C(1)	-1262(16)	6153(13)	2544(13)	72(4)
C(2)	-149(22)	7445(18)	2882(20)	106(6)
C(3)	757(24)	7828(16)	2253(24)	120(8)
C(4)	540(18)	6866(21)	1173(21)	99(6)
C(5)	-647(16)	5559(15)	878(14)	74(4)
C(6)	-2282(16)	5459(14)	3155(12)	73(4)
C(7)	-3978(15)	3685(16)	3543(11)	68(4)
C(8)	-3562(28)	5118(29)	4441(15)	125(8)
C(9)	-1142(14)	4330(15)	-121(12)	65(3)
C(10)	-2501(15)	2127(15)	-1279(10)	66(3)
C(11)	-1225(21)	2995(24)	-1763(17)	95(6)
C(12)	-6583(14)	1677(13)	-310(10)	58(3)
C(13)	-5623(16)	831(12)	229(11)	63(3)
C(14)	-6412(14)	4106(13)	-373(11)	63(3)
C(15)	-5543(13)	5577(12)	342(11)	57(3)
C(16)	-4496(17)	6471(16)	-25(15)	73(4)
C(17)	-3617(19)	7899(16)	739(18)	90(5)
C(18)	-3852(18)	8315(15)	1745(15)	82(4)
C(19)	-4890(18)	7409(15)	2091(14)	80(4)
C(20)	-5759(16)	6056(13)	1401(12)	69(3)
C(21)	-3456(18)	2554(19)	4108(11)	76(4)
C(22)	-1912(24)	2688(27)	4510(17)	123(8)
C(23)	-1462(37)	1581(40)	5031(23)	174(15)
C(24)	-2428(47)	542(32)	5212(20)	156(13)
C(25)	-4106(38)	434(27)	4800(17)	138(8)
C(26)	-4520(24)	1466(22)	4282(12)	99(5)
C(27)	-4150(17)	1679(16)	-2163(10)	73(4)
C(28)	-4820(19)	2575(18)	-2707(11)	79(4)
C(29)	-6362(23)	2094(21)	-3488(14)	96(5)
C(30)	-7189(23)	704(21)	-3736(14)	95(5)
C(31)	-6591(22)	-288(22)	-3192(18)	119(7)
C(32)	-5036(21)	249(21)	-2412(13)	99(6)
C(1S)	-6398(24)	5940(24)	-4028(32)	155(11)
Cl(1S)	-7174(13)	6573(8)	-5404(7)	186(3)
Cl(2S)	-7656(15)	5624(11)	-3358(11)	206(4)

[a]U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 27. Interatomic Distances (Å) for $C_{33}H_{31}Cl_2CuF_{12}N_3O_4Sb_2$.

Cu(1)-N(1)	1.952(10)	Cu(1)-O(3)	1.986(8)
Cu(1)-N(3)	1.989(10)	Cu(1)-N(2)	2.014(9)
Cu(1)-O(4)	2.328(8)	Cu(1)-F(1)	2.619(7)
Sb(1)-F(6)	1.829(9)	Sb(1)-F(5)	1.840(10)
Sb(1)-F(4)	1.847(9)	Sb(1)-F(2)	1.847(9)
Sb(1)-F(1)	1.855(6)	Sb(1)-F(3)	1.877(6)
Sb(2)-F(12)	1.734(14)	Sb(2)-F(9)	1.770(13)
Sb(2)-F(8)	1.826(10)	Sb(2)-F(7)	1.828(14)
Sb(2)-F(10)	1.858(10)	Sb(2)-F(11)	1.865(13)
O(1)-C(6)	1.33(2)	O(1)-C(8)	1.46(3)
O(2)-C(9)	1.33(2)	O(2)-C(11)	1.46(2)
N(1)-C(1)	1.31(2)	N(1)-C(5)	1.34(2)
N(2)-C(9)	1.29(2)	N(2)-C(10)	1.46(2)
N(3)-C(6)	1.29(2)	N(3)-C(7)	1.51(2)
O(3)-C(13)	1.20(2)	O(4)-C(12)	1.42(2)
O(4)-C(14)	1.425(14)	C(1)-C(2)	1.35(2)
C(1)-C(6)	1.47(2)	C(2)-C(3)	1.32(3)
C(3)-C(4)	1.44(3)	C(4)-C(5)	1.40(2)
C(5)-C(9)	1.47(2)	C(7)-C(21)	1.50(2)

C(7)-C(8)	1.56(3)	C(10)-C(27)	1.50(2)
C(10)-C(11)	1.60(2)	C(12)-C(13)	1.46(2)
C(14)-C(15)	1.48(2)	C(15)-C(16)	1.37(2)
C(15)-C(20)	1.40(2)	C(16)-C(17)	1.47(2)
C(17)-C(18)	1.33(2)	C(18)-C(19)	1.35(2)
C(19)-C(20)	1.38(2)	C(21)-C(26)	1.36(3)
C(21)-C(22)	1.36(2)	C(22)-C(23)	1.43(3)
C(23)-C(24)	1.28(4)	C(24)-C(25)	1.48(4)
C(25)-C(26)	1.35(3)	C(27)-C(28)	1.35(2)
C(27)-C(32)	1.39(3)	C(28)-C(29)	1.38(2)
C(29)-C(30)	1.34(3)	C(30)-C(31)	1.40(3)
C(31)-C(32)	1.39(2)	C(1S)-Cl(2S)	1.62(3)
C(1S)-Cl(1S)	1.85(3)		

Table 28. Bond Angles (deg) for $C_{33}H_{31}Cl_2CuF_{12}N_3O_4Sb_2$.

