Title: Experimental Crystal Structure Determination: Copper(II)-Monensin Complex

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Computing details

Data collection: Collect (Nonius BV, 1997-2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor 1997); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1986); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

Crystal data

$C_{72}H_{122}Cl_2CuNa_2O_{22}\cdot C_2H_6O$	$F(000)$ = 1682
M_r = 1566.18	D_x = 1.308 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 15717 reflections
a = 19.0390 (3) Å	θ = 3.4–26.0°
b = 15.7362 (3) Å	μ = 0.43 mm^{-1}
c = 13.2719 (2) Å	*T* = 173 K
β = 90.704 (1)°	Prism, blue
V = 3975.98 (12) Å^3	0.2 × 0.2 × 0.2 mm
Z = 2	

Data collection

KappaCCD diffractometer	7815 independent reflections
Radiation source: Enraf Nonius FR590	7314 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.037$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 26.1°$, $\theta_{min} = 3.5°$
CCD rotation images, thick slices scans	$h = -23 \rightarrow 23$
Absorption correction: multi-scan [c.f. r.h. blessing, acta cryst. (1995), a51, 33-38]	$k = -19 \rightarrow 19$
$T_{min} = 0.889$, $T_{max} = 0.928$	$l = -16 \rightarrow 15$
29805 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 2.7057P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.002$
7815 reflections	$\Delta\rangle_{max} = 0.41$ e $Å^{-3}$
477 parameters	$\Delta\rangle_{min} = -0.45$ e $Å^{-3}$
1 restraint	Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: -0.004 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for (mar1905)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu	0	0.35612 (2)	0	0.02368 (9)	

Cl	-0.10778 (4)	0.32110 (8)	-0.04517 (5)	0.0895 (4)	
Na	-0.08676 (4)	0.64565 (5)	0.23976 (6)	0.02511 (18)	
O1	0.01249 (8)	0.41340 (9)	0.29115 (11)	0.0267 (3)	
O2	-0.02360 (8)	0.40019 (9)	0.13293 (10)	0.0250 (3)	
O3	-0.10595 (8)	0.18473 (9)	0.33382 (12)	0.0299 (3)	
O4	-0.22369 (7)	0.44964 (9)	0.33157 (11)	0.0220 (3)	
O5	-0.07813 (8)	0.58149 (10)	0.39681 (12)	0.0287 (3)	
H5X	-0.0402 (17)	0.560 (2)	0.398 (2)	0.049 (9)*	
O6	-0.19647 (7)	0.58177 (9)	0.26114 (10)	0.0217 (3)	
O7	-0.17481 (7)	0.72522 (9)	0.14358 (12)	0.0260 (3)	
O8	-0.07756 (7)	0.79279 (9)	0.28599 (11)	0.0258 (3)	
O9	0.03370 (7)	0.70303 (9)	0.23317 (10)	0.0209 (3)	
O10	-0.02053 (7)	0.57112 (10)	0.12244 (11)	0.0245 (3)	
H10X	-0.0265 (14)	0.5215 (19)	0.125 (2)	0.038 (8)*	
O11	0.05778 (8)	0.57234 (10)	0.30500 (11)	0.0244 (3)	
H11X	0.0467 (13)	0.5284 (17)	0.2882 (19)	0.025 (7)*	
C1	-0.01269 (10)	0.37049 (13)	0.22183 (14)	0.0205 (4)	
C2	-0.03345 (10)	0.27862 (13)	0.24316 (15)	0.0223 (4)	
H2	-0.0537	0.253	0.1802	0.027*	
C3	-0.08862 (10)	0.27355 (13)	0.32715 (15)	0.0221 (4)	
H3	-0.0661	0.2916	0.3921	0.027*	
C4	-0.15723 (10)	0.32444 (13)	0.31194 (15)	0.0206 (4)	
H4	-0.1917	0.2997	0.36	0.025*	
C5	-0.15172 (10)	0.41888 (13)	0.33823 (15)	0.0210 (4)	
H5	-0.123	0.4482	0.2861	0.025*	
C6	-0.12109 (11)	0.43876 (13)	0.44296 (15)	0.0225 (4)	
H6	-0.0705	0.4218	0.4432	0.027*	
C7	-0.12448 (11)	0.53496 (14)	0.46156 (16)	0.0246 (5)	
H7	-0.1111	0.5467	0.5333	0.03*	
C8	-0.19825 (11)	0.56888 (14)	0.44165 (15)	0.0247 (4)	
H8B	-0.1967	0.6318	0.4418	0.03*	
H8A	-0.229	0.5508	0.4973	0.03*	
C9	-0.23033 (10)	0.53885 (13)	0.34207 (15)	0.0225 (4)	
C10	-0.30834 (10)	0.55908 (15)	0.32832 (17)	0.0275 (5)	
H10B	-0.3379	0.5121	0.3537	0.033*	
H10A	-0.3209	0.6121	0.3639	0.033*	
C11	-0.31722 (11)	0.56922 (15)	0.21486 (17)	0.0281 (5)	

