10)
Cu(7)-O(61)	1.941(9)
Cu(7)-O(16)	1.967(11)
Cu(7)-O(204)	2.113(9)
Cu(7)-Cu(8)	2.649(2)
Cu(8)-O(49)	1.948(10)
Cu(8)-O(46)	1.950(9)
Cu(8)-O(62)	1.962(10)
Cu(8)-O(15)	1.969(11)
Cu(8)-O(202)	2.128(8)
Cu(9)-O(33)	1.925(10)
Cu(9)-O(14)	1.947(10)
Cu(9)-O(37)	1.949(9)
Cu(9)-O(68)	1.975(9)
Cu(9)-O(100)	2.118(11)
Cu(9)-Cu(10)	2.647(3)
Cu(10)-O(38)	1.947(9)
Cu(10)-O(34)	1.951(9)
Cu(10)-O(67)	1.959(9)
Cu(10)-O(13)	1.966(10)
Cu(10)-O(110)	2.082(12)
Cu(11)-O(56)	1.945(11)
Cu(11)-O(69)	1.949(10)
Cu(11)-O(63)	1.955(9)
Cu(11)-O(28)	1.975(10)
Cu(11)-O(205)	2.095(11)
Cu(11)-Cu(12)	2.644(2)
Cu(12)-O(27)	1.961(10)
Cu(12)-O(64)	1.965(9)
Cu(12)-O(70)	1.967(10)
Cu(12)-O(55)	1.970(10)
Cu(12)-O(201)	2.087(8)
C(1)-C(2)	1.35(2)

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C(1)-C(6)	1.36(2)
C(1)-C(9)	1.50(2)
C(2)-C(3)	1.39(2)
C(3)-C(4)	1.38(2)
C(3)-C(10)	1.50(2)
C(4)-C(5)	1.35(2)
C(5)-O(5)	1.360(17)
C(5)-C(6)	1.42(2)
C(9)-O(2)	1.229(17)
C(9)-O(1)	1.267(18)
C(10)-O(4)	1.240(17)
C(10)-O(3)	1.253(18)
C(12)-C(13)	1.34(2)
C(12)-C(11)	1.41(2)
C(13)-C(14)	1.39(2)
C(13)-C(20)	1.48(2)
C(19)-O(7)	1.252(17)
C(19)-O(8)	1.276(17)
C(19)-C(11)	1.45(2)
C(20)-O(9)	1.24(2)
C(20)-O(10)	1.271(19)
C(21)-C(22)	1.38(2)
C(21)-C(26)	1.42(2)
C(21)-C(29)	1.47(2)
C(22)-C(23)	1.386(19)
C(24)-C(25)	1.38(3)
C(24)-C(23)	1.38(2)
C(25)-C(26)	1.38(2)
C(25)-O(17)	1.390(18)
C(29)-O(13)	1.242(19)
C(29)-O(14)	1.266(19)
C(31)-C(32)	1.36(2)
C(31)-C(36)	1.39(2)
C(31)-C(39)	1.45(2)
C(32)-C(33)#1	1.42(2)
C(33)-C(34)	1.36(2)

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C(33)-C(32)#1	1.42(2)
C(33)-C(40)	1.48(2)
C(35)-C(34)	1.37(2)
C(35)-O(23)	1.375(17)
C(35)-C(36)#1	1.38(2)
C(39)-O(19)	1.267(19)
C(39)-O(20)	1.274(19)
C(40)-O(21)	1.228(18)
C(40)-O(22)	1.284(16)
C(41)-C(46)	1.369(19)
C(41)-C(42)	1.41(2)
C(41)-C(49)	1.41(2)
C(42)-C(43)	1.38(2)
C(43)-C(44)	1.384(18)
C(43)-C(50)	1.48(2)
C(44)-C(45)	1.38(2)
C(45)-O(29)	1.363(15)
C(45)-C(46)	1.41(2)
C(49)-O(25)	1.229(16)
C(49)-O(26)	1.289(19)
C(50)-O(27)	1.244(18)
C(50)-O(28)	1.256(16)
C(51)-C(52)	1.36(2)
C(51)-C(56)	1.40(2)
C(51)-C(59)#1	1.55(2)
C(52)-C(53)	1.35(2)
C(53)-C(54)	1.40(2)
C(53)-C(60)	1.51(2)
C(54)-C(55)	1.38(2)
C(55)-C(56)	1.37(2)
C(55)-O(35)	1.386(17)
C(59)-O(31)	1.222(18)
C(59)-O(32)	1.239(18)
C(59)-C(51)#1	1.55(2)
C(60)-O(33)	1.248(19)
C(60)-O(34)	1.288(18)

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C(61)-C(62)	1.35(2)
C(61)-C(66)	1.38(2)
C(61)-C(69)#1	1.48(2)
C(62)-C(63)	1.400(19)
C(63)-C(64)	1.41(2)
C(63)-C(70)	1.46(2)
C(64)-C(65)	1.36(2)
C(65)-C(66)	1.34(2)
C(65)-O(41)	1.389(15)
C(69)-O(37)	1.239(19)
C(69)-O(38)	1.284(19)
C(69)-C(61)#1	1.48(2)
C(70)-O(39)	1.247(17)
C(70)-O(40)	1.251(15)
C(71)-C(76)	1.35(2)
C(71)-C(72)	1.39(2)
C(71)-C(79)	1.49(2)
C(72)-C(73)	1.406(18)
C(73)-C(74)	1.40(2)
C(73)-C(80)	1.47(2)
C(74)-C(75)	1.36(2)
C(75)-O(47)	1.350(15)
C(75)-C(76)	1.40(2)
C(77)-O(47)	1.430(14)
C(77)-C(78)	1.477(18)
C(79)-O(43)	1.240(18)
C(79)-O(44)	1.280(18)
C(80)-O(46)	1.272(15)
C(80)-O(45)	1.291(17)
C(81)-C(86)	1.357(19)
C(81)-C(82)	1.38(2)
C(81)-C(89)	1.51(2)
C(82)-C(83)	1.34(2)
C(83)-C(84)	1.37(2)
C(83)-C(90)	1.50(2)
C(84)-C(85)	1.34(2)

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C(85)-O(53)	1.402(16)
C(85)-C(86)	1.42(2)
C(89)-O(50)	1.255(18)
C(89)-O(49)	1.275(17)
C(90)-O(51)	1.227(17)
C(90)-O(52)	1.254(17)
C(91)-C(92)	1.343(19)
C(91)-C(96)	1.39(2)
C(91)-C(99)#1	1.49(2)
C(92)-C(93)	1.41(2)
C(93)-C(94)	1.37(2)
C(93)-C(100)	1.458(19)
C(94)-C(95)	1.36(2)
C(96)-C(95)	1.41(2)
C(99)-O(55)	1.252(16)
C(99)-O(56)	1.27(2)
C(99)-C(91)#1	1.49(2)
C(100)-O(57)	1.267(18)
C(100)-O(58)	1.269(17)
C(101)-C(106)	1.346(18)
C(101)-C(102)	1.412(19)
C(101)-C(109)	1.50(2)
C(102)-C(103)	1.37(2)
C(103)-C(104)	1.361(18)
C(103)-C(110)	1.483(19)
C(105)-C(106)	1.352(19)
C(105)-O(65)	1.376(13)
C(105)-C(104)	1.413(19)
C(107)-O(65)	1.438(15)
C(107)-C(108)	1.507(16)
C(108)-O(66)	1.403(17)
C(109)-O(61)	1.245(15)
C(109)-O(62)	1.268(16)
C(110)-O(63)	1.222(15)
C(110)-O(64)	1.275(16)
C(111)-C(116)	1.34(2)

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C(111)-C(112)	1.35(2)
C(111)-C(119)	1.51(2)
C(112)-C(113)	1.372(19)
C(113)-C(114)	1.42(2)
C(113)-C(120)	1.48(2)
C(114)-C(115)	1.35(2)
C(115)-C(116)	1.36(2)
C(115)-O(71)	1.372(17)
C(119)-O(68)	1.226(18)
C(119)-O(67)	1.261(17)
C(120)-O(69)	1.262(18)
C(120)-O(70)	1.276(16)
C(201)-S(1)	1.781(13)
C(202)-S(1)	1.762(14)
C(203)-S(2)	1.736(15)
C(204)-S(2)	1.736(16)
C(205)-S(3)	1.753(13)
C(206)-S(3)	1.757(15)
C(36)-C(35)#1	1.38(2)
O(5)-C(407)	1.44(2)
O(5)-C(7)	1.44(2)
O(15)-C(30)	1.246(16)
O(16)-C(30)	1.259(18)
O(17)-C(27)	1.49(2)
O(23)-C(37)	1.480(19)
O(29)-C(47)	1.49(2)
O(29)-C(447)	1.61(5)
O(35)-C(457)	1.44(2)
O(35)-C(57)	1.48(3)
O(41)-C(67)	1.402(18)
O(41)-C(367)	1.50(2)
O(53)-C(87)	1.47(2)
O(59)-C(95)	1.372(16)
O(59)-C(497)	1.44(2)
O(59)-C(97)	1.47(2)
O(71)-C(117)	1.48(2)

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O(71)-C(417)	1.49(2)
O(806)-C(806)	1.53(3)
O(805)-C(805)	1.463(17)
O(201)-S(1)	1.496(10)
O(202)-S(2)	1.483(10)
O(203)-S(3)	1.499(9)
O(204)-S(4)	1.456(11)
S(16)-O(216)	1.492(15)
S(16)-C(231)	1.70(2)
S(16)-C(232)	1.757(18)
S(17)-O(217)	1.494(14)
S(17)-C(233)	1.729(16)
S(17)-C(234)	1.755(18)
S(18)-O(218)	1.461(18)
S(18)-C(235)	1.75(2)
S(18)-C(236)	1.786(18)
S(19)-O(219)	1.61(2)
S(19)-C(238)	1.70(2)
S(19)-C(237)	1.83(2)
O(106)-S(6)	1.417(16)
O(106)-S(7)	1.455(14)
O(48)-C(78)	1.36(2)
S(4)-C(207)	1.753(19)
S(4)-C(208)	1.77(2)
O(11)-C(15)	1.350(16)
O(11)-C(17)	1.47(2)
C(14)-C(15)	1.41(2)
C(15)-C(16)	1.37(2)
C(16)-C(11)	1.36(2)
C(30)-C(23)	1.47(2)
S(10)-O(210)	1.53(2)
S(10)-C(220)	1.84(3)
S(10)-C(219)	1.84(2)
S(13)-O(213)	1.575(18)
S(13)-C(225)	1.77(2)
S(13)-C(226)	1.82(2)

