Supplementary Information

Synthesis and Reactions of a Hybrid Tristibine Ligand

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Table S1 Crystal Data and Structure Refinement Details[a]

Compound	$[(Me_2Sb\text{-}2\text{-}C_6H_4CH_2)N(CH_2\text{-}2\text{-}C_6H_4)_2SbMe_2]I\cdot CH_2Cl_2$	$[Mn(CO)_3\{N(CH_2\text{-}2\text{-}C_6H_4SbMe_2)_3\}][CF_3SO_3]\cdot CHCl_3\cdot C_7H_8$	$[Mn(CO)_2(MeCN)\{N(CH_2\text{-}2\text{-}C_6H_4SbMe_2)_3\}][CF_3SO_3]\cdot Et_2O$
Formula	$C_{26}H_{32}Cl_2INSb_2$	$C_{39}H_{45}Cl_3F_3MnNO_6SSb_3$	$C_{36}H_{49}F_3MnN_2O_6SSb_3$
M	799.83	1239.36	1115.02
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1 (no. 2)	$P2_1/c$ (no. 14)	$P\ 2_1/n$ (no. 14)
a/Å	9.6461(13)	16.758(4)	9.644(2)
b/Å	11.2438(16)	14.392(3)	22.7495(12)
c/Å	13.686(2)	19.233(7)	19.7761(14)
α/°	102.791(7)	90	90
β/°	93.471(7)	93.825(7)	102.835(11)
γ/°	102.749(7)	90	90
U/Å^3	1402.5(3)	4628(2)	4230.4(10)
Z	2	4	4
μ(Mo-Kα)/mm^{-1}	3.232	2.272	2.292
F(000)	768	2424	2192
θ(max)	26.0	27.5	27.5
Temperature/K	120	100	100
Total no. reflections	17910	21676	20281
Unique reflections	6321	10508	9581
R_{int}	0.0279	0.0523	0.0486
Min., max. transmission	0.500, 1.000	0.655, 1.000	0.481, 1.000
No. of parameters, restraints	289, 0	468, 1	472, 0
R_1[b] [$I_o > 2\sigma(I_o)$]	0.0383	0.0688	0.0520
R_1 (all data)	0.0425	0.1118	0.0816
wR_2[b] [$I_o > 2\sigma(I_o)$]	0.1024	0.1436	0.1022
wR_2 (all data)	0.1063	0.1614	0.1153

[a] Common item: wavelength (Mo-Kα) = 0.71073 Å.

[b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]^{1/2}$.

Compound	$[Cu_3Br_2\{N(CH_2\text{-}2\text{-}C_6H_4SbMe_2)_3\}_2][BF_4]\cdot 1.5CH_2Cl_2$	$[Cu_4Br_4\{N(CH_2\text{-}2\text{-}C_6H_4SbMe_2)_3\}_2]$	$[Cu_4Br_4\{N(CH_2\text{-}2\text{-}C_6H_4SbMe_2)_3\}_2]\cdot 4CH_2Cl_2$
Formula	$C_{55.5}H_{75}BBr_2Cl_3Cu_3F_4N_2Sb_6$	$C_{54}H_{72}Br_4Cu_4N_2Sb_6$	$C_{58}H_{80}Br_4Cl_8Cu_4N_2Sb_6$
M	2044.27	2053.44	2393.1
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$ (no. 14)	$C2/c$ (no. 15)	P-1 (no. 2)
a/Å	16.636(8)	17.908(6)	11.755(3)
b/Å	12.192(6)	14.592(4)	12.875(4)
c/Å	18.546(9)	26.275(9)	13.094(5)
α/°	90	90	100.987(7)
β/°	104.656(8)	109.250(8)	93.589(7)
γ/°	90	90	101.211(7)
U/Å^3	3639(3)	6482(3)	1898.1(10)
Z	2	4	1
μ(Mo-Kα)/mm^{-1}	4.299	6.242	5.617
F(000)	1954	3888	1140
θ(max)	27.5	27.5	27.5
Temperature/K	100	100	100
Total no. reflections	23331	21141	17942
Unique reflections	8252	7306	8666
R_{int}	0.0623	0.0306	0.0453
Min., max. transmission	0.615, 1.000	0.708, 1.000	0.831, 1.000
No. of parameters, restraints	371, 7	322, 0	370, 0
R_1[b] [$I_o > 2\sigma(I_o)$]	0.0648	0.0311	0.0401
R_1 (all data)	0.0834	0.0398	0.0634
wR_2[b] [$I_o > 2\sigma(I_o)$]	0.1637	0.0650	0.0688
wR_2 (all data)	0.1784	0.0683	0.0751

[a] Common item: wavelength (Mo-Kα) = 0.71073 Å.

[b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]^{1/2}$.

The structure of $[Cu_4Br_4\{N(CH_2\text{-}2\text{-}C_6H_4SbMe_2)_3\}_2]\cdot 4CH_2Cl_2$ is very similar to the unsolvated complex reported above (Figure 6). The same atom numbering scheme has been employed. Selected bond lengths (Å) and angles (deg): Sb1-Cu1 = 2.5246(9), Sb2-Cu1 = 2.5352(8), Sb3-Cu1 = 2.5226(8), Br1-Cu2 = 2.3510(10), Br1-Cu1 = 2.4556(11), Br2-Cu2 = 2.4057(11), Br2-Cu2a = 2.4169(11), Cu2···Cu2a = 2.6321(14); Cu2-Br1-Cu1 = 101.06(3), Cu2-Br2-Cu2a = 66.16(4), Br1-Cu1-Sb2 = 113.42(3), Br1-Cu1-Sb1 = 112.88(3), Sb2-Cu1-Sb1 = 107.73(3), Br1-Cu1-Sb3 = 105.41(3), Sb2-Cu1-Sb3 = 109.59(3), Sb1-Cu1-Sb3 = 107.63(3), Br1-Cu2-Br2 = 125.66(4), Br1-Cu2-Br2a = 120.49(4), Br2-Cu2-Br2a = 113.84(4), Br1-Cu2···Cu2a = 177.08(5).