Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1996, 35(26), 7500-7507, DOI:10.1021/ic9610748

Table S1. Crystal Data and Intensity Data Collection Parameters for $[Ni(OEP^{\bullet/2})]_2SbCl_6$.

Parameter	Value
compound	$[Ni(OEP^{\bullet/2})]_2SbCl_6 \bullet CH_2Cl_2$
empirical formula	$C_{72}H_{88}SbNi_2Cl_6N_8 \bullet CH_2Cl_2$
formula weight, Daltons	1602.38
crystal dimensions, mm	0.23 x 0.43 x 0.46
crystal color	brown
crystal shape	fragment from a large plate
temperature, deg K	124±2
crystal system	orthorhombic
space group	*Pbcn* (No. 60)
a, Å	16.744(6)
b, Å	14.785(2)
c, Å	29.173(5)
V, A^3	7221.9
lattice parameter refinement	25 reflns; 17.4°<2θ<34.4°
Z	4
calculated density, g/cm^3	1.47
μ(MoKα), cm^{-1}	12.38
diffractometer	Enraf-Nonius CAD4
radiation	graphite crystal, incident beam monochromated MoKα, $\bar{\lambda}$=0.71073Å
attenuator	Zr foil, factor 19.3
take-off angle, deg	2.8
detector aperture, mm	horizontal 2.0-2.5 vertical 4.0
crystal-detector distance, cm	21
omega width at half-height, deg	0.32
scan type	ω/2θ
scan rate, deg/min in omega	4.12
scan width, deg	0.90+0.344tanθ
2θ range, deg	3.0 to 54.9
sinθ/λ maximum	0.649
data total measured	11061
unique measured	7528
unique $F_o>3\sigma(F_o)$	3960
corrections, on I	Lorentz-polarization absorption (transmission: 0.788 to 1.000) absorption (transmission: 1.000 to 1.068)
reflection averaging (3033 multiply measured)	$R_{merge}(I)$=0.016 $R_{merge}(F)$=0.026
refinement	full-matrix least-squares
hydrogen atom	idealized riding; d[CH]=1.00Å; $U_{ij}[H]=1.0U_{ij}[C_{attached}]$
minimization function	$\Sigma w(\|F_o\|-\|F_c\|)^2$
p, weight=$[\sigma^2(F)^2+p^2F^2]^{-1/2}$	0.03
anomalous dispersion	all nonhydrogen atoms
data:variable ratio	9.5

$R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ 0.073

$R_2=(\Sigma w(F_o-F_c)^2/\Sigma wF_o^2)^{1/2}$ 0.075

goodness of fit 2.43

computer hardware VAXstation 3200

computer software RAELS90 and SDP/VAX

Table S2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Ni(OEP^{\bullet/2})]_2SbCl_6 \cdot CH_2Cl_2$.[a]

atom	x	y	z	U(eq)
Sb[b]	0.0221(1)	0.5720(1)	0.4599(1)	0.034(1)
Cl(1)[b]	-0.0010(2)	0.6058(3)	0.5367(1)	0.066(1)
Cl(2)[b]	0.1040(3)	0.4532(4)	0.4815(2)	0.117(3)
Cl(3)[b]	0.0459(3)	0.5374(3)	0.3814(2)	0.116(2)
Cl(4)[b]	-0.0609(3)	0.6926(4)	0.4380(2)	0.151(4)
Cl(5)[b]	0.1324(3)	0.6690(4)	0.4599(1)	0.086(2)
Cl(6)[b]	-0.0887(2)	0.4745(3)	0.4600(1)	0.107(2)
Ni	0.09678(5)	0.07249(7)	0.23056(3)	0.018(1)
N(1)	0.0979(3)	0.0825(3)	0.2972(2)	0.018(1)
N(2)	0.1003(3)	0.2044(4)	0.2259(2)	0.021(1)
N(3)	0.0967(4)	0.0635(4)	0.1638(2)	0.020(1)
N(4)	0.0971(4)	-0.0592(4)	0.2349(2)	0.019(1)
C(a1)	0.1073(5)	0.0133(6)	0.3288(2)	0.025(2)
C(a2)	0.0908(4)	0.1596(5)	0.3237(2)	0.020(2)
C(a3)	0.0939(5)	0.2665(5)	0.2610(2)	0.023(2)
C(a4)	0.1083(4)	0.2549(6)	0.1865(2)	0.025(2)
C(a5)	0.1048(5)	0.1310(5)	0.1334(2)	0.023(2)
C(a6)	0.0868(5)	-0.0143(5)	0.1372(2)	0.023(2)
C(a7)	0.0896(5)	-0.1210(5)	0.2004(3)	0.026(2)
C(a8)	0.1068(5)	-0.1108(5)	0.2735(3)	0.024(2)
C(b1)	0.1073(5)	0.0475(5)	0.3749(2)	0.023(2)
C(b2)	0.0946(5)	0.1362(5)	0.3718(2)	0.024(2)
C(b3)	0.0994(5)	0.3578(5)	0.2432(3)	0.025(2)
C(b4)	0.1096(4)	0.3513(5)	0.1980(3)	0.026(2)
C(b5)	0.1042(5)	0.0966(6)	0.0861(2)	0.028(2)

Table S2. continued (page 2)

C(b6)	0.0897(5)	0.0069(6)	0.0889(3)	0.029(2)
C(b7)	0.0949(5)	-0.2135(5)	0.2174(3)	0.028(2)
C(b8)	0.1071(4)	-0.2072(6)	0.2626(3)	0.029(2)
C(m1)	0.0866(4)	0.2454(5)	0.3067(2)	0.022(2)
C(m2)	0.1131(5)	0.2213(5)	0.1432(2)	0.026(2)
C(m3)	0.0818(5)	-0.0988(5)	0.1540(3)	0.026(2)
C(m4)	0.1135(4)	-0.0763(5)	0.3176(2)	0.021(2)
C(11)	0.1211(5)	-0.0109(6)	0.4163(2)	0.032(2)
C(21)	0.0900(5)	0.2042(6)	0.4101(2)	0.031(2)
C(31)	0.1002(5)	0.4408(5)	0.2728(3)	0.031(2)
C(41)	0.1214(5)	0.4260(6)	0.1631(3)	0.035(2)
C(51)	0.1177(5)	0.1549(7)	0.0446(3)	0.059(3)
C(61)	0.0819(5)	-0.0632(7)	0.0509(2)	0.036(2)
C(71)	0.0949(5)	-0.2966(5)	0.1880(3)	0.035(2)
C(81)	0.1200(5)	-0.2791(5)	0.2968(3)	0.033(2)
C(12)	0.2087(6)	-0.0266(8)	0.4236(3)	0.051(3)
C(22)	0.1698(5)	0.2487(7)	0.4202(3)	0.042(2)
C(32)	0.1835(6)	0.4592(6)	0.2924(4)	0.049(3)
C(42)	0.2099(6)	0.4344(7)	0.1492(3)	0.048(2)
C(52)	0.2094(6)	0.1743(8)	0.0392(3)	0.057(2)
C(62)	0.1635(6)	-0.1047(7)	0.0397(3)	0.051(2)
C(72)	0.1765(6)	-0.3179(7)	0.1677(4)	0.054(3)
C(82)	0.2075(6)	-0.2899(6)	0.3102(3)	0.042(2)
C(s1)	0.0267(0)	0.6196(6)	0.4286(4)	0.103(3)
Cl(s1)	0.0719(6)	0.7276(4)	0.4293(2)	0.110(2)
Cl(s2)	0.0648(6)	0.5601(5)	0.3808(3)	0.104(2)

[a] U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. The estimated standard deviations of the least significant digits are given in parentheses. [b] Occupancy factor 0.5.