H11B	-0.3551	0.6103	0.1986	0.034*	
H11A	-0.3286	0.5141	0.1827	0.034*	
C12	-0.24566 (10)	0.60257 (14)	0.17926 (15)	0.0231 (4)	
C13	-0.24544 (11)	0.69935 (14)	0.16816 (17)	0.0262 (5)	
H13	-0.278	0.7158	0.1117	0.031*	
C14	-0.26171 (12)	0.75284 (15)	0.25987 (19)	0.0331 (5)	
H14B	-0.2445	0.7247	0.3222	0.04*	
H14A	-0.3129	0.7625	0.2653	0.04*	
C15	-0.22300 (11)	0.83683 (14)	0.2428 (2)	0.0355 (6)	
H15B	-0.1989	0.8558	0.3054	0.043*	
H15A	-0.2561	0.8817	0.2203	0.043*	
C16	-0.16914 (11)	0.81679 (14)	0.15973 (18)	0.0279 (5)	
C17	-0.09224 (11)	0.82903 (13)	0.18831 (17)	0.0265 (5)	
H17	-0.0641	0.7963	0.1384	0.032*	
C18	-0.05998 (12)	0.91824 (14)	0.19497 (19)	0.0324 (5)	
H18	-0.0524	0.9417	0.1259	0.039*	
C19	0.01038 (12)	0.89428 (14)	0.24429 (19)	0.0320 (5)	
H19B	0.0315	0.9435	0.2798	0.038*	
H19A	0.0438	0.8732	0.1935	0.038*	
C20	-0.00902 (11)	0.82375 (14)	0.31880 (17)	0.0260 (4)	
H20	-0.0137	0.8494	0.3873	0.031*	
C21	0.04230 (11)	0.74910 (13)	0.32587 (15)	0.0224 (4)	
H21	0.0283	0.7116	0.383	0.027*	
C22	0.11885 (11)	0.77639 (14)	0.34186 (16)	0.0258 (4)	
H22	0.1311	0.8185	0.2884	0.031*	
C23	0.16596 (11)	0.69851 (14)	0.33010 (17)	0.0274 (5)	
H23B	0.2157	0.7169	0.3331	0.033*	
H23A	0.158	0.6595	0.3874	0.033*	
C24	0.15312 (10)	0.65029 (14)	0.23198 (16)	0.0251 (4)	
H24	0.164	0.6893	0.1748	0.03*	
C25	0.07521 (10)	0.62665 (13)	0.22453 (15)	0.0204 (4)	
C26	0.05255 (10)	0.58955 (13)	0.12324 (15)	0.0228 (4)	
H26B	0.0631	0.6306	0.069	0.027*	
H26A	0.0793	0.5369	0.1102	0.027*	
C27	0.20191 (12)	0.57304 (16)	0.2251 (2)	0.0360 (5)	
H27C	0.1918	0.5335	0.2801	0.054*	
H27B	0.2509	0.5918	0.2304	0.054*	

H27A	0.1943	0.5444	0.1603	0.054*	
C28	0.13042 (13)	0.81816 (18)	0.44464 (19)	0.0402 (6)	
H28C	0.1193	0.7774	0.498	0.06*	
H28B	0.0998	0.8679	0.4503	0.06*	
H28A	0.1796	0.8359	0.4516	0.06*	
C29	-0.10080 (14)	0.98181 (16)	0.2590 (2)	0.0475 (7)	
H29C	-0.1102	0.9567	0.325	0.071*	
H29B	-0.1453	0.9957	0.2251	0.071*	
H29A	-0.0729	1.0337	0.2679	0.071*	
C30	-0.18755 (12)	0.86293 (17)	0.06182 (18)	0.0390 (5)	
H30B	-0.2368	0.8494	0.0432	0.047*	
H30A	-0.1848	0.9249	0.0741	0.047*	
C31	-0.14156 (15)	0.8416 (2)	-0.02608 (19)	0.0501 (7)	
H31C	-0.0927	0.8564	-0.0096	0.075*	
H31B	-0.1571	0.8739	-0.0854	0.075*	
H31A	-0.1448	0.7807	-0.0405	0.075*	
C32	-0.22096 (12)	0.55937 (15)	0.08358 (17)	0.0320 (5)	
H32C	-0.2524	0.5745	0.0275	0.048*	
H32B	-0.2214	0.4976	0.093	0.048*	
H32A	-0.1731	0.5781	0.0686	0.048*	
C33	-0.15693 (12)	0.39130 (15)	0.52949 (16)	0.0309 (5)	
H33C	-0.2068	0.4068	0.531	0.046*	
H33B	-0.1344	0.407	0.5936	0.046*	
H33A	-0.1525	0.3299	0.519	0.046*	
C34	-0.18881 (11)	0.31078 (15)	0.20594 (16)	0.0272 (5)	
H34C	-0.1551	0.3295	0.1553	0.041*	
H34B	-0.2322	0.3438	0.1989	0.041*	
H34A	-0.1992	0.2503	0.1961	0.041*	
C35	-0.12406 (16)	0.15751 (17)	0.43175 (19)	0.0424 (6)	
H35C	-0.0846	0.1679	0.4782	0.064*	
H35B	-0.1349	0.0966	0.4305	0.064*	
H35A	-0.1653	0.1892	0.4544	0.064*	
C36	0.03223 (12)	0.22824 (14)	0.27476 (19)	0.0314 (5)	
H36C	0.0666	0.23	0.2204	0.047*	
H36B	0.0192	0.1691	0.2882	0.047*	
H36A	0.0528	0.2534	0.3359	0.047*	
C1S	-0.4664 (2)	0.5857 (3)	0.0300 (3)	0.0752 (10)	