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C(27)-C(28)	1.53(3)
C(48)-O(430)	1.13(6)
C(48)-O(30)	1.51(3)
C(48)-C(447)	1.56(3)
C(48)-C(47)	1.59(3)
C(18)-O(12)	1.46(2)
C(18)-C(17)	1.60(3)
C(7)-C(8)	1.56(3)
C(8)-O(6)	1.45(3)
C(407)-C(408)	1.52(3)
C(408)-O(406)	1.39(3)
C(38)-O(24)	1.43(3)
C(38)-C(37)	1.60(3)
C(67)-C(68)	1.50(3)
C(68)-O(42)	1.43(2)
C(367)-C(368)	1.51(3)
C(368)-O(442)	1.40(3)
C(457)-C(458)	1.53(2)
C(458)-O(436)	1.41(3)
C(57)-C(58)	1.53(3)
C(58)-O(36)	1.41(3)
O(18)-C(28)	1.46(3)
S(6)-C(212)	1.69(2)
S(6)-C(211)	1.76(2)
S(7)-C(214)	1.76(3)
S(7)-C(213)	1.78(3)
C(117)-C(118)	1.55(3)
C(118)-O(72)	1.44(3)
C(417)-C(418)	1.50(3)
C(418)-O(472)	1.46(3)
S(12)-O(212)	1.478(16)
S(12)-C(223)	1.67(2)
S(12)-C(224)	1.692(19)
S(8)-O(110)	1.360(14)
S(8)-C(216)	1.65(2)
S(8)-C(215)	1.66(3)

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S(9)-O(110)	1.436(15)
S(9)-C(217)	1.69(2)
S(9)-C(218)	1.743(19)
C(801)-O(801)	1.52(3)
C(87)-C(88)	1.57(3)
C(88)-O(54)	1.45(3)
C(497)-C(498)	1.52(3)
C(498)-O(460)	1.42(3)
C(97)-C(98)	1.52(3)
C(98)-O(60)	1.43(3)
C(239)-S(20)	1.68(3)
S(20)-O(220)	1.52(3)
S(20)-C(240)	1.79(3)
O(803)-C(803)	1.52(3)
O(802)-C(802)	1.56(3)
O(804)-C(804)	1.48(3)
O(811)-C(811)	1.48(3)
O(812)-C(812)	1.47(3)
O(807)-C(807)	1.55(3)
O(815)-C(815)	1.47(2)
O(816)-C(816)	1.56(3)
O(814)-C(814)	1.41(3)
O(818)-C(818)	1.48(3)
O(810)-C(810)	1.48(3)
O(819)-C(819)	1.51(3)
S(15)-O(215)	1.53(3)
S(15)-C(230)	1.68(3)
S(15)-C(229)	1.76(3)
S(14)-O(214)	1.50(3)
S(14)-C(228)	1.76(3)
S(14)-C(227)	1.82(3)
O(813)-C(813)	1.42(3)
C(808)-O(808)	1.46(3)
C(809)-O(809)	1.47(3)
O(817)-C(817)	1.48(3)
S(11)-O(211)	1.49(3)

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S(11)-C(221)	1.73(3)
S(11)-C(222)	1.78(3)
S(5)-O(205)	1.569(13)
S(5)-C(210)	1.710(18)
S(5)-C(209)	1.796(19)

O(7)-Cu(1)-O(21)	170.6(4)
O(7)-Cu(1)-O(39)	89.3(5)
O(21)-Cu(1)-O(39)	90.0(5)
O(7)-Cu(1)-O(25)	90.8(5)
O(21)-Cu(1)-O(25)	87.3(5)
O(39)-Cu(1)-O(25)	164.1(4)
O(7)-Cu(1)-O(806)	93.7(5)
O(21)-Cu(1)-O(806)	95.7(5)
O(39)-Cu(1)-O(806)	98.3(5)
O(25)-Cu(1)-O(806)	97.6(5)
O(7)-Cu(1)-Cu(2)	83.9(3)
O(21)-Cu(1)-Cu(2)	86.7(3)
O(39)-Cu(1)-Cu(2)	82.0(3)
O(25)-Cu(1)-Cu(2)	82.2(3)
O(806)-Cu(1)-Cu(2)	177.5(4)
O(26)-Cu(2)-O(40)	170.3(4)
O(26)-Cu(2)-O(22)	87.9(5)
O(40)-Cu(2)-O(22)	88.5(5)
O(26)-Cu(2)-O(8)	90.5(5)
O(40)-Cu(2)-O(8)	90.6(5)
O(22)-Cu(2)-O(8)	164.4(4)
O(26)-Cu(2)-O(203)	94.0(4)
O(40)-Cu(2)-O(203)	95.6(4)
O(22)-Cu(2)-O(203)	102.1(4)
O(8)-Cu(2)-O(203)	93.5(4)
O(26)-Cu(2)-Cu(1)	85.2(3)
O(40)-Cu(2)-Cu(1)	85.3(3)
O(22)-Cu(2)-Cu(1)	80.8(3)
O(8)-Cu(2)-Cu(1)	83.6(3)
O(203)-Cu(2)-Cu(1)	177.0(3)

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O(32)-Cu(3)-O(52)	166.5(5)
O(32)-Cu(3)-O(1)	89.8(5)
O(52)-Cu(3)-O(1)	88.7(5)
O(32)-Cu(3)-O(10)	88.2(5)
O(52)-Cu(3)-O(10)	90.3(5)
O(1)-Cu(3)-O(10)	167.3(5)
O(32)-Cu(3)-O(805)	96.9(5)
O(52)-Cu(3)-O(805)	96.6(5)
O(1)-Cu(3)-O(805)	97.4(5)
O(10)-Cu(3)-O(805)	95.3(5)
O(32)-Cu(3)-Cu(4)	83.6(3)
O(52)-Cu(3)-Cu(4)	82.9(3)
O(1)-Cu(3)-Cu(4)	84.2(3)
O(10)-Cu(3)-Cu(4)	83.1(3)
O(805)-Cu(3)-Cu(4)	178.3(4)
O(9)-Cu(4)-O(51)	89.1(5)
O(9)-Cu(4)-O(2)	167.7(4)
O(51)-Cu(4)-O(2)	90.5(4)
O(9)-Cu(4)-O(31)	88.7(5)
O(51)-Cu(4)-O(31)	168.0(4)
O(2)-Cu(4)-O(31)	89.1(4)
O(9)-Cu(4)-O(803)	102(2)
O(51)-Cu(4)-O(803)	94.3(15)
O(2)-Cu(4)-O(803)	90(2)
O(31)-Cu(4)-O(803)	97.7(15)
O(9)-Cu(4)-O(802)	90.3(9)
O(51)-Cu(4)-O(802)	96.7(12)
O(2)-Cu(4)-O(802)	102.0(9)
O(31)-Cu(4)-O(802)	95.1(12)
O(9)-Cu(4)-O(804)	101.2(16)
O(51)-Cu(4)-O(804)	105.3(13)
O(2)-Cu(4)-O(804)	90.7(16)
O(31)-Cu(4)-O(804)	86.7(13)
O(9)-Cu(4)-Cu(3)	84.5(3)
O(51)-Cu(4)-Cu(3)	84.1(3)
O(2)-Cu(4)-Cu(3)	83.3(3)

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O(31)-Cu(4)-Cu(3)	83.9(3)
O(803)-Cu(4)-Cu(3)	173.3(19)
O(802)-Cu(4)-Cu(3)	174.7(9)
O(804)-Cu(4)-Cu(3)	168.9(10)
O(19)-Cu(5)-O(44)	90.6(4)
O(19)-Cu(5)-O(57)	87.8(4)
O(44)-Cu(5)-O(57)	165.9(5)
O(19)-Cu(5)-O(3)	169.5(5)
O(44)-Cu(5)-O(3)	88.1(4)
O(57)-Cu(5)-O(3)	91.1(5)
O(19)-Cu(5)-O(801)	95.7(6)
O(44)-Cu(5)-O(801)	95.0(5)
O(57)-Cu(5)-O(801)	99.1(6)
O(3)-Cu(5)-O(801)	94.8(6)
O(19)-Cu(5)-Cu(6)	86.9(3)
O(44)-Cu(5)-Cu(6)	82.1(3)
O(57)-Cu(5)-Cu(6)	83.8(3)
O(3)-Cu(5)-Cu(6)	82.6(3)
O(801)-Cu(5)-Cu(6)	176.2(4)
O(43)-Cu(6)-O(20)	90.7(4)
O(43)-Cu(6)-O(58)	169.3(4)
O(20)-Cu(6)-O(58)	88.8(4)
O(43)-Cu(6)-O(4)	88.6(4)
O(20)-Cu(6)-O(4)	166.1(5)
O(58)-Cu(6)-O(4)	89.3(4)
O(43)-Cu(6)-O(106)	97.5(4)
O(20)-Cu(6)-O(106)	93.6(5)
O(58)-Cu(6)-O(106)	93.2(4)
O(4)-Cu(6)-O(106)	100.3(4)
O(43)-Cu(6)-Cu(5)	85.5(3)
O(20)-Cu(6)-Cu(5)	81.5(4)
O(58)-Cu(6)-Cu(5)	83.9(3)
O(4)-Cu(6)-Cu(5)	84.6(3)
O(106)-Cu(6)-Cu(5)	174.3(3)
O(45)-Cu(7)-O(50)	89.7(5)
O(45)-Cu(7)-O(61)	167.0(4)