Table S3. General Atomic Displacement Parameters (in $Å^2$)[a] for the Atoms Refined Anisotropically For $[Ni(OEP^{+/2})]_2SbCl_6$.[a]

Name	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni	0.016(1)	0.021(1)	0.016(1)	0.001(1)	0.001(1)	-0.001(1)
N(1)	0.017(3)	0.021(3)	0.017(3)	0.002(3)	0.001(2)	0.003(2)
C(a1)	0.012(4)	0.039(5)	0.024(4)	-0.004(4)	0.002(3)	0.002(3)
C(a2)	0.012(4)	0.031(4)	0.015(3)	0.002(3)	-0.003(3)	-0.004(3)
C(b1)	0.024(5)	0.025(4)	0.021(3)	0.002(3)	0.003(3)	0.006(3)
C(b2)	0.018(4)	0.033(4)	0.021(3)	-0.001(4)	0.001(3)	-0.004(3)
C(m1)	0.017(4)	0.026(4)	0.022(4)	0.005(3)	0.003(3)	-0.005(3)
N(2)	0.015(3)	0.024(3)	0.024(3)	-0.001(3)	-0.002(3)	-0.002(3)
C(a3)	0.009(4)	0.030(4)	0.029(4)	-0.001(4)	-0.001(3)	0.000(3)
C(a4)	0.009(4)	0.039(4)	0.027(4)	0.004(3)	-0.003(3)	0.006(3)
C(b3)	0.015(4)	0.025(4)	0.035(4)	0.005(4)	-0.003(3)	0.002(3)
C(b4)	0.012(4)	0.033(4)	0.034(4)	0.001(3)	0.002(3)	0.004(4)
C(m2)	0.023(5)	0.032(5)	0.023(4)	0.003(4)	0.001(3)	0.005(3)
N(3)	0.014(3)	0.028(3)	0.019(3)	0.005(3)	0.001(2)	0.000(3)
C(a5)	0.011(4)	0.032(4)	0.025(4)	0.002(4)	0.004(3)	0.001(3)
C(a6)	0.019(4)	0.031(4)	0.018(3)	-0.001(4)	-0.003(3)	-0.009(3)
C(b5)	0.022(4)	0.041(5)	0.020(3)	0.007(4)	0.002(3)	0.000(3)
C(b6)	0.013(4)	0.048(5)	0.026(4)	0.008(4)	0.003(3)	-0.007(4)
C(m3)	0.019(5)	0.030(4)	0.029(4)	0.001(3)	-0.005(3)	-0.011(3)
N(4)	0.014(3)	0.020(3)	0.023(3)	-0.003(3)	0.003(3)	-0.005(3)
C(a7)	0.017(4)	0.031(4)	0.030(4)	0.000(4)	0.003(3)	-0.009(3)
C(a8)	0.008(4)	0.030(4)	0.034(4)	0.003(3)	0.004(3)	0.006(3)
C(b7)	0.016(4)	0.037(4)	0.030(4)	-0.003(4)	0.004(4)	-0.013(3)
C(b8)	0.006(4)	0.043(5)	0.039(4)	-0.004(3)	0.002(4)	-0.001(4)
C(m4)	0.018(4)	0.022(4)	0.023(3)	0.000(4)	0.003(3)	0.008(3)
C(11)	0.040(5)	0.043(5)	0.013(3)	0.005(4)	0.001(3)	0.003(3)
C(21)	0.033(5)	0.042(5)	0.019(3)	0.005(4)	0.000(4)	-0.001(3)
C(31)	0.026(4)	0.025(4)	0.042(4)	0.002(4)	-0.007(4)	0.001(4)
C(41)	0.030(5)	0.027(4)	0.048(5)	0.006(4)	0.010(3)	0.006(4)
C(51)	0.058(6)	0.085(7)	0.034(4)	-0.014(5)	0.010(4)	0.002(4)
C(61)	0.030(5)	0.061(6)	0.017(3)	0.012(5)	0.000(3)	-0.003(4)
C(71)	0.029(5)	0.031(4)	0.046(5)	-0.008(4)	0.002(4)	-0.010(4)
C(81)	0.033(5)	0.021(4)	0.045(5)	-0.010(4)	-0.003(4)	0.002(4)
C(12)	0.041(6)	0.082(7)	0.029(4)	0.022(6)	-0.005(4)	0.011(5)
C(22)	0.030(5)	0.057(6)	0.040(5)	-0.010(5)	-0.004(4)	-0.028(5)
C(32)	0.036(6)	0.034(5)	0.076(7)	-0.005(4)	-0.008(5)	-0.016(5)
C(42)	0.037(5)	0.043(4)	0.065(6)	0.004(4)	0.020(4)	0.010(4)
C(52)	0.045(5)	0.090(6)	0.036(4)	-0.016(5)	0.013(5)	0.006(3)
C(62)	0.046(6)	0.071(6)	0.036(4)	0.016(5)	0.009(4)	-0.022(5)
C(72)	0.041(7)	0.042(6)	0.078(7)	-0.005(5)	0.025(5)	-0.010(5)
C(82)	0.030(5)	0.032(5)	0.065(6)	0.002(4)	-0.009(5)	0.010(5)
Sb	0.029(2)	0.046(2)	0.026(1)	-0.001(1)	0.001(1)	-0.004(1)
Cl(1)	0.087(3)	0.073(3)	0.038(1)	-0.035(2)	0.026(1)	-0.024(1)
Cl(2)	0.098(3)	0.104(2)	0.149(4)	0.070(3)	0.074(3)	0.061(3)
Cl(3)	0.158(6)	0.153(6)	0.036(2)	-0.084(4)	0.035(2)	-0.033(2)
Cl(4)	0.108(4)	0.181(5)	0.164(4)	0.089(3)	0.052(4)	0.121(4)
Cl(5)	0.084(3)	0.111(3)	0.063(2)	-0.062(3)	0.028(2)	-0.022(2)
Cl(6)	0.093(2)	0.178(4)	0.051(3)	-0.094(3)	0.006(2)	-0.025(2)

Table S3 -- continued

Name	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(s1)	0.191(7)	0.056(3)	0.063(4)	-0.013(3)	-0.015(4)	0.000(3)
Cl(s1)	0.206(8)	0.060(3)	0.066(4)	-0.020(4)	-0.008(4)	-0.003(3)
Cl(s2)	0.191(7)	0.058(3)	0.064(3)	-0.014(4)	-0.014(4)	-0.001(3)
H-s1	0.191	0.062	0.066	-0.012	-0.015	-0.004
H-s2	0.199	0.057	0.063	-0.011	-0.016	0.000

a. Estimated standard deviations in the least significant digits are given in parentheses. The form of the anisotropic displacement parameter is: $\exp[-2\pi^2\{h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23}\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table S4. Fractional Monoclinic Coordinates for the Hydrogen Atoms for $[Ni(OEP^{\bullet/2})]_2SbCl_6$.[a]