N(1)-Cu(1)-O(3)	169.0(4)	N(1)-Cu(1)-N(3)	78.9(5)
O(3)-Cu(1)-N(3)	101.3(4)	N(1)-Cu(1)-N(2)	80.5(4)
O(3)-Cu(1)-N(2)	98.3(4)	N(3)-Cu(1)-N(2)	159.1(5)
N(1)-Cu(1)-O(4)	117.4(3)	O(3)-Cu(1)-O(4)	73.6(3)
N(3)-Cu(1)-O(4)	91.9(4)	N(2)-Cu(1)-O(4)	100.5(3)
N(1)-Cu(1)-F(1)	78.2(3)	O(3)-Cu(1)-F(1)	90.8(3)
N(3)-Cu(1)-F(1)	84.2(3)	N(2)-Cu(1)-F(1)	88.4(3)
O(4)-Cu(1)-F(1)	163.0(3)	F(6)-Sb(1)-F(5)	178.6(8)
F(6)-Sb(1)-F(4)	90.9(8)	F(5)-Sb(1)-F(4)	87.7(6)
F(6)-Sb(1)-F(2)	90.7(7)	F(5)-Sb(1)-F(2)	90.7(6)
F(4)-Sb(1)-F(2)	177.8(7)	F(6)-Sb(1)-F(1)	91.2(4)
F(5)-Sb(1)-F(1)	88.6(5)	F(4)-Sb(1)-F(1)	89.5(4)
F(2)-Sb(1)-F(1)	91.9(4)	F(6)-Sb(1)-F(3)	89.6(4)
F(5)-Sb(1)-F(3)	90.5(5)	F(4)-Sb(1)-F(3)	88.5(4)
F(2)-Sb(1)-F(3)	90.0(4)	F(1)-Sb(1)-F(3)	177.9(4)
F(12)-Sb(2)-F(9)	102.1(14)	F(12)-Sb(2)-F(8)	94.8(7)
F(9)-Sb(2)-F(8)	91.9(7)	F(12)-Sb(2)-F(7)	85.0(14)
F(9)-Sb(2)-F(7)	172.8(12)	F(8)-Sb(2)-F(7)	87.7(7)
F(12)-Sb(2)-F(10)	89.2(7)	F(9)-Sb(2)-F(10)	89.2(7)
F(8)-Sb(2)-F(10)	175.5(7)	F(7)-Sb(2)-F(10)	90.7(7)
F(12)-Sb(2)-F(11)	171.0(13)	F(9)-Sb(2)-F(11)	86.9(10)
F(8)-Sb(2)-F(11)	84.3(6)	F(7)-Sb(2)-F(11)	86.0(9)
F(10)-Sb(2)-F(11)	91.4(7)	Sb(1)-F(1)-Cu(1)	136.5(4)
C(6)-O(1)-C(8)	107.3(13)	C(9)-O(2)-C(11)	104.7(12)
C(1)-N(1)-C(5)	121.0(12)	C(1)-N(1)-Cu(1)	120.5(9)
C(5)-N(1)-Cu(1)	118.2(9)	C(9)-N(2)-C(10)	109.9(10)
C(9)-N(2)-Cu(1)	111.5(9)	C(10)-N(2)-Cu(1)	137.9(8)
C(6)-N(3)-C(7)	107.3(11)	C(6)-N(3)-Cu(1)	113.5(10)
C(7)-N(3)-Cu(1)	139.2(9)	C(13)-O(3)-Cu(1)	122.2(8)
C(12)-O(4)-C(14)	114.7(9)	C(12)-O(4)-Cu(1)	110.5(6)
C(14)-O(4)-Cu(1)	132.9(7)	N(1)-C(1)-C(2)	121(2)
N(1)-C(1)-C(6)	108.2(11)	C(2)-C(1)-C(6)	131(2)
C(3)-C(2)-C(1)	121(2)	C(2)-C(3)-C(4)	120(2)
C(5)-C(4)-C(3)	115(2)	N(1)-C(5)-C(4)	121(2)
N(1)-C(5)-C(9)	108.9(11)	C(4)-C(5)-C(9)	130(2)
N(3)-C(6)-O(1)	118(2)	N(3)-C(6)-C(1)	118.7(12)
O(1)-C(6)-C(1)	123.5(13)	C(21)-C(7)-N(3)	111.6(9)
C(21)-C(7)-C(8)	114.6(13)	N(3)-C(7)-C(8)	102.1(14)
O(1)-C(8)-C(7)	104.1(12)	N(2)-C(9)-O(2)	119.2(14)
N(2)-C(9)-C(5)	120.6(11)	O(2)-C(9)-C(5)	120.2(13)
N(2)-C(10)-C(27)	110.5(9)	N(2)-C(10)-C(11)	99.9(12)
C(27)-C(10)-C(11)	113.7(11)	O(2)-C(11)-C(10)	106.1(11)

O(4)-C(12)-C(13)	107.8(10)	O(3)-C(13)-C(12)	124.4(11)
O(4)-C(14)-C(15)	110.3(9)	C(16)-C(15)-C(20)	119.7(12)
C(16)-C(15)-C(14)	119.7(11)	C(20)-C(15)-C(14)	120.6(11)
C(15)-C(16)-C(17)	117.7(13)	C(18)-C(17)-C(16)	121(2)
C(17)-C(18)-C(19)	120.3(14)	C(18)-C(19)-C(20)	121.3(13)
C(19)-C(20)-C(15)	120.1(12)	C(26)-C(21)-C(22)	121(2)
C(26)-C(21)-C(7)	119.6(13)	C(22)-C(21)-C(7)	119(2)
C(21)-C(22)-C(23)	118(2)	C(24)-C(23)-C(22)	123(2)
C(23)-C(24)-C(25)	119(2)	C(26)-C(25)-C(24)	118(3)
C(25)-C(26)-C(21)	122(2)	C(28)-C(27)-C(32)	119(2)
C(28)-C(27)-C(10)	124(2)	C(32)-C(27)-C(10)	117.3(12)
C(27)-C(28)-C(29)	121(2)	C(30)-C(29)-C(28)	120(2)
C(29)-C(30)-C(31)	123(2)	C(32)-C(31)-C(30)	115(2)
C(31)-C(32)-C(27)	123(2)	Cl(2S)-C(1S)-Cl(1S)	110.9(13)

Table 29. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{33}H_{31}Cl_2CuF_{12}N_3O_4Sb_2$.[a]

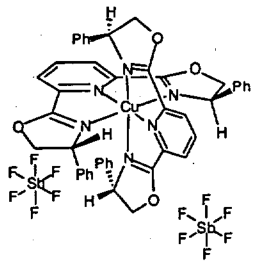
atom	U11	U22	U33	U23	U13	U12
Cu(1)	54(1)	38(1)	47(1)	9(1)	11(1)	13(1)
Sb(1)	49(1)	49(1)	69(1)	22(1)	14(1)	15(1)
Sb(2)	72(1)	72(1)	70(1)	17(1)	6(1)	14(1)
F(1)	82(5)	107(6)	100(5)	47(5)	44(5)	61(5)
F(2)	164(10)	165(11)	117(7)	97(8)	82(8)	113(9)
F(3)	85(5)	72(5)	81(5)	15(4)	29(4)	43(4)
F(4)	122(8)	134(9)	227(13)	138(10)	112(10)	77(7)
F(5)	97(7)	106(8)	118(8)	-9(7)	12(6)	-17(6)
F(6)	74(6)	107(8)	200(12)	-79(9)	-10(7)	27(6)
F(7)	316(24)	98(10)	164(13)	31(9)	-86(14)	59(12)
F(8)	86(6)	158(11)	118(7)	51(7)	11(6)	42(7)
F(9)	227(18)	106(10)	241(18)	-58(11)	-70(15)	89(12)
F(10)	97(7)	140(11)	143(10)	62(9)	-30(7)	-2(7)
F(11)	160(12)	241(18)	125(9)	75(11)	66(9)	79(13)
F(12)	134(13)	641(55)	147(13)	196(22)	75(11)	81(21)
O(1)	123(9)	91(8)	67(6)	-23(6)	7(6)	55(7)
O(2)	79(6)	108(9)	100(7)	63(7)	42(6)	42(6)
N(1)	64(6)	41(6)	68(6)	20(5)	11(5)	14(5)
N(2)	60(6)	62(6)	51(5)	22(5)	15(4)	28(5)
N(3)	70(7)	70(8)	60(6)	13(6)	10(5)	38(6)
O(3)	74(6)	34(4)	64(5)	9(4)	17(5)	13(4)
O(4)	47(4)	39(5)	62(5)	10(4)	8(4)	9(4)
C(1)	69(8)	41(7)	77(9)	12(7)	-9(7)	13(6)
C(2)	89(12)	55(10)	140(16)	14(10)	7(11)	12(9)
C(3)	94(13)	31(9)	185(22)	20(12)	-5(14)	7(8)
C(4)	55(9)	78(12)	156(16)	68(12)	19(9)	12(8)
C(5)	54(7)	58(8)	101(10)	41(8)	10(7)	16(6)
C(6)	75(8)	46(8)	73(8)	-11(7)	-10(7)	32(7)
C(7)	54(7)	84(10)	67(7)	-4(7)	27(6)	28(7)
C(8)	133(17)	173(23)	63(10)	-14(12)	25(11)	70(18)
C(9)	55(7)	85(10)	75(8)	52(8)	26(6)	37(7)
C(10)	71(8)	79(9)	55(7)	19(6)	21(6)	35(7)
C(11)	87(11)	144(18)	97(11)	59(13)	55(10)	62(12)
C(12)	51(6)	56(8)	51(6)	0(6)	12(5)	7(6)
C(13)	71(8)	34(6)	72(8)	2(6)	24(7)	1(6)
C(14)	52(7)	67(8)	66(7)	11(6)	18(6)	20(6)
C(15)	49(6)	44(6)	75(7)	21(6)	13(6)	17(5)
C(16)	72(9)	76(10)	94(10)	34(8)	45(8)	39(8)
C(17)	83(10)	50(9)	128(15)	42(10)	22(10)	15(7)
C(18)	88(10)	42(8)	99(11)	5(8)	14(9)	21(7)