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O(50)-Cu(7)-O(61)	90.5(4)
O(45)-Cu(7)-O(16)	89.5(5)
O(50)-Cu(7)-O(16)	169.0(4)
O(61)-Cu(7)-O(16)	87.8(5)
O(45)-Cu(7)-O(204)	96.8(4)
O(50)-Cu(7)-O(204)	93.6(4)
O(61)-Cu(7)-O(204)	96.2(4)
O(16)-Cu(7)-O(204)	97.4(4)
O(45)-Cu(7)-Cu(8)	85.1(3)
O(50)-Cu(7)-Cu(8)	81.8(3)
O(61)-Cu(7)-Cu(8)	82.1(3)
O(16)-Cu(7)-Cu(8)	87.2(3)
O(204)-Cu(7)-Cu(8)	175.0(3)
O(49)-Cu(8)-O(46)	91.3(4)
O(49)-Cu(8)-O(62)	90.2(4)
O(46)-Cu(8)-O(62)	168.8(4)
O(49)-Cu(8)-O(15)	165.9(4)
O(46)-Cu(8)-O(15)	88.6(4)
O(62)-Cu(8)-O(15)	87.3(5)
O(49)-Cu(8)-O(202)	93.5(4)
O(46)-Cu(8)-O(202)	93.2(4)
O(62)-Cu(8)-O(202)	97.7(4)
O(15)-Cu(8)-O(202)	100.6(4)
O(49)-Cu(8)-Cu(7)	86.0(3)
O(46)-Cu(8)-Cu(7)	83.4(3)
O(62)-Cu(8)-Cu(7)	85.6(3)
O(15)-Cu(8)-Cu(7)	79.9(3)
O(202)-Cu(8)-Cu(7)	176.6(3)
O(33)-Cu(9)-O(14)	169.0(5)
O(33)-Cu(9)-O(37)	88.4(4)
O(14)-Cu(9)-O(37)	91.0(5)
O(33)-Cu(9)-O(68)	91.1(5)
O(14)-Cu(9)-O(68)	86.9(4)
O(37)-Cu(9)-O(68)	166.1(4)
O(33)-Cu(9)-O(100)	94.5(5)
O(14)-Cu(9)-O(100)	96.5(5)

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O(37)-Cu(9)-O(100)	93.0(5)
O(68)-Cu(9)-O(100)	100.9(5)
O(33)-Cu(9)-Cu(10)	83.2(3)
O(14)-Cu(9)-Cu(10)	85.8(3)
O(37)-Cu(9)-Cu(10)	82.8(3)
O(68)-Cu(9)-Cu(10)	83.3(3)
O(100)-Cu(9)-Cu(10)	175.3(3)
O(38)-Cu(10)-O(34)	89.8(4)
O(38)-Cu(10)-O(67)	168.9(5)
O(34)-Cu(10)-O(67)	89.6(4)
O(38)-Cu(10)-O(13)	89.9(5)
O(34)-Cu(10)-O(13)	167.1(5)
O(67)-Cu(10)-O(13)	88.2(4)
O(38)-Cu(10)-O(110)	95.1(4)
O(34)-Cu(10)-O(110)	98.3(4)
O(67)-Cu(10)-O(110)	96.0(5)
O(13)-Cu(10)-O(110)	94.6(5)
O(38)-Cu(10)-Cu(9)	85.3(3)
O(34)-Cu(10)-Cu(9)	85.3(3)
O(67)-Cu(10)-Cu(9)	83.6(3)
O(13)-Cu(10)-Cu(9)	81.7(3)
O(110)-Cu(10)-Cu(9)	176.4(3)
O(56)-Cu(11)-O(69)	90.1(5)
O(56)-Cu(11)-O(63)	168.3(4)
O(69)-Cu(11)-O(63)	87.5(4)
O(56)-Cu(11)-O(28)	88.0(5)
O(69)-Cu(11)-O(28)	167.1(4)
O(63)-Cu(11)-O(28)	91.8(4)
O(56)-Cu(11)-O(205)	92.1(5)
O(69)-Cu(11)-O(205)	98.7(4)
O(63)-Cu(11)-O(205)	99.6(5)
O(28)-Cu(11)-O(205)	94.2(4)
O(56)-Cu(11)-Cu(12)	84.1(3)
O(69)-Cu(11)-Cu(12)	86.9(3)
O(63)-Cu(11)-Cu(12)	84.3(3)
O(28)-Cu(11)-Cu(12)	80.2(3)

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O(205)-Cu(11)-Cu(12)	173.3(4)
O(27)-Cu(12)-O(64)	91.1(4)
O(27)-Cu(12)-O(70)	168.7(4)
O(64)-Cu(12)-O(70)	87.9(4)
O(27)-Cu(12)-O(55)	89.4(4)
O(64)-Cu(12)-O(55)	167.1(4)
O(70)-Cu(12)-O(55)	89.1(4)
O(27)-Cu(12)-O(201)	91.2(4)
O(64)-Cu(12)-O(201)	97.8(4)
O(70)-Cu(12)-O(201)	100.0(4)
O(55)-Cu(12)-O(201)	95.1(4)
O(27)-Cu(12)-Cu(11)	87.0(3)
O(64)-Cu(12)-Cu(11)	83.2(3)
O(70)-Cu(12)-Cu(11)	81.7(3)
O(55)-Cu(12)-Cu(11)	83.9(3)
O(201)-Cu(12)-Cu(11)	178.0(3)
C(2)-C(1)-C(6)	122.1(15)
C(2)-C(1)-C(9)	120.4(16)
C(6)-C(1)-C(9)	117.4(15)
C(1)-C(2)-C(3)	119.8(16)
C(4)-C(3)-C(2)	119.2(15)
C(4)-C(3)-C(10)	119.7(15)
C(2)-C(3)-C(10)	121.1(16)
C(5)-C(4)-C(3)	120.8(16)
C(4)-C(5)-O(5)	116.8(16)
C(4)-C(5)-C(6)	120.1(17)
O(5)-C(5)-C(6)	122.7(16)
O(2)-C(9)-O(1)	124.9(15)
O(2)-C(9)-C(1)	119.9(16)
O(1)-C(9)-C(1)	115.2(14)
O(4)-C(10)-O(3)	125.5(16)
O(4)-C(10)-C(3)	118.5(16)
O(3)-C(10)-C(3)	116.0(14)
C(13)-C(12)-C(11)	120.3(15)
C(12)-C(13)-C(14)	120.3(15)
C(12)-C(13)-C(20)	121.1(15)

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C(14)-C(13)-C(20)	118.4(17)
O(7)-C(19)-O(8)	123.6(17)
O(7)-C(19)-C(11)	119.4(15)
O(8)-C(19)-C(11)	117.1(15)
O(9)-C(20)-O(10)	124.3(15)
O(9)-C(20)-C(13)	121.4(17)
O(10)-C(20)-C(13)	114.3(18)
C(22)-C(21)-C(26)	121.1(14)
C(22)-C(21)-C(29)	121.8(15)
C(26)-C(21)-C(29)	116.9(16)
C(21)-C(22)-C(23)	120.1(15)
C(25)-C(24)-C(23)	118.7(16)
C(26)-C(25)-C(24)	123.1(17)
C(26)-C(25)-O(17)	112.1(18)
C(24)-C(25)-O(17)	123.7(17)
C(25)-C(26)-C(21)	115.9(17)
O(13)-C(29)-O(14)	124.8(14)
O(13)-C(29)-C(21)	117.7(17)
O(14)-C(29)-C(21)	117.5(16)
C(32)-C(31)-C(36)	117.4(15)
C(32)-C(31)-C(39)	122.2(16)
C(36)-C(31)-C(39)	120.3(16)
C(31)-C(32)-C(33)#1	121.2(16)
C(34)-C(33)-C(32)#1	119.4(15)
C(34)-C(33)-C(40)	121.0(14)
C(32)#1-C(33)-C(40)	119.6(14)
C(34)-C(35)-O(23)	125.4(16)
C(34)-C(35)-C(36)#1	119.2(15)
O(23)-C(35)-C(36)#1	115.4(17)
O(19)-C(39)-O(20)	125.2(14)
O(19)-C(39)-C(31)	117.3(17)
O(20)-C(39)-C(31)	117.5(16)
O(21)-C(40)-O(22)	124.6(15)
O(21)-C(40)-C(33)	120.2(13)
O(22)-C(40)-C(33)	115.2(15)
C(46)-C(41)-C(42)	117.0(15)

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C(46)-C(41)-C(49)	123.6(15)
C(42)-C(41)-C(49)	118.8(14)
C(43)-C(42)-C(41)	122.5(14)
C(42)-C(43)-C(44)	119.4(14)
C(42)-C(43)-C(50)	119.7(13)
C(44)-C(43)-C(50)	120.9(14)
C(45)-C(44)-C(43)	119.0(15)
O(29)-C(45)-C(44)	114.7(15)
O(29)-C(45)-C(46)	124.4(14)
C(44)-C(45)-C(46)	120.8(14)
C(41)-C(46)-C(45)	121.1(15)
O(25)-C(49)-O(26)	124.3(17)
O(25)-C(49)-C(41)	120.2(16)
O(26)-C(49)-C(41)	115.5(13)
O(27)-C(50)-O(28)	124.0(15)
O(27)-C(50)-C(43)	119.6(13)
O(28)-C(50)-C(43)	116.4(15)
C(52)-C(51)-C(56)	120.7(16)
C(52)-C(51)-C(59)#1	122.1(18)
C(56)-C(51)-C(59)#1	117.2(16)
C(53)-C(52)-C(51)	121.2(17)
C(52)-C(53)-C(54)	119.2(15)
C(52)-C(53)-C(60)	118.9(16)
C(54)-C(53)-C(60)	121.9(14)
C(55)-C(54)-C(53)	119.6(15)
C(56)-C(55)-C(54)	120.6(17)
C(56)-C(55)-O(35)	124.8(16)
C(54)-C(55)-O(35)	114.6(16)
C(55)-C(56)-C(51)	118.5(16)
O(31)-C(59)-O(32)	128.8(15)
O(31)-C(59)-C(51)#1	117.4(16)
O(32)-C(59)-C(51)#1	113.9(16)
O(33)-C(60)-O(34)	126.1(13)
O(33)-C(60)-C(53)	117.6(14)
O(34)-C(60)-C(53)	116.2(16)
C(62)-C(61)-C(66)	118.0(14)