Atom	x	y	z
H1C(m1)	0.0777	0.2960	0.3289
H1C(m2)	0.1232	0.2642	0.1173
H1C(m3)	0.0719	-0.1492	0.1318
H1C(m4)	0.1237	-0.1202	0.3431
H1C(11)	0.0938	-0.0704	0.4117
H2C(11)	0.0983	0.0199	0.4439
H1C(12)	0.2398	0.0053	0.3992
H2C(12)	0.2246	-0.0027	0.4544
H3C(12)	0.2201	-0.0930	0.4222
H1C(21)	0.0711	0.1726	0.4385
H2C(21)	0.0506	0.2522	0.4014
H1C(22)	0.2115	0.2239	0.3990
H2C(22)	0.1651	0.3155	0.4156
H3C(22)	0.1856	0.2360	0.4527
H1C(31)	0.0618	0.4321	0.2988
H2C(31)	0.0832	0.4940	0.2540
H1C(32)	0.2216	0.4116	0.2815
H2C(32)	0.2025	0.5200	0.2819
H3C(32)	0.1811	0.4581	0.3267
H1C(41)	0.1033	0.4847	0.1767
H2C(41)	0.0888	0.4122	0.1352
H1C(42)	0.2422	0.3883	0.1662
H2C(42)	0.2152	0.4239	0.1154
H3C(42)	0.2297	0.4964	0.1569
H1C(51)	0.0882	0.2134	0.0484
H2C(51)	0.0976	0.1229	0.0166
H1C(52)	0.2394	0.1437	0.0645
H2C(52)	0.2284	0.1506	0.0090
H3C(52)	0.2191	0.2411	0.0407
H1C(61)	0.0599	-0.0335	0.0228
H2C(61)	0.0446	-0.1122	0.0611
H1C(62)	0.2054	-0.0769	0.0598
H2C(62)	0.1617	-0.1715	0.0452
H3C(62)	0.1769	-0.0928	0.0068
H1C(71)	0.0561	-0.2874	0.1622
H2C(71)	0.0774	-0.3492	0.2071
H1C(72)	0.2160	-0.2713	0.1781
H2C(72)	0.1942	-0.3791	0.1783
H3C(72)	0.1730	-0.3173	0.1335
H1C(81)	0.1006	-0.3377	0.2837
H2C(81)	0.0885	-0.2642	0.3250
H1C(82)	0.2407	-0.2451	0.2929
H2C(82)	0.2137	-0.2791	0.3439
H3C(82)	0.2258	-0.3526	0.3026
H-s1	-0.0326	0.6259	0.4259
H-s2	0.0401	0.5863	0.4575

a. Hydrogen atoms included using an idealized riding model.

Table S5. Crystal Data and Intensity Data Collection Parameters for $[Cu(OEP^{\bullet/2})]_2SbCl_6$.

Parameter	Value
compound	$[Cu(OEP^{\bullet/2})]_2SbCl_6 \cdot 1/2CH_2Cl_2 \cdot 1/2CHCl_3$
empirical formula	$C_{72}H_{88}SbCu_2Cl_6N_8 \cdot 1/2CH_2Cl_2 \cdot 1/2CHCl_3$
formula weight, Daltons	1556.01
crystal dimensions, mm	0.08 x 0.28 x 0.33
crystal color	brown-violet
crystal shape	truncated hexagonal bipyramidal
temperature, deg K	125±2
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
a, Å	14.791(3)
b, Å	17.042(5)
c, Å	14.796(3)
b, Å	99.87(2)
V, A^3	3674.4(28)
lattice parameter refinement	25 reflns; 8.4°<2q<35.4°
Z	2
calculated density, g/cm^3	1.41
m(MoKa), cm^{-1}	12.78
diffractometer	Enraf-Nonius CAD4
radiation	graphite crystal, incident beam monochromated MoKa, `1=0.71073Å
attenuator	Zr foil, factor 19.3
take-off angle, deg	2.8
detector aperture, mm	horizontal 2.0-2.4 vertical 4.0
crystal-detector distance, cm	21
omega width at half-height, deg	0.20
scan type	q/2q
scan rate, deg/min in omega	2.35-8.24
scan width, deg	0.76+0.344tanq
2q range, deg	3.0 to 56.8
sinq/l maximum	0.689
total data measured	10320
unique data, measured	9804
$F_o>3s(F_o)$	5623
corrections, on I	Lorentz-polarization linear decay (factors: 1.000 to 1.039) absorption (transmission: 0.904 to 1.000)
reflection averaging	$R_{merge}(I)=0.032$
(515 multiply measured)	$R_{merge}(F)=0.043$
refinement	full-matrix least-squares
hydrogen atom	idealized; d[CH]=0.98Å; $B[H]=1.1B[C_{attached}]$
minimization function	$Sw(\|F_o\|-\|F_c\|)^2$
p, weight=$[s^2(F)^2+p^2F^2]^{-1/2}$	0.035
anomalous dispersion	all nonhydrogen atoms
data:variable ratio	12.1

$R_1=S\|\|F_o\|-\|F_c\|\|/S\|F_o\|$	0.072
$R_2=(Sw(F_o-F_c)^2/SwF_o^2)^{1/2}$	0.077
goodness of fit	2.06
convergence, largest shift/error	0.08
high peak in final diff. map	1.5(2)$e^-/Å^3$
computer hardware	VAXstation 3200
computer software	SDP/VAX

Table S6. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Cu(OEP^{\bullet/2})]_2SbCl_6 \cdot 1/2CH_2Cl_2 \cdot 1/2CHCl_3$.[a]

atom	x	y	z	U(eq)
Sb[b]	1.41358(6)	0.00094(5)	0.07369(5)	0.025(1)
Cl(1)[b]	1.2566(2)	0.0076(2)	1.0435(2)	0.029(6)
Cl(2)[b]	1.3941(2)	-0.0550(2)	0.2201(2)	0.034(6)
Cl(3)[b]	1.5746(3)	-0.0099(3)	0.1050(3)	0.068(1)
Cl(4)[b]	1.4162(3)	0.0615(3)	0.9300(3)	0.073(1)
Cl(5)[b]	1.4125(4)	0.1216(2)	0.1477(3)	0.073(1)
Cl(6)[b]	1.4091(4)	-0.1219(3)	0.0007(4)	0.090(1)
Cu	0.99880(4)	0.09551(4)	0.46971(4)	0.012(1)
N(1)	1.0021(3)	0.0808(3)	0.6038(3)	0.015(9)
N(2)	1.1348(3)	0.0982 3)	0.4906(3)	0.013(8)
N(3)	0.9951(3)	0.1125(3)	0.3370(3)	0.015(9)
N(4)	0.8626(3)	0.0985(3)	0.4505(3)	0.015(8)
C(a1)	0.9282(4)	0.0787(3)	0.6495(4)	0.016(1)
C(a2)	1.0784(4)	0.0775(3)	0.6716(3)	0.015(1)
C(a3)	1.1941(4)	0.0908(3)	0.5727(3)	0.016(1)
C(a4)	1.1896(4)	0.1083(3)	0.4263(4)	0.015(1)
C(a5)	1.0695(4)	0.1182(3)	0.2909(4)	0.015(1)
C(a6)	1.9194(4)	0.1178(3)	0.2689(3)	0.015(1)
C(a7)	0.8036(4)	0.1094(3)	0.3695(4)	0.015(1)
C(a8)	0.8076(4)	0.0909(3)	0.5159(4)	0.016(1)
C(b1)	0.9596(4)	0.0745(3)	0.7485(4)	0.018(1)
C(b2)	1.0520(4)	0.0739(3)	0.7618(3)	0.019(1)
C(b3)	1.2888(4)	0.0967(3)	0.5601(4)	0.018(1)
C(b4)	1.2861(4)	0.1080(3)	0.4685(4)	0.018(1)
C(b5)	1.0390(4)	0.1269(3)	0.1922(3)	0.016(1)