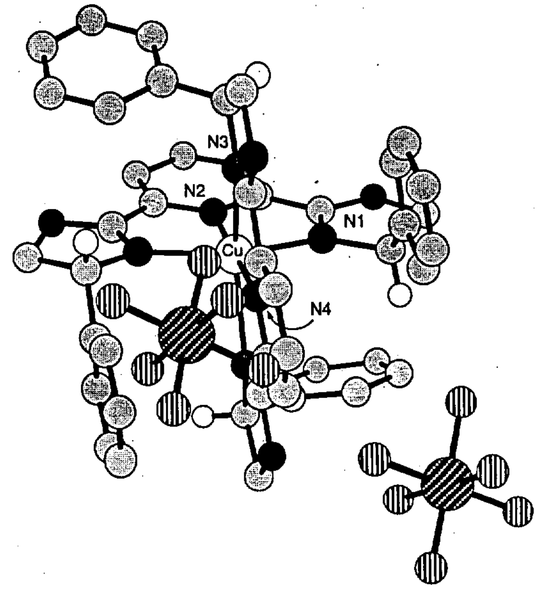
C(19)	100(10)	53(8)	92(10)	1(7)	44(9)	28(8)
C(20)	85(9)	54(8)	85(9)	21(7)	47(7)	27(7)
C(21)	82(9)	122(13)	47(6)	25(8)	36(7)	53(9)
C(22)	113(14)	213(24)	113(13)	105(15)	66(12)	104(16)
C(23)	209(29)	315(41)	158(22)	169(27)	126(23)	214(33)
C(24)	293(40)	170(24)	101(14)	83(17)	110(22)	157(28)
C(25)	208(28)	131(19)	70(11)	33(12)	33(14)	62(19)
C(26)	122(14)	122(15)	48(8)	12(9)	27(9)	38(12)
C(27)	85(9)	78(10)	44(6)	-6(7)	7(6)	34(8)
C(28)	95(10)	96(11)	53(7)	7(7)	12(7)	61(9)
C(29)	120(14)	117(15)	69(9)	29(10)	26(10)	74(13)
C(30)	105(12)	86(12)	69(9)	7(9)	0(8)	35(10)
C(31)	102(13)	93(13)	116(14)	-38(11)	3(11)	29(11)
C(32)	108(12)	118(15)	66(9)	-22(9)	13(9)	71(12)
C(1S)	80(12)	87(14)	305(37)	43(19)	81(19)	23(11)
Cl(1S)	284(10)	129(5)	145(5)	26(4)	47(6)	102(7)
Cl(2S)	271(12)	179(8)	250(10)	94(8)	150(10)	113(9)

[a]The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11} + ... + 2hka^*b^*U_{12}]$.

Table 30. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal Parameters (Å^2 x 10^3) for $C_{33}H_{31}Cl_2CuF_{12}N_3O_4Sb_2$.

atom	x	y	z	U(eq)
H(2A)	-16(22)	8085(18)	3579(20)	127
H(3A)	1537(24)	8724(16)	2510(24)	144
H(4A)	1153(18)	7099(21)	699(21)	119
H(7A)	-5122(15)	3319(16)	3100(11)	81
H(8A)	-4475(28)	5447(29)	4317(15)	150
H(8B)	-3175(28)	5017(29)	5273(15)	150
H(10A)	-2235(15)	1294(15)	-1012(10)	79
H(11A)	-488(21)	2479(24)	-1806(17)	115
H(11B)	-1734(21)	3135(24)	-2565(17)	115
H(12A)	-6924(14)	1416(13)	-1187(10)	69
H(12B)	-7513(14)	1503(13)	-84(10)	69
H(13A)	-6101(16)	-160(12)	77(11)	75
H(14A)	-7485(14)	3835(13)	-376(11)	75
H(14B)	-6462(14)	4059(13)	-1205(11)	75
H(16A)	-4347(17)	6178(16)	-742(15)	87
H(17A)	-2878(19)	8529(16)	516(18)	108
H(18A)	-3295(18)	9242(15)	2217(15)	99
H(19A)	-5021(18)	7708(15)	2815(14)	96
H(20A)	-6497(16)	5455(13)	1645(12)	82
H(22A)	-1165(24)	3480(27)	4448(17)	148
H(23A)	-409(37)	1618(40)	5252(23)	209
H(24A)	-2079(47)	-139(32)	5598(20)	187
H(25A)	-4856(38)	-327(27)	4897(17)	165
H(26A)	-5573(24)	1433(22)	4033(12)	119
H(28A)	-4234(19)	3542(18)	-2556(11)	95
H(29A)	-6827(23)	2735(21)	-3843(14)	115
H(30A)	-8215(23)	386(21)	-4300(14)	114
H(31A)	-7193(22)	-1249(22)	-3342(18)	142
H(32A)	-4567(21)	-380(21)	-2039(13)	118
H(1SA)	-6156(24)	5067(24)	-4238(32)	186
H(1SB)	-5426(24)	6664(24)	-3482(32)	186





[Cu{(*S,S*)-phenyl-bis(oxazolinyl)pyridine}{(*R,R*)-phenyl-bis(oxazolinyl)pyridine}](SbF_6)$_2$. A 1:1 mixture of [Cu{(*S,S*)-Ph-pybox}](SbF_6)$_2$ and [Cu({*R,R*)-Ph-pybox}](SbF_6)$_2$ was prepared following method C using racemic ligand. The single crystal X-ray structure[39] was determined for the blue crystals obtained by slow evaporation of the resultant CH_2Cl_2 solution in a septum-sealed vial.

