Table S1. Crystallographic Data and Data Collection Parameters.

Molecule	[Cu(2,7-dioxoOEiBC)][$SbCl_6$] · 0.5 $CHCl_3$	[Cu(2,7,12-trioxoOEHP)][$SbCl_6$]·1.25(CH_2Cl_2)
Formula	Cu N_4 $C_{36.5}$ $H_{44.5}$ O_2 Sb $Cl_{7.5}$	Cu $N_4C_{37.25}H_{46.50}$ $O_3SbCl_{8.50}$
FW, amu	1022.43	1077.34
a, Å	9.655(4)	31.085 (14)
b, Å	20.592(8)	—
c, Å	43.347(17)	9.410 (4)
β, °	89.97(1)	—
V, $Å^3$	8618(6)	9093 (7)
Space group	$P2_1/n$	$P4_2/n$
Z	8	8
D_c, g/cm^3	1.576	1.574
F(000)	4120	4312.00
μ, mm^{-1}	1.622	1.601
Radiation	MoKα, λ = 0.71073 Å	MoKα, λ = 0.71073 Å
Temp, K	100 (2)	127 (1)
Diffractometer	Bruker Apex	FAST
Total collected data	63639	28222
Unique collected data	15176	8981
Unique observed data [I>2σ(I)]	11785	7338
Variables refined	977	509
max(Δ_ρ), $eÅ^{-3}$	0.96	1.156
min(Δ_ρ), $eÅ^{-3}$	– 1.24	– 1.429
Final R indices [I>2σ(I)]	R_1 = 0.0525, wR_2 = 0.0948	R_1 = 0.0397; wR_2 = 0.1000
Final R indices (all data)	R_1 = 0.0753, wR_2 = 0.1145	R_1 = 0.0553; wR_2 = 0.1171
Goodness-of-fit on F^2	1.06	1.089

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (A^2) for [Cu(trioxoOEHP)][$SbCl_6$]·1.25-[CH_2Cl_2]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.[a]

	x	y	z	U(eq)
Cu	0.98475(1)	0.20920(1)	0.22463(4)	0.01264(10)
N(1)	0.98290(9)	0.14380(9)	0.2428(3)	0.0151(6)
N(3)	0.98699(9)	0.27416(9)	0.2047(3)	0.0151(6)
N(2)	1.04990(9)	0.20743(9)	0.2442(3)	0.0165(6)
N(4)	0.92074(9)	0.21125(9)	0.2082(3)	0.0145(6)
C(a1)	0.94595(11)	0.11985(11)	0.2285(4)	0.0173(7)
C(a2)	1.01607(12)	0.11672(11)	0.2704(4)	0.0188(7)
C(a3)	1.07321(11)	0.17046(11)	0.2660(4)	0.0176(7)
C(a4)	1.07770(11)	0.24129(11)	0.2362(4)	0.0182(7)
C(a5)	1.02403(11)	0.29748(11)	0.1984(4)	0.0174(7)
C(a6)	0.95264(11)	0.30158(11)	0.1881(4)	0.0171(7)
C(a7)	0.89544(10)	0.24741(11)	0.1975(4)	0.0155(7)
C(a8)	0.89277(11)	0.17718(11)	0.2019(4)	0.0156(7)
C(b1)	0.95566(12)	0.07325(12)	0.2432(4)	0.0213(8)
C(b2)	1.00169(12)	0.07023(12)	0.2909(5)	0.0272(9)
C(b3)	1.12033(12)	0.18067(12)	0.2736(5)	0.0235(8)
C(b4)	1.12468(11)	0.22889(12)	0.2547(5)	0.0240(8)
C(b5)	1.01438(11)	0.34386(11)	0.1721(4)	0.0195(7)
C(b6)	0.96610(11)	0.34813(11)	0.1629(4)	0.0201(7)
C(b7)	0.84985(11)	0.23563(12)	0.1876(4)	0.0174(7)
C(b8)	0.84830(11)	0.19202(12)	0.1887(4)	0.0178(7)
C(m1)	1.05874(11)	0.12902(11)	0.2793(4)	0.0187(7)
C(m2)	1.06578(11)	0.28351(11)	0.2124(4)	0.0201(7)

Table S2. (cont.)

C(m3)	0.91039(11)	0.28930(11)	0.1890(4)	0.0178(7)
C(m4)	0.90474(11)	0.13433(11)	0.2093(4)	0.0170(7)
O(1)	0.93084(9)	0.04354(8)	0.2242(3)	0.0270(6)
O(2)	1.14906(9)	0.15471(9)	0.2912(4)	0.0358(8)
O(3)	1.04102(8)	0.37233(8)	0.1608(3)	0.0275(6)
C(11)	1.02681(14)	0.03743(13)	0.2069(6)	0.0357(11)
C(21)	0.99787(13)	0.06026(13)	0.4594(5)	0.0352(10)
C(31)	1.14476(13)	0.24945(13)	0.3881(5)	0.0319(10)
C(41)	1.15158(12)	0.23910(13)	0.1206(5)	0.0309(10)
C(51)	0.94910(13)	0.37909(12)	0.2771(5)	0.0292(9)
C(61)	0.95311(13)	0.36423(12)	0.0130(5)	0.0271(9)
C(71)	0.81341(11)	0.26703(12)	0.1694(4)	0.0208(7)
C(81)	0.81021(11)	0.16256(12)	0.1723(4)	0.0218(7)
C(12)	1.02815(15)	0.04760(15)	0.0483(7)	0.0491(15)
C(22)	1.04030(15)	0.0556(2)	0.5363(6)	0.0411(11)
C(32)	1.1206(2)	0.2396(2)	0.5275(6)	0.0443(11)
C(42)	1.1338(2)	0.2210(2)	-0.0178(6)	0.0441(12)
C(52)	0.9630(2)	0.36783(15)	0.4284(5)	0.0382(11)
C(62)	0.9663(2)	0.33500(14)	-0.1090(5)	0.0383(11)
C(72)	0.80590(14)	0.27987(15)	0.0160(5)	0.0339(10)
C(82)	0.80529(14)	0.14613(14)	0.0207(5)	0.0328(9)
Sb	0.69392(1)	0.03816(1)	0.22591(3)	0.02179(9)
Cl(1)	0.72406(3)	-0.00808(3)	0.40070(11)	0.0333(2)
Cl(2)	0.63035(4)	0.04182(4)	0.36343(13)	0.0435(3)
Cl(3)	0.72228(4)	0.09898(4)	0.34490(12)	0.0407(3)
Cl(4)	0.66258(4)	0.08462(4)	0.05459(11)	0.0402(3)
Cl(5)	0.75699(4)	0.03280(5)	0.08612(14)	0.0511(3)
Cl(6)	0.66682(5)	-0.02277(4)	0.10523(14)	0.0496(3)

Table S2. (cont.)

CS(1)	1.0897(6)	0.3843(7)	0.7036(21)	0.100(5)
CS(2)	1.0634(6)	0.3483(6)	0.6861(19)	0.088(5)
Cl(11)	1.09096(6)	0.35745(6)	0.5273(2)	0.0733(5)
Cl(12)	1.1030(3)	0.3466(3)	0.8330(8)	0.077(2)
Cl(13)	1.1207(5)	0.3366(5)	0.8244(14)	0.089(3)
Cl(14)	1.1171(8)	0.3577(7)	0.8393(23)	0.099(6)
Cl(15)	1.0936(4)	0.3337(4)	0.8258(14)	0.079(4)
Cl(16)	1.0614(14)	0.4009(14)	0.7711(46)	0.085(11)
CS(3)	1.2532(11)	0.2249(8)	0.7620(33)	0.069(7)
Cl(17)	1.2500	0.2500	0.5906(5)	0.0462(10)
Cl(18)	1.2345(2)	0.2449(2)	0.6070(8)	0.0570(14)

[a] The estimated standard deviations of the least significant digits are given in parentheses.

Table S3. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for [Cu(2,7-DioxoOEiBC)][$SbCl_6$] · 0.5 $CHCl_3$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu	0.7508(1)	0.3386(1)	0.1284(1)	0.015
O(1)	0.7814(8)	0.5488(2)	0.0536(1)	0.025
O(2)	0.7225(8)	0.1832(2)	0.0284(1)	0.042
N(1)	0.7570(7)	0.3977(3)	0.0907(1)	0.016
N(2)	0.7413(7)	0.2599(3)	0.1006(1)	0.017
N(3)	0.7382(6)	0.2806(2)	0.1653(1)	0.015
N(4)	0.7699(8)	0.4158(2)	0.1562(1)	0.017
CA1	0.7747(9)	0.4644(3)	0.0918(2)	0.018
CA2	0.7379(9)	0.3800(3)	0.0608(1)	0.016
CA3	0.7315(9)	0.2634(3)	0.0691(2)	0.019
CA4	0.7409(9)	0.1963(3)	0.1092(2)	0.019
CA5	0.7295(9)	0.2146(3)	0.1651(2)	0.017
CA6	0.7337(9)	0.2990(3)	0.1957(1)	0.017
CA7	0.7670(9)	0.4163(3)	0.1878(1)	0.014
CA8	0.7914(8)	0.4792(3)	0.1477(2)	0.018
CB1	0.7679(8)	0.4921(3)	0.0602(2)	0.016
CB2	0.7385(9)	0.4365(3)	0.0384(1)	0.018
C(11)	0.5927(9)	0.4454(3)	0.0241(2)	0.021
CB3	0.7321(9)	0.1960(3)	0.0557(1)	0.026
C(12)	0.4751(8)	0.4455(3)	0.0471(2)	0.027
CB4	0.7511(9)	0.1493(4)	0.0823(2)	0.020
CB5	0.7154(8)	0.1900(4)	0.1969(2)	0.016
CB6	0.7195(7)	0.2420(3)	0.2153(2)	0.019
CB7	0.7861(9)	0.4819(3)	0.1992(2)	0.020
CB8	0.8043(8)	0.5204(3)	0.1751(2)	0.014
CM1	0.7272(9)	0.3168(3)	0.0503(1)	0.019
CM2	0.7335(8)	0.1746(3)	0.1394(2)	0.019
CM3	0.7462(8)	0.3624(4)	0.2058(2)	0.021
CM4	0.7935(8)	0.5014(4)	0.1172(2)	0.015
C(21)	0.8499(9)	0.4307(4)	0.0136(2)	0.022
C(22)	0.9961(9)	0.4224(4)	0.0255(2)	0.027
C(31)	0.9011(10)	0.1197(4)	0.0805(2)	0.030
C(32)	1.0163(9)	0.1687(4)	0.0804(2)	0.045
C(41)	0.6383(9)	0.0955(4)	0.0818(2)	0.031
C(42)	0.4899(11)	0.1216(5)	0.0830(2)	0.044
C(51)	0.7056(8)	0.1180(3)	0.2043(2)	0.022
C(52)	0.8470(8)	0.0841(4)	0.2027(2)	0.028
C(61)	0.7092(9)	0.2422(4)	0.2501(2)	0.023
C(62)	0.5584(9)	0.2445(4)	0.2617(2)	0.031
C(71)	0.7906(8)	0.4987(4)	0.2331(2)	0.020