Table S6. continued (page 2)

C(b6)	0.9460(4)	0.1265(3)	0.1792(4)	0.019(1)
C(b7)	0.7091(4)	0.1098(3)	0.3836(4)	0.021(1)
C(b8)	0.7113(4)	0.0972(4)	0.4742(4)	0.021(1)
C(m1)	1.1666(4)	0.0799(3)	0.6566(4)	0.018(1)
C(m2)	1.1594(4)	0.1169(3)	0.3329(4)	0.016(1)
C(m3)	0.8301(4)	0.1172(3)	0.2841(4)	0.018(1)
C(m4)	0.8384(4)	0.0808(3)	0.6076(4)	0.019(1)
C(11)	0.8968(4)	0.0767(4)	0.8175(4)	0.025(1)
C(21)	1.1183(4)	0.0752(4)	0.8500(4)	0.024(1)
C(31)	1.3695(4)	0.0913(4)	0.6358(4)	0.021(1)
C(41)	1.3650(4)	0.1212 4)	0.4192(4)	0.027(1)
C(51)	1.1003(4)	0.1372(4)	0.1237(4)	0.024(1)
C(61)	0.8797(4)	0.8797(4)	0.0910(4)	0.024(1)
C(71)	0.6283(4)	0.1258(4)	0.3089(4)	0.030(1)
C(81)	0.6326(4)	0.0929(4)	0.5261(4)	0.029(1)
C(12)	0.8646(5)	0.1597(4)	0.8331(4)	0.035(1)
C(22)	1.1516(5)	0.1582(4)	0.8781(4)	0.038(2)
C(32)	1.3860(4)	0.1685(4)	0.6874(4)	0.030(1)
C(42)	1.3806(4)	0.2074 4)	0.4019(5)	0.039(2)
C(52)	1.1349(5)	0.2216(4)	0.1217(4)	0.030(1)
C(62)	0.8500(5)	0.2210(4)	0.0746(4)	0.030(1)
C(72)	0.6169(5)	0.2120(4)	0.2874(5)	0.043(2)
C(82)	0.6106(4)	0.1709(4)	0.1709(4)	0.035(1)
C(s1)	1.6232(9)	-0.0191(8)	-0.1294(9)	0.040(3)
Cl(s1)	1.7235(3)	0.0172(3)	-0.0555(3)	0.037(8)
Cl(s2)	1.6337(3)	-0.1171(3)	-0.1532(3)	0.045(9)
Cl(s3)	1.5846(5)	0.0318(4)	-0.2254(4)	0.016(1)

[a] U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. The estimated standard deviations of the least significant digits are given in parentheses. [b] Occupancy factor 0.5.

Table S7. General Atomic Displacement Parameters (in $Å^2$)[a] for the Atoms Refined Anisotropically for $[Cu(OEP^{\bullet/2})]_2SbCl_6$.

Name	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	0.0101(3)	0.0185(3)	0.0096(2)	0.0005(3)	0.0023(2)	0.0003(3)
N(1)	0.018(2)	0.018(2)	0.011(2)	0.003(2)	0.006(2)	0.001(2)
N(2)	0.009(2)	0.018(2)	0.011(2)	0.000(2)	-0.002(2)	-0.001(2)
N(3)	0.016(2)	0.017(2)	0.011(2)	0.001(2)	0.002(2)	0.000(2)
N(4)	0.014(2)	0.015(2)	0.016(2)	-0.002(2)	0.003(2)	0.002(2)
C(a1)	0.018(3)	0.016(3)	0.017(2)	-0.000(2)	0.006(2)	0.001(2)
C(a2)	0.022(3)	0.010(3)	0.012(2)	-0.002(2)	0.001(2)	-0.001(2)
C(a3)	0.020(3)	0.013(3)	0.016(2)	-0.002(2)	0.001(2)	-0.002(2)
C(a4)	0.012(2)	0.017(3)	0.016(2)	-0.000(2)	0.004(2)	-0.002(2)
C(a5)	0.019(3)	0.013(3)	0.014(2)	0.001(2)	0.005(2)	0.002(2)
C(a6)	0.016(3)	0.018(3)	0.012(2)	0.001(2)	0.002(2)	-0.002(2)
C(a7)	0.014(3)	0.014(3)	0.019(2)	-0.002(2)	0.001(2)	-0.000(2)
C(a8)	0.014(2)	0.015(3)	0.021(2)	0.002(2)	0.006(2)	-0.001(2)
C(b1)	0.024(3)	0.019(3)	0.013(2)	0.003(2)	0.007(2)	-0.000(2)
C(b2)	0.027(3)	0.020(3)	0.008(2)	-0.003(2)	-0.000(2)	0.002(2)
C(b3)	0.014(3)	0.014(3)	0.024(3)	-0.001(2)	0.001(2)	-0.002(2)
C(b4)	0.010(2)	0.022(3)	0.020(3)	0.001(2)	0.004(2)	0.000(2)
C(b5)	0.028(3)	0.013(3)	0.011(2)	0.003(2)	0.007(2)	-0.001(2)
C(b6)	0.030(3)	0.015(3)	0.010(2)	0.001(3)	0.001(2)	-0.001(2)
C(b7)	0.013(3)	0.023(3)	0.025(3)	-0.000(2)	-0.001(2)	0.003(2)
C(b8)	0.017(3)	0.018(3)	0.030(3)	-0.003(3)	0.007(2)	0.002(3)
C(m1)	0.019(3)	0.018(3)	0.013(2)	0.003(2)	-0.002(2)	0.001(2)
C(m2)	0.017(3)	0.018(3)	0.018(2)	0.001(2)	0.011(2)	0.002(2)
C(m3)	0.021(3)	0.021(3)	0.011(2)	0.002(2)	-0.003(2)	0.000(2)
C(m4)	0.019(3)	0.023(3)	0.017(2)	0.000(2)	0.008(2)	0.001(2)
C(11)	0.031(3)	0.031(3)	0.016(2)	0.007(3)	0.012(2)	0.005(2)
C(12)	0.049(4)	0.039(4)	0.022(3)	0.006(3)	0.019(3)	-0.003(3)
C(21)	0.029(3)	0.030(3)	0.012(2)	-0.007(3)	-0.001(2)	0.001(2)
C(22)	0.060(5)	0.032(4)	0.019(3)	-0.010(4)	-0.003(3)	-0.004(3)
C(31)	0.011(3)	0.022(3)	0.028(3)	-0.003(3)	-0.001(2)	0.001(3)
C(32)	0.019(3)	0.036(4)	0.033(3)	0.003(3)	-0.002(3)	-0.008(3)
C(41)	0.012(3)	0.041(4)	0.029(3)	-0.000(3)	0.009(2)	0.004(3)
C(42)	0.027(3)	0.048(4)	0.044(3)	-0.005(3)	0.017(3)	0.015(3)
C(51)	0.035(3)	0.027(3)	0.014(3)	0.003(3)	0.009(2)	0.000(2)
C(52)	0.047(4)	0.036(4)	0.023(3)	-0.002(3)	0.014(3)	0.007(3)
C(61)	0.034(3)	0.029(3)	0.008(2)	0.006(3)	-0.000(2)	0.001(2)
C(62)	0.048(4)	0.035(4)	0.019(3)	0.014(3)	0.001(3)	0.005(3)
C(71)	0.013(3)	0.042(4)	0.033(3)	-0.003(3)	-0.002(3)	0.010(3)
C(72)	0.021(3)	0.052(4)	0.056(4)	0.009(3)	0.006(3)	0.025(4)
C(81)	0.015(3)	0.036(3)	0.037(3)	-0.006(3)	0.009(2)	0.002(3)
C(82)	0.025(3)	0.046(4)	0.038(3)	-0.002(3)	0.017(3)	-0.010(3)
Sb	0.0215(4)	0.0351(4)	0.0181(3)	0.0056(4)	0.0036(3)	-0.0024(4)
Cl(1)	0.029(2)	0.035(2)	0.023(1)	0.002(1)	0.004(1)	0.002(1)
Cl(2)	0.030(2)	0.053(2)	0.016(1)	-0.012(1)	-0.006(1)	0.028(1)
Cl(3)	0.029(2)	0.116(4)	0.059(2)	0.014(2)	0.011(2)	0.006(3)
Cl(4)	0.083(2)	0.095(3)	0.057(2)	0.040(2)	0.050(2)	0.045(2)
Cl(5)	0.079(3)	0.042(2)	0.090(3)	0.005(2)	-0.018(3)	-0.038(2)
Cl(6)	0.123(4)	0.052(2)	0.090(3)	0.035(3)	0.004(3)	-0.031(2)