Table 31. Crystal and Data Collection Parameters for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

Empirical formula	$C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$
Formula weight	1358.79
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	$I\bar{4}2d$ (space group #122)
a, alpha	20.351(3) Å, 90 deg.
b, beta	20.351(3) Å, 90 deg.
c, gamma	24.758(5) Å, 90 deg.
Volume, Z	10254(3) Å^3, 8
Density (calculated)	1.760 mg/mm^3
Absorption coefficient	1.655 mm^{-1}
F(000)	5400
Crystal size	0.05 x 0.10 x 0.19 mm
θ range for data collection	1.30 to 24.72 deg.
Limiting indices	$-23 \leq h \leq 23$, $-23 \leq k \leq 15$, $-29 \leq l \leq 29$
Reflections collected	26342
Independent reflections	4385 [R_{int} = 0.0658]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9218 and 0.7438
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4385 / 6 / 343
Goodness-of-fit on F^2	1.106
Final R indices [$I>2\sigma(I)$]	R1 = 0.0448, wR2 = 0.1188
R indices (all data)	R1 = 0.0537, wR2 = 0.1309

Absolute structure parameter	-0.06(3)
Extinction coefficient	0.00024(5)
Largest diff. peak and hole	0.910 and -0.865 eA^{-3}

Table 32. Atomic Coordinates (x 10^4) and Isotropic Thermal Parameters ($Å^2$ x 10^3) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

atom	x	y	z	U(eq)[a]
Cu	7411(1)	2500	1250	38(1)
N(1)	7624(3)	3492(3)	1190(2)	41(1)
N(2)	8389(4)	2500	1250	40(2)
N(3)	7109(3)	2329(3)	323(2)	47(1)
N(4)	6418(4)	2500	1250	42(2)
O(1)	8443(3)	4228(3)	1132(2)	53(1)
O(2)	6172(3)	2203(3)	-159(2)	72(2)
C(1)	8239(3)	3619(3)	1176(3)	41(2)
C(2)	7277(3)	4135(3)	1156(3)	44(2)
C(3)	7842(4)	4626(4)	1051(3)	56(2)
C(4)	8697(3)	3068(3)	1218(3)	40(1)
C(5)	9389(4)	3087(4)	1207(3)	55(2)
C(6)	9726(5)	2500	1250	57(3)
C(7)	6754(3)	4099(3)	719(3)	45(2)
C(8)	6093(4)	4161(4)	862(4)	56(2)
C(9)	5602(4)	4085(5)	489(5)	71(3)
C(10)	5769(5)	3958(5)	-34(4)	73(3)
C(11)	6430(5)	3895(4)	-179(4)	66(2)
C(12)	6909(4)	3973(4)	188(3)	51(2)
C(13)	6485(4)	2312(3)	305(3)	51(2)
C(14)	7343(4)	2201(4)	-230(3)	59(2)
C(15)	6713(6)	2160(6)	-561(4)	86(3)
C(16)	6074(3)	2398(3)	788(3)	48(2)
C(17)	5386(4)	2387(4)	778(4)	64(2)
C(18)	5055(6)	2500	1250	71(3)
C(19)	7767(5)	1594(4)	-240(3)	58(2)
C(20)	7508(5)	982(4)	-90(3)	67(2)
C(21)	7897(6)	428(5)	-74(4)	78(3)
C(22)	8569(8)	482(7)	-230(5)	102(4)
C(23)	8797(6)	1054(7)	-393(6)	103(4)
C(24)	8409(6)	1617(6)	-393(5)	86(3)
Sb	3732(1)	997(1)	543(1)	54(1)
F(1)	3164(3)	1231(4)	-16(2)	107(2)
F(2)	4426(3)	1297(4)	126(3)	104(2)
F(3)	3807(4)	173(3)	249(3)	117(3)
F(4)	3016(4)	738(4)	950(3)	112(3)
F(5)	3626(4)	1843(3)	830(3)	94(2)
F(6)	4305(4)	789(4)	1092(3)	111(2)
Cl(1)	9393(5)	613(5)	-1648(4)	304(5)
C(1S)	10000	0	-1177(5)	55(3)
C(1SA)	10000	0	-1886(11)	148(10)

[a]U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 33. Interatomic Distances (Å) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.[a]

Cu-N(2)	1.990(8)	Cu-N(4)	2.022(8)
Cu-N(1)	2.071(5)	Cu-N(1)#1	2.071(5)
Cu-N(3)	2.402(6)	Cu-N(3)#1	2.402(6)
N(1)-C(1)	1.278(9)	N(1)-C(2)	1.490(8)
N(2)-C(4)#1	1.317(7)	N(2)-C(4)	1.317(7)

N(3)-C(13)	1.271(10)	N(3)-C(14)	1.471(10)
N(4)-C(16)	1.356(8)	N(4)-C(16)#1	1.356(8)
O(1)-C(1)	1.311(8)	O(1)-C(3)	1.480(10)
O(2)-C(13)	1.332(9)	O(2)-C(15)	1.489(12)
C(1)-C(4)	1.461(10)	C(2)-C(7)	1.521(10)
C(2)-C(3)	1.545(10)	C(4)-C(5)	1.410(9)
C(5)-C(6)	1.381(10)	C(6)-C(5)#1	1.381(10)
C(7)-C(12)	1.376(11)	C(7)-C(8)	1.396(11)
C(8)-C(9)	1.369(13)	C(9)-C(10)	1.37(2)
C(10)-C(11)	1.398(14)	C(11)-C(12)	1.341(12)
C(13)-C(16)	1.469(11)	C(14)-C(19)	1.507(12)
C(14)-C(15)	1.525(13)	C(16)-C(17)	1.402(11)
C(17)-C(18)	1.369(11)	C(18)-C(17)#1	1.369(11)
C(19)-C(24)	1.360(14)	C(19)-C(20)	1.403(12)
C(20)-C(21)	1.378(14)	C(21)-C(22)	1.43(2)
C(22)-C(23)	1.32(2)	C(23)-C(24)	1.39(2)
Sb-F(3)	1.834(6)	Sb-F(6)	1.839(6)
Sb-F(4)	1.847(6)	Sb-F(2)	1.853(6)
Sb-F(1)	1.865(6)	Sb-F(5)	1.875(5)
Cl(1)-C(1SA)	1.852(12)	Cl(1)-C(1S)	2.11(2)
C(1S)-Cl(1)#2	2.11(2)	C(1SA)-Cl(1)#2	1.852(12)

[a]Symmetry transformations used to generate equivalent atoms: #1 x+1-1,-y+1/2,-z+1/4 #2 -x+2,-y,z.