O1S	-0.4059 (3)	0.6051 (4)	-0.0210 (4)	0.0832 (15)	0.5

Atomic displacement parameters (Å^2) for (mar1905)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.02401 (18)	0.02643 (19)	0.02065 (17)	0	0.00175 (13)	0
Cl	0.0392 (4)	0.1918 (12)	0.0377 (4)	-0.0536 (5)	0.0103 (3)	-0.0404 (5)
Na	0.0192 (4)	0.0221 (4)	0.0340 (4)	-0.0003 (3)	-0.0002 (3)	-0.0007 (4)
O1	0.0302 (8)	0.0248 (7)	0.0249 (7)	-0.0073 (6)	-0.0031 (6)	-0.0006 (6)
O2	0.0311 (8)	0.0213 (8)	0.0226 (7)	0.0005 (6)	0.0007 (6)	-0.0004 (6)
O3	0.0401 (9)	0.0179 (7)	0.0318 (8)	-0.0045 (7)	0.0102 (7)	0.0012 (6)
O4	0.0157 (7)	0.0234 (7)	0.0269 (7)	-0.0001 (6)	-0.0010 (6)	-0.0034 (6)
O5	0.0208 (8)	0.0312 (9)	0.0341 (8)	-0.0016 (7)	-0.0018 (6)	-0.0019 (7)
O6	0.0147 (6)	0.0259 (8)	0.0245 (7)	0.0013 (6)	-0.0030 (5)	0.0013 (6)
O7	0.0218 (7)	0.0213 (7)	0.0349 (8)	0.0014 (6)	0.0008 (6)	0.0005 (6)
O8	0.0211 (7)	0.0254 (8)	0.0310 (8)	-0.0011 (6)	0.0001 (6)	-0.0005 (6)
O9	0.0211 (7)	0.0201 (7)	0.0215 (7)	0.0012 (6)	-0.0027 (6)	-0.0011 (6)
O10	0.0262 (8)	0.0222 (8)	0.0250 (8)	-0.0009 (6)	-0.0035 (6)	-0.0020 (6)
O11	0.0293 (8)	0.0200 (8)	0.0237 (8)	-0.0073 (7)	-0.0011 (6)	0.0027 (6)
C1	0.0171 (9)	0.0223 (11)	0.0223 (9)	0.0007 (8)	0.0034 (7)	-0.0015 (8)
C2	0.0225 (10)	0.0221 (10)	0.0224 (10)	-0.0010 (8)	0.0017 (8)	-0.0027 (8)
C3	0.0253 (10)	0.0180 (10)	0.0232 (10)	-0.0040 (8)	0.0023 (8)	-0.0014 (8)
C4	0.0184 (9)	0.0228 (10)	0.0208 (10)	-0.0047 (8)	0.0030 (7)	-0.0022 (8)
C5	0.0167 (9)	0.0225 (10)	0.0236 (10)	0.0023 (8)	-0.0006 (8)	-0.0011 (8)
C6	0.0209 (10)	0.0253 (11)	0.0213 (10)	0.0016 (8)	-0.0022 (8)	-0.0046 (8)
C7	0.0239 (10)	0.0290 (12)	0.0210 (11)	0.0004 (9)	-0.0002 (8)	-0.0057 (9)
C8	0.0248 (10)	0.0258 (11)	0.0236 (10)	0.0010 (9)	0.0024 (8)	-0.0058 (9)
C9	0.0169 (10)	0.0247 (11)	0.0259 (11)	-0.0006 (8)	0.0020 (8)	-0.0025 (9)
C10	0.0158 (10)	0.0327 (12)	0.0340 (12)	0.0021 (9)	0.0028 (9)	-0.0045 (10)
C11	0.0177 (10)	0.0309 (12)	0.0356 (12)	0.0009 (9)	-0.0045 (9)	-0.0034 (10)
C12	0.0156 (9)	0.0286 (11)	0.0250 (10)	0.0011 (8)	-0.0061 (8)	-0.0027 (9)
C13	0.0182 (10)	0.0274 (11)	0.0327 (12)	0.0030 (8)	-0.0050 (9)	-0.0003 (9)
C14	0.0253 (11)	0.0297 (12)	0.0445 (14)	0.0039 (9)	0.0023 (10)	-0.0069 (10)
C15	0.0259 (11)	0.0290 (13)	0.0516 (14)	0.0063 (9)	0.0034 (10)	-0.0052 (10)
C16	0.0265 (11)	0.0183 (10)	0.0387 (12)	0.0059 (9)	-0.0009 (9)	0.0002 (9)
C17	0.0257 (11)	0.0211 (10)	0.0327 (12)	0.0049 (8)	0.0005 (9)	0.0014 (9)
C18	0.0281 (12)	0.0208 (11)	0.0482 (14)	0.0003 (9)	0.0005 (10)	-0.0004 (10)