C(1s)	0.037(7)	0.048(8)	0.041(6)	0.022(6)	0.021(5)	-0.016(6)

a. Estimated standard deviations in the least significant digits are given in parentheses. The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2\{h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23}\}]$
where
a^*, b^*, and c^* are reciprocal lattice constants.

Table S8. Fractional Monoclinic Coordinates and Isotropic Atomic Displacement Parameters for the Hydrogen Atoms for $[Cu(OEP^{\bullet/2})]_2SbCl_6$.[a]

Atom	x	y	z	Ueq
H(m1)	1.215	0.073	0.710	0.019
H(m2)	1.206	0.123	0.294	0.019
H(m3)	0.782	0.123	0.231	0.020
H(m4)	0.792	0.075	0.647	0.021
H(11a)	0.929	0.056	0.876	0.028
H(11b)	0.843	0.044	0.796	0.028
H(12a)	0.824	0.159	0.879	0.039
H(12b)	0.918	0.193	0.855	0.039
H(12c)	0.832	0.181	0.775	0.039
H(21a)	1.171	0.043	0.843	0.027
H(21b)	1.088	0.053	0.899	0.027
H(22a)	1.195	0.156	0.936	0.042
H(22b)	1.182	0.181	0.830	0.042
H(22c)	1.099	0.191	0.886	0.042
H(31a)	1.424	0.078	0.610	0.023
H(31b)	1.358	0.050	0.679	0.023
H(32a)	1.439	0.163	0.736	0.033
H(32b)	1.398	0.210	0.645	0.033
H(32c)	1.332	0.182	0.714	0.033
H(41a)	1.353	0.094	0.360	0.029
H(41b)	1.421	0.100	0.456	0.029
H(42a)	1.433	0.213	0.370	0.043
H(42b)	1.326	0.229	0.364	0.043
H(42c)	1.393	0.235	0.461	0.043
H(51a)	1.066	0.124	0.063	0.027
H(51b)	1.153	0.102	0.139	0.027
H(52a)	1.175	0.226	0.076	0.038
H(52b)	1.083	0.257	0.106	0.038
H(52c)	1.169	0.235	0.182	0.038
H(61a)	0.825	0.104	0.094	0.027
H(61b)	0.909	0.119	0.040	0.027
H(62a)	0.807	0.225	0.017	0.038
H(62b)	0.820	0.239	0.125	0.038
H(62c)	0.904	0.254	0.071	0.038
H(71a)	0.573	0.106	0.329	0.033
H(71b)	0.637	0.098	0.253	0.033
H(72a)	0.564	0.220	0.239	0.048
H(72b)	0.607	0.240	0.343	0.048
H(72c)	0.672	0.232	0.267	0.048
H(81a)	0.648	0.055	0.576	0.032
H(81b)	0.578	0.075	0.484	0.032
H(82a)	0.559	0.164	0.600	0.038
H(82b)	0.664	0.189	0.610	0.038
H(82c)	0.595	0.210	0.518	0.038

a. Hydrogen atoms included as fixed contributors: d[C-H]=0.98Å; B[H]=1.1B[attached atom].

Table S9. Complete Crystallographic details for $[Zn(OEP^{\bullet/2})H_2(OEP^{\bullet/2})]SbCl_6 \cdot 1/3CH_2Cl_2 \cdot 2/3CHCl_3$.

molecule	$[Zn(OEP^{\bullet/2})H_2(OEP^{\bullet/2})]SbCl_6 \cdot 1/3CH_2Cl_2 \cdot 2/3CHCl_3$
Formula	$C_{72}H_{90}Cl_6N_8ZnSb$
FW, amu	1684.50
a, Å	14.744 (4)
b, Å	17.156 (9)
c, Å	14.887 (6)
β, deg	99.95 (10)
V, Å^3	3709.0 (27)
Space group	$P2_1/a$
Z	2
D_c, g/cm^3	1.508
F(000)	1726
μ, mm^{-1}	1.411
Detector dist., mm	40.080
Detector tilt angle, deg	–24.949
Image time, sec	10
Increment, deg	0.20
Cryst dimens, mm	0.49 x 0.19 x 0.10
Rel. trans. coeffic. (I)	1.00 -- 0.54
Radiation	MoKα, λ = 0.71073 Å
Temp, K	127 (2)
Diffractometer	FAST
Theta range for collected data, deg	2.37 -- 30.09
Index range	$-12 \le h \le 20$
	$-23 \le k \le 17$
	$-20 \le l \le 18$
Total data collected	27257
Unique data	9782 (R_{int} = 0.089)
Unique observed data [I > 2 σ(I)]	5687
Refinement method	on F^2 (SHELXL-93)
Variables refined	479
Goodness-of-fit (on F^2)	1.052
max(Δρ), eÅ^{-3}	1.200
min(Δρ), eÅ^{-3}	0.885
Final R indices [I > 2 σ(I)]	R_1 = 0.0773; wR_2 = 0.1507
Final R indices [for all data]	R_1 = 0.1450; wR_2 = 0.1919