Table 34. Bond Angles (deg) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.[a]

N(2)-Cu-N(4)	180.0	N(2)-Cu-N(1)	77.9(2)
N(4)-Cu-N(1)	102.1(2)	N(2)-Cu-N(1)#1	77.9(2)
N(4)-Cu-N(1)#1	102.1(2)	N(1)-Cu-N(1)#1	155.8(3)
N(2)-Cu-N(3)	104.8(2)	N(4)-Cu-N(3)	75.2(2)
N(1)-Cu-N(3)	97.3(2)	N(1)#1-Cu-N(3)	88.9(2)
N(2)-Cu-N(3)#1	104.8(2)	N(4)-Cu-N(3)#1	75.2(2)
N(1)-Cu-N(3)#1	88.9(2)	N(1)#1-Cu-N(3)#1	97.3(2)
N(3)-Cu-N(3)#1	150.3(3)	C(1)-N(1)-C(2)	106.6(5)
C(1)-N(1)-Cu	113.8(5)	C(2)-N(1)-Cu	139.6(4)
C(4)#1-N(2)-C(4)	123.2(8)	C(4)#1-N(2)-Cu	118.4(4)
C(4)-N(2)-Cu	118.4(4)	C(13)-N(3)-C(14)	106.7(6)
C(13)-N(3)-Cu	107.0(5)	C(14)-N(3)-Cu	146.2(5)
C(16)-N(4)-C(16)#1	118.0(9)	C(16)-N(4)-Cu	121.0(4)
C(16)#1-N(4)-Cu	121.0(4)	C(1)-O(1)-C(3)	105.5(6)
C(13)-O(2)-C(15)	103.5(7)	N(1)-C(1)-O(1)	120.2(6)
N(1)-C(1)-C(4)	117.9(6)	O(1)-C(1)-C(4)	122.0(6)
N(1)-C(2)-C(7)	109.2(5)	N(1)-C(2)-C(3)	102.9(5)
C(7)-C(2)-C(3)	115.7(6)	O(1)-C(3)-C(2)	103.8(6)
N(2)-C(4)-C(5)	120.0(7)	N(2)-C(4)-C(1)	112.0(6)
C(5)-C(4)-C(1)	127.9(7)	C(6)-C(5)-C(4)	118.1(8)
C(5)#1-C(6)-C(5)	120.4(9)	C(12)-C(7)-C(8)	118.7(7)
C(12)-C(7)-C(2)	122.0(7)	C(8)-C(7)-C(2)	119.3(7)
C(9)-C(8)-C(7)	121.5(8)	C(10)-C(9)-C(8)	118.6(9)
C(9)-C(10)-C(11)	120.1(8)	C(12)-C(11)-C(10)	121.0(9)
C(11)-C(12)-C(7)	120.2(8)	N(3)-C(13)-O(2)	120.8(7)
N(3)-C(13)-C(16)	122.6(6)	O(2)-C(13)-C(16)	116.7(7)

N(3)-C(14)-C(19)	110.3(7)	N(3)-C(14)-C(15)	103.7(7)
C(19)-C(14)-C(15)	115.3(8)	O(2)-C(15)-C(14)	105.0(7)
N(4)-C(16)-C(17)	122.2(8)	N(4)-C(16)-C(13)	114.3(6)
C(17)-C(16)-C(13)	123.5(7)	C(18)-C(17)-C(16)	118.2(8)
C(17)#1-C(18)-C(17)	121.1(10)	C(24)-C(19)-C(20)	117.7(9)
C(24)-C(19)-C(14)	121.7(9)	C(20)-C(19)-C(14)	120.6(8)
C(21)-C(20)-C(19)	121.2(10)	C(20)-C(21)-C(22)	118.7(10)
C(23)-C(22)-C(21)	119.2(12)	C(22)-C(23)-C(24)	122.0(12)
C(19)-C(24)-C(23)	121.1(11)	F(3)-Sb-F(6)	91.7(4)
F(3)-Sb-F(4)	91.3(4)	F(6)-Sb-F(4)	91.8(3)
F(3)-Sb-F(2)	90.9(4)	F(6)-Sb-F(2)	90.2(4)
F(4)-Sb-F(2)	177.0(4)	F(3)-Sb-F(1)	89.5(4)
F(6)-Sb-F(1)	178.3(4)	F(4)-Sb-F(1)	89.4(3)
F(2)-Sb-F(1)	88.5(3)	F(3)-Sb-F(5)	177.9(3)
F(6)-Sb-F(5)	90.3(3)	F(4)-Sb-F(5)	88.0(3)
F(2)-Sb-F(5)	89.8(3)	F(1)-Sb-F(5)	88.6(3)
C(1SA)-Cl(1)-C(1S)	52.1(9)	Cl(1)#2-C(1S)-Cl(1)	112.9(6)
Cl(1)#2-C(1SA)-Cl(1)	143(2)		

[a]Symmetry transformations used to generate equivalent atoms: #1 x+1-1,-y+1/2,-z+1/4 #2 -x+2,-y,z.

Table 35. Anisotropic Displacement Parameters (Å^2 x 10^3) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.[a]

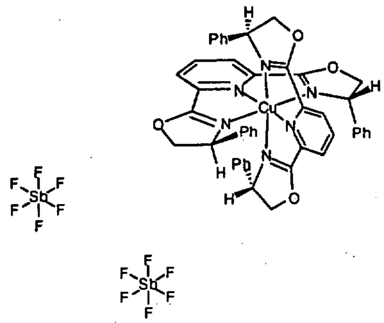
atom	U11	U22	U33	U23	U13	U12
Cu	33(1)	39(1)	42(1)	2(1)	0	0
N(1)	42(3)	42(3)	38(3)	3(2)	-1(2)	2(2)
N(2)	39(4)	49(4)	32(4)	7(3)	0	0
N(3)	59(4)	48(3)	33(3)	-1(2)	-2(3)	-1(3)
N(4)	46(4)	30(4)	51(5)	-3(4)	0	0
O(1)	51(3)	47(3)	61(3)	1(2)	-5(2)	-10(2)
O(2)	78(4)	84(4)	55(3)	-12(3)	-28(3)	9(3)
C(1)	47(4)	39(4)	36(3)	-4(3)	-7(3)	-9(3)
C(2)	46(4)	35(3)	52(4)	-2(3)	2(3)	3(3)
C(3)	62(5)	43(4)	64(5)	6(3)	-11(4)	2(4)
C(4)	38(3)	46(3)	37(3)	7(3)	-6(3)	-7(3)
C(5)	40(4)	69(5)	55(4)	5(4)	1(3)	-16(3)
C(6)	39(5)	68(7)	66(7)	-2(6)	0	0
C(7)	45(4)	33(3)	56(4)	7(3)	-4(3)	8(3)
C(8)	57(5)	48(4)	62(5)	10(3)	6(4)	5(3)
C(9)	49(5)	67(5)	99(7)	24(5)	-7(5)	-4(4)
C(10)	72(6)	61(5)	85(7)	13(5)	-37(5)	-7(4)
C(11)	90(7)	59(5)	48(4)	6(4)	-15(4)	9(4)
C(12)	58(4)	42(4)	53(4)	5(3)	-2(3)	5(3)
C(13)	63(5)	41(4)	50(4)	-7(3)	-17(4)	6(3)
C(14)	77(6)	61(5)	39(4)	0(3)	2(4)	1(4)
C(15)	120(9)	95(7)	44(4)	-9(5)	-17(6)	34(7)
C(16)	48(4)	36(3)	61(4)	1(3)	-16(3)	-5(3)
C(17)	41(4)	58(5)	93(6)	2(4)	-26(4)	-5(4)
C(18)	36(5)	64(7)	114(11)	7(8)	0	0
C(19)	77(5)	65(5)	33(4)	-9(3)	-8(4)	1(4)
C(20)	95(6)	58(4)	46(4)	-4(4)	12(4)	-6(5)
C(21)	112(8)	53(5)	69(6)	-6(4)	9(6)	-3(5)
C(22)	136(12)	96(9)	72(7)	-30(7)	-7(7)	30(8)
C(23)	71(6)	103(9)	135(11)	-30(8)	17(7)	16(7)