C19	0.0308 (12)	0.0211 (11)	0.0440 (13)	-0.0045 (9)	0.0026 (10)	0.0001 (10)
C20	0.0225 (10)	0.0235 (10)	0.0320 (11)	-0.0032 (8)	0.0022 (8)	-0.0063 (9)
C21	0.0234 (10)	0.0244 (11)	0.0195 (10)	-0.0053 (8)	-0.0009 (8)	-0.0003 (8)
C22	0.0242 (10)	0.0266 (11)	0.0265 (11)	-0.0076 (9)	-0.0032 (8)	-0.0005 (9)
C23	0.0188 (10)	0.0317 (12)	0.0316 (12)	-0.0070 (9)	-0.0055 (9)	0.0067 (10)
C24	0.0206 (10)	0.0257 (11)	0.0289 (11)	0.0006 (9)	0.0005 (8)	0.0073 (9)
C25	0.0192 (10)	0.0199 (10)	0.0223 (10)	0.0017 (8)	0.0019 (8)	0.0026 (8)
C26	0.0222 (10)	0.0232 (11)	0.0230 (10)	0.0000 (8)	0.0015 (8)	-0.0012 (8)
C27	0.0243 (11)	0.0370 (14)	0.0467 (14)	0.0079 (10)	-0.0016 (10)	0.0037 (11)
C28	0.0348 (13)	0.0478 (15)	0.0376 (13)	-0.0105 (11)	-0.0076 (10)	-0.0099 (11)
C29	0.0418 (14)	0.0221 (12)	0.079 (2)	0.0041 (11)	0.0038 (14)	-0.0100 (13)
C30	0.0347 (12)	0.0309 (12)	0.0513 (14)	0.0036 (11)	-0.0090 (10)	0.0113 (13)
C31	0.0616 (17)	0.0526 (19)	0.0358 (13)	-0.0024 (14)	-0.0121 (12)	0.0070 (13)
C32	0.0337 (12)	0.0338 (13)	0.0285 (12)	-0.0027 (10)	-0.0026 (9)	-0.0063 (10)
C33	0.0379 (13)	0.0314 (12)	0.0233 (10)	-0.0027 (10)	0.0005 (9)	0.0012 (9)
C34	0.0239 (10)	0.0308 (12)	0.0270 (11)	-0.0038 (9)	-0.0020 (8)	-0.0043 (9)
C35	0.0628 (17)	0.0288 (13)	0.0361 (13)	-0.0024 (12)	0.0164 (12)	0.0100 (11)
C36	0.0271 (11)	0.0265 (11)	0.0407 (13)	0.0054 (9)	0.0052 (10)	0.0045 (10)
C1S	0.074 (2)	0.079 (3)	0.072 (2)	-0.014 (2)	-0.0273 (19)	-0.006 (2)
O1S	0.085 (4)	0.093 (4)	0.072 (3)	0.010 (3)	0.008 (3)	-0.002 (3)

Geometric parameters (Å, º) for (mar1905)

Cu—O2	1.9531 (14)	C14—H14A	0.99
Cu—O2^{i}	1.9531 (14)	C15—C16	1.548 (3)
Cu—Cl	2.2008 (7)	C15—H15B	0.99
Cu—Cl^{i}	2.2008 (7)	C15—H15A	0.99
Na—O5	2.3200 (18)	C16—C17	1.520 (3)
Na—O10	2.3320 (17)	C16—C30	1.526 (3)
Na—O6	2.3386 (15)	C17—C18	1.534 (3)
Na—O8	2.4012 (16)	C17—H17	1
Na—O7	2.4404 (16)	C18—C29	1.531 (3)
Na—O9	2.4673 (15)	C18—C19	1.531 (3)
O1—C1	1.233 (2)	C18—H18	1
O2—C1	1.284 (2)	C19—C20	1.535 (3)
O3—C35	1.415 (3)	C19—H19B	0.99
O3—C3	1.439 (2)	C19—H19A	0.99