C(72)	0.9335(9)	0.4900(4)	0.2466(2)	0.027
C(81)	0.8356(8)	0.5918(4)	0.1737(2)	0.021
C(82)	0.9878(8)	0.6060(4)	0.1674(2)	0.034
Cu'	0.2541(1)	0.3321(1)	0.3709(1)	0.017
O(1')	0.3290(8)	0.5418(3)	0.4446(1)	0.038
O(2')	0.1557(7)	0.1838(3)	0.4711(1)	0.029
N(1')	0.2758(8)	0.3911(3)	0.4082(1)	0.021
N(2')	0.2195(7)	0.2554(3)	0.3995(1)	0.016
N(3')	0.2356(7)	0.2733(3)	0.3345(1)	0.021
N(4')	0.2770(6)	0.4090(2)	0.3428(1)	0.017
C(11')	0.4228(8)	0.4209(3)	0.4808(2)	0.030
C(12')	0.5587(9)	0.4164(3)	0.4633(2)	0.046
C(21')	0.1641(9)	0.4420(3)	0.4811(2)	0.028
CA1'	0.2956(7)	0.4580(3)	0.4064(2)	0.017
C(22')	0.0316(8)	0.4496(3)	0.4632(2)	0.037
CA2'	0.2726(8)	0.3740(3)	0.4387(2)	0.019
CA3'	0.2149(9)	0.2590(3)	0.4310(2)	0.018
CA4'	0.1893(8)	0.1921(3)	0.3905(2)	0.017
CA5'	0.2070(9)	0.2080(4)	0.3346(2)	0.015
CA6'	0.2386(9)	0.2912(3)	0.3038(2)	0.017
CA7'	0.2734(8)	0.4081(4)	0.3111(2)	0.019
CA8'	0.2918(8)	0.4731(3)	0.3509(2)	0.020
CB1'	0.3104(8)	0.4853(4)	0.4382(2)	0.027
CB2'	0.2920(9)	0.4292(4)	0.4603(2)	0.024
C(31')	0.0063(8)	0.1224(4)	0.4164(2)	0.028
CB3'	0.1731(8)	0.1952(4)	0.4440(2)	0.020
C(32')	-0.1042(9)	0.1740(3)	0.4099(2)	0.035
CB4'	0.1554(8)	0.1481(4)	0.4175(2)	0.018
CB5'	0.1932(9)	0.1829(3)	0.3027(2)	0.021
CB6'	0.2139(9)	0.2341(4)	0.2842(2)	0.023
CB7'	0.2841(9)	0.4739(4)	0.2989(2)	0.022
CB8'	0.2948(9)	0.5139(4)	0.3233(2)	0.025
CM1'	0.2423(9)	0.3117(4)	0.4490(2)	0.020
CM2'	0.1869(9)	0.1701(4)	0.3606(2)	0.018
CM3'	0.2582(10)	0.3533(4)	0.2929(2)	0.018
CM4'	0.3008(9)	0.4954(4)	0.3812(2)	0.024
C(41')	0.2600(9)	0.0913(3)	0.4210(2)	0.031
C(42')	0.4081(10)	0.1117(4)	0.4234(2)	0.036
C(51')	0.1491(8)	0.1147(4)	0.2960(2)	0.023
C(52')	-0.0069(8)	0.1060(4)	0.3012(2)	0.028
C(61')	0.2055(9)	0.2364(4)	0.2495(2)	0.026
C(62')	0.0643(9)	0.2563(5)	0.2380(2)	0.041
C(71')	0.2824(9)	0.4885(4)	0.2651(2)	0.026
C(72')	0.4162(9)	0.4717(4)	0.2483(2)	0.025
C(81')	0.3002(8)	0.5861(4)	0.3238(2)	0.031
C(82')	0.1572(9)	0.6170(4)	0.3263(2)	0.044

Cl(31)	0.3652(40)	0.2033(8)	-0.0159(6)	0.047
Cl(32)	0.2866(8)	0.2888(3)	0.0361(2)	0.084
Cl(33)	0.0822(14)	0.2564(4)	-0.0093(3)	0.094
Cl(41)	0.3080(7)	0.2612(3)	0.0412(2)	0.110
Cl(42)	0.3039(30)	0.3371(14)	-0.0136(7)	0.062
Cl(43)	0.3510(20)	0.2008(7)	-0.0114(4)	0.213
C(1S)	0.2240(7)	0.2729(3)	-0.0054(1)	0.111
C(2S)	0.3830(30)	0.2689(12)	0.0049(6)	0.069
Sb	0.2677(1)	0.3768(1)	0.1465(1)	0.020
Cl(1)	0.3887(2)	0.3321(1)	0.1889(1)	0.034
Cl(2)	0.4139(2)	0.3161(1)	0.1132(1)	0.040
Cl(3)	0.1475(2)	0.4208(1)	0.1040(1)	0.039
Cl(4)	0.1061(2)	0.2902(1)	0.1484(1)	0.038
Cl(5)	0.4271(2)	0.4652(1)	0.1444(1)	0.036
Cl(6)	0.1286(2)	0.4375(1)	0.1810(1)	0.041
Sb'	0.7661(1)	0.3729(1)	0.3497(1)	0.021
Cl(1')	0.6471(3)	0.4578(1)	0.3752(1)	0.048
Cl(2')	0.8820(3)	0.2870(1)	0.3240(1)	0.050
Cl(3')	0.9333(2)	0.4492(1)	0.3325(1)	0.046
Cl(4')	0.9034(3)	0.3533(1)	0.3937(1)	0.046
Cl(5')	0.5958(3)	0.2981(1)	0.3672(1)	0.049
Cl(6')	0.6338(2)	0.3929(1)	0.3047(1)	0.038

Table S4. Bond Lengths [Å] and Angles [deg] for [Cu(trioxoOEHP)][$SbCl_6$]·1.25-(CH_2Cl_2).[a]

Cu-N(1)	2.041(3)	C(a7)-C(m3)	1.385(5)
Cu-N(2)	2.035(3)	C(a8)-C(m4)	1.385(5)
Cu-N(3)	2.029(3)	C(b1)-C(b2)	1.503(5)
Cu-N(4)	1.997(3)	C(b3)-C(b4)	1.515(5)
N(1)-C(a1)	1.375(4)	C(b5)-C(b6)	1.509(5)
N(1)-C(a2)	1.356(5)	C(b7)-C(b8)	1.356(5)
N(2)-C(a3)	1.374(4)	C(b1)-O(1)	1.217(5)
N(2)-C(a4)	1.364(4)	C(b3)-O(2)	1.217(4)
N(3)-C(a5)	1.375(4)	C(b5)-O(3)	1.215(5)
N(3)-C(a6)	1.362(4)	C(b2)-C(11)	1.508(6)
N(4)-C(a7)	1.375(4)	C(b2)-C(21)	1.620(7)
N(4)-C(a8)	1.372(4)	C(b4)-C(31)	1.541(6)
C(a1)-C(b1)	1.486(5)	C(b4)-C(41)	1.547(6)
C(a2)-C(b2)	1.525(5)	C(b6)-C(51)	1.536(5)
C(a3)-C(b3)	1.500(5)	C(b6)-C(61)	1.550(6)
C(a4)-C(b4)	1.521(5)	C(b7)-C(71)	1.505(5)
C(a5)-C(b5)	1.493(5)	C(b8)-C(81)	1.505(5)
C(a6)-C(b6)	1.525(5)	C(11)-C(12)	1.526(8)
C(a7)-C(b7)	1.467(5)	C(21)-C(22)	1.511(6)
C(a8)-C(b8)	1.462(5)	C(31)-C(32)	1.543(7)
C(a1)-C(m4)	1.370(5)	C(41)-C(42)	1.523(7)
C(a2)-C(m1)	1.383(5)	C(51)-C(52)	1.528(7)
C(a3)-C(m1)	1.370(5)	C(61)-C(62)	1.520(6)
C(a4)-C(m2)	1.382(5)	C(71)-C(72)	1.516(6)
C(a5)-C(m2)	1.375(5)	C(81)-C(82)	1.523(6)
C(a6)-C(m3)	1.368(5)		

Table S4. (cont.)