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C(62)-C(61)-C(69)#1	119.1(15)
C(66)-C(61)-C(69)#1	122.6(15)
C(61)-C(62)-C(63)	122.6(14)
C(62)-C(63)-C(64)	116.5(14)
C(62)-C(63)-C(70)	121.6(14)
C(64)-C(63)-C(70)	121.9(13)
C(65)-C(64)-C(63)	120.4(13)
C(66)-C(65)-C(64)	120.4(14)
C(66)-C(65)-O(41)	116.8(15)
C(64)-C(65)-O(41)	122.8(14)
C(65)-C(66)-C(61)	122.0(15)
O(37)-C(69)-O(38)	125.4(14)
O(37)-C(69)-C(61)#1	117.7(15)
O(38)-C(69)-C(61)#1	116.9(15)
O(39)-C(70)-O(40)	125.7(14)
O(39)-C(70)-C(63)	116.9(13)
O(40)-C(70)-C(63)	117.4(14)
C(76)-C(71)-C(72)	121.4(14)
C(76)-C(71)-C(79)	120.5(14)
C(72)-C(71)-C(79)	118.0(14)
C(71)-C(72)-C(73)	118.4(14)
C(74)-C(73)-C(72)	119.7(13)
C(74)-C(73)-C(80)	121.5(13)
C(72)-C(73)-C(80)	118.8(14)
C(75)-C(74)-C(73)	120.0(13)
O(47)-C(75)-C(74)	122.9(13)
O(47)-C(75)-C(76)	116.9(14)
C(74)-C(75)-C(76)	120.2(14)
C(71)-C(76)-C(75)	120.2(15)
O(47)-C(77)-C(78)	111.5(13)
O(43)-C(79)-O(44)	124.5(14)
O(43)-C(79)-C(71)	118.9(15)
O(44)-C(79)-C(71)	116.5(14)
O(46)-C(80)-O(45)	123.8(13)
O(46)-C(80)-C(73)	117.4(14)
O(45)-C(80)-C(73)	118.8(12)

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C(86)-C(81)-C(82)	121.9(15)
C(86)-C(81)-C(89)	118.4(15)
C(82)-C(81)-C(89)	119.6(14)
C(83)-C(82)-C(81)	119.9(14)
C(82)-C(83)-C(84)	120.7(15)
C(82)-C(83)-C(90)	118.7(14)
C(84)-C(83)-C(90)	120.4(15)
C(85)-C(84)-C(83)	119.4(16)
C(84)-C(85)-O(53)	118.1(17)
C(84)-C(85)-C(86)	121.9(14)
O(53)-C(85)-C(86)	120.0(15)
C(81)-C(86)-C(85)	116.0(15)
O(50)-C(89)-O(49)	124.3(17)
O(50)-C(89)-C(81)	117.1(14)
O(49)-C(89)-C(81)	118.6(15)
O(51)-C(90)-O(52)	125.1(14)
O(51)-C(90)-C(83)	119.0(14)
O(52)-C(90)-C(83)	115.9(15)
C(92)-C(91)-C(96)	122.7(14)
C(92)-C(91)-C(99)#1	119.8(16)
C(96)-C(91)-C(99)#1	117.5(14)
C(91)-C(92)-C(93)	119.0(16)
C(94)-C(93)-C(92)	118.5(13)
C(94)-C(93)-C(100)	122.4(14)
C(92)-C(93)-C(100)	119.1(16)
C(95)-C(94)-C(93)	122.8(14)
C(91)-C(96)-C(95)	118.3(14)
O(55)-C(99)-O(56)	125.1(15)
O(55)-C(99)-C(91)#1	118.3(17)
O(56)-C(99)-C(91)#1	116.6(14)
O(57)-C(100)-O(58)	123.6(13)
O(57)-C(100)-C(93)	118.7(14)
O(58)-C(100)-C(93)	117.6(15)
C(106)-C(101)-C(102)	120.1(14)
C(106)-C(101)-C(109)	122.1(13)
C(102)-C(101)-C(109)	117.8(13)

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C(103)-C(102)-C(101)	120.0(13)
C(104)-C(103)-C(102)	119.9(13)
C(104)-C(103)-C(110)	121.0(14)
C(102)-C(103)-C(110)	118.9(12)
C(106)-C(105)-O(65)	116.6(13)
C(106)-C(105)-C(104)	121.0(12)
O(65)-C(105)-C(104)	122.3(13)
C(101)-C(106)-C(105)	120.0(13)
O(65)-C(107)-C(108)	107.4(12)
O(66)-C(108)-C(107)	109.7(13)
O(61)-C(109)-O(62)	125.3(14)
O(61)-C(109)-C(101)	119.6(13)
O(62)-C(109)-C(101)	115.1(13)
O(63)-C(110)-O(64)	125.6(13)
O(63)-C(110)-C(103)	118.9(13)
O(64)-C(110)-C(103)	115.5(13)
C(116)-C(111)-C(112)	120.8(14)
C(116)-C(111)-C(119)	119.4(15)
C(112)-C(111)-C(119)	119.8(15)
C(111)-C(112)-C(113)	119.8(15)
C(112)-C(113)-C(114)	119.2(15)
C(112)-C(113)-C(120)	122.2(15)
C(114)-C(113)-C(120)	118.7(14)
C(115)-C(114)-C(113)	119.1(14)
C(114)-C(115)-C(116)	119.7(16)
C(114)-C(115)-O(71)	123.9(14)
C(116)-C(115)-O(71)	116.4(17)
C(111)-C(116)-C(115)	121.3(17)
O(68)-C(119)-O(67)	124.4(14)
O(68)-C(119)-C(111)	117.6(14)
O(67)-C(119)-C(111)	118.0(16)
O(69)-C(120)-O(70)	125.3(14)
O(69)-C(120)-C(113)	117.7(13)
O(70)-C(120)-C(113)	117.1(15)
C(35)#1-C(36)-C(31)	122.3(16)
C(103)-C(104)-C(105)	119.1(13)

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C(9)-O(1)-Cu(3)	122.8(9)
C(9)-O(2)-Cu(4)	124.8(10)
C(10)-O(3)-Cu(5)	125.0(10)
C(10)-O(4)-Cu(6)	122.3(11)
C(5)-O(5)-C(407)	121.1(19)
C(5)-O(5)-C(7)	120.1(17)
C(19)-O(7)-Cu(1)	125.8(10)
C(19)-O(8)-Cu(2)	123.0(11)
C(20)-O(9)-Cu(4)	123.9(10)
C(20)-O(10)-Cu(3)	124.1(11)
C(29)-O(13)-Cu(10)	125.9(11)
C(29)-O(14)-Cu(9)	121.5(11)
C(30)-O(15)-Cu(8)	129.0(11)
C(30)-O(16)-Cu(7)	120.0(10)
C(25)-O(17)-C(27)	114.2(16)
C(39)-O(19)-Cu(5)	120.3(11)
C(39)-O(20)-Cu(6)	126.0(10)
C(40)-O(21)-Cu(1)	121.8(9)
C(40)-O(22)-Cu(2)	126.0(11)
C(35)-O(23)-C(37)	115.6(14)
C(49)-O(25)-Cu(1)	125.5(11)
C(49)-O(26)-Cu(2)	122.3(10)
C(50)-O(27)-Cu(12)	120.8(10)
C(50)-O(28)-Cu(11)	127.9(11)
C(45)-O(29)-C(47)	112.1(14)
C(45)-O(29)-C(447)	111(2)
C(59)-O(31)-Cu(4)	121.1(11)
C(59)-O(32)-Cu(3)	122.5(10)
C(60)-O(33)-Cu(9)	125.0(9)
C(60)-O(34)-Cu(10)	120.3(10)
C(55)-O(35)-C(457)	119.2(15)
C(55)-O(35)-C(57)	114(2)
C(69)-O(37)-Cu(9)	125.2(10)
C(69)-O(38)-Cu(10)	121.3(10)
C(70)-O(39)-Cu(1)	124.6(9)
C(70)-O(40)-Cu(2)	122.3(10)

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C(65)-O(41)-C(67)	123.0(15)
C(65)-O(41)-C(367)	112.7(18)
C(79)-O(43)-Cu(6)	122.5(10)
C(79)-O(44)-Cu(5)	125.3(10)
C(80)-O(45)-Cu(7)	123.0(9)
C(80)-O(46)-Cu(8)	124.6(9)
C(75)-O(47)-C(77)	119.3(11)
C(89)-O(49)-Cu(8)	120.9(11)
C(89)-O(50)-Cu(7)	127.1(11)
C(90)-O(51)-Cu(4)	123.0(9)
C(90)-O(52)-Cu(3)	124.6(10)
C(85)-O(53)-C(87)	110.7(17)
C(99)-O(55)-Cu(12)	123.0(11)
C(99)-O(56)-Cu(11)	123.7(9)
C(100)-O(57)-Cu(5)	124.3(9)
C(100)-O(58)-Cu(6)	124.2(10)
C(95)-O(59)-C(497)	120(2)
C(95)-O(59)-C(97)	118.6(18)
C(109)-O(61)-Cu(7)	126.2(9)
C(109)-O(62)-Cu(8)	120.2(9)
C(110)-O(63)-Cu(11)	123.4(9)
C(110)-O(64)-Cu(12)	122.8(8)
C(105)-O(65)-C(107)	119.6(11)
C(119)-O(67)-Cu(10)	123.8(11)
C(119)-O(68)-Cu(9)	124.3(10)
C(120)-O(69)-Cu(11)	120.6(9)
C(120)-O(70)-Cu(12)	125.5(10)
C(115)-O(71)-C(117)	114.8(15)
C(115)-O(71)-C(417)	114.9(15)
C(806)-O(806)-Cu(1)	128(2)
C(805)-O(805)-Cu(3)	126.8(11)
S(1)-O(201)-Cu(12)	132.2(5)
S(2)-O(202)-Cu(8)	131.9(6)
S(3)-O(203)-Cu(2)	132.0(6)
S(4)-O(204)-Cu(7)	136.3(8)
O(201)-S(1)-C(202)	105.1(7)