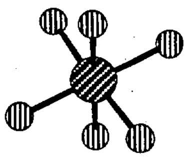
C(24)	88(7)	81(7)	88(8)	-26(6)	28(6)	-25(6)
Sb	61(1)	53(1)	47(1)	-1(1)	2(1)	-4(1)
F(1)	94(4)	164(7)	62(3)	-12(4)	-21(3)	22(5)
F(2)	103(5)	124(5)	86(4)	2(4)	35(4)	-31(4)
F(3)	141(6)	71(4)	140(6)	-44(4)	16(5)	-11(4)
F(4)	99(5)	124(6)	114(5)	17(4)	44(4)	-23(4)
F(5)	119(5)	61(3)	102(4)	-22(3)	-14(4)	6(3)
F(6)	116(5)	137(6)	80(4)	0(4)	-27(4)	43(5)
Cl(1)	263(8)	323(9)	327(9)	-190(8)	140(7)	-184(7)
C(1S)	63(7)	62(6)	40(6)	0	0	-35(5)
C(1SA)	104(15)	220(3)	116(18)	0	0	-10(19)

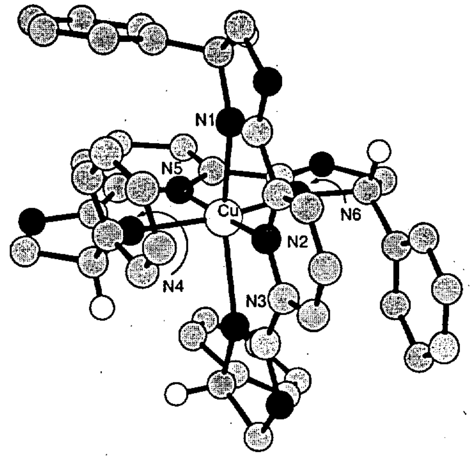
[a]The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11} + ... + 2hka^*b^*U_{12}]$.

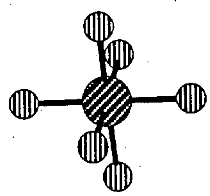
Table 36. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal Parameters ($Å^2$ x 10^3) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

atom	x	y	z	U(eq)
H(2B)	7068	4235	1508	53
H(3A)	7822	4800	682	68
H(3B)	7826	4993	1307	68
H(5A)	9615	3488	1172	66
H(6A)	10188	2500	1250	69
H(8A)	5984	4257	1222	67
H(9A)	5158	4120	592	86
H(10A)	5439	3912	-297	87
H(11A)	6540	3798	-539	79
H(12A)	7351	3940	82	61
H(14A)	7606	2581	-355	71
H(15A)	6688	2524	-820	104
H(15B)	6692	1744	-760	104
H(17A)	5157	2304	455	77
H(18A)	4593	2500	1250	86
H(20A)	7061	949	3	80
H(21A)	7722	22	37	93
H(22A)	8847	113	-216	122
H(23A)	9234	1083	-513	124
H(24A)	8593	2020	-501	103
H(1SA)	9729	-268	-949	66
H(1SC)	10265	262	-2123	178









[Cu{(*S*,*S*)-phenyl-bis(oxazolinyl)pyridine}$_2$](SbF$_6$)$_2$. The single crystal X-ray structure[40] was determined for the blue crystals obtained by slow evaporation of a CH_2Cl_2 solution of [Cu{(*S*,*S*)-Ph-pybox}]$(SbF_6)_2$ (method C) in a septum-sealed vial.

Table 37. Crystal and Data Collection Parameters for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

Empirical formula	$C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$
Formula weight	1358.79
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P*2(1)
a, alpha	9.988(2) Å, 90 deg.
b, beta	22.739(4) Å, 99.62 deg.
c, gamma	11.224(2) Å, 90 deg.
Volume, Z	2513.4(9) Å^3, 2
Density (calculated)	1.795 mg/mm^3
Absorption coefficient	1.688 mm^{-1}
F(000)	1338
Crystal size	0.10 x 0.20 x 0.25 mm
θ range for data collection	1.84 to 28.22 deg.
Limiting indices	$-13 \le h \le 12$, $-25 \le k \le 29$, $-14 \le l \le 13$
Reflections collected	12994
Independent reflections	7368 [R_{int} = 0.0342]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.8494 and 0.6777
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	7368 / 1 / 677
Goodness-of-fit on F^2	1.084
Final R indices [I>2σ(I)]	R1 = 0.0428, wR2 = 0.0872
R indices (all data)	R1 = 0.0634, wR2 = 0.1004
Absolute structure parameter	-0.02(2)
Largest diff. peak and hole	0.417 and -0.528 eA^{-3}

Table 38. Atomic Coordinates (x 10^4) and Isotropic Thermal Parameters (Å^2 x 10^3) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

atom	x	y	z	U(eq)[a]
Cu(1)	17172(1)	6358(1)	12020(1)	32(1)
O(1)	21288(5)	5791(3)	12602(6)	59(2)
O(2)	15708(6)	6802(2)	8314(5)	45(1)
O(3)	14931(7)	4936(3)	12774(5)	59(2)
O(4)	17108(6)	7854(2)	14043(5)	50(2)
N(1)	19221(6)	6025(3)	13010(6)	40(2)
N(2)	18291(6)	6304(3)	10705(5)	33(1)
N(3)	15671(6)	6627(3)	10281(5)	35(1)
N(4)	16284(6)	5525(3)	11901(6)	37(2)
N(5)	16184(6)	6373(3)	13386(5)	31(1)
N(6)	17588(7)	7199(3)	12675(6)	38(2)
C(1)	20001(7)	5972(3)	12236(8)	41(2)
C(2)	20016(9)	5868(4)	14224(8)	51(2)
C(3)	21367(10)	5671(5)	13894(9)	72(3)
C(4)	19574(8)	6120(3)	10951(7)	39(2)
C(5)	20379(9)	6064(3)	10070(8)	47(2)
C(6)	19832(9)	6230(4)	8908(8)	54(2)
C(7)	18515(9)	6431(4)	8636(7)	46(2)
C(8)	17769(8)	6461(3)	9570(7)	38(2)
C(9)	16334(7)	6639(3)	9421(6)	31(2)
C(10)	14262(8)	6791(4)	9773(7)	39(2)
C(11)	14336(10)	6974(4)	8464(8)	58(3)
C(12)	19251(9)	5448(4)	14878(8)	44(2)
C(13)	18519(9)	5668(4)	15700(8)	50(2)
C(14)	17731(11)	5308(6)	16279(9)	72(3)
C(15)	17685(13)	4723(5)	16056(10)	78(3)
C(16)	18435(16)	4487(5)	15232(13)	92(4)
C(17)	19237(13)	4851(5)	14664(11)	75(3)
C(18)	13717(8)	7243(4)	10584(8)	46(2)
C(19)	13588(10)	7834(4)	10361(11)	68(3)
C(20)	13181(12)	8214(5)	11157(13)	89(4)
C(21)	12917(11)	8014(5)	12216(12)	80(4)
C(22)	13005(10)	7429(6)	12502(9)	74(3)
C(23)	13404(9)	7031(4)	11683(8)	55(2)
C(24)	15608(8)	5442(3)	12757(8)	42(2)
C(25)	16032(8)	5028(4)	11056(7)	47(2)
C(26)	15174(13)	4604(5)	11710(10)	75(3)
C(27)	15540(7)	5897(3)	13657(7)	36(2)
C(28)	14923(8)	5872(4)	14674(7)	46(2)
C(29)	14956(9)	6368(5)	15365(8)	57(2)
C(30)	15605(9)	6870(4)	15056(7)	49(2)
C(31)	16209(8)	6859(3)	14057(7)	37(2)
C(32)	16986(8)	7329(3)	13563(7)	36(2)
C(33)	18415(8)	7728(3)	12481(7)	41(2)
C(34)	17895(10)	8193(4)	13261(8)	53(2)