N(1)-Cu-N(2)	89.62(11)	O(1)-C(b1)-C(b2)	126.9(3)
N(1)-Cu-N(3)	179.39(12)	C(a2)-C(b2)-C(11)	115.0(4)
N(1)-Cu-N(4)	90.59(11)	C(a2)-C(b2)-C(21)	109.1(3)
N(2)-Cu-N(3)	90.06(11)	C(a2)-C(b2)-C(b1)	100.5(3)
N(2)-Cu-N(4)	179.19(12)	C(b1)-C(b2)-C(11)	112.2(3)
N(3)-Cu-N(4)	89.73(11)	C(b1)-C(b2)-C(21)	103.6(3)
C(a1)-N(1)-Cu	123.7(2)	C(11)-C(b2)-C(21)	114.9(3)
C(a2)-N(1)-Cu	127.8(2)	C(a3)-C(b3)-C(b4)	106.9(3)
C(a3)-N(2)-Cu	124.1(2)	O(2)-C(b3)-C(a3)	125.7(3)
C(a4)-N(2)-Cu	127.2(2)	O(2)-C(b3)- C(b4)	127.4(3)
C(a5)-N(3)-Cu	124.3(2)	C(a4)-C(b4)-C(31)	112.1(3)
C(a6)-N(3)-Cu	126.9(2)	C(a4)-C(b4)-C(41)	112.0(3)
C(a7)-N(4)-Cu	127.0(2)	C(a4)-C(b4)-C(b3)	100.3(3)
C(a8)-N(4)-Cu	127.6(2)	C(b3)-C(b4)-C(31)	110.6(3)
C(a1)-N(1)-C(a2)	108.5(3)	C(b3)-C(b4)- C(41)	110.3(3)
C(a3)-N(2)-C(a4)	108.6(3)	C(31)-C(b4)-C(41)	111.1(3)
C(a5)-N(3)-C(a6)	108.8(3)	C(a5)-C(b5)-C(b6)	107.1(3)
C(a7)-N(4)-C(a8)	105.4(3)	O(3)-C(b5)-C(a5)	125.4(3)
N(1)-C(a2)-C(m1)	124.7(3)	O(3)-C(b5)-C(b6)	127.5(3)
N(1)-C(a1)-C(m4)	128.0(3)	C(a6)-C(b6)-C(51)	113.0(3)
N(1)-C(a1)-C(b1)	110.4(3)	C(a6)-C(b6)-C(61)	112.1(3)
N(1)-C(a2)-C(b2)	112.9(3)	C(a6)-C(b6)-C(b5)	100.4(3)
N(2)-C(a3)-C(m1)	128.8(3)	C(b5)-C(b6)-C(51)	110.9(3)
N(2)-C(a4)-C(m2)	124.9(3))	C(b5)-C(b6)-C(61)	109.8(3)
N(2)-C(a3)-C(b3)	110.2(3)	C(51)-C(b6)-C(61)	110.2(3)
N(2)-C(a4)-C(b4)	114.0(3)	C(a7)-C(b7)-C(71)	124.9(3)
N(3)-C(a5)-C(m2)	128.7(3))	C(a7)-C(b7)-C(b8)	106.5(3)

Table S4. (cont.)

N(3)-C(a6)-C(m3)	124.9(3)	C(b8)-C(b7)-C(71)	128.5(3)
N(3)-C(a5)-C(b5)	110.6(3)	C(a8)-C(b8)-C(81)	129.4(3)
N(3)-C(a6)-C(b6)	113.1(3)	C(a8)-C(b8)-C(b7)	106.4(3)
N(4)-C(a7)-C(m3)	125.5(3)	C(b7)-C(b8)-C(81)	129.4(3)
N(4)-C(a8)-C(m4)	124.8(3)	C(a2)-C(m1)-C(a3)	124.7(3)
N(4)-C(a7)-C(b7)	110.7(3)	C(a4)-C(m2)-C(a5)	124.7(3)
N(4)-C(a8)-C(b8)	111.1(3)	C(a6)-C(m3)-C(a7)	125.8(3)
C(m4)-C(a1)-C(b1)	121.5(3)	C(a8)-C(m4)-C(a1)	125.0(3)
C(m1)-C(a2)-C(b2)	122.4(3)	C(b2)-C(11)-C(12)	112.8(4)
C(m1)-C(a3)-C(b3)	121.0(3)	C(b2)-C(21)-C(22)	115.0(4)
C(m2)-C(a4)-C(b4)	121.1(3)	C(b4)-C(31)-C(32)	114.4(3)
C(m2)-C(a5)-C(b5)	120.7(3)	C(b4)-C(41)-C(42)	115.2(3)
C(m3)-C(a6)-C(b6)	122.0(3)	C(b6)-C(51)-C(52)	115.1(3)
C(m3)-C(a7)-C(b7)	123.7(3)	C(b6)-C(61)-C(62)	114.3(3)
C(m4)-C(a8)-C(b8)	124.2(3)	C(b7)-C(71)-C(72)	113.3(3)
C(a1)-C(b1)-C(b2)	106.4(3)	C(b8)-C(81)-C(82)	112.3(3)
O(1)-C(b1)- C(a1)	126.7(3)		

[a] The estimated standard deviations of the least significant digits are given in parentheses.

Table S5. Bond lengths [Å] for [Cu(2,7-dioxoP)][$SbCl_6$] 0.5 $CHCl_3$.

atom-atom	distance	atom-atom	distance
Cu-N(1)	2.037(5)	Cu-N(2)	2.020(5)
Cu-N(3)	1.998(5)	Cu-N(4)	2.004(5)
N(1)-CA1	1.387(8)	N(1)-CA2	1.362(8)
N(2)-CA3	1.371(8)	N(2)-CA4	1.360(8)
N(3)-CA5	1.363(8)	N(3)-CA6	1.373(8)
N(4)-CA7	1.368(8)	N(4)-CA8	1.372(9)
CA1-CB1	1.485(9)	CA2-CB2	1.514(9)
CA3-CB3	1.503(9)	CA4-CB4	1.519(9)
CA5-CB5	1.476(9)	CA6-CB6	1.455(9)
CA7-CB7	1.449(9)	CA8-CB8	1.463(9)
CA1-CM4	1.351(9)	CA2-CM1	1.381(9)
CA3-CM1	1.370(9)	CA4-CM2	1.384(9)
CA5-CM2	1.388(9)	CA6-CM3	1.383(9)
CA7-CM3	1.374(9)	CA8-CM4	1.401(10)
O(1)-CB1	1.208(8)	O(2)-CB3	1.216(8)
CB1-CB2	1.510(9)	CB3-CB4	1.511(9)
CB5-CB6	1.334(9)	CB7-CB8	1.322(10)
CB2-C(11)	1.550(11)	CB2-C(21)	1.527(10)
CB4-C(31)	1.573(12)	CB4-C(41)	1.555(11)
CB5-C(51)	1.520(9)	CB6-C(61)	1.512(9)
CB7-C(71)	1.510(9)	CB8-C(81)	1.502(10)
C(11)-C(12)	1.510(11)	C(21)-C(22)	1.513(11)
C(31)-C(32)	1.501(12)	C(41)-C(42)	1.531(14)
C(51)-C(52)	1.535(10)	C(61)-C(62)	1.542(12)
C(71)-C(72)	1.511(11)	C(81)-C(82)	1.524(11)
C(1S)-Cl(31)	2.03(3)	C(1S)-Cl(32)	1.93(3)
C(1S)-Cl(33)	1.42(3)	C(1S)-Cl(41)	2.19(3)
C(1S)-Cl(42)	1.57(2)	C(1S)-Cl(43)	1.95(3)
C(1S)-C(2S)	1.60(4)	C(2S)-Cl(31)	1.63(3)
C(2S)-Cl(32)	1.69(3)	C(2S)-Cl(41)	1.73(4)
C(2S)-Cl(42)	1.79(3)	C(2S)-Cl(43)	1.60(3)
Cu'-N(1')	2.033(6)	Cu'-N(2')	2.033(6)
Cu'-N(3')	1.997(6)	Cu'-N(4')	2.012(5)
N(1')-CA1'	1.392(9)	N(1')-CA2'	1.371(9)
N(2')-CA3'	1.370(8)	N(2')-CA4'	1.393(9)
N(3')-CA5'	1.373(9)	N(3')-CA6'	1.383(8)
N(4')-CA7'	1.373(9)	N(4')-CA8'	1.372(9)
CA1'-CB1'	1.494(10)	CA2'-CB2'	1.484(10)
CA3'-CB3'	1.485(10)	CA4'-CB4'	1.514(10)
CA5'-CB5'	1.483(10)	CA6'-CB6'	1.470(10)
CA7'-CB7'	1.460(10)	CA8'-CB8'	1.462(10)
CA1'-CM4'	1.338(10)	CA2'-CM1'	1.389(9)

CA3'-CM1'	1.364(9)	CA4'-CM2'	1.373(10)
CA5'-CM2'	1.383(10)	CA6'-CM3'	1.376(9)
CA7'-CM3'	1.386(10)	CA8'-CM4'	1.396(11)
O(1')-CB1'	1.210(9)	O(2')-CB3'	1.212(8)
CB1'-CB2'	1.510(10)	CB3'-CB4'	1.512(10)
CB5'-CB6'	1.340(10)	CB7'-CB8'	1.345(11)
CB2'-C(11')	1.553(11)	CB2'-C(21')	1.552(11)
CB4'-C(31')	1.535(12)	CB4'-C(41')	1.553(10)
CB5'-C(51')	1.495(10)	CB6'-C(61')	1.507(10)
CB7'-C(71')	1.497(10)	CB8'-C(81')	1.489(10)
C(11')-C(12')	1.517(12)	C(21')-C(22')	1.506(12)
C(32')-C(31')	1.532(12)	C(41')-C(42')	1.493(12)
C(51')-C(52')	1.534(10)	C(61')-C(62')	1.509(12)
C(71')-C(72')	1.522(11)	C(81')-C(82')	1.523(11)
Sb-Cl(1)	2.365(2)	Sb-Cl(2)	2.375(2)
Sb-Cl(3)	2.359(2)	Sb-Cl(4)	2.371(2)
Sb-Cl(5)	2.386(2)	Sb-Cl(6)	2.366(2)
Sb'-Cl(1')	2.367(2)	Sb'-Cl(2')	2.370(2)
Sb'-Cl(3')	2.371(2)	Sb'-Cl(4')	2.359(2)
Sb'-Cl(5')	2.379(2)	Sb'-Cl(6')	2.366(2)
C(11)-H(11B)	0.9600	C(11)-H(11A)	0.9600
C(12)-H(12B)	0.9600	C(12)-H(12C)	0.9600
C(12)-H(12A)	0.9600	CM1-HM1A	0.9600
CM2-HM2A	0.9600	CM3-HM3A	0.9600
CM4-HM4A	0.9600	C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600	C(22)-H(22C)	0.9600
C(22)-H(22B)	0.9600	C(22)-H(22A)	0.9600
C(31)-H(31A)	0.9600	C(31)-H(31B)	0.9600
C(32)-H(32A)	0.9600	C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600	C(41)-H(41B)	0.9600
C(41)-H(41A)	0.9600	C(42)-H(42B)	0.9600
C(42)-H(42A)	0.9600	C(42)-H(42C)	0.9600
C(51)-H(51A)	0.9600	C(51)-H(51B)	0.9600
C(52)-H(52A)	0.9600	C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600	C(61)-H(61B)	0.9600
C(61)-H(61A)	0.9600	C(62)-H(62B)	0.9600
C(62)-H(62A)	0.9600	C(62)-H(62C)	0.9600
C(71)-H(71A)	0.9600	C(71)-H(71B)	0.9600
C(72)-H(72B)	0.9600	C(72)-H(72A)	0.9600
C(72)-H(72C)	0.9600	C(81)-H(81A)	0.9600
C(81)-H(81B)	0.9600	C(82)-H(82A)	0.9600
C(82)-H(82C)	0.9600	C(82)-H(82B)	0.9600
C(11')-H(11D)	0.9600	C(11')-H(11C)	0.9600
C(12')-H(12E)	0.9600	C(12')-H(12F)	0.9600
C(12')-H(12D)	0.9600	C(21')-H(21C)	0.9600
C(21')-H(21D)	0.9600	C(22')-H(22E)	0.9600