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O(201)-S(1)-C(201)	105.2(7)
C(202)-S(1)-C(201)	98.7(8)
O(202)-S(2)-C(203)	106.8(7)
O(202)-S(2)-C(204)	106.9(9)
C(203)-S(2)-C(204)	97.1(9)
O(203)-S(3)-C(205)	105.2(7)
O(203)-S(3)-C(206)	105.5(8)
C(205)-S(3)-C(206)	99.5(9)
O(216)-S(16)-C(231)	111.1(14)
O(216)-S(16)-C(232)	103.0(11)
C(231)-S(16)-C(232)	100.9(13)
O(217)-S(17)-C(233)	106.5(10)
O(217)-S(17)-C(234)	104.0(11)
C(233)-S(17)-C(234)	100.2(11)
O(218)-S(18)-C(235)	109.4(15)
O(218)-S(18)-C(236)	105.2(13)
C(235)-S(18)-C(236)	96.4(12)
O(219)-S(19)-C(238)	101.6(17)
O(219)-S(19)-C(237)	92.9(14)
C(238)-S(19)-C(237)	101.5(15)
S(6)-O(106)-Cu(6)	134.4(9)
S(7)-O(106)-Cu(6)	126.4(8)
O(48)-C(78)-C(77)	114.0(16)
O(204)-S(4)-C(207)	108.2(10)
O(204)-S(4)-C(208)	108.7(13)
C(207)-S(4)-C(208)	101.4(13)
C(15)-O(11)-C(17)	118.9(16)
C(13)-C(14)-C(15)	119.0(17)
O(11)-C(15)-C(16)	117.6(16)
O(11)-C(15)-C(14)	122.0(17)
C(16)-C(15)-C(14)	120.3(14)
C(11)-C(16)-C(15)	119.5(15)
O(15)-C(30)-O(16)	123.8(16)
O(15)-C(30)-C(23)	118.7(15)
O(16)-C(30)-C(23)	117.4(14)
C(24)-C(23)-C(22)	120.2(16)

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C(24)-C(23)-C(30)	118.0(14)
C(22)-C(23)-C(30)	121.6(15)
C(16)-C(11)-C(12)	120.5(17)
C(16)-C(11)-C(19)	120.4(16)
C(12)-C(11)-C(19)	118.9(15)
O(210)-S(10)-C(220)	99.6(18)
O(210)-S(10)-C(219)	100.1(16)
C(220)-S(10)-C(219)	87.2(15)
O(213)-S(13)-C(225)	93.4(15)
O(213)-S(13)-C(226)	92.6(15)
C(225)-S(13)-C(226)	97.8(16)
O(17)-C(27)-C(28)	103(3)
O(430)-C(48)-C(447)	140(7)
O(30)-C(48)-C(447)	125(4)
O(430)-C(48)-C(47)	128(4)
O(30)-C(48)-C(47)	96(2)
O(29)-C(47)-C(48)	105(3)
C(48)-C(447)-O(29)	101(4)
O(12)-C(18)-C(17)	102(2)
O(11)-C(17)-C(18)	103(2)
O(5)-C(7)-C(8)	97(2)
O(6)-C(8)-C(7)	109(2)
O(5)-C(407)-C(408)	111(3)
O(406)-C(408)-C(407)	115(3)
O(24)-C(38)-C(37)	101(2)
O(23)-C(37)-C(38)	101.6(18)
O(41)-C(67)-C(68)	112(2)
O(42)-C(68)-C(67)	111(2)
O(41)-C(367)-C(368)	105(4)
O(442)-C(368)-C(367)	112(3)
O(35)-C(457)-C(458)	110(2)
O(436)-C(458)-C(457)	111(2)
O(35)-C(57)-C(58)	105(4)
O(36)-C(58)-C(57)	111(3)
O(18)-C(28)-C(27)	101(3)
C(94)-C(95)-O(59)	117.4(15)

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C(94)-C(95)-C(96)	118.6(15)
O(59)-C(95)-C(96)	123.9(14)
O(106)-S(6)-C(212)	111.7(17)
O(106)-S(6)-C(211)	111.1(14)
C(212)-S(6)-C(211)	100.8(15)
O(106)-S(7)-C(214)	107(2)
O(106)-S(7)-C(213)	102(2)
C(214)-S(7)-C(213)	97(2)
O(71)-C(117)-C(118)	112(2)
O(72)-C(118)-C(117)	109(2)
O(71)-C(417)-C(418)	112(2)
O(472)-C(418)-C(417)	109(2)
O(212)-S(12)-C(223)	108.3(15)
O(212)-S(12)-C(224)	116.8(15)
C(223)-S(12)-C(224)	105.6(14)
O(110)-S(8)-C(216)	123(2)
O(110)-S(8)-C(215)	119(2)
C(216)-S(8)-C(215)	109.6(19)
O(110)-S(9)-C(217)	110.9(15)
O(110)-S(9)-C(218)	109.8(12)
C(217)-S(9)-C(218)	100.6(14)
S(8)-O(110)-Cu(10)	133.4(9)
S(9)-O(110)-Cu(10)	138.3(9)
C(1)-C(6)-C(5)	117.9(15)
C(801)-O(801)-Cu(5)	122(2)
C(33)-C(34)-C(35)	120.5(15)
O(53)-C(87)-C(88)	94(4)
O(54)-C(88)-C(87)	106(3)
O(59)-C(497)-C(498)	129(4)
O(460)-C(498)-C(497)	112(3)
O(59)-C(97)-C(98)	109(5)
O(60)-C(98)-C(97)	111(3)
O(220)-S(20)-C(239)	110(3)
O(220)-S(20)-C(240)	101(2)
C(239)-S(20)-C(240)	96.7(19)
C(803)-O(803)-Cu(4)	120(4)

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C(802)-O(802)-Cu(4)	117(3)
C(804)-O(804)-Cu(4)	123(3)
O(215)-S(15)-C(230)	106(3)
O(215)-S(15)-C(229)	102(2)
C(230)-S(15)-C(229)	112(3)
O(214)-S(14)-C(228)	104(2)
O(214)-S(14)-C(227)	105(2)
C(228)-S(14)-C(227)	95.3(18)
O(211)-S(11)-C(221)	107.7(13)
O(211)-S(11)-C(222)	104.4(13)
C(221)-S(11)-C(222)	97.8(13)
O(205)-S(5)-C(210)	102.4(12)
O(205)-S(5)-C(209)	106.7(13)
C(210)-S(5)-C(209)	94.9(14)
S(5)-O(205)-Cu(11)	121.8(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z-1

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Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	40(1)	44(1)	49(1)	14(1)	11(1)	14(1)
Cu(2)	36(1)	41(1)	40(1)	7(1)	8(1)	11(1)
Cu(3)	48(1)	30(1)	31(1)	1(1)	0(1)	-3(1)
Cu(4)	44(1)	30(1)	32(1)	0(1)	-1(1)	-2(1)
Cu(5)	32(1)	39(1)	38(1)	-7(1)	2(1)	3(1)
Cu(6)	28(1)	34(1)	36(1)	-8(1)	0(1)	2(1)
Cu(7)	31(1)	43(1)	34(1)	-9(1)	5(1)	-4(1)
Cu(8)	27(1)	37(1)	35(1)	-7(1)	6(1)	-4(1)
Cu(9)	33(1)	40(1)	35(1)	8(1)	-1(1)	-1(1)
Cu(10)	31(1)	40(1)	35(1)	7(1)	-2(1)	-4(1)
Cu(11)	26(1)	39(1)	48(1)	-4(1)	4(1)	-2(1)
Cu(12)	24(1)	32(1)	45(1)	-4(1)	3(1)	-1(1)
C(1)	56(10)	35(9)	38(11)	1(8)	4(8)	6(8)
C(2)	44(9)	42(9)	38(10)	-7(8)	2(8)	4(7)
C(3)	26(8)	59(11)	56(13)	-1(10)	-1(8)	4(7)
C(4)	81(12)	52(11)	41(12)	-3(10)	-1(10)	30(9)
C(5)	95(14)	91(16)	46(14)	-7(12)	14(11)	42(12)
C(9)	49(9)	37(9)	41(11)	-9(9)	5(9)	-12(7)
C(10)	16(7)	49(11)	63(13)	-11(10)	4(8)	-2(7)
C(12)	46(9)	33(9)	52(12)	0(8)	9(8)	3(7)
C(13)	48(9)	42(10)	44(11)	8(9)	5(8)	-1(8)
C(19)	47(10)	38(10)	66(14)	5(10)	9(9)	9(8)
C(20)	43(10)	36(10)	77(16)	-7(11)	6(10)	-3(8)
C(21)	46(9)	55(11)	43(12)	-9(9)	2(8)	-11(8)
C(22)	39(8)	50(10)	31(10)	-3(8)	2(7)	8(7)
C(24)	170(20)	74(15)	42(14)	4(12)	-31(15)	-43(15)
C(25)	98(15)	91(16)	81(17)	27(14)	-33(14)	-52(13)
C(26)	99(15)	106(17)	28(11)	-7(11)	-16(11)	-21(13)
C(29)	53(10)	69(13)	22(10)	-3(9)	-8(8)	10(9)
C(31)	33(8)	66(12)	45(12)	-7(10)	-4(8)	6(8)