O4—C9	1.416 (2)	C20—C21	1.530 (3)
O4—C5	1.455 (2)	C20—H20	1
O5—C7	1.439 (3)	C21—C22	1.532 (3)
O5—H5X	0.80 (3)	C21—H21	1
O6—C9	1.429 (3)	C22—C28	1.528 (3)
O6—C12	1.463 (2)	C22—C23	1.528 (3)
O7—C13	1.446 (2)	C22—H22	1
O7—C16	1.461 (3)	C23—C24	1.524 (3)
O8—C17	1.441 (3)	C23—H23B	0.99
O8—C20	1.455 (2)	C23—H23A	0.99
O9—C21	1.436 (2)	C24—C25	1.531 (3)
O9—C25	1.444 (2)	C24—C27	1.533 (3)
O10—C26	1.421 (2)	C24—H24	1
O10—H10X	0.79 (3)	C25—C26	1.523 (3)
O11—C25	1.411 (2)	C26—H26B	0.99
O11—H11X	0.76 (3)	C26—H26A	0.99
C1—C2	1.526 (3)	C27—H27C	0.98
C2—C36	1.535 (3)	C27—H27B	0.98
C2—C3	1.543 (3)	C27—H27A	0.98
C2—H2	1	C28—H28C	0.98
C3—C4	1.543 (3)	C28—H28B	0.98
C3—H3	1	C28—H28A	0.98
C4—C5	1.530 (3)	C29—H29C	0.98
C4—C34	1.538 (3)	C29—H29B	0.98
C4—H4	1	C29—H29A	0.98
C5—C6	1.533 (3)	C30—C31	1.505 (4)
C5—H5	1	C30—H30B	0.99
C6—C7	1.535 (3)	C30—H30A	0.99
C6—C33	1.537 (3)	C31—H31C	0.98
C6—H6	1	C31—H31B	0.98
C7—C8	1.522 (3)	C31—H31A	0.98
C7—H7	1	C32—H32C	0.98
C8—C9	1.524 (3)	C32—H32B	0.98
C8—H8B	0.99	C32—H32A	0.98
C8—H8A	0.99	C33—H33C	0.98
C9—C10	1.528 (3)	C33—H33B	0.98
C10—C11	1.522 (3)	C33—H33A	0.98

C10—H10B	0.99	C34—H34C	0.98
C10—H10A	0.99	C34—H34B	0.98
C11—C12	1.540 (3)	C34—H34A	0.98
C11—H11B	0.99	C35—H35C	0.98
C11—H11A	0.99	C35—H35B	0.98
C12—C32	1.520 (3)	C35—H35A	0.98
C12—C13	1.530 (3)	C36—H36C	0.98
C13—C14	1.515 (3)	C36—H36B	0.98
C13—H13	1	C36—H36A	0.98
C14—C15	1.531 (3)	C1S—O1S	1.378 (7)
C14—H14B	0.99	C1S—C1S^{ii}	1.498 (7)
O2—Cu—O2^{i}	138.41 (8)	H15B—C15—H15A	108.9
O2—Cu—Cl	96.37 (5)	O7—C16—C17	103.35 (16)
O2^{i}—Cu—Cl	93.84 (5)	O7—C16—C30	109.19 (19)
O2—Cu—Cl^{i}	93.84 (5)	C17—C16—C30	111.27 (19)
O2^{i}—Cu—Cl^{i}	96.37 (5)	O7—C16—C15	104.90 (17)
Cl—Cu—Cl^{i}	150.99 (7)	C17—C16—C15	116.2 (2)
O5—Na—O10	110.38 (7)	C30—C16—C15	111.26 (18)
O5—Na—O6	75.96 (6)	O8—C17—C16	110.49 (18)
O10—Na—O6	110.85 (6)	O8—C17—C18	103.73 (17)
O5—Na—O8	100.71 (6)	C16—C17—C18	120.93 (17)
O10—Na—O8	128.11 (6)	O8—C17—H17	107
O6—Na—O8	116.48 (6)	C16—C17—H17	107
O5—Na—O7	137.21 (6)	C18—C17—H17	107
O10—Na—O7	106.40 (6)	C29—C18—C19	111.8 (2)
O6—Na—O7	71.04 (5)	C29—C18—C17	115.10 (19)
O8—Na—O7	71.72 (5)	C19—C18—C17	98.44 (17)
O5—Na—O9	97.79 (6)	C29—C18—H18	110.3
O10—Na—O9	69.51 (5)	C19—C18—H18	110.3
O6—Na—O9	173.54 (6)	C17—C18—H18	110.3
O8—Na—O9	65.87 (5)	C18—C19—C20	103.74 (18)
O7—Na—O9	115.25 (6)	C18—C19—H19B	111
C1—O2—Cu	131.65 (13)	C20—C19—H19B	111
C35—O3—C3	114.14 (17)	C18—C19—H19A	111
C9—O4—C5	114.13 (15)	C20—C19—H19A	111
C7—O5—Na	136.10 (13)	H19B—C19—H19A	109