C(22')-H(22F)	0.9600	C(22')-H(22D)	0.9600
C(31')-H(31D)	0.9600	C(31')-H(31C)	0.9600
C(32')-H(32E)	0.9600	C(32')-H(32D)	0.9600
C(32')-H(32F)	0.9600	CM1'-HM1B	0.9600
CM2'-HM2B	0.9600	CM3'-HM3B	0.9600
CM4'-HM4B	0.9600	C(41')-H(41C)	0.9600
C(41')-H(41D)	0.9600	C(42')-H(42F)	0.9600
C(42')-H(42D)	0.9600	C(42')-H(42E)	0.9600
C(51')-H(51D)	0.9600	C(51')-H(51C)	0.9600
C(52')-H(52F)	0.9600	C(52')-H(52E)	0.9600
C(52')-H(52D)	0.9600	C(61')-H(61C)	0.9600
C(61')-H(61D)	0.9600	C(62')-H(62E)	0.9600
C(62')-H(62F)	0.9600	C(62')-H(62D)	0.9600
C(71')-H(71C)	0.9600	C(71')-H(71D)	0.9600
C(72')-H(72D)	0.9600	C(72')-H(72F)	0.9600
C(72')-H(72E)	0.9600	C(81')-H(81D)	0.9600
C(81')-H(81C)	0.9600	C(82')-H(82E)	0.9600
C(82')-H(82F)	0.9600	C(82')-H(82D)	0.9600
C(1S)-H(1SA)	0.9600	C(2S)-H(2SA)	0.9600

Symmetry transformations used to generate equivalent atoms:

Table S6. Bond angles [°] for [Cu(2,7-dioxoP)][$SbCl_6$] 0.5 $CHCl_3$.

atom-atom-atom	angle	atom-atom-atom	angle
N(1)-Cu-N(2)	90.2(2)	N(1)-Cu-N(3)	178.2(3)
N(1)-Cu-N(4)	90.3(2)	N(2)-Cu-N(3)	89.7(2)
N(2)-Cu-N(4)	177.3(3)	N(3)-Cu-N(4)	89.9(2)
CA1-N(1)-Cu	124.7(4)	CA2-N(1)-Cu	126.9(4)
CA3-N(2)-Cu	123.7(4)	CA4-N(2)-Cu	127.6(4)
CA5-N(3)-Cu	126.6(4)	CA6-N(3)-Cu	127.3(5)
CA7-N(4)-Cu	127.3(4)	CA8-N(4)-Cu	127.4(5)
CA2-N(1)-CA1	108.2(5)	CA4-N(2)-CA3	108.7(5)
CA5-N(3)-CA6	106.1(6)	CA7-N(4)-CA8	105.3(6)
N(1)-CA2-CM1	125.0(6)	N(1)-CA2-CB2	113.8(6)
N(1)-CA1-CB1	110.2(6)	CM4-CA1-N(1)	127.0(6)
N(2)-CA4-CM2	124.6(6)	N(2)-CA4-CB4	113.9(5)
N(2)-CA3-CB3	109.7(6)	CM1-CA3-N(2)	129.6(6)
N(3)-CA5-CM2	126.4(6)	N(3)-CA5-CB5	110.1(6)
N(3)-CA6-CM3	124.2(6)	N(3)-CA6-CB6	109.9(6)
N(4)-CA7-CM3	124.5(6)	N(4)-CA7-CB7	110.2(6)
N(4)-CA8-CM4	124.5(6)	N(4)-CA8-CB8	110.3(6)
O(1)-CB1-CA1	125.8(6)	O(1)-CB1-CB2	127.2(6)
O(2)-CB3-CA3	125.2(7)	O(2)-CB3-CB4	127.7(6)
CA1-CB1-CB2	107.0(5)	CB1-CB2-CA2	100.7(5)
CB1-CB2-C(21)	111.6(6)	CA2-CB2-C(21)	113.1(6)
CB1-CB2-C(11)	109.4(6)	CA2-CB2-C(11)	110.1(7)
C(21)-CB2-C(11)	111.4(6)	CM1-CA2-CB2	121.1(6)
CA3-CM1-CA2	124.0(6)	CM1-CA3-CB3	120.7(6)
CA3-CB3-CB4	107.0(6)	CB3-CB4-CA4	99.8(5)
CB3-CB4-C(41)	111.1(7)	CA4-CB4-C(41)	114.8(6)
CB3-CB4-C(31)	108.8(7)	CA4-CB4-C(31)	110.1(7)
C(41)-CB4-C(31)	111.6(6)	CM2-CA4-CB4	121.5(6)
CA4-CM2-CA5	124.8(6)	CM2-CA5-CB5	123.5(6)
CB6-CB5-CA5	106.2(6)	CB6-CB5-C(51)	131.2(6)
CA5-CB5-C(51)	122.5(6)	CB5-CB6-CA6	107.6(6)
CB5-CB6-C(61)	126.5(7)	CA6-CB6-C(61)	125.8(6)
CM3-CA6-CB6	125.8(6)	CA7-CM3-CA6	126.5(6)
CM3-CA7-CB7	125.3(6)	CB8-CB7-CA7	107.8(6)
CB8-CB7-C(71)	128.8(7)	CA7-CB7-C(71)	123.3(7)
CB7-CB8-CA8	106.3(6)	CB7-CB8-C(81)	130.0(7)
CA8-CB8-C(81)	123.6(6)	CM4-CA8-CB8	125.1(6)
CA1-CM4-CA8	125.8(6)	CM4-CA1-CB1	122.8(6)
CB5-C(51)-C(52)	112.2(6)	CB6-C(61)-C(62)	112.9(7)
CB7-C(71)-C(72)	112.2(7)	CB8-C(81)-C(82)	112.9(7)
C(12)-C(11)-CB2	114.7(6)	C(22)-C(21)-CB2	115.1(6)
C(32)-C(31)-CB4	115.0(6)	C(42)-C(41)-CB4	113.8(7)

Cl(33)-C(1S)-Cl(42)	130(2)	Cl(33)-C(1S)-Cl(32)	117.0(15)
Cl(33)-C(1S)-Cl(31)	116.9(11)	Cl(42)-C(1S)-Cl(32)	85.0(13)
Cl(33)-C(1S)-Cl(43)	114.3(14)	Cl(42)-C(1S)-Cl(43)	107.6(19)
Cl(32)-C(1S)-Cl(43)	93.2(17)	Cl(42)-C(1S)-Cl(31)	102.4(16)
Cl(32)-C(1S)-Cl(31)	96.7(15)	Cl(33)-C(1S)-Cl(41)	116.3(14)
Cl(42)-C(1S)-Cl(41)	96.7(16)	Cl(43)-C(1S)-Cl(41)	78.7(15)
Cl(31)-C(1S)-Cl(41)	83.0(13)	Cl(43)-C(2S)-Cl(32)	117(2)
Cl(31)-C(2S)-Cl(32)	125.7(19)	Cl(43)-C(2S)-Cl(41)	104.0(19)
Cl(31)-C(2S)-Cl(41)	112.3(18)	Cl(43)-C(2S)-Cl(42)	114(2)
Cl(31)-C(2S)-Cl(42)	110.9(17)	Cl(32)-C(2S)-Cl(42)	86.2(13)
Cl(41)-C(2S)-Cl(42)	107.6(16)	Cl(3)-Sb-Cl(1)	179.54(8)
Cl(3)-Sb-Cl(6)	90.71(9)	Cl(1)-Sb-Cl(6)	89.71(8)
Cl(3)-Sb-Cl(4)	89.48(8)	Cl(1)-Sb-Cl(4)	90.32(8)
N(1')-Cu'-N(2')	89.9(2)	N(1')-Cu'-N(3')	179.1(3)
N(1')-Cu'-N(4')	89.9(2)	N(2')-Cu'-N(3')	89.8(2)
N(2')-Cu'-N(4')	176.8(3)	N(3')-Cu'-N(4')	90.5(2)
CA1'-N(1')-Cu'	124.3(5)	CA2'-N(1')-Cu'	127.7(5)
CA3'-N(2')-Cu'	124.9(5)	CA4'-N(2')-Cu'	126.3(5)
CA5'-N(3')-Cu'	127.5(5)	CA6'-N(3')-Cu'	126.7(5)
CA7'-N(4')-Cu'	126.3(5)	CA8'-N(4')-Cu'	127.9(5)
CA2'-N(1')-CA1'	108.0(6)	CA3'-N(2')-CA4'	108.8(6)
CA5'-N(3')-CA6'	105.6(6)	CA8'-N(4')-CA7'	105.8(6)
N(1')-CA1'-CB1'	109.6(6)	CM4'-CA1'-N(1')	128.2(7)
N(1')-CA2'-CM1'	123.6(6)	N(1')-CA2'-CB2'	114.1(6)
N(2')-CA4'-CB4'	112.9(6)	N(2')-CA3'-CB3'	109.8(6)
CM1'-CA3'-N(2')	127.4(6)	CM2'-CA4'-N(2')	125.1(7)
N(3')-CA6'-CB6'	109.8(6)	N(3')-CA5'-CM2'	125.7(6)
N(3')-CA5'-CB5'	110.8(6)	CM3'-CA6'-N(3')	125.6(6)
N(4')-CA8'-CM4'	124.3(6)	N(4')-CA8'-CB8'	110.2(7)
N(4')-CA7'-CM3'	125.8(6)	N(4')-CA7'-CB7'	110.4(6)
O(1')-CB1'-CA1'	125.9(7)	O(1')-CB1'-CB2'	127.5(7)
O(2')-CB3'-CA3'	125.1(7)	O(2')-CB3'-CB4'	126.8(7)
CA2'-CB2'-CB1'	101.6(6)	CA2'-CB2'-C(21')	113.4(7)
CB1'-CB2'-C(21')	109.4(6)	CA2'-CB2'-C(11')	112.2(7)
CB1'-CB2'-C(11')	110.5(7)	C(21')-CB2'-C(11')	109.5(6)
CA1'-CB1'-CB2'	106.6(7)	CA4'-CM2'-CA5'	125.5(7)
CB3'-CB4'-CA4'	100.3(6)	CB3'-CB4'-C(31')	110.5(7)
CA4'-CB4'-C(31')	112.7(6)	CB3'-CB4'-C(41')	109.5(6)
CA4'-CB4'-C(41')	112.7(6)	C(31')-CB4'-C(41')	110.7(6)
C(22')-C(21')-CB2'	113.1(7)	CA3'-CB3'-CB4'	108.1(6)
CB5'-CB6'-CA6'	107.9(6)	CB5'-CB6'-C(61')	128.0(7)
CA6'-CB6'-C(61')	124.0(7)	CA1'-CM4'-CA8'	125.3(7)
CB8'-CB7'-CA7'	106.7(6)	CB8'-CB7'-C(71')	130.5(7)
CA7'-CB7'-C(71')	122.8(7)	CB7'-CB8'-CA8'	106.9(7)
CB7'-CB8'-C(81')	128.7(7)	CA8'-CB8'-C(81')	124.3(7)
CB8'-C(81')-C(82')	112.7(7)	C(32')-C(31')-CB4'	114.8(6)