Table S10. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $Zn(OEP^{\bullet/2})H_2(OEP^{\bullet/2})]SbCl_6 \cdot 1/3CH_2Cl_2 \cdot 2/3CHCl_3$.[a]

atom	x	y	z	U(eq)
Sb[b]	-0.42658(4)	-0.00012(4)	0.41077(5)	0.0321(2)
Cl(1)[b]	-0.3966(3)	0.0102(3)	0.5712(2)	0.0686(11)
Cl(2)[b]	-0.2799(7)	0.0567(6)	0.3990(5)	0.059(2)
Cl(3)[b]	-0.3597(4)	-0.1237(3)	0.4165(4)	0.0730(15)
Cl(4)[b]	-0.4544(5)	-0.0025(4)	0.2536(5)	0.0470(11)
Cl(5)[b]	-0.5729(3)	-0.0565(3)	0.4139(3)	0.0680(11)
Cl(6)[b]	-0.4959(3)	0.1237(2)	0.4033(3)	0.0816(13)
Zn[c]	0.03845(6)	0.08816(6)	0.00111(6)	0.0247(3)
N(1)	0.1735(2)	0.1161(2)	0.0044(3)	0.0280(8)
N(2)	0.0146(2)	0.0968(2)	-0.1393(2)	0.0252(8)
N(3)	-0.0992(2)	0.0710(2)	-0.0023(2)	0.0275(8)
N(4)	0.0566(2)	0.0968(2)	0.1413(2)	0.0236(8)
C(a1)	0.2399(3)	0.1223(3)	0.0808(3)	0.0284(10)
C(a2)	0.2172(3)	0.1226(3)	-0.0693(3)	0.0293(10)
C(a3)	0.0798(3)	0.1101(3)	-0.1924(3)	0.0272(9)
C(a4)	-0.0679(3)	0.0879(3)	-0.1963(3)	0.0252(9)
C(a5)	-0.1667(3)	0.0705(3)	-0.0780(3)	0.0273(9)
C(a6)	-0.1439(3)	0.0710(3)	0.0710(3)	0.0259(9)
C(a7)	-0.0085(3)	0.0880(3)	0.1946(3)	0.0261(9)
C(a8)	0.1385(3)	0.1105(3)	0.1980(3)	0.0272(9)
C(b1)	0.3287(3)	0.1321(3)	0.0542(3)	0.0298(10)
C(b2)	0.3148(3)	0.1322(3)	-0.0389(3)	0.0291(10)
C(b3)	0.0361(3)	0.1095(3)	-0.2876(3)	0.0289(10)
C(b4)	-0.0547(3)	0.0958(3)	-0.2899(3)	0.0274(9)
C(b5)	-0.2567(3)	0.0691(3)	-0.0522(3)	0.0291(10)
C(b6)	-0.2433(3)	0.0696(3)	0.0403(3)	0.0298(10)

Table S10. continued (page 2)

C(b7)	0.0331(3)	0.0967(3)	0.2896(3)	0.0307(10)
C(b8)	0.1238(3)	0.1106(3)	0.2919(3)	0.0301(10)
C(m1)	0.1732(3)	0.1204(3)	-0.1603(3)	0.0324(10)
C(m2)	-0.1515(3)	0.0747(3)	-0.1675(3)	0.0284(10)
C(m3)	-0.1023(3)	0.0755(3)	0.1621(3)	0.0287(10)
C(m4)	0.2232(3)	0.1200(3)	0.1695(3)	0.0301(10)
C(11)	0.4171(3)	0.1424(3)	0.1200(4)	0.0363(11)
C(21)	0.3843(3)	0.1442(3)	-0.0998(4)	0.0389(12)
C(31)	0.0840(4)	0.1254(3)	-0.3662(3)	0.0385(12)
C(41)	-0.1308(3)	0.0912(3)	-0.3710(3)	0.0318(10)
C(51)	-0.3457(3)	0.0723(3)	-0.1185(4)	0.0350(11)
C(61)	-0.3121(3)	0.0738(3)	0.1026(4)	0.0367(11)
C(71)	-0.0178(4)	0.0920(3)	0.3685(3)	0.0362(11)
C(81)	0.1961(4)	0.1285(3)	0.3723(3)	0.0439(14)
C(12)	0.4338(4)	0.2261(3)	0.1492(4)	0.0497(15)
C(22)	0.3859(4)	0.2274(3)	-0.1341(4)	0.0485(14)
C(32)	0.0987(4)	0.2114(4)	-0.3820(4)	0.052(2)
C(42)	-0.1848(4)	0.1666(3)	-0.3883(4)	0.0415(13)
C(52)	-0.3710(4)	0.1546(4)	-0.1528(5)	0.051(2)
C(62)	-0.3250(4)	0.1565(4)	0.1362(5)	0.050(2)
C(72)	-0.0623(4)	0.1683(4)	0.3876(4)	0.0476(14)
C(82)	0.2162(5)	0.2151(4)	0.3837(4)	0.059(2)
C(S)	-0.3704(7)	-0.0192(8)	0.3776(9)	0.053(3)
Cl(7)	-0.4443(7)	0.0093(7)	0.2763(7)	0.111(4)
Cl(8)	-0.3501(4)	-0.1180(3)	0.3692(3)	0.0677(12)
Cl(9)	-0.2729(8)	0.0333(6)	0.4020(8)	0.092(4)

[a] U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. The estimated standard deviations of the least significant digits are given in parentheses. [b] Occupancy factor 0.5. [c] Occupancy factor 0.588(3).

Table S11. Anisotropic displacement parameters ($Å^2$) for $[Zn(OEP^{\cdot/2})H_2(OEP^{\cdot/2})]SbCl_6 \cdot 1/3CH_2Cl_2 \cdot 2/3CHCl_3$.[a] The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