C7—O5—H5X	109 (2)	O8—C20—C21	109.34 (16)
Na—O5—H5X	105 (2)	O8—C20—C19	105.75 (17)
C9—O6—C12	111.94 (14)	C21—C20—C19	115.87 (18)
C9—O6—Na	134.92 (11)	O8—C20—H20	108.6
C12—O6—Na	112.23 (11)	C21—C20—H20	108.6
C13—O7—C16	108.18 (15)	C19—C20—H20	108.6
C13—O7—Na	111.86 (12)	O9—C21—C20	105.61 (16)
C16—O7—Na	112.35 (12)	O9—C21—C22	111.01 (17)
C17—O8—C20	107.47 (15)	C20—C21—C22	113.52 (17)
C17—O8—Na	97.99 (11)	O9—C21—H21	108.9
C20—O8—Na	117.50 (12)	C20—C21—H21	108.9
C21—O9—C25	115.57 (15)	C22—C21—H21	108.9
C21—O9—Na	104.52 (11)	C28—C22—C23	110.97 (18)
C25—O9—Na	102.01 (10)	C28—C22—C21	111.76 (18)
C26—O10—Na	115.45 (12)	C23—C22—C21	108.65 (17)
C26—O10—H10X	110 (2)	C28—C22—H22	108.5
Na—O10—H10X	113 (2)	C23—C22—H22	108.5
C25—O11—H11X	113 (2)	C21—C22—H22	108.5
O1—C1—O2	122.92 (18)	C24—C23—C22	113.48 (17)
O1—C1—C2	118.64 (17)	C24—C23—H23B	108.9
O2—C1—C2	118.42 (17)	C22—C23—H23B	108.9
C1—C2—C36	109.15 (16)	C24—C23—H23A	108.9
C1—C2—C3	111.30 (16)	C22—C23—H23A	108.9
C36—C2—C3	109.60 (17)	H23B—C23—H23A	107.7
C1—C2—H2	108.9	C23—C24—C25	108.73 (17)
C36—C2—H2	108.9	C23—C24—C27	110.79 (18)
C3—C2—H2	108.9	C25—C24—C27	112.99 (18)
O3—C3—C2	104.67 (16)	C23—C24—H24	108.1
O3—C3—C4	108.52 (15)	C25—C24—H24	108.1
C2—C3—C4	117.46 (16)	C27—C24—H24	108.1
O3—C3—H3	108.6	O11—C25—O9	108.07 (15)
C2—C3—H3	108.6	O11—C25—C26	111.67 (16)
C4—C3—H3	108.6	O9—C25—C26	103.87 (15)
C5—C4—C34	111.67 (17)	O11—C25—C24	109.57 (16)
C5—C4—C3	114.74 (16)	O9—C25—C24	108.87 (16)
C34—C4—C3	111.59 (16)	C26—C25—C24	114.44 (16)
C5—C4—H4	106	O10—C26—C25	110.58 (16)

C34—C4—H4	106	O10—C26—H26B	109.5
C3—C4—H4	106	C25—C26—H26B	109.5
O4—C5—C4	104.32 (15)	O10—C26—H26A	109.5
O4—C5—C6	109.55 (16)	C25—C26—H26A	109.5
C4—C5—C6	115.42 (17)	H26B—C26—H26A	108.1
O4—C5—H5	109.1	C24—C27—H27C	109.5
C4—C5—H5	109.1	C24—C27—H27B	109.5
C6—C5—H5	109.1	H27C—C27—H27B	109.5
C5—C6—C7	109.31 (17)	C24—C27—H27A	109.5
C5—C6—C33	114.27 (17)	H27C—C27—H27A	109.5
C7—C6—C33	109.83 (17)	H27B—C27—H27A	109.5
C5—C6—H6	107.7	C22—C28—H28C	109.5
C7—C6—H6	107.7	C22—C28—H28B	109.5
C33—C6—H6	107.7	H28C—C28—H28B	109.5
O5—C7—C8	106.80 (17)	C22—C28—H28A	109.5
O5—C7—C6	112.23 (17)	H28C—C28—H28A	109.5
C8—C7—C6	110.99 (17)	H28B—C28—H28A	109.5
O5—C7—H7	108.9	C18—C29—H29C	109.5
C8—C7—H7	108.9	C18—C29—H29B	109.5
C6—C7—H7	108.9	H29C—C29—H29B	109.5
C7—C8—C9	113.63 (17)	C18—C29—H29A	109.5
C7—C8—H8B	108.8	H29C—C29—H29A	109.5
C9—C8—H8B	108.8	H29B—C29—H29A	109.5
C7—C8—H8A	108.8	C31—C30—C16	115.1 (2)
C9—C8—H8A	108.8	C31—C30—H30B	108.5
H8B—C8—H8A	107.7	C16—C30—H30B	108.5
O4—C9—O6	110.66 (16)	C31—C30—H30A	108.5
O4—C9—C8	110.94 (17)	C16—C30—H30A	108.5
O6—C9—C8	109.00 (16)	H30B—C30—H30A	107.5
O4—C9—C10	106.41 (16)	C30—C31—H31C	109.5
O6—C9—C10	104.98 (16)	C30—C31—H31B	109.5
C8—C9—C10	114.68 (17)	H31C—C31—H31B	109.5
C11—C10—C9	103.66 (17)	C30—C31—H31A	109.5
C11—C10—H10B	111	H31C—C31—H31A	109.5
C9—C10—H10B	111	H31B—C31—H31A	109.5
C11—C10—H10A	111	C12—C32—H32C	109.5
C9—C10—H10A	111	C12—C32—H32B	109.5