C(35)	17362(9)	4776(4)	10779(8)	48(2)
C(36)	18181(13)	4450(5)	11606(9)	78(4)
C(37)	19415(15)	4262(6)	11340(10)	98(5)
C(38)	19806(12)	4370(5)	10230(11)	76(3)
C(39)	18913(10)	4679(4)	9407(9)	57(2)
C(40)	17703(9)	4876(3)	9664(7)	45(2)
C(41)	18311(9)	7868(3)	11160(8)	46(2)
C(42)	19405(9)	7767(4)	10600(9)	53(2)
C(43)	19333(13)	7847(4)	9365(11)	70(3)
C(44)	18159(15)	8040(4)	8707(11)	75(3)
C(45)	17059(13)	8159(5)	9227(10)	77(3)
C(46)	17138(10)	8074(4)	10470(9)	55(2)
Sb(1)	8895(1)	2594(1)	3960(1)	47(1)
Sb(2)	6859(1)	89(1)	12218(1)	45(1)
F(1)	8810(7)	3001(3)	5373(5)	85(2)
F(2)	7762(7)	2026(3)	4387(6)	88(2)
F(3)	10016(7)	3182(3)	3555(6)	98(2)
F(4)	10401(7)	2196(3)	4727(9)	126(4)
F(5)	7428(8)	3002(3)	3141(8)	111(3)
F(6)	8953(8)	2178(3)	2563(7)	108(3)
F(7)	7817(8)	765(4)	12780(8)	126(3)
F(8)	7052(7)	299(4)	10665(6)	109(3)
F(9)	8431(7)	-340(4)	12427(7)	105(3)
F(10)	5257(6)	531(3)	11988(6)	81(2)
F(11)	5867(8)	-555(3)	11643(8)	102(2)
F(12)	6655(8)	-38(4)	13781(5)	122(3)
Cl(2)	2677(4)	4019(2)	3988(4)	77(1)
Cl(1)	5316(5)	3490(2)	4188(5)	85(1)
C(1S)	4296(13)	3991(5)	4814(12)	58(3)
Cl(1B)	4601(15)	3530(7)	3952(17)	85(1)
Cl(2B)	2390(11)	4300(5)	3070(12)	77(1)
C(1SB)	3180(5)	3860(2)	4210(5)	58(3)

[a]U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 39. Interatomic Distances (Å) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

Cu(1)-N(5)	1.957(5)	Cu(1)-N(2)	1.999(6)
Cu(1)-N(6)	2.066(6)	Cu(1)-N(4)	2.085(6)
Cu(1)-N(1)	2.288(6)	Cu(1)-N(3)	2.335(6)
O(1)-C(1)	1.347(9)	O(1)-C(3)	1.465(11)
O(2)-C(9)	1.346(8)	O(2)-C(11)	1.461(11)
O(3)-C(24)	1.335(9)	O(3)-C(26)	1.467(12)
O(4)-C(32)	1.308(9)	O(4)-C(34)	1.487(10)
N(1)-C(1)	1.266(10)	N(1)-C(2)	1.501(10)
N(2)-C(4)	1.332(9)	N(2)-C(8)	1.342(9)
N(3)-C(9)	1.259(9)	N(3)-C(10)	1.475(9)
N(4)-C(24)	1.278(10)	N(4)-C(25)	1.471(10)
N(5)-C(27)	1.320(9)	N(5)-C(31)	1.336(10)
N(6)-C(32)	1.281(10)	N(6)-C(33)	1.496(10)
C(1)-C(4)	1.473(11)	C(2)-C(12)	1.490(12)
C(2)-C(3)	1.525(13)	C(4)-C(5)	1.381(11)
C(5)-C(6)	1.381(12)	C(6)-C(7)	1.378(12)
C(7)-C(8)	1.386(10)	C(8)-C(9)	1.472(10)
C(10)-C(18)	1.532(11)	C(10)-C(11)	1.541(12)
C(12)-C(13)	1.364(12)	C(12)-C(17)	1.377(12)
C(13)-C(14)	1.374(13)	C(14)-C(15)	1.35(2)
C(15)-C(16)	1.39(2)	C(16)-C(17)	1.38(2)
C(18)-C(19)	1.368(12)	C(18)-C(23)	1.408(12)

C(19)-C(20)	1.354(14)	C(20)-C(21)	1.34(2)
C(21)-C(22)	1.37(2)	C(22)-C(23)	1.396(13)
C(24)-C(27)	1.456(11)	C(25)-C(35)	1.525(12)
C(25)-C(26)	1.553(12)	C(27)-C(28)	1.386(11)
C(28)-C(29)	1.366(13)	C(29)-C(30)	1.386(12)
C(30)-C(31)	1.359(11)	C(31)-C(32)	1.481(11)
C(33)-C(41)	1.503(11)	C(33)-C(34)	1.519(12)
C(35)-C(36)	1.352(12)	C(35)-C(40)	1.370(11)
C(36)-C(37)	1.38(2)	C(37)-C(38)	1.39(2)
C(38)-C(39)	1.367(13)	C(39)-C(40)	1.364(12)
C(41)-C(42)	1.369(12)	C(41)-C(46)	1.374(12)
C(42)-C(43)	1.388(13)	C(43)-C(44)	1.35(2)
C(44)-C(45)	1.36(2)	C(45)-C(46)	1.398(14)
Sb(1)-F(2)	1.832(6)	Sb(1)-F(6)	1.840(6)
Sb(1)-F(4)	1.841(7)	Sb(1)-F(5)	1.845(7)
Sb(1)-F(3)	1.850(6)	Sb(1)-F(1)	1.851(6)
Sb(2)-F(12)	1.822(6)	Sb(2)-F(11)	1.825(6)
Sb(2)-F(9)	1.830(6)	Sb(2)-F(8)	1.848(6)
Sb(2)-F(7)	1.864(7)	Sb(2)-F(10)	1.871(5)
Cl(2)-C(1S)	1.726(14)	Cl(1)-C(1S)	1.751(13)
Cl(1B)-C(1SB)	1.68(5)	Cl(2B)-C(1SB)	1.71(5)