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C(32)	41(9)	69(12)	42(11)	4(10)	2(8)	-4(8)
C(33)	44(9)	48(10)	28(10)	2(8)	-8(7)	10(8)
C(35)	98(14)	58(13)	56(14)	-4(11)	11(12)	33(11)
C(39)	30(8)	66(12)	38(12)	17(10)	-7(8)	-13(8)
C(40)	39(9)	76(13)	16(9)	8(9)	-11(7)	-5(9)
C(41)	39(9)	31(9)	56(12)	-8(8)	5(8)	1(7)
C(42)	48(10)	39(10)	58(12)	-16(9)	2(9)	-1(8)
C(43)	31(8)	33(9)	44(10)	-8(8)	3(7)	-4(7)
C(44)	26(8)	39(9)	67(12)	5(9)	14(8)	0(7)
C(45)	54(11)	48(11)	78(14)	6(11)	5(10)	-1(9)
C(46)	52(10)	48(10)	47(11)	4(9)	11(8)	14(8)
C(49)	44(10)	54(11)	50(12)	-6(10)	-6(9)	13(9)
C(50)	39(9)	40(10)	44(11)	-23(8)	1(8)	-1(8)
C(51)	59(11)	69(13)	49(13)	13(10)	-4(10)	-6(9)
C(52)	61(10)	42(10)	40(11)	4(8)	-2(9)	-12(8)
C(53)	49(9)	48(10)	47(12)	7(9)	-2(8)	-11(8)
C(54)	76(12)	97(16)	36(12)	8(11)	13(10)	-56(11)
C(55)	101(15)	140(20)	27(12)	4(13)	4(11)	-68(15)
C(56)	95(14)	73(13)	36(12)	7(10)	-13(11)	-45(11)
C(59)	45(9)	43(10)	52(13)	19(10)	12(9)	9(8)
C(60)	30(8)	50(10)	45(12)	-8(9)	-16(8)	5(8)
C(61)	30(8)	55(11)	43(11)	3(9)	1(7)	-4(8)
C(62)	50(9)	34(9)	31(10)	3(7)	-4(7)	-2(7)
C(63)	43(9)	36(9)	58(12)	-7(9)	11(8)	7(7)
C(64)	23(8)	57(11)	68(13)	-11(10)	-4(8)	8(8)
C(65)	49(10)	30(9)	98(16)	-8(10)	9(10)	-12(8)
C(66)	23(8)	58(11)	82(14)	10(10)	-8(8)	-13(8)
C(69)	30(9)	69(13)	43(11)	-3(10)	-10(8)	-4(9)
C(70)	39(9)	40(10)	46(11)	-2(8)	14(8)	10(8)
C(71)	38(9)	41(10)	46(11)	-8(8)	-6(8)	11(7)
C(72)	36(8)	49(10)	31(9)	-2(8)	4(7)	-3(7)
C(73)	33(8)	50(10)	32(10)	10(8)	6(7)	11(7)
C(74)	24(8)	50(11)	71(13)	7(10)	7(8)	-3(7)
C(75)	42(9)	51(11)	53(12)	-16(9)	-10(8)	7(8)
C(76)	25(8)	60(12)	82(14)	1(11)	0(8)	15(8)
C(77)	29(8)	55(11)	85(14)	-27(10)	5(8)	-6(8)

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C(79)	27(8)	63(12)	39(11)	4(9)	0(8)	6(8)
C(80)	31(8)	52(10)	36(10)	19(8)	-15(7)	9(7)
C(81)	56(10)	44(10)	33(10)	1(8)	6(8)	6(8)
C(82)	40(9)	44(10)	47(11)	14(9)	-2(8)	-10(7)
C(83)	49(9)	45(10)	44(11)	5(9)	9(8)	-4(8)
C(84)	72(12)	77(13)	29(10)	16(9)	3(9)	-33(10)
C(85)	73(12)	79(15)	53(13)	-1(11)	-3(11)	-16(11)
C(86)	57(10)	48(10)	47(12)	9(9)	9(9)	-12(8)
C(89)	30(9)	40(10)	95(16)	-6(11)	12(9)	0(7)
C(90)	57(10)	35(9)	38(11)	5(9)	8(9)	-9(8)
C(91)	56(10)	43(10)	29(10)	0(8)	-2(8)	-12(8)
C(92)	37(8)	44(10)	47(11)	-3(8)	-5(8)	-12(7)
C(93)	35(8)	41(9)	49(11)	-6(8)	-11(8)	-11(7)
C(94)	58(11)	63(12)	38(11)	-26(9)	-2(9)	-19(9)
C(96)	42(9)	64(12)	65(13)	-19(10)	2(9)	-23(9)
C(99)	51(10)	51(11)	38(11)	2(9)	-17(9)	-12(9)
C(100)	43(9)	48(10)	25(9)	-3(8)	-8(8)	-4(8)
C(101)	43(9)	26(8)	44(10)	-10(7)	-3(8)	11(7)
C(102)	31(8)	40(9)	44(10)	8(8)	10(7)	-2(7)
C(103)	28(8)	32(8)	45(10)	3(8)	8(7)	3(6)
C(105)	40(9)	31(9)	47(11)	-1(8)	4(8)	-9(7)
C(106)	35(8)	35(9)	53(11)	-24(8)	6(8)	0(7)
C(107)	37(9)	45(10)	87(14)	-17(10)	23(9)	4(7)
C(108)	44(10)	38(11)	150(20)	-5(13)	18(11)	-3(8)
C(109)	48(10)	32(9)	37(10)	-4(8)	8(8)	4(7)
C(110)	46(9)	16(7)	41(10)	3(7)	14(8)	10(7)
C(111)	28(8)	42(10)	58(12)	-9(9)	-2(8)	2(7)
C(112)	25(8)	32(9)	62(12)	-7(8)	-3(7)	-6(6)
C(113)	48(10)	48(10)	38(10)	-1(8)	8(8)	-2(8)
C(114)	41(9)	51(11)	86(15)	25(11)	13(9)	20(8)
C(115)	36(10)	97(17)	120(20)	35(15)	13(11)	10(11)
C(116)	44(10)	60(12)	71(14)	12(10)	-14(10)	1(9)
C(119)	53(10)	35(9)	33(10)	-4(8)	-14(8)	-7(8)
C(120)	40(10)	41(10)	50(12)	-6(9)	-7(9)	0(8)
C(201)	68(12)	104(17)	68(14)	-10(13)	12(11)	3(12)
C(202)	34(9)	62(12)	132(19)	15(13)	-10(11)	-2(8)

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C(203)	160(20)	91(17)	67(16)	38(13)	-26(15)	-63(16)
C(204)	127(18)	130(20)	46(14)	-8(14)	14(13)	-29(16)
C(205)	107(15)	53(12)	95(17)	4(12)	-27(14)	-11(11)
C(206)	86(14)	78(15)	99(18)	12(13)	40(12)	28(11)
C(36)	54(10)	61(12)	29(10)	3(9)	7(8)	-6(9)
C(104)	24(8)	46(10)	65(12)	-17(9)	2(7)	17(7)
O(1)	61(7)	43(7)	49(8)	1(6)	-13(6)	20(5)
O(2)	64(7)	43(6)	21(6)	-2(5)	-8(5)	11(5)
O(3)	64(7)	41(7)	37(7)	4(6)	-10(6)	25(5)
O(4)	68(7)	52(7)	33(7)	-9(6)	-3(6)	17(6)
O(5)	195(16)	106(12)	46(9)	15(9)	31(10)	81(11)
O(7)	78(7)	31(6)	51(8)	1(6)	16(6)	17(6)
O(8)	64(7)	46(7)	64(8)	-14(6)	4(6)	13(6)
O(9)	61(7)	36(6)	44(8)	-4(6)	10(6)	16(5)
O(10)	62(7)	44(7)	52(8)	-6(6)	6(6)	20(6)
O(13)	62(7)	59(7)	34(7)	-1(6)	-8(6)	-11(6)
O(14)	46(6)	66(8)	38(7)	7(6)	-7(5)	-8(6)
O(15)	63(7)	54(7)	38(7)	-3(6)	-4(6)	-11(6)
O(16)	51(6)	63(8)	29(6)	-6(6)	-12(5)	-19(6)
O(17)	181(15)	157(16)	65(10)	24(11)	-31(11)	-127(14)
O(19)	54(6)	60(8)	35(7)	3(6)	-5(5)	9(6)
O(20)	52(6)	64(8)	27(7)	14(6)	-4(5)	9(5)
O(21)	66(7)	71(9)	32(7)	8(6)	-1(6)	31(7)
O(22)	70(7)	64(8)	23(6)	0(6)	4(5)	20(6)
O(23)	147(13)	94(11)	55(9)	-13(9)	-8(9)	55(10)
O(25)	41(6)	49(7)	75(9)	23(6)	20(6)	15(5)
O(26)	42(6)	51(7)	73(9)	16(7)	13(6)	9(5)
O(27)	41(6)	39(6)	50(7)	17(5)	12(5)	-2(5)
O(28)	40(6)	38(6)	62(8)	9(6)	16(5)	-4(5)
O(29)	48(7)	84(10)	113(12)	55(9)	44(7)	26(6)
O(31)	64(7)	56(7)	25(6)	-8(5)	-8(5)	-25(6)
O(32)	48(6)	47(7)	47(8)	-7(6)	-3(6)	-20(5)
O(33)	62(7)	44(7)	33(7)	4(6)	-13(6)	-16(5)
O(34)	56(6)	52(7)	33(7)	1(5)	-8(5)	-18(6)
O(35)	160(14)	114(13)	57(10)	-30(9)	17(10)	-59(11)
O(37)	39(6)	43(7)	60(8)	25(6)	20(5)	9(5)