H10B—C10—H10A	109	H32C—C32—H32B	109.5
C10—C11—C12	104.56 (16)	C12—C32—H32A	109.5
C10—C11—H11B	110.8	H32C—C32—H32A	109.5
C12—C11—H11B	110.8	H32B—C32—H32A	109.5
C10—C11—H11A	110.8	C6—C33—H33C	109.5
C12—C11—H11A	110.8	C6—C33—H33B	109.5
H11B—C11—H11A	108.9	H33C—C33—H33B	109.5
O6—C12—C32	108.59 (16)	C6—C33—H33A	109.5
O6—C12—C13	106.96 (16)	H33C—C33—H33A	109.5
C32—C12—C13	111.31 (19)	H33B—C33—H33A	109.5
O6—C12—C11	104.87 (16)	C4—C34—H34C	109.5
C32—C12—C11	112.83 (17)	C4—C34—H34B	109.5
C13—C12—C11	111.86 (17)	H34C—C34—H34B	109.5
O7—C13—C14	102.99 (17)	C4—C34—H34A	109.5
O7—C13—C12	107.79 (16)	H34C—C34—H34A	109.5
C14—C13—C12	118.34 (19)	H34B—C34—H34A	109.5
O7—C13—H13	109.1	O3—C35—H35C	109.5
C14—C13—H13	109.1	O3—C35—H35B	109.5
C12—C13—H13	109.1	H35C—C35—H35B	109.5
C13—C14—C15	104.90 (19)	O3—C35—H35A	109.5
C13—C14—H14B	110.8	H35C—C35—H35A	109.5
C15—C14—H14B	110.8	H35B—C35—H35A	109.5
C13—C14—H14A	110.8	C2—C36—H36C	109.5
C15—C14—H14A	110.8	C2—C36—H36B	109.5
H14B—C14—H14A	108.8	H36C—C36—H36B	109.5
C14—C15—C16	104.70 (18)	C2—C36—H36A	109.5
C14—C15—H15B	110.8	H36C—C36—H36A	109.5
C16—C15—H15B	110.8	H36B—C36—H36A	109.5
C14—C15—H15A	110.8	O1S—C1S—C1S^{ii}	116.9 (5)
C16—C15—H15A	110.8		

Symmetry codes: (i) -*x*, *y*, -*z*; (ii) -*x*-1, *y*, -*z*.