atom	U11	U22	U33	U23	U13	U12
Sb	0.0279(3)	0.0352(4)	0.0325(3)	-0.0068(3)	0.0031(2)	0.0016(3)
Cl(1)	0.064(2)	0.101(3)	0.039(2)	-0.011(2)	0.0041(15)	-0.006(2)
Cl(2)	0.049(3)	0.070(6)	0.058(3)	-0.012(2)	0.007(2)	-0.026(3)
Cl(3)	0.093(3)	0.042(2)	0.074(3)	0.000(2)	-0.014(3)	0.026(2)
Cl(4)	0.037(2)	0.058(2)	0.048(3)	0.023(2)	0.012(2)	0.012(2)
Cl(5)	0.053(2)	0.085(3)	0.071(2)	-0.021(2)	0.026(2)	-0.029(2)
Cl(6)	0.084(3)	0.046(2)	0.111(3)	-0.027(2)	0.008(2)	0.023(2)
Zn	0.0200(4)	0.0353(6)	0.0182(4)	0.0002(4)	0.0017(3)	-0.0023(3)
N(1)	0.024(2)	0.037(2)	0.023(2)	0.001(2)	0.0034(14)	-0.006(2)
N(2)	0.025(2)	0.030(2)	0.021(2)	0.002(2)	0.0035(14)	-0.0010(15)
N(3)	0.024(2)	0.038(2)	0.020(2)	0.002(2)	0.0029(14)	-0.001(2)
N(4)	0.023(2)	0.025(2)	0.023(2)	-0.0023(15)	0.0037(13)	-0.0027(14)
C(a1)	0.026(2)	0.026(2)	0.031(2)	0.000(2)	-0.001(2)	-0.003(2)
C(a2)	0.029(2)	0.030(3)	0.029(2)	-0.001(2)	0.005(2)	-0.002(2)
C(a3)	0.031(2)	0.028(2)	0.024(2)	0.000(2)	0.010(2)	-0.005(2)
C(a4)	0.026(2)	0.026(2)	0.023(2)	0.003(2)	0.002(2)	0.000(2)
C(a5)	0.028(2)	0.025(2)	0.027(2)	-0.001(2)	-0.001(2)	-0.001(2)
C(a6)	0.027(2)	0.027(2)	0.023(2)	0.000(2)	0.006(2)	0.002(2)
C(a7)	0.029(2)	0.027(2)	0.022(2)	0.000(2)	0.003(2)	0.004(2)
C(a8)	0.031(2)	0.032(3)	0.018(2)	-0.001(2)	0.004(2)	-0.005(2)
C(b1)	0.024(2)	0.026(2)	0.037(3)	0.001(2)	0.000(2)	-0.001(2)
C(b2)	0.024(2)	0.025(2)	0.037(3)	0.002(2)	0.003(2)	-0.001(2)
C(b3)	0.034(2)	0.029(2)	0.023(2)	-0.002(2)	0.005(2)	-0.001(2)
C(b4)	0.037(2)	0.024(2)	0.021(2)	-0.002(2)	0.003(2)	-0.001(2)
C(b5)	0.024(2)	0.031(3)	0.032(2)	0.004(2)	0.004(2)	0.002(2)
C(b6)	0.027(2)	0.030(2)	0.034(2)	0.001(2)	0.008(2)	-0.001(2)
C(b7)	0.044(3)	0.028(3)	0.020(2)	0.002(2)	0.006(2)	0.000(2)
C(b8)	0.040(3)	0.028(2)	0.021(2)	0.001(2)	0.002(2)	-0.006(2)
C(m1)	0.035(2)	0.036(3)	0.026(2)	0.004(2)	0.005(2)	-0.004(2)
C(m2)	0.029(2)	0.030(3)	0.023(2)	0.001(2)	-0.005(2)	-0.001(2)
C(m3)	0.031(2)	0.036(3)	0.022(2)	0.006(2)	0.014(2)	-0.003(2)
C(m4)	0.027(2)	0.029(2)	0.032(2)	0.000(2)	-0.003(2)	-0.005(2)
C(11)	0.028(2)	0.037(3)	0.042(3)	-0.006(2)	0.001(2)	0.001(2)
C(21)	0.031(2)	0.039(3)	0.048(3)	0.001(2)	0.010(2)	0.003(2)
C(31)	0.044(3)	0.049(3)	0.022(2)	-0.004(2)	0.007(2)	-0.006(2)
C(41)	0.038(2)	0.036(3)	0.020(2)	0.001(2)	0.001(2)	-0.004(2)
C(51)	0.024(2)	0.037(3)	0.042(3)	0.008(2)	0.001(2)	-0.003(2)
C(61)	0.029(2)	0.037(3)	0.046(3)	-0.003(2)	0.012(2)	-0.005(2)
C(71)	0.045(3)	0.041(3)	0.025(2)	-0.002(2)	0.009(2)	0.000(2)
C(81)	0.054(3)	0.052(4)	0.023(2)	0.004(2)	-0.002(2)	-0.018(3)
C(12)	0.044(3)	0.041(3)	0.062(4)	-0.015(3)	0.001(3)	-0.002(2)
C(22)	0.050(3)	0.039(3)	0.061(4)	0.008(3)	0.022(3)	-0.005(3)
C(32)	0.069(4)	0.055(4)	0.035(3)	0.001(3)	0.019(3)	-0.028(3)
C(42)	0.049(3)	0.041(3)	0.032(3)	0.002(2)	-0.003(2)	0.007(2)
C(52)	0.033(3)	0.049(4)	0.067(4)	0.012(3)	-0.004(3)	0.004(2)
C(62)	0.038(3)	0.048(4)	0.069(4)	-0.013(3)	0.018(3)	-0.001(2)
C(72)	0.055(3)	0.056(4)	0.034(3)	-0.002(3)	0.017(2)	0.010(3)
C(82)	0.085(5)	0.061(4)	0.028(3)	-0.009(3)	0.004(3)	-0.039(4)
C(S)	0.034(5)	0.064(9)	0.069(8)	0.015(7)	0.028(6)	0.007(5)
Cl(7)	0.080(5)	0.188(10)	0.070(6)	0.048(5)	0.025(4)	0.041(5)
Cl(8)	0.077(3)	0.054(2)	0.072(3)	0.004(3)	0.013(3)	0.008(2)
Cl(9)	0.053(3)	0.067(6)	0.151(7)	-0.037(4)	0.002(3)	-0.016(3)

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

Table S12. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Zn(OEP^{\bullet/2})H_2(OEP^{\bullet/2})]SbCl_6 \cdot 1/3CH_2Cl_2 \cdot 2/3CHCl_3$.[a]

atom	x	y	z	U(eq)
H(m1)	0.2106(3)	0.1264(3)	-0.2041(3)	0.039
H(m2)	-0.2027(3)	0.0679(3)	-0.2130(3)	0.034
H(m3)	-0.1403(3)	0.0696(3)	0.2055(3)	0.034
H(m4)	0.2743(3)	0.1254(3)	0.2153(3)	0.036
H(11a)	0.4679(3)	0.1245(3)	0.0918(4)	0.044
H(11b)	0.4155(3)	0.1105(3)	0.1735(4)	0.044
H(21a)	0.3705(3)	0.1093(3)	-0.1517(4)	0.047
H(21b)	0.4448(3)	0.1308(3)	-0.0667(4)	0.047
H(31a)	0.0480(4)	0.1032(3)	-0.4209(3)	0.046
H(31b)	0.1433(4)	0.0995(3)	-0.3555(3)	0.046
H(41a)	-0.1725(3)	0.0496(3)	-0.3614(3)	0.038
H(41b)	-0.1046(3)	0.0784(3)	-0.4246(3)	0.038
H(51a)	-0.3946(3)	0.0520(3)	-0.0892(4)	0.042
H(51b)	-0.3409(3)	0.0391(3)	-0.1702(4)	0.042
H(61a)	-0.2922(3)	0.0403(3)	0.1548(4)	0.044
H(61b)	-0.3708(3)	0.0544(3)	0.0710(4)	0.044
H(71a)	0.0248(4)	0.0762(3)	0.4225(3)	0.043
H(71b)	-0.0651(4)	0.0523(3)	0.3558(3)	0.043
H(81a)	0.2523(4)	0.1014(3)	0.3657(3)	0.053
H(81b)	0.1763(4)	0.1089(3)	0.4269(3)	0.053
H(12a)	0.4892(16)	0.2295(5)	0.1937(21)	0.074
H(12b)	0.3827(14)	0.2448(8)	0.1753(26)	0.074
H(12c)	0.4401(29)	0.2574(5)	0.0971(7)	0.074
H(22a)	0.4326(19)	0.2325(7)	-0.1714(23)	0.073
H(22b)	0.3992(28)	0.2623(4)	-0.0831(4)	0.073
H(22c)	0.3270(10)	0.2402(9)	-0.1694(23)	0.073
H(32a)	0.1271(27)	0.2178(4)	-0.4349(17)	0.078
H(32b)	0.1379(24)	0.2331(7)	-0.3298(13)	0.078
H(32c)	0.0404(5)	0.2378(6)	-0.3914(29)	0.078
H(42a)	-0.2315(17)	0.1608(8)	-0.4415(15)	0.062
H(42b)	-0.1439(6)	0.2082(5)	-0.3979(26)	0.062
H(42c)	-0.2133(22)	0.1785(12)	-0.3366(11)	0.062
H(52a)	-0.4282(15)	0.1532(5)	-0.1949(23)	0.077
H(52b)	-0.3235(15)	0.1747(10)	-0.1830(26)	0.077
H(52c)	-0.3773(29)	0.1876(7)	-0.1022(6)	0.077
H(62a)	-0.3681(22)	0.1558(5)	0.1777(22)	0.076
H(62b)	-0.3480(27)	0.1893(6)	0.0851(5)	0.076
H(62c)	-0.2670(7)	0.1763(10)	0.1669(26)	0.076
H(72a)	-0.0937(24)	0.1618(7)	0.4385(18)	0.071
H(72b)	-0.1056(21)	0.1837(13)	0.3349(10)	0.071
H(72c)	-0.0157(5)	0.2077(7)	0.4017(27)	0.071
H(82a)	0.2653(22)	0.2231(4)	0.4343(20)	0.088
H(82b)	0.1620(11)	0.2418(5)	0.3948(32)	0.088
H(82c)	0.2341(31)	0.2352(7)	0.3291(13)	0.088
H	-0.4043(7)	-0.0119(8)	0.4281(9)	0.064

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

Table S1. Positional and Equivalent Isotropic Thermal Parameters for $[Cu(trpn)(NO_3)]_2(NO_3)_2$.