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O(38)	28(5)	38(6)	71(8)	17(6)	7(5)	3(5)
O(39)	24(5)	54(7)	84(9)	16(7)	3(5)	4(5)
O(40)	34(5)	45(6)	55(7)	13(6)	19(5)	7(5)
O(41)	60(7)	47(8)	165(15)	30(9)	9(8)	8(6)
O(43)	21(5)	49(7)	61(8)	-15(6)	3(5)	-3(5)
O(44)	23(5)	51(7)	63(8)	-19(6)	11(5)	1(5)
O(45)	30(5)	48(7)	66(8)	-16(6)	-1(5)	-12(5)
O(46)	19(5)	47(6)	58(7)	-15(6)	3(5)	3(4)
O(47)	34(6)	41(7)	107(11)	-23(7)	13(6)	-2(5)
O(49)	51(6)	45(6)	29(6)	6(5)	3(5)	-15(5)
O(50)	49(6)	44(6)	37(7)	-3(5)	-1(5)	-18(5)
O(51)	51(6)	53(7)	39(7)	1(6)	0(5)	-17(5)
O(52)	74(7)	45(7)	43(7)	10(6)	-3(6)	-29(6)
O(53)	85(9)	129(13)	73(10)	11(9)	-16(8)	-61(9)
O(55)	31(5)	55(7)	55(8)	-14(6)	-1(5)	-12(5)
O(56)	35(6)	60(8)	65(9)	-29(7)	7(6)	-17(5)
O(57)	33(6)	62(8)	56(8)	-24(6)	-2(5)	-12(5)
O(58)	28(5)	51(7)	52(7)	-16(6)	6(5)	-13(5)
O(59)	54(8)	149(15)	114(13)	-74(11)	42(8)	-39(8)
O(61)	28(5)	45(6)	56(7)	-15(6)	12(5)	2(5)
O(62)	22(5)	57(7)	60(8)	-20(6)	12(5)	0(5)
O(63)	28(5)	44(6)	58(8)	-24(6)	12(5)	-3(5)
O(64)	35(5)	40(6)	51(7)	-24(5)	5(5)	0(5)
O(65)	48(6)	43(7)	91(10)	-24(7)	15(6)	2(5)
O(66)	89(10)	72(10)	144(15)	0(10)	26(9)	-16(8)
O(67)	29(5)	58(7)	61(8)	18(6)	2(5)	11(5)
O(68)	27(5)	44(6)	63(8)	17(6)	9(5)	8(5)
O(69)	20(5)	54(7)	63(8)	16(6)	6(5)	10(5)
O(70)	27(5)	40(6)	68(8)	7(6)	-1(5)	0(5)
O(71)	40(7)	134(14)	240(20)	127(14)	50(9)	45(8)
O(806)	87(9)	88(10)	105(11)	46(9)	37(8)	46(8)
O(805)	107(10)	84(10)	43(7)	7(7)	-1(7)	-14(8)
O(100)	82(8)	91(10)	97(11)	43(9)	6(8)	-37(8)
O(201)	22(5)	44(6)	58(7)	-2(6)	3(5)	0(4)
O(202)	54(6)	36(6)	53(7)	-2(5)	-7(5)	-22(5)
O(203)	45(6)	42(6)	47(7)	3(5)	-2(5)	23(5)

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O(204)	41(6)	79(9)	96(10)	-25(8)	-10(6)	-38(6)
S(1)	31(2)	60(3)	78(3)	13(3)	15(2)	-1(2)
S(2)	77(3)	61(3)	78(4)	-8(3)	1(3)	-23(3)
S(3)	73(3)	44(3)	50(3)	5(2)	-2(2)	21(2)
S(16)	111(5)	138(6)	102(6)	-19(5)	-1(4)	-30(5)
O(216)	163(17)	280(30)	210(20)	-90(20)	59(16)	-130(20)
C(231)	150(30)	270(40)	290(50)	190(40)	-120(30)	-80(30)
C(232)	310(40)	90(20)	100(20)	-4(18)	-30(30)	0(20)
S(17)	97(4)	123(6)	98(5)	20(4)	18(4)	41(4)
C(233)	140(20)	150(30)	84(19)	10(18)	11(17)	-26(19)
O(217)	113(12)	153(17)	142(17)	42(13)	44(12)	45(12)
C(234)	200(30)	130(30)	140(30)	-40(20)	80(20)	-20(20)
S(18)	202(10)	160(9)	170(10)	17(8)	22(8)	-10(8)
C(236)	170(20)	91(19)	130(20)	1(18)	-30(20)	4(18)
O(218)	152(19)	280(30)	360(40)	-120(30)	-30(20)	100(20)
O(106)	69(7)	71(8)	43(8)	-35(6)	-11(6)	13(6)
O(48)	99(10)	80(11)	129(14)	18(10)	25(10)	11(9)
C(78)	51(11)	57(13)	140(20)	1(14)	7(12)	2(10)
S(4)	121(6)	194(10)	173(9)	2(7)	8(6)	-67(6)
O(11)	127(12)	134(14)	73(11)	5(10)	13(9)	70(11)
C(14)	69(11)	67(13)	49(12)	-12(10)	3(10)	2(10)
C(15)	67(12)	63(13)	69(15)	0(12)	-20(11)	21(10)
C(16)	55(10)	39(10)	67(14)	10(10)	-1(10)	18(8)
C(30)	37(9)	56(11)	50(12)	-15(10)	8(8)	1(8)
C(23)	48(9)	62(11)	33(10)	10(9)	-12(8)	5(9)
C(11)	44(9)	53(11)	68(14)	-6(10)	16(9)	3(8)
C(38)	230(30)	250(40)	160(30)	120(30)	30(30)	90(30)
C(37)	310(40)	70(18)	100(20)	0(17)	-10(30)	70(20)
C(95)	46(10)	88(15)	58(13)	-26(11)	8(9)	-11(10)
S(12)	271(15)	276(18)	330(20)	-127(16)	-140(15)	37(13)
O(212)	152(16)	200(20)	116(16)	45(15)	-13(13)	-42(15)
C(223)	230(40)	190(40)	200(40)	-110(30)	20(30)	-50(30)
C(224)	260(40)	150(30)	90(20)	10(20)	-50(20)	40(30)
C(6)	85(13)	67(13)	49(13)	16(11)	-6(11)	38(11)
O(801)	146(13)	98(12)	134(15)	-63(11)	69(11)	7(10)
C(34)	49(10)	91(15)	50(13)	12(11)	-15(9)	13(10)

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S(5)	129(6)	160(9)	275(13)	26(9)	112(7)	-5(6)
C(209)	500(60)	100(30)	170(30)	-80(30)	110(40)	-70(30)
C(210)	90(20)	360(60)	440(60)	220(50)	70(30)	60(30)
O(205)	46(7)	108(11)	105(11)	28(9)	16(7)	-16(7)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Tetracosakis(μ_4-5-(2-hydroxyethoxy)benzene-1,3-dicarboxylato)-diaqua-tetradecakis(dimethylsulfoxid)-octamethanol-tetracosa-copper(II) dimethylsulfoxide methanol solvate (**2**).

	x	y	z	U(eq)
H(2)	-218	823	7903	50
H(4)	-969	1466	8749	70
H(12)	1671	-875	7650	52
H(22)	1766	1675	4835	48
H(24)	2789	2353	5481	118
H(26)	2346	2422	3988	95
H(32)	-1545	1790	5237	61
H(42)	2969	-970	5646	58
H(44)	4465	-1038	5455	52
H(46)	3815	-1711	6354	58
H(52)	332	851	2121	58
H(54)	1271	1370	1299	83
H(56)	280	688	627	83
H(62)	319	-1790	6775	47
H(64)	1100	-2665	7096	60
H(66)	-383	-2606	7259	66
H(72)	580	1736	6785	46
H(74)	1532	2538	7155	58
H(76)	25	2612	7302	67
H(77A)	1394	3105	6990	68
H(77B)	1573	3057	7572	68
H(82)	1784	741	7703	53
H(84)	2314	628	9144	72
H(86)	2977	1313	8274	61
H(92)	-2383	900	6370	52
H(94)	-2824	1543	7428	64
H(96)	-3821	862	6766	69
H(102)	3073	658	5756	46
H(106)	4049	1383	6329	49

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H(10A)	5148	1018	5363	66
H(10B)	5353	824	5869	66
H(10C)	5755	1356	6159	91
H(10D)	6003	1190	5695	91
H(112)	2466	716	3667	48
H(114)	3956	641	3409	71
H(116)	3060	1365	2745	71
H(20A)	4729	-242	3266	120
H(20B)	4864	149	3193	120
H(20C)	4356	47	3433	120
H(20D)	5115	473	4507	116
H(20E)	4585	468	4167	116
H(20F)	5093	571	3929	116
H(20G)	2500	2762	6925	162
H(20H)	2542	2540	6432	162
H(20I)	2812	2903	6489	162
H(20J)	3893	2324	6487	152
H(20K)	3616	2651	6237	152
H(20L)	3348	2288	6179	152
H(20M)	2212	-3011	6895	131
H(20N)	2501	-3136	6433	131
H(20O)	2200	-2784	6401	131
H(20P)	3546	-2499	6392	129
H(20Q)	2988	-2475	6107	129
H(20R)	3287	-2828	6129	129
H(36)	-1856	2596	6073	57
H(104)	4537	628	5463	54
H(66A)	5822	1728	5555	151
H(101)	1525	-884	5857	137
H(80A)	637	-836	5825	434
H(80B)	785	-804	6414	434
H(80C)	608	-1161	6176	434
H(103)	731	159	7058	118
H(109)	882	957	4061	135
H(999)	471	888	3580	135
H(20S)	2883	-4060	9782	365

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H(20T)	2885	-4028	10375	365
H(20U)	2648	-4357	10092	365
H(20V)	3779	-4713	10844	256
H(20W)	3173	-4725	10750	256
H(20$)	3449	-4404	11019	256
H(201)	-1469	-2709	10187	188
H(202)	-1341	-3106	10196	188
H(203)	-1883	-2977	10333	188
H(21A)	-2206	-3450	9139	230
H(21B)	-2322	-3422	9709	230
H(21C)	-1776	-3546	9576	230
H(21D)	1206	-5213	8882	199
H(21E)	1431	-5067	8394	199
H(21F)	1735	-5352	8724	199
H(21G)	1396	-5802	7534	293
H(21H)	1841	-5710	7959	293
H(21I)	1561	-5415	7629	293
H(21J)	622	-4296	7846	255
H(21K)	899	-4567	8222	255
H(21L)	651	-4685	7683	255
H(21M)	2062	-4795	7543	424
H(21N)	1519	-4976	7480	424
H(21O)	1769	-4871	8024	424
H(48)	613	3570	7058	153
H(78A)	1116	3550	7749	99
H(78B)	1566	3627	7410	99
H(14)	2080	-892	9136	74
H(16)	2654	-1599	8235	65
H(99A)	363	-240	6558	132
H(99B)	42	-350	7006	132
H(99C)	585	-517	6955	132
H(21P)	1030	675	6945	242
H(21Q)	456	770	6753	242
H(21R)	866	1064	6874	242
H(21S)	646	1183	5489	354
H(215)	705	1377	6014	354