CA6'-CM3'-CA7'	125.1(6)	CA3'-CM1'-CA2'	126.4(6)
CB7'-C(71')-C(72')	114.5(7)	CM4'-CA8'-CB8'	125.5(7)
CM4'-CA1'-CB1'	122.2(7)	CM1'-CA2'-CB2'	122.1(6)
CB6'-CB5'-CA5'	105.8(7)	CB6'-CB5'-C(51')	131.7(7)
CA5'-CB5'-C(51')	122.3(7)	CM2'-CA5'-CB5'	123.4(6)
CM3'-CA7'-CB7'	123.7(6)	CM3'-CA6'-CB6'	124.6(6)
C(42')-C(41')-CB4'	114.7(7)	CM1'-CA3'-CB3'	122.8(6)
CB6'-C(61')-C(62')	112.8(7)	CM2'-CA4'-CB4'	121.9(6)
CB5'-C(51')-C(52')	111.2(7)	C(12')-C(11')-CB2'	115.2(7)
Cl(6)-Sb-Cl(4)	90.15(9)	Cl(3)-Sb-Cl(2)	91.11(9)
Cl(1)-Sb-Cl(2)	88.47(9)	Cl(6)-Sb-Cl(2)	177.92(9)
Cl(4)-Sb-Cl(2)	90.87(9)	Cl(3)-Sb-Cl(5)	89.70(8)
Cl(1)-Sb-Cl(5)	90.49(8)	Cl(6)-Sb-Cl(5)	89.32(8)
Cl(4)-Sb-Cl(5)	179.02(9)	Cl(2)-Sb-Cl(5)	89.69(9)
Cl(4')-Sb'-Cl(6')	178.50(9)	Cl(4')-Sb'-Cl(1')	91.19(9)
Cl(6')-Sb'-Cl(1')	89.68(9)	Cl(4')-Sb'-Cl(2')	89.23(9)
Cl(6')-Sb'-Cl(2')	89.91(8)	Cl(1')-Sb'-Cl(2')	179.10(10)
Cl(4')-Sb'-Cl(3')	89.08(9)	Cl(6')-Sb'-Cl(3')	89.71(8)
Cl(1')-Sb'-Cl(3')	89.27(10)	Cl(2')-Sb'-Cl(3')	91.53(10)
Cl(4')-Sb'-Cl(5')	91.06(9)	Cl(6')-Sb'-Cl(5')	90.17(9)
Cl(1')-Sb'-Cl(5')	89.61(10)	Cl(2')-Sb'-Cl(5')	89.59(10)
Cl(3')-Sb'-Cl(5')	178.88(10)	C(12)-C(11)-H(11A)	109.00
C(12)-C(11)-H(11B)	109.00	CB2-C(11)-H(11A)	109.00
CB2-C(11)-H(11B)	109.00	H(11A)-C(11)-H(11B)	108.00
H(12A)-C(12)-H(12C)	109.00	H(12B)-C(12)-H(12C)	109.00
H(12A)-C(12)-H(12B)	109.00	C(11)-C(12)-H(12C)	109.00
C(11)-C(12)-H(12B)	109.00	C(11)-C(12)-H(12A)	109.00
CA2-CM1-HM1A	118.00	CA3-CM1-HM1A	118.00
CA4-CM2-HM2A	118.00	CA5-CM2-HM2A	118.00
CA6-CM3-HM3A	117.00	CA7-CM3-HM3A	117.00
CA1-CM4-HM4A	117.00	CA8-CM4-HM4A	117.00
CB2-C(21)-H(21A)	108.00	CB2-C(21)-H(21B)	108.00
C(22)-C(21)-H(21B)	108.00	H(21A)-C(21)-H(21B)	107.00
C(22)-C(21)-H(21A)	108.00	C(21)-C(22)-H(22B)	109.00
C(21)-C(22)-H(22C)	109.00	C(21)-C(22)-H(22A)	109.00
H(22A)-C(22)-H(22C)	109.00	H(22B)-C(22)-H(22C)	109.00
H(22A)-C(22)-H(22B)	109.00	CB4-C(31)-H(31A)	109.00
H(31A)-C(31)-H(31B)	108.00	C(32)-C(31)-H(31A)	109.00
CB4-C(31)-H(31B)	109.00	C(32)-C(31)-H(31B)	109.00
C(31)-C(32)-H(32B)	109.00	H(32A)-C(32)-H(32C)	109.00
H(32B)-C(32)-H(32C)	109.00	C(31)-C(32)-H(32A)	109.00
C(31)-C(32)-H(32C)	109.00	H(32A)-C(32)-H(32B)	109.00
CB4-C(41)-H(41A)	109.00	CB4-C(41)-H(41B)	109.00
C(42)-C(41)-H(41A)	109.00	C(42)-C(41)-H(41B)	109.00
H(41A)-C(41)-H(41B)	108.00	H(42B)-C(42)-H(42C)	109.00
H(42A)-C(42)-H(42B)	109.00	H(42A)-C(42)-H(42C)	109.00

C(41)-C(42)-H(42C)	109.00	C(41)-C(42)-H(42A)	109.00
C(41)-C(42)-H(42B)	109.00	C(52)-C(51)-H(51A)	109.00
CB5-C(51)-H(51A)	109.00	C(52)-C(51)-H(51B)	109.00
H(51A)-C(51)-H(51B)	108.00	CB5-C(51)-H(51B)	109.00
C(51)-C(52)-H(52C)	109.00	H(52B)-C(52)-H(52C)	109.00
C(51)-C(52)-H(52B)	109.00	C(51)-C(52)-H(52A)	109.00
H(52A)-C(52)-H(52B)	109.00	H(52A)-C(52)-H(52C)	109.00
C(62)-C(61)-H(61B)	109.00	C(62)-C(61)-H(61A)	109.00
CB6-C(61)-H(61A)	109.00	CB6-C(61)-H(61B)	109.00
H(61A)-C(61)-H(61B)	108.00	C(61)-C(62)-H(62A)	109.00
C(61)-C(62)-H(62B)	109.00	H(62A)-C(62)-H(62C)	109.00
H(62B)-C(62)-H(62C)	109.00	H(62A)-C(62)-H(62B)	109.00
C(61)-C(62)-H(62C)	109.00	C(72)-C(71)-H(71A)	109.00
C(72)-C(71)-H(71B)	109.00	H(71A)-C(71)-H(71B)	108.00
CB7-C(71)-H(71B)	109.00	CB7-C(71)-H(71A)	109.00
C(71)-C(72)-H(72B)	109.00	H(72A)-C(72)-H(72B)	109.00
H(72B)-C(72)-H(72C)	109.00	H(72A)-C(72)-H(72C)	109.00
C(71)-C(72)-H(72A)	109.00	C(71)-C(72)-H(72C)	109.00
C(82)-C(81)-H(81A)	109.00	CB8-C(81)-H(81B)	109.00
CB8-C(81)-H(81A)	109.00	H(81A)-C(81)-H(81B)	108.00
C(82)-C(81)-H(81B)	109.00	H(82B)-C(82)-H(82C)	109.00
H(82A)-C(82)-H(82C)	109.00	C(81)-C(82)-H(82A)	109.00
H(82A)-C(82)-H(82B)	109.00	C(81)-C(82)-H(82B)	109.00
C(81)-C(82)-H(82C)	109.00	C(12')-C(11')-H(11C)	109.00
H(11C)-C(11')-H(11D)	108.00	CB2'-C(11')-H(11D)	109.00
C(12')-C(11')-H(11D)	109.00	CB2'-C(11')-H(11C)	109.00
C(11')-C(12')-H(12F)	109.00	C(11')-C(12')-H(12D)	109.00
C(11')-C(12')-H(12E)	109.00	H(12D)-C(12')-H(12F)	109.00
H(12E)-C(12')-H(12F)	109.00	H(12D)-C(12')-H(12E)	109.00
C(22')-C(21')-H(21D)	109.00	C(22')-C(21')-H(21C)	109.00
H(21C)-C(21')-H(21D)	108.00	CB2'-C(21')-H(21C)	109.00
CB2'-C(21')-H(21D)	109.00	H(22D)-C(22')-H(22F)	109.00
H(22D)-C(22')-H(22E)	109.00	H(22E)-C(22')-H(22F)	109.00
C(21')-C(22')-H(22D)	109.00	C(21')-C(22')-H(22F)	109.00
C(21')-C(22')-H(22E)	109.00	CB4'-C(31')-H(31C)	109.00
C(32')-C(31')-H(31D)	109.00	CB4'-C(31')-H(31D)	109.00
H(31C)-C(31')-H(31D)	108.00	C(32')-C(31')-H(31C)	109.00
C(31')-C(32')-H(32F)	109.00	H(32D)-C(32')-H(32F)	109.00
C(31')-C(32')-H(32D)	109.00	H(32E)-C(32')-H(32F)	109.00
H(32D)-C(32')-H(32E)	109.00	C(31')-C(32')-H(32E)	109.00
CA3'-CM1'-HM1B	117.00	CA2'-CM1'-HM1B	117.00
CA5'-CM2'-HM2B	117.00	CA4'-CM2'-HM2B	117.00
CA6'-CM3'-HM3B	117.00	CA7'-CM3'-HM3B	117.00
CA1'-CM4'-HM4B	117.00	CA8'-CM4'-HM4B	117.00
CB4'-C(41')-H(41D)	109.00	C(42')-C(41')-H(41D)	109.00
CB4'-C(41')-H(41C)	109.00	H(41C)-C(41')-H(41D)	108.00