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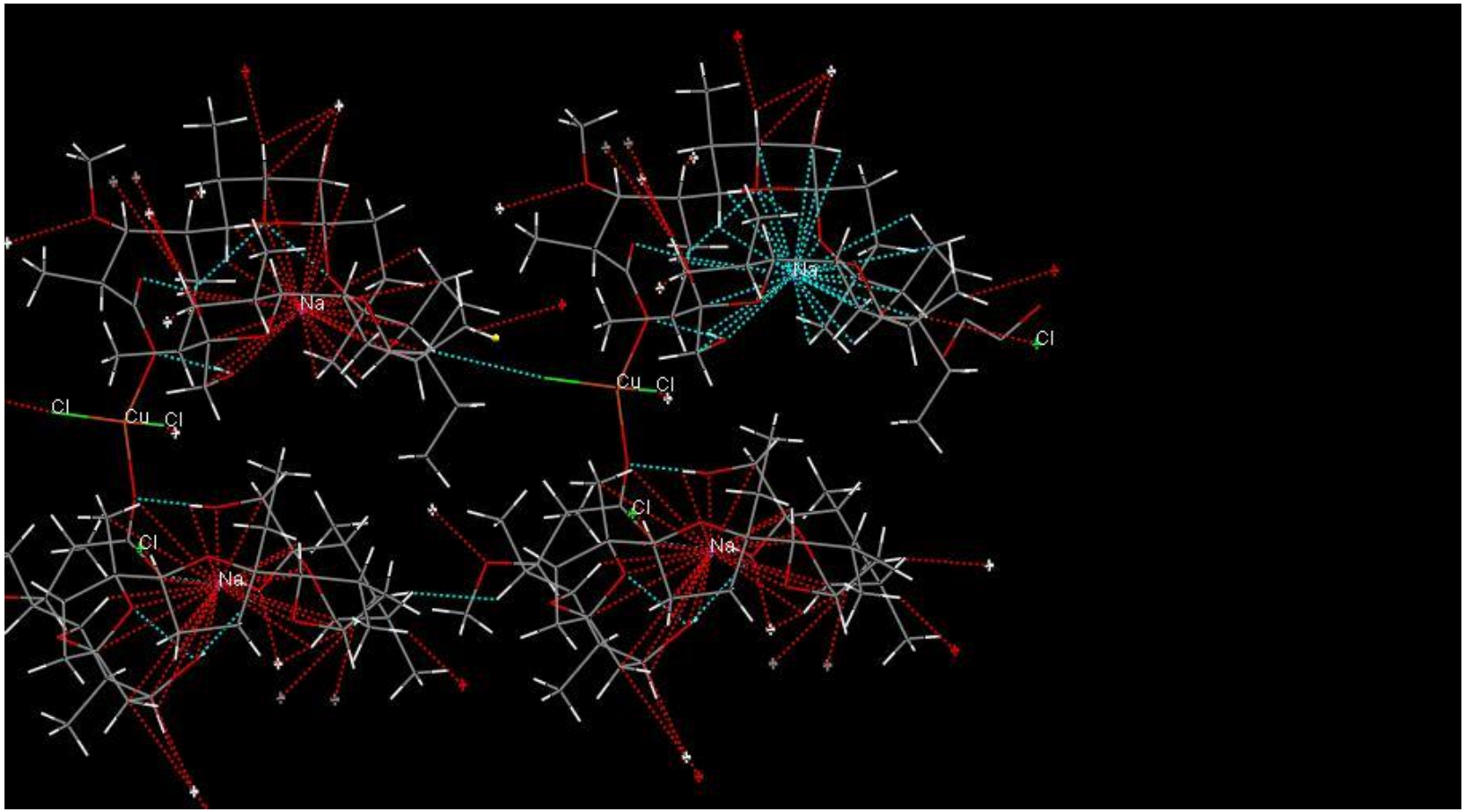
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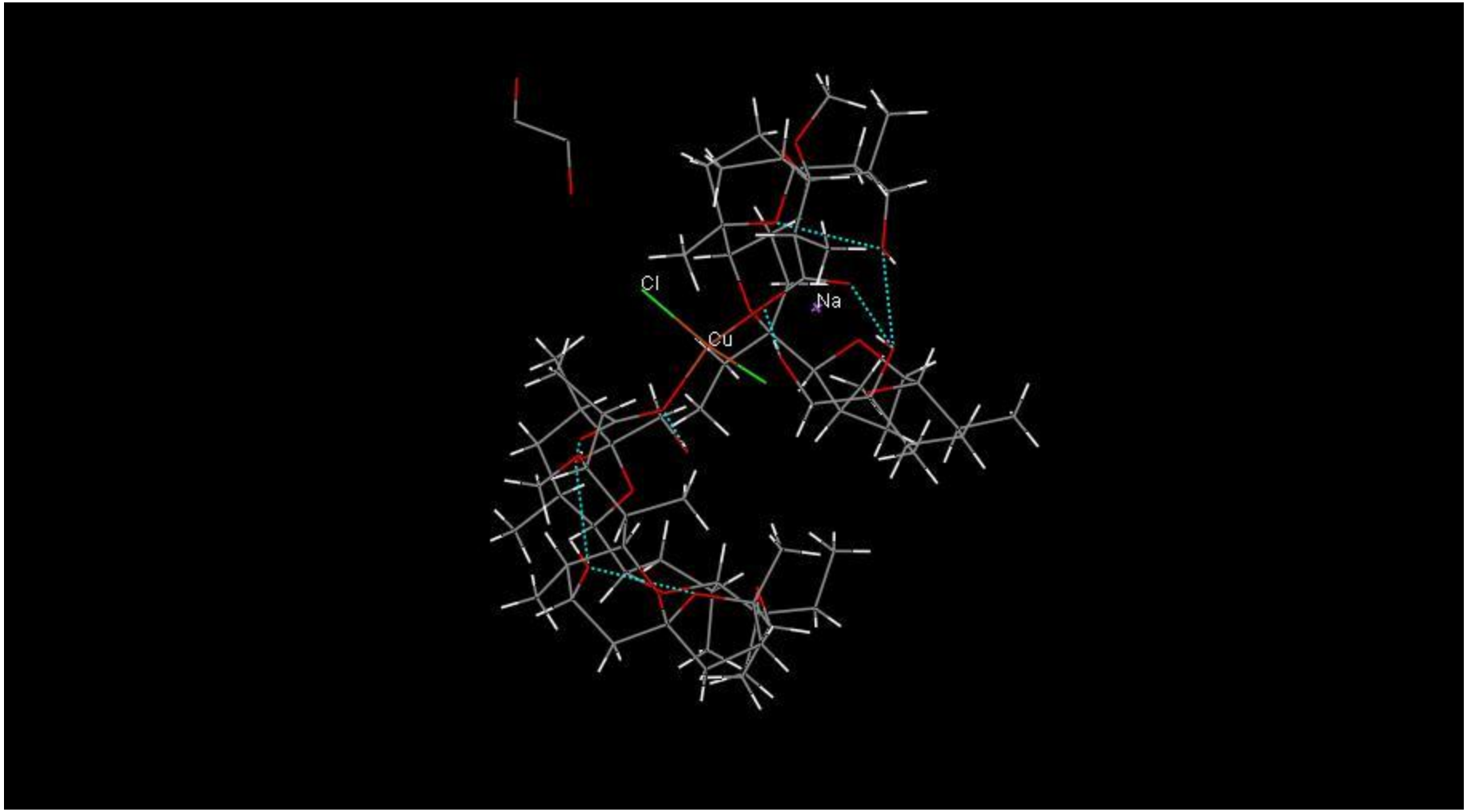
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