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H(21U)	237	1126	5882	354
H(21V)	3199	-4863	7747	201
H(21W)	3373	-4714	8290	201
H(211)	2806	-4653	8041	201
H(22A)	2722	-5091	9197	671
H(22B)	2376	-4854	8819	671
H(22C)	2963	-4765	8956	671
H(22D)	919	-1393	7600	429
H(22E)	652	-1208	8034	429
H(22F)	317	-1418	7612	429
H(22G)	95	-1955	8700	509
H(22H)	-158	-1745	8231	509
H(22I)	132	-1550	8695	509
H(27A)	3637	2586	5088	188
H(27B)	3201	2757	5383	188
H(48A)	5205	-2294	6320	328
H(48B)	5262	-2054	5840	328
H(471)	4389	-2003	6209	172
H(473)	4699	-1797	6657	172
H(472)	4391	-2039	6207	178
H(474)	4556	-2055	5646	178
H(30)	5521	-1856	6819	322
H(430)	5728	-1998	5947	103
H(18A)	2771	-1671	10316	259
H(18B)	2786	-1891	9812	259
H(17A)	2184	-1394	9651	244
H(17B)	2657	-1142	9783	244
H(12A)	3583	-1702	10102	455
H(7A)	-321	1145	10244	111
H(7B)	-489	786	9983	111
H(8A)	-1073	953	10626	142
H(8B)	-1234	1278	10289	142
H(6)	-1394	633	9977	286
H(40A)	-445	822	10008	90
H(40B)	-1053	812	9946	90
H(40C)	-985	1030	10704	145

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H(40D)	-417	1154	10667	145
H(406)	-1030	1556	10725	161
H(38A)	2540	-3729	5078	257
H(38B)	2213	-3614	4568	257
H(37A)	2213	-3174	5294	195
H(37B)	2785	-3089	5176	195
H(67A)	670	-3388	7753	70
H(67B)	1024	-3068	7675	70
H(68A)	1057	-3226	6824	136
H(68B)	1291	-3515	7196	136
H(42A)	348	-3537	6738	260
H(36A)	1100	-3114	7504	65
H(36B)	892	-3219	6943	65
H(36C)	1033	-3678	7618	127
H(36D)	476	-3567	7736	127
H(442)	208	-3711	6974	259
H(45A)	567	963	-99	91
H(45B)	932	653	77	91
H(45C)	1604	879	-310	125
H(45D)	1121	906	-716	125
H(436)	1530	1415	-168	265
H(57A)	736	751	-49	99
H(57B)	1176	572	316	99
H(58A)	1410	722	-539	104
H(58B)	1423	1107	-349	104
H(36E)	2024	943	237	273
H(18)	4167	2923	4730	604
H(28A)	3265	3249	4764	482
H(28B)	3705	3230	5223	482
H(23A)	-2187	2882	8116	114
H(23B)	-1617	2995	8052	114
H(23C)	-1781	2911	8595	114
H(23D)	-918	2189	8461	348
H(23E)	-1119	2445	8858	348
H(23F)	-864	2589	8387	348
H(23G)	-1377	2952	7316	447

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H(23H)	-1257	3157	7828	447
H(23I)	-1825	3037	7654	447
H(23J)	-1667	2495	8741	777
H(23K)	-2094	2653	8347	777
H(23L)	-1660	2891	8616	777
H(11A)	4562	853	2998	93
H(11B)	4492	1154	3386	93
H(11C)	4810	1558	2815	128
H(11D)	5226	1267	2946	128
H(72A)	4572	1263	2115	165
H(41A)	4245	691	2641	66
H(41B)	4612	909	3026	66
H(41C)	4976	878	2267	91
H(41D)	4467	1023	1969	91
H(475)	5034	1446	2158	94
H(22J)	1016	1080	-2003	316
H(22K)	1021	1423	-2320	316
H(22L)	493	1257	-2206	316
H(22M)	520	2032	-1404	258
H(22N)	191	1835	-1844	258
H(22O)	712	2015	-1949	258
H(24B)	1080	2200	1784	346
H(24C)	1363	2342	1328	346
H(24D)	1065	2596	1659	346
H(23M)	1877	2917	2498	567
H(23N)	1641	2994	1939	567
H(23O)	2236	2925	2054	567
H(24E)	1899	1836	1537	195
H(24F)	2161	2104	1198	195
H(24G)	1627	2190	1399	195
H(24H)	2456	2818	2083	43
H(24I)	1934	2768	1739	43
H(24J)	2462	2701	1514	43
H(6A)	-114	697	9396	81
H(99D)	-746	559	5994	450
H(99E)	-1263	712	6161	450

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H(99F)	-841	566	6572	450
H(105)	-350	1082	6152	183
H(34)	2255	-2614	5414	77
H(87A)	3443	1475	9026	339
H(87B)	3599	1153	8697	339
H(88A)	3888	850	9495	755
H(88B)	4228	1184	9447	755
H(54A)	3453	1118	10014	525
H(49A)	-4023	911	7641	141
H(49B)	-4373	1137	7265	141
H(49C)	-4853	1270	7825	639
H(49D)	-4563	984	8163	639
H(460)	-4392	1646	8220	1034
H(97A)	-4332	1213	7007	76
H(97B)	-4463	1473	7434	76
H(98A)	-4192	976	8011	265
H(98B)	-4764	997	7760	265
H(60)	-4115	670	7250	347
H(24K)	-578	-2352	10782	243
H(24L)	-988	-2451	10329	243
H(24M)	-1013	-2088	10590	243
H(24N)	-755	-1893	9312	437
H(24O)	-1112	-1803	9740	437
H(24P)	-1117	-2177	9510	437
H(10E)	1347	156	9959	58
H(80D)	964	-205	10500	58
H(80E)	862	-472	10054	58
H(80F)	464	-174	10117	58
H(11E)	1448	-260	9942	66
H(80G)	1015	69	10518	131
H(80H)	532	71	10112	131
H(80I)	956	359	10102	131
H(124)	687	-67	9994	78
H(80J)	1406	-82	10535	49
H(80K)	1723	60	10102	49
H(80L)	1623	-339	10148	49

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H(503)	-288	160	5607	357
H(81G)	160	313	4773	91
H(81H)	-59	-54	4889	91
H(81I)	436	87	5213	91
H(504)	461	2363	5284	830
H(81J)	725	2837	5840	495
H(81K)	873	2823	5278	495
H(81L)	1260	2684	5725	495
H(534)	-687	1412	5344	1095
H(83A)	-103	1872	5531	1006
H(83B)	269	1654	5223	1006
H(83C)	98	1511	5737	1006
H(507)	-46	-1258	5147	281
H(81P)	515	-1690	5579	222
H(81Q)	-81	-1676	5631	222
H(81R)	307	-1487	6032	222
H(508)	2232	-5063	6412	705
H(81M)	1470	-5544	6266	392
H(81N)	1752	-5388	5819	392
H(81O)	1377	-5157	6105	392
H(506)	3970	1915	1180	178
H(81S)	4867	2018	1357	150
H(811)	4647	1662	1151	150
H(81U)	4772	1718	1738	150
H(536)	3933	1517	1272	291
H(83D)	4116	1723	2050	309
H(83E)	3547	1825	1853	309
H(83F)	3997	2093	1825	309
H(516)	1027	2828	3890	526
H(82A)	1446	2983	3162	524
H(82B)	1728	2733	3568	524
H(82C)	1850	3130	3589	524
H(511)	1386	-420	2871	1700
H(814)	568	-131	3214	1143
H(813)	642	-209	2642	1143
H(812)	904	117	2911	1143

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H(22V)	167	-2460	9733	229
H(22W)	284	-2854	9825	229
H(223)	-268	-2735	9596	229
H(23P)	-343	-2483	8514	497
H(23Q)	-477	-2867	8643	497
H(23R)	-99	-2789	8229	497
H(222)	-1939	1744	8664	549
H(225)	-2512	1701	8795	549
H(226)	-2375	1643	8235	549
H(221)	-2800	789	8605	910
H(224)	-2860	1084	8194	910
H(227)	-3002	1155	8749	910
H(515)	4188	2401	9288	386
H(82D)	4743	1919	9659	618
H(82E)	4869	2170	9221	618
H(82F)	4540	1836	9092	618
H(82G)	2607	704	1471	560
H(82H)	2235	971	1174	560
H(82I)	2234	931	1766	560
H(517)	2819	1321	1317	674
H(82J)	2577	-55	2292	827
H(82K)	2810	-301	2730	827
H(82L)	2890	-385	2162	827
H(518)	3427	40	2753	648
H(519)	4618	385	2202	795
H(82M)	4592	-185	1644	579
H(82N)	4358	-147	2168	579
H(82O)	4960	-158	2151	579
H(22P)	2076	-3514	10297	283
H(22Q)	1769	-3864	10258	283
H(22R)	1879	-3678	10786	283
H(22S)	471	-3642	10532	248
H(228)	932	-3762	10922	248
H(22U)	838	-3941	10387	248
H(204)	2210	-936	4697	379
H(205)	1683	-772	4475	379

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H(206)	1708	-999	4969	379
H(212)	1375	-108	5251	436
H(213)	1270	-476	5469	436
H(214)	1204	-413	4879	436
H(241)	3034	-3708	4435	557

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Table 7. Values for the restrained bond lengths to fix the geometries by DFIX instructions

Restrained group	**X-X bond length set to… [pm]**
dimethylsulfoxide	*S-O*: 149, *S-C*: 174, *C-C*: 266, *C-O*: 258.
C^{Ar}-O^{a}-$C^{a}H_2$-$C^{b}H_2$-$O^{b}H$	O^{a}-C^{a}: 145, C^{a}-C^{b}: 153, C^{b}-O^{b}: 143, C^{a}-O^{b}: 243, C^{Ar}-O^{a}: 139, C^{Ar}-C^{a}: 244.
(2-hydroxyethoxy-sidechain of linker)	
methanol	*C-O*: 149, *Cu-O*: 224.
water	*Cu-O*: 216.

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