C(42')-C(41')-H(41C)	109.00	H(42D)-C(42')-H(42F)	109.00
H(42E)-C(42')-H(42F)	109.00	H(42D)-C(42')-H(42E)	109.00
C(41')-C(42')-H(42F)	109.00	C(41')-C(42')-H(42E)	109.00
C(41')-C(42')-H(42D)	109.00	CB5'-C(51')-H(51D)	109.00
C(52')-C(51')-H(51C)	109.00	CB5'-C(51')-H(51C)	109.00
H(51C)-C(51')-H(51D)	108.00	C(52')-C(51')-H(51D)	109.00
H(52D)-C(52')-H(52F)	109.00	C(51')-C(52')-H(52F)	109.00
H(52D)-C(52')-H(52E)	109.00	C(51')-C(52')-H(52D)	109.00
H(52E)-C(52')-H(52F)	109.00	C(51')-C(52')-H(52E)	109.00
CB6'-C(61')-H(61C)	109.00	CB6'-C(61')-H(61D)	109.00
H(61C)-C(61')-H(61D)	108.00	C(62')-C(61')-H(61D)	109.00
C(62')-C(61')-H(61C)	109.00	C(61')-C(62')-H(62D)	109.00
H(62D)-C(62')-H(62E)	109.00	C(61')-C(62')-H(62E)	109.00
C(61')-C(62')-H(62F)	109.00	H(62E)-C(62')-H(62F)	109.00
H(62D)-C(62')-H(62F)	109.00	CB7'-C(71')-H(71D)	109.00
C(72')-C(71')-H(71C)	109.00	H(71C)-C(71')-H(71D)	108.00
C(72')-C(71')-H(71D)	109.00	CB7'-C(71')-H(71C)	109.00
H(72E)-C(72')-H(72F)	109.00	H(72D)-C(72')-H(72F)	109.00
C(71')-C(72')-H(72F)	109.00	C(71')-C(72')-H(72E)	109.00
H(72D)-C(72')-H(72E)	109.00	C(71')-C(72')-H(72D)	109.00
CB8'-C(81')-H(81D)	109.00	H(81C)-C(81')-H(81D)	108.00
C(82')-C(81')-H(81C)	109.00	C(82')-C(81')-H(81D)	109.00
CB8'-C(81')-H(81C)	109.00	H(82E)-C(82')-H(82F)	109.00
C(81')-C(82')-H(82D)	109.00	H(82D)-C(82')-H(82F)	109.00
C(81')-C(82')-H(82F)	109.00	H(82D)-C(82')-H(82E)	109.00
C(81')-C(82')-H(82E)	109.00	Cl(33)-C(1S)-H(1SA)	108.00
Cl(31)-C(1S)-H(1SA)	108.00	Cl(32)-C(1S)-H(1SA)	108.00
C(2S)-C(1S)-H(1SA)	90.00	Cl(42)-C(1S)-H(1SA)	25.00
Cl(43)-C(1S)-H(1SA)	115.00	C(1S)-C(2S)-H(2SA)	164.00
Cl(31)-C(2S)-H(2SA)	105.00	Cl(32)-C(2S)-H(2SA)	116.00
Cl(41)-C(2S)-H(2SA)	110.00	Cl(42)-C(2S)-H(2SA)	110.00
Cl(43)-C(2S)-H(2SA)	110.00		

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters (A^2) for [Cu(trioxoOEHP)][$SbCl_6$]·1.25[CH_2Cl_2].[a] The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu	0.0090(2)	0.0091(2)	0.0198(2)	0.0005(2)	-0.0014(2)	-0.0005(1)
N(1)	0.0140(14)	0.0100(13)	0.0212(15)	0.0013(11)	-0.0018(11)	-0.0016(10)
N(2)	0.0119(13)	0.0115(13)	0.026(2)	-0.0006(11)	-0.0010(11)	0.0007(11)
N(3)	0.0118(13)	0.0113(13)	0.022(2)	-0.0001(11)	0.0010(11)	0.0010(10)
N(4)	0.0129(13)	0.0154(14)	0.0153(14)	0.0003(11)	-0.0007(11)	-0.0024(11)
C(a1)	0.021(2)	0.013(2)	0.018(2)	0.0026(13)	-0.0030(14)	-0.0055(13)
C(a2)	0.020(2)	0.012(2)	0.024(2)	0.0014(13)	-0.0041(14)	-0.0006(13)
C(a3)	0.012(2)	0.013(2)	0.028(2)	0.0002(14)	-0.0010(14)	0.0003(12)
C(a4)	0.010(2)	0.015(2)	0.029(2)	0.0005(14)	-0.0015(14)	-0.0012(13)
C(a5)	0.015(2)	0.011(2)	0.026(2)	-0.0005(13)	0.0003(14)	-0.0003(13)
C(a6)	0.017(2)	0.012(2)	0.023(2)	-0.0022(13)	0.0008(14)	0.0013(12)
C(a7)	0.009(2)	0.021(2)	0.016(2)	-0.0001(13)	-0.0003(12)	0.0023(12)
C(a8)	0.012(2)	0.020(2)	0.015(2)	0.0006(13)	-0.0001(12)	-0.0026(13)
C(b1)	0.020(2)	0.017(2)	0.027(2)	0.0020(14)	-0.0051(15)	-0.0037(14)
C(b2)	0.020(2)	0.011(2)	0.051(3)	0.004(2)	-0.013(2)	-0.0034(14)
C(b3)	0.014(2)	0.016(2)	0.040(2)	-0.001(2)	-0.003(2)	-0.0011(13)
C(b4)	0.011(2)	0.014(2)	0.047(2)	0.002(2)	-0.003(2)	0.0003(13)
C(b5)	0.017(2)	0.013(2)	0.028(2)	-0.0009(14)	0.0001(14)	0.0004(13)
C(b6)	0.014(2)	0.012(2)	0.035(2)	-0.0007(15)	-0.0008(15)	0.0009(12)
C(b7)	0.013(2)	0.024(2)	0.015(2)	0.0011(13)	-0.0006(13)	-0.0003(13)
C(b8)	0.012(2)	0.025(2)	0.016(2)	0.0009(14)	0.0002(13)	-0.0018(13)
C(m1)	0.014(2)	0.013(2)	0.029(2)	-0.0011(14)	-0.0041(14)	0.0031(13)
C(m2)	0.012(2)	0.012(2)	0.036(2)	0.0014(15)	0.0014(14)	-0.0035(12)
C(m3)	0.013(2)	0.015(2)	0.025(2)	-0.0004(14)	0.0001(13)	0.0049(12)
C(m4)	0.014(2)	0.019(2)	0.018(2)	0.0003(13)	0.0006(13)	-0.0070(13)
O(1)	0.0239(14)	0.0156(13)	0.042(2)	0.0010(12)	-0.0035(12)	-0.0078(10)

Table S7. (cont.)

O(2)	0.0164(13)	0.0177(13)	0.073(2)	0.0054(14)	-0.0039(14)	0.0046(11)
O(3)	0.0204(13)	0.0114(12)	0.051(2)	0.0026(12)	0.0010(12)	-0.0035(10)
C(11)	0.022(2)	0.018(2)	0.067(3)	-0.007(2)	-0.007(2)	-0.001(2)
C(21)	0.025(2)	0.020(2)	0.060(3)	0.018(2)	-0.006(2)	-0.005(2)
C(31)	0.018(2)	0.024(2)	0.054(3)	0.000(2)	-0.011(2)	-0.0014(15)
C(41)	0.011(2)	0.022(2)	0.060(3)	0.004(2)	0.006(2)	-0.0001(14)
C(51)	0.024(2)	0.014(2)	0.050(3)	-0.009(2)	0.008(2)	0.0002(14)
C(61)	0.026(2)	0.014(2)	0.041(2)	0.008(2)	-0.005(2)	0.0014(14)
C(71)	0.010(2)	0.026(2)	0.025(2)	0.000(2)	0.0004(14)	0.0013(14)
C(81)	0.013(2)	0.026(2)	0.027(2)	0.000(2)	0.0001(14)	-0.0053(14)
C(12)	0.026(2)	0.028(2)	0.093(4)	-0.030(3)	0.015(2)	-0.002(2)
C(22)	0.035(2)	0.039(3)	0.050(3)	0.012(2)	-0.002(2)	-0.001(2)
C(32)	0.042(3)	0.047(3)	0.043(3)	0.001(2)	-0.007(2)	-0.002(2)
C(42)	0.033(2)	0.052(3)	0.047(3)	-0.002(2)	0.011(2)	0.001(2)
C(52)	0.041(3)	0.031(2)	0.043(3)	-0.013(2)	0.011(2)	-0.006(2)
C(62)	0.053(3)	0.027(2)	0.035(2)	0.007(2)	-0.005(2)	0.000(2)
C(72)	0.032(2)	0.040(2)	0.029(2)	0.004(2)	-0.005(2)	0.014(2)
C(82)	0.032(2)	0.036(2)	0.030(2)	-0.009(2)	-0.007(2)	-0.009(2)
Sb	0.0239(1)	0.0254(1)	0.0161(1)	-0.0020(1)	-0.0023(1)	0.0025(1)
Cl(1)	0.0358(5)	0.0325(5)	0.0317(5)	0.0064(4)	-0.0105(4)	0.0019(4)
Cl(2)	0.0325(6)	0.0569(7)	0.0412(6)	0.0092(5)	0.0103(5)	0.0117(5)
Cl(3)	0.0604(7)	0.0305(5)	0.0313(6)	-0.0003(4)	-0.0086(5)	-0.0136(5)
Cl(4)	0.0516(7)	0.0445(6)	0.0245(5)	0.0053(4)	-0.0065(5)	0.0143(5)
Cl(5)	0.0397(6)	0.0725(9)	0.0412(7)	0.0078(6)	0.0165(5)	0.0138(6)
Cl(6)	0.0652(8)	0.0393(6)	0.0442(7)	-0.0149(5)	-0.0246(6)	0.0011(6)

[a] The estimated standard deviations of the least significant digits are given in parentheses.