Atom	x	y	z	U_{eq} [Å^2] [a]
Cu	0.42080(3)	0.34550(3)	0.75461(2)	0.029(1)
N1	0.2002(3)	0.1319(2)	0.7830(2)	0.033(1)
N2	0.2647(3)	0.4563(2)	0.7068(2)	0.036(1)
N3	0.5862(3)	0.2415(3)	0.7821(2)	0.042(1)
N4	0.3412(2)	0.4165(2)	1.2010(2)	0.034(1)
N5	0.4926(3)	0.3065(3)	0.5003(2)	0.041(1)
N6	0.1387(3)	0.6503(3)	0.9225(2)	0.042(1)
O1	0.3651(3)	0.2668(3)	0.5473(2)	0.057(1)
O2	0.4533(3)	0.2634(3)	0.3916(2)	0.060(1)
O3	0.6580(3)	0.3872(4)	0.5630(2)	0.085(1)
O4	0.2914(3)	0.6518(3)	0.9457(2)	0.057(1)
O5	0.1164(4)	0.7455(4)	0.9885(3)	0.082(1)
O6	0.0117(3)	0.5539(4)	0.8308(2)	0.082(1)
C1	0.0173(3)	0.1312(3)	0.7395(2)	0.042(1)
C2	-0.0161(3)	0.1715(3)	0.6174(2)	0.046(1)
C3	0.0765(3)	0.3577(3)	0.6163(2)	0.047(1)
C4	0.1747(4)	-0.0307(3)	0.7195(2)	0.047(1)
C5	0.3421(4)	-0.0590(3)	0.7508(3)	0.053(1)
C6	0.5102(4)	0.0643(4)	0.7185(3)	0.053(1)
C7	0.2363(3)	0.1289(3)	0.9123(2)	0.036(1)
C8	0.2815(3)	0.2897(3)	0.9931(2)	0.037(1)
C9	0.3168(3)	0.2702(3)	1.1204(2)	0.035(1)
Hn21	0.2486	0.4933	0.7704	0.04
Hn22	0.3309	0.5452	0.6815	0.04
Hn31	0.6868	0.3059	0.7641	0.05
Hn32	0.6209	0.2450	0.8574	0.05
Hn41	0.2462	0.4309	1.1710	0.04
Hn42	0.3295	0.3950	1.2669	0.04
H11	0.0159	0.2125	0.7939	0.05
H12	-0.0826	0.0226	0.7371	0.05
H21	0.0280	0.1186	0.5705	0.06
H22	-0.1474	0.1228	0.5814	0.06
H31	0.0898	0.3717	0.5403	0.06

Table S1. Continued.

Atom	x	y	z	U_{eq} [Å^2] [a]
H32	-0.0015	0.4015	0.6306	0.06
H41	0.1399	-0.0349	0.6371	0.06
H42	0.0727	-0.1227	0.7344	0.06
H51	0.3792	-0.0525	0.8334	0.07
H52	0.3038	-0.1709	0.7121	0.07
H61	0.6051	0.0333	0.7373	0.07
H62	0.4753	0.0580	0.6358	0.07
H71	0.3378	0.1074	0.9370	0.05
H72	0.1286	0.0367	0.9219	0.05
H81	0.3896	0.3834	0.9852	0.05
H82	0.1797	0.3115	0.9714	0.05
H91	0.4263	0.2599	1.1441	0.05
H92	0.2141	0.1690	1.1260	0.05

[a]The equivalent isotropic thermal parameter U_{eq} is defined as $1/3[\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i a_j]$. All hydrogen positions are calculated ($d_{C\text{-}H}$ = 0.95 Å, $d_{N\text{-}H}$ = 0.87 Å see M. R. Churchill, *Inorg. Chem.* **1973**, *12*, 1213). The isotropic U_{eq} for hydrogens were fixed to be 1.3 U_{eq} of the parent atom.

Table S2. Bond Distances [Å] in $[Cu(trpn)(NO_3)]_2(NO_3)_2$.

Atom	Atom	Distance	Atom	Atom	Distance
Cu	N1	2.100(2)	N5	O1	1.249(3)
Cu	N2	2.008(2)	N5	O2	1.242(3)
Cu	N3	1.998(2)	N5	O3	1.236(3)
Cu	N4*[a]	2.075(2)	N6	O4	1.245(3)
Cu	O1	2.391(2)	N6	O5	1.231(3)
N1	C1	1.505(3)	N6	O6	1.244(3)
N1	C4	1.501(3)	C1	C2	1.523(3)
N1	C7	1.506(3)	C2	C3	1.503(4)
N2	C3	1.491(3)	C4	C5	1.517(4)
N3	C6	1.485(4)	C5	C6	1.508(4)
N4	C9	1.478(3)	C7	C8	1.517(3)
C8	C9	1.519(3)			
Cu·····Cu*		5.8517(9)			

[a]Starred atoms represent transformed coordinates related by an inversion center (see Fig. S1).

Table S3. Bond Angles [deg] in $[Cu(trpn)(NO_3)]_2(NO_3)_2$.

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
O1	Cu	N1	101.58(8)	Cu	N3	C6	118.4(2)
O1	Cu	N2	84.84(8)	Cu	N4*	C9*	122.84(13)
O1	Cu	N3	88.30(9)	O1	N5	O2	120.3(2)
O1	Cu	N4*	101.61(8)	O1	N5	O3	119.3(2)
N1	Cu	N2	93.60(8)	O2	N5	O3	120.4(2)
N1	Cu	N3	91.50(8)	O4	N6	O5	120.1(2)
N1	Cu	N4*	156.82(8)	O4	N6	O6	119.0(2)
N2	Cu	N3	172.15(8)	O5	N6	O6	121.0(2)
N2	Cu	N4*	88.68(8)	Cu	O1	N5	123.7(2)
N3	Cu	N4*	88.97(9)	N1	C1	C2	113.1(2)
Cu	N1	C1	111.18(14)	C1	C2	C3	114.9(2)
Cu	N1	C4	111.59(15)	N2	C3	C2	112.2(2)
Cu	N1	C7	111.15(13)	N1	C4	C5	116.7(2)
C1	N1	C4	107.4(2)	C4	C5	C6	115.2(2)
C1	N1	C7	107.8(2)	N3	C6	C5	111.6(2)
C4	N1	C7	107.5(2)	N1	C7	C8	115.5(2)
Cu	N2	C3	120.0(2)	C7	C8	C9	110.0(2)
N4	C9	C8	111.8(2)				

[a]Starred atoms represent transformed coordinates related by an inversion center (see Fig. S1).