Table S8. Anisotropic displacement parameters ($Å^2$) for [Cu(2,7-DioxoOEiBC)] $[SbCl_6] \cdot 0.5\ CHCl_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu	0.0190	0.0150	0.0100	0.0000	-0.0010	0.0010
O(1)	0.0370	0.0160	0.0210	0.0040	-0.0020	-0.0040
O(2)	0.0970	0.0220	0.0080	-0.0020	0.0070	-0.0070
N(1)	0.0150	0.0160	0.0160	-0.0030	0.0020	-0.0030
N(2)	0.0240	0.0120	0.0140	0.0000	-0.0090	-0.0020
N(3)	0.0130	0.0190	0.0120	-0.0010	0.0020	-0.0050
N(4)	0.0190	0.0150	0.0170	-0.0010	-0.0030	0.0000
CA1	0.0250	0.0100	0.0190	0.0010	0.0000	0.0060
CA2	0.0110	0.0230	0.0150	0.0010	-0.0030	0.0050
CA3	0.0220	0.0230	0.0130	-0.0060	-0.0010	-0.0020
CA4	0.0230	0.0190	0.0160	0.0030	0.0000	0.0000
CA5	0.0190	0.0190	0.0130	0.0060	0.0000	-0.0020
CA6	0.0110	0.0280	0.0120	0.0020	-0.0020	-0.0030
CA7	0.0100	0.0260	0.0070	0.0010	0.0010	0.0040
CA8	0.0150	0.0190	0.0210	-0.0050	0.0040	-0.0040
CB1	0.0140	0.0180	0.0170	0.0000	-0.0010	0.0040
CB2	0.0260	0.0180	0.0090	0.0010	0.0050	-0.0030
C(11)	0.0280	0.0180	0.0180	0.0050	-0.0050	0.0030
CB3	0.0360	0.0210	0.0200	0.0010	0.0110	0.0030
C(12)	0.0310	0.0210	0.0280	0.0040	-0.0070	-0.0020
CB4	0.0300	0.0150	0.0140	0.0010	-0.0010	0.0040
CB5	0.0110	0.0170	0.0200	0.0070	0.0040	0.0010
CB6	0.0180	0.0270	0.0110	0.0010	-0.0060	-0.0010
CB7	0.0180	0.0260	0.0160	-0.0110	-0.0040	0.0020
CB8	0.0090	0.0150	0.0180	-0.0050	0.0020	0.0000
CM1	0.0300	0.0150	0.0120	-0.0040	0.0000	0.0030
CM2	0.0280	0.0140	0.0160	0.0040	0.0020	0.0030
CM3	0.0170	0.0360	0.0090	-0.0060	0.0000	0.0030
CM4	0.0160	0.0130	0.0160	0.0000	-0.0030	-0.0020
C(21)	0.0380	0.0150	0.0130	0.0020	0.0020	-0.0070
C(22)	0.0340	0.0250	0.0220	0.0020	0.0050	0.0010
C(31)	0.0430	0.0120	0.0350	-0.0100	-0.0010	0.0090
C(32)	0.0360	0.0390	0.0590	-0.0250	0.0070	0.0060
C(41)	0.0520	0.0220	0.0180	-0.0040	-0.0030	-0.0090
C(42)	0.0440	0.0470	0.0410	-0.0130	0.0070	-0.0150
C(51)	0.0260	0.0260	0.0140	0.0060	-0.0070	-0.0030
C(52)	0.0340	0.0300	0.0190	0.0060	0.0070	0.0050
C(61)	0.0300	0.0300	0.0100	0.0060	-0.0010	-0.0050
C(62)	0.0220	0.0430	0.0290	0.0070	0.0000	0.0010
C(71)	0.0170	0.0270	0.0160	-0.0070	-0.0060	0.0020

C(72)	0.0310	0.0320	0.0170	-0.0030	-0.0030	0.0070
C(81)	0.0200	0.0190	0.0230	-0.0070	0.0020	-0.0060
C(82)	0.0250	0.0410	0.0350	-0.0050	0.0070	-0.0050
Cu'	0.0200	0.0170	0.0130	0.0020	0.0020	-0.0010
O(1')	0.0680	0.0190	0.0270	-0.0040	0.0030	-0.0100
O(2')	0.0520	0.0220	0.0120	0.0070	0.0000	-0.0010
N(1')	0.0230	0.0180	0.0220	0.0000	0.0060	0.0000
N(2')	0.0170	0.0160	0.0150	0.0000	-0.0090	-0.0010
N(3')	0.0210	0.0310	0.0110	0.0010	0.0030	0.0100
N(4')	0.0120	0.0260	0.0140	0.0120	0.0020	0.0100
C(11')	0.0440	0.0210	0.0250	-0.0020	-0.0080	-0.0030
C(12')	0.0450	0.0400	0.0520	-0.0050	-0.0120	0.0010
C(21')	0.0410	0.0170	0.0260	-0.0020	0.0060	0.0010
CA1'	0.0190	0.0100	0.0230	-0.0030	0.0000	0.0000
C(22')	0.0390	0.0350	0.0370	-0.0070	0.0090	0.0030
CA2'	0.0130	0.0180	0.0250	-0.0010	0.0080	-0.0030
CA3'	0.0250	0.0170	0.0120	-0.0010	-0.0060	0.0010
CA4'	0.0190	0.0120	0.0210	0.0010	-0.0020	0.0010
CA5'	0.0150	0.0090	0.0220	-0.0040	0.0030	-0.0020
CA6'	0.0020	0.0320	0.0170	0.0030	-0.0010	-0.0030
CA7'	0.0060	0.0260	0.0260	0.0100	0.0030	0.0030
CA8'	0.0150	0.0130	0.0310	0.0080	0.0050	0.0020
CB1'	0.0300	0.0290	0.0210	0.0020	0.0020	0.0070
CB2'	0.0420	0.0140	0.0160	-0.0030	0.0020	0.0000
C(31')	0.0380	0.0110	0.0340	0.0000	0.0040	-0.0070
CB3'	0.0240	0.0210	0.0140	0.0020	0.0040	0.0040
C(32')	0.0350	0.0380	0.0310	0.0100	0.0020	-0.0090
CB4'	0.0310	0.0170	0.0060	-0.0040	-0.0040	0.0030
CB5'	0.0170	0.0330	0.0140	-0.0090	0.0060	-0.0030
CB6'	0.0100	0.0400	0.0190	-0.0030	0.0000	-0.0040
CB7'	0.0090	0.0360	0.0210	0.0110	-0.0010	-0.0010
CB8'	0.0160	0.0210	0.0390	0.0110	0.0070	0.0050
CM1'	0.0200	0.0240	0.0150	-0.0020	-0.0030	-0.0030
CM2'	0.0200	0.0160	0.0190	-0.0040	-0.0020	-0.0020
CM3'	0.0090	0.0340	0.0120	0.0050	0.0040	0.0010
CM4'	0.0290	0.0100	0.0330	0.0030	0.0090	-0.0020
C(41')	0.0370	0.0240	0.0310	0.0020	-0.0060	0.0060
C(42')	0.0410	0.0380	0.0290	0.0040	-0.0060	0.0080
C(51')	0.0230	0.0310	0.0160	-0.0110	0.0060	-0.0040
C(52')	0.0240	0.0280	0.0310	-0.0080	-0.0030	0.0010
C(61')	0.0170	0.0420	0.0190	0.0030	-0.0010	-0.0010
C(62')	0.0250	0.0880	0.0110	0.0100	-0.0090	-0.0120
C(71')	0.0250	0.0290	0.0240	0.0140	0.0020	-0.0010
C(72')	0.0260	0.0340	0.0160	0.0070	0.0000	-0.0080
C(81')	0.0260	0.0270	0.0400	0.0160	0.0090	-0.0050
C(82')	0.0450	0.0220	0.0650	0.0110	0.0110	0.0050

Cl(31)	0.0560	0.0300	0.0540	-0.0080	0.0190	-0.0040
Cl(32)	0.0900	0.0780	0.0830	-0.0430	-0.0040	-0.0210
Cl(33)	0.1020	0.0640	0.1150	-0.0460	-0.0620	0.0120
Cl(41)	0.1430	0.1160	0.0720	0.0190	0.0260	0.0050
Cl(42)	0.0630	0.0660	0.0560	0.0060	0.0030	0.0030
Cl(43)	0.2800	0.1690	0.1900	-0.0460	0.0640	-0.0690
C(1S)	0.2200	0.0110	0.1030	-0.0110	0.0800	-0.0210
C(2S)	0.0480	0.0800	0.0800	0.0100	-0.0130	0.0000
Sb	0.0170	0.0260	0.0180	-0.0010	0.0010	0.0020
Cl(1)	0.0290	0.0500	0.0220	0.0100	-0.0020	0.0030
Cl(2)	0.0420	0.0460	0.0320	-0.0030	0.0160	0.0130
Cl(3)	0.0350	0.0490	0.0340	0.0080	-0.0130	0.0030
Cl(4)	0.0390	0.0430	0.0310	-0.0020	0.0010	-0.0170
Cl(5)	0.0300	0.0320	0.0460	0.0060	-0.0040	-0.0070
Cl(6)	0.0270	0.0590	0.0380	-0.0230	0.0030	0.0080
Sb'	0.0200	0.0250	0.0180	-0.0010	-0.0030	0.0030
Cl(1')	0.0440	0.0430	0.0560	-0.0240	0.0070	0.0090
Cl(2')	0.0470	0.0560	0.0470	-0.0210	-0.0150	0.0290
Cl(3')	0.0250	0.0580	0.0560	0.0250	-0.0030	-0.0090
Cl(4')	0.0620	0.0440	0.0320	0.0030	-0.0230	-0.0010
Cl(5')	0.0440	0.0410	0.0630	0.0120	0.0000	-0.0140
Cl(6')	0.0320	0.0480	0.0330	0.0000	-0.0140	0.0080

Table S9.Hydrogen coordinates and isotropic displacement parameters (A^2) for [Cu(trioxoOEHP)][$SbCl_6$]·1.25[CH_2Cl_2].[a]

	x	y	z	U(eq)
H(m1)	1.07907(11)	0.10763(11)	0.2955(4)	0.022
H(m2)	1.08755(11)	0.30391(11)	0.2053(4)	0.024
H(m3)	0.88987(11)	0.31101(11)	0.1834(4)	0.021
H(m4)	0.88314(11)	0.11380(11)	0.2005(4)	0.020
H(1A)	1.01390(14)	0.00931(13)	0.2204(6)	0.043
H(1B)	1.05600(14)	0.03621(13)	0.2431(6)	0.043
H(2A)	0.98167(13)	0.08332(13)	0.5038(5)	0.042
H(2B)	0.98158(13)	0.03392(13)	0.4718(5)	0.042
H(4A)	1.15386(12)	0.27009(13)	0.1113(5)	0.037
H(4B)	1.18041(12)	0.22791(13)	0.1343(5)	0.037
H(5A)	0.95901(13)	0.40792(12)	0.2552(5)	0.035
H(5B)	0.91792(13)	0.37930(12)	0.2731(5)	0.035
H(6A)	0.92211(13)	0.36776(12)	0.0105(5)	0.033
H(6B)	0.96588(13)	0.39233(12)	-0.0021(5)	0.033
H(7A)	0.81953(11)	0.29266(12)	0.2246(4)	0.025
H(7B)	0.78728(11)	0.25430(12)	0.2068(4)	0.025
H(8A)	0.78429(11)	0.17787(12)	0.1994(4)	0.026
H(8B)	0.81349(11)	0.13825(12)	0.2360(4)	0.026
H(1C)	1.0433(11)	0.0251(6)	-0.0008(9)	0.074
H(1D)	1.0427(11)	0.0745(6)	0.0337(7)	0.074
H(1E)	0.99933(15)	0.0496(13)	0.0123(11)	0.074
H(2C)	1.03510(15)	0.0484(12)	0.6340(11)	0.062
H(2D)	1.0558(5)	0.0823(4)	0.5312(34)	0.062
H(2E)	1.0569(5)	0.0332(8)	0.4924(25)	0.062
H(4C)	1.1521(7)	0.2292(10)	-0.0952(8)	0.066
H(4D)	1.1054(5)	0.2321(10)	-0.0336(21)	0.066
H(4E)	1.1326(11)	0.1901(2)	-0.0119(16)	0.066

Table S9. (cont.)

H(5C)	0.9505(9)	0.3880(7)	0.4938(6)	0.057
H(5D)	0.9938(2)	0.3691(11)	0.4351(11)	0.057
H(5E)	0.9534(10)	0.3393(4)	0.4514(14)	0.057
H(6C)	0.9603(11)	0.3490(5)	-0.1977(5)	0.057
H(6D)	0.9504(8)	0.3086(5)	-0.1038(22)	0.057
H(6E)	0.9965(3)	0.3290(9)	-0.1026(22)	0.057
H(7C)	0.7818(7)	0.2991(8)	0.0108(6)	0.051
H(7D)	0.8001(10)	0.2547(2)	-0.0396(8)	0.051
H(7E)	0.8311(4)	0.2940(9)	-0.0203(11)	0.051
H(8C)	0.7806(6)	0.1276(8)	0.0150(9)	0.049
H(8D)	0.8306(5)	0.1304(9)	-0.0059(13)	0.049
H(8E)	0.8015(10)	0.1701(2)	-0.0426(6)	0.049

[a] The estimated standard deviations of the least significant digits are given in parentheses.

Table S10. Fixed atomic coordinates for hydrogen atoms of [Cu(2,7-dioxoP)][$SbCl_6$] 0.5 $CHCl_3$

	x	y	z	U(eq)
HM1A	0.71610	0.30995	0.02854	0.023
HM2A	0.73096	0.12854	0.14277	0.023
HM3A	0.73965	0.36942	0.22765	0.025
HM4A	0.80972	0.54691	0.11404	0.018
H(11A)	0.57720	0.41110	0.00951	0.026
H(11B)	0.59108	0.48568	0.01295	0.026
H(12A)	0.38889	0.45122	0.03642	0.040
H(12B)	0.47381	0.40493	0.05801	0.040
H(12C)	0.48786	0.48042	0.06150	0.040
H(21A)	0.84682	0.46892	0.00094	0.026
H(21B)	0.82797	0.39426	0.00068	0.026
H(22A)	1.05889	0.41918	0.00839	0.041
H(22B)	1.02064	0.45918	0.03796	0.041
H(22C)	1.00155	0.38358	0.03770	0.041
H(31A)	0.90793	0.09397	0.06209	0.036
H(31B)	0.91394	0.09114	0.09777	0.036
H(32A)	1.10374	0.14663	0.07926	0.067
H(32B)	1.00636	0.19683	0.06288	0.067
H(32C)	1.01244	0.19397	0.09899	0.067
H(41A)	0.65259	0.06714	0.09909	0.037
H(41B)	0.64928	0.07018	0.06337	0.037
H(42A)	0.42589	0.08594	0.08262	0.066
H(42B)	0.47706	0.14608	0.10163	0.066
H(42C)	0.47371	0.14915	0.06550	0.066
H(51A)	0.64350	0.09765	0.18997	0.026
H(51B)	0.66774	0.11271	0.22463	0.026
H(52A)	0.83604	0.03889	0.20751	0.041
H(52B)	0.88445	0.08850	0.18229	0.041
H(52C)	0.90895	0.10371	0.21730	0.041
H(61A)	0.75832	0.27915	0.25801	0.028
H(61B)	0.75313	0.20385	0.25803	0.028
H(62A)	0.55761	0.24454	0.28385	0.047
H(62B)	0.51444	0.28324	0.25423	0.047
H(62C)	0.50919	0.20715	0.25425	0.047
H(71A)	0.72647	0.47152	0.24405	0.024
H(71B)	0.76194	0.54297	0.23582	0.024
H(72A)	0.93186	0.50115	0.26810	0.040
H(72B)	0.96185	0.44558	0.24430	0.040
H(72C)	0.99767	0.51774	0.23599	0.040
H(81A)	0.80970	0.61147	0.19293	0.025
H(81B)	0.78052	0.61124	0.15775	0.025
H(82A)	1.00203	0.65212	0.16674	0.051

H(82B)	1.04340	0.58754	0.18352	0.051
H(82C)	1.01392	0.58730	0.14796	0.051
HM1B	0.24049	0.30515	0.47092	0.024
HM2B	0.16986	0.12465	0.35746	0.022
HM3B	0.26160	0.35908	0.27094	0.022
HM4B	0.31160	0.54131	0.38422	0.029
H(11C)	0.42793	0.45701	0.49476	0.036
H(11D)	0.41202	0.38228	0.49297	0.036
H(12D)	0.63357	0.41137	0.47767	0.068
H(12E)	0.55618	0.37966	0.44968	0.068
H(12F)	0.57229	0.45532	0.45149	0.068
H(21C)	0.15404	0.40657	0.49532	0.034
H(21D)	0.17993	0.48072	0.49292	0.034
H(22D)	-0.04356	0.45738	0.47723	0.056
H(22E)	0.04000	0.48561	0.44926	0.056
H(22F)	0.01383	0.41065	0.45169	0.056
H(31C)	0.00066	0.08958	0.40072	0.033
H(31D)	-0.01444	0.10209	0.43579	0.033
H(32D)	-0.19397	0.15397	0.40960	0.052
H(32E)	-0.10158	0.20651	0.42576	0.052
H(32F)	-0.08629	0.19385	0.39026	0.052
H(41C)	0.25040	0.06290	0.40357	0.037
H(41D)	0.23621	0.06689	0.43911	0.037
H(42D)	0.46569	0.07395	0.42549	0.054
H(42E)	0.43407	0.13511	0.40514	0.054
H(42F)	0.41970	0.13915	0.44111	0.054
H(51C)	0.19898	0.08538	0.30915	0.028
H(51D)	0.17134	0.10419	0.27500	0.028
H(52D)	-0.03244	0.06193	0.29675	0.041
H(52E)	-0.02902	0.11582	0.32228	0.041
H(52F)	-0.05691	0.13480	0.28782	0.041
H(61C)	0.22776	0.19431	0.24137	0.031
H(61D)	0.27320	0.26657	0.24190	0.031
H(62D)	0.06448	0.25700	0.21586	0.062
H(62E)	-0.00368	0.22577	0.24515	0.062
H(62F)	0.04224	0.29879	0.24568	0.062
H(71C)	0.26388	0.53394	0.26234	0.031
H(71D)	0.20774	0.46483	0.25575	0.031
H(72D)	0.40711	0.48240	0.22684	0.038
H(72E)	0.49134	0.49601	0.25707	0.038
H(72F)	0.43452	0.42609	0.25040	0.038
H(81C)	0.34434	0.60117	0.30529	0.037
H(81D)	0.35558	0.59988	0.34098	0.037
H(82D)	0.16632	0.66342	0.32653	0.066
H(82E)	0.10192	0.60417	0.30894	0.066
H(82F)	0.11328	0.60287	0.34501	0.066

H(1SA)	0.24350	0.31067	-0.01764	0.134
H(2SA)	0.48112	0.27539	0.00672	0.083