Table 40. Bond Angles (deg) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

N(5)-Cu(1)-N(2)	175.5(3)	N(5)-Cu(1)-N(6)	78.6(3)
N(2)-Cu(1)-N(6)	102.5(3)	N(5)-Cu(1)-N(4)	78.6(3)
N(2)-Cu(1)-N(4)	100.4(2)	N(6)-Cu(1)-N(4)	157.1(3)
N(5)-Cu(1)-N(1)	98.7(2)	N(2)-Cu(1)-N(1)	76.9(2)
N(6)-Cu(1)-N(1)	91.3(3)	N(4)-Cu(1)-N(1)	93.8(2)
N(5)-Cu(1)-N(3)	108.3(2)	N(2)-Cu(1)-N(3)	76.1(2)
N(6)-Cu(1)-N(3)	96.8(2)	N(4)-Cu(1)-N(3)	88.7(2)
N(1)-Cu(1)-N(3)	152.8(2)	C(1)-O(1)-C(3)	104.4(7)
C(9)-O(2)-C(11)	105.5(6)	C(24)-O(3)-C(26)	106.2(7)
C(32)-O(4)-C(34)	104.6(6)	C(1)-N(1)-C(2)	107.9(7)
C(1)-N(1)-Cu(1)	107.5(5)	C(2)-N(1)-Cu(1)	144.5(5)
C(4)-N(2)-C(8)	119.3(6)	C(4)-N(2)-Cu(1)	120.2(5)
C(8)-N(2)-Cu(1)	120.5(5)	C(9)-N(3)-C(10)	106.7(6)
C(9)-N(3)-Cu(1)	107.5(5)	C(10)-N(3)-Cu(1)	145.8(5)
C(24)-N(4)-C(25)	108.4(6)	C(24)-N(4)-Cu(1)	111.0(5)
C(25)-N(4)-Cu(1)	139.9(5)	C(27)-N(5)-C(31)	120.8(6)
C(27)-N(5)-Cu(1)	119.7(5)	C(31)-N(5)-Cu(1)	119.5(5)
C(32)-N(6)-C(33)	105.7(6)	C(32)-N(6)-Cu(1)	113.4(6)
C(33)-N(6)-Cu(1)	140.8(5)	N(1)-C(1)-O(1)	119.0(8)
N(1)-C(1)-C(4)	122.7(7)	O(1)-C(1)-C(4)	118.3(7)
C(12)-C(2)-N(1)	111.3(7)	C(12)-C(2)-C(3)	118.6(8)
N(1)-C(2)-C(3)	101.9(7)	O(1)-C(3)-C(2)	106.4(7)
N(2)-C(4)-C(5)	122.4(8)	N(2)-C(4)-C(1)	112.7(7)
C(5)-C(4)-C(1)	124.9(8)	C(4)-C(5)-C(6)	117.8(8)
C(7)-C(6)-C(5)	120.8(7)	C(6)-C(7)-C(8)	117.6(8)
N(2)-C(8)-C(7)	122.2(7)	N(2)-C(8)-C(9)	113.5(6)
C(7)-C(8)-C(9)	124.3(7)	N(3)-C(9)-O(2)	119.5(7)
N(3)-C(9)-C(8)	122.2(6)	O(2)-C(9)-C(8)	118.3(6)
N(3)-C(10)-C(18)	110.5(6)	N(3)-C(10)-C(11)	104.0(6)
C(18)-C(10)-C(11)	117.6(7)	O(2)-C(11)-C(10)	103.4(6)
C(13)-C(12)-C(17)	119.3(10)	C(13)-C(12)-C(2)	118.4(8)
C(17)-C(12)-C(2)	122.4(10)	C(12)-C(13)-C(14)	121.0(10)
C(15)-C(14)-C(13)	120.3(12)	C(14)-C(15)-C(16)	119.8(12)
C(17)-C(16)-C(15)	119.7(11)	C(12)-C(17)-C(16)	120.0(12)

C(19)-C(18)-C(23)	117.9(9)	C(19)-C(18)-C(10)	125.7(9)
C(23)-C(18)-C(10)	116.3(8)	C(20)-C(19)-C(18)	122.5(11)
C(21)-C(20)-C(19)	119.5(12)	C(20)-C(21)-C(22)	121.7(10)
C(21)-C(22)-C(23)	119.4(11)	C(22)-C(23)-C(18)	118.9(9)
N(4)-C(24)-O(3)	118.1(8)	N(4)-C(24)-C(27)	120.5(7)
O(3)-C(24)-C(27)	121.3(7)	N(4)-C(25)-C(35)	111.0(7)
N(4)-C(25)-C(26)	102.8(6)	C(35)-C(25)-C(26)	115.6(8)
O(3)-C(26)-C(25)	104.1(7)	N(5)-C(27)-C(28)	121.6(7)
N(5)-C(27)-C(24)	110.0(6)	C(28)-C(27)-C(24)	128.4(7)
C(29)-C(28)-C(27)	117.6(8)	C(28)-C(29)-C(30)	120.4(7)
C(31)-C(30)-C(29)	118.8(8)	N(5)-C(31)-C(30)	120.8(8)
N(5)-C(31)-C(32)	110.3(6)	C(30)-C(31)-C(32)	128.9(8)
N(6)-C(32)-O(4)	120.5(8)	N(6)-C(32)-C(31)	117.9(7)
O(4)-C(32)-C(31)	121.5(7)	N(6)-C(33)-C(41)	111.5(6)
N(6)-C(33)-C(34)	103.0(6)	C(41)-C(33)-C(34)	116.5(7)
O(4)-C(34)-C(33)	104.2(6)	C(36)-C(35)-C(40)	120.2(9)
C(36)-C(35)-C(25)	120.9(8)	C(40)-C(35)-C(25)	118.9(7)
C(35)-C(36)-C(37)	118.7(10)	C(36)-C(37)-C(38)	122.2(10)
C(39)-C(38)-C(37)	116.6(10)	C(40)-C(39)-C(38)	121.8(10)
C(39)-C(40)-C(35)	120.3(8)	C(42)-C(41)-C(46)	118.0(9)
C(42)-C(41)-C(33)	119.2(8)	C(46)-C(41)-C(33)	122.7(8)
C(41)-C(42)-C(43)	121.6(10)	C(44)-C(43)-C(42)	119.0(10)
C(43)-C(44)-C(45)	121.4(11)	C(44)-C(45)-C(46)	119.3(11)
C(41)-C(46)-C(45)	120.6(10)	F(2)-Sb(1)-F(6)	88.3(3)
F(2)-Sb(1)-F(4)	91.4(4)	F(6)-Sb(1)-F(4)	90.4(4)
F(2)-Sb(1)-F(5)	90.6(4)	F(6)-Sb(1)-F(5)	88.3(4)
F(4)-Sb(1)-F(5)	177.5(5)	F(2)-Sb(1)-F(3)	178.3(3)
F(6)-Sb(1)-F(3)	93.2(3)	F(4)-Sb(1)-F(3)	89.4(4)
F(5)-Sb(1)-F(3)	88.7(4)	F(2)-Sb(1)-F(1)	90.5(3)
F(6)-Sb(1)-F(1)	178.8(3)	F(4)-Sb(1)-F(1)	89.7(4)
F(5)-Sb(1)-F(1)	91.7(4)	F(3)-Sb(1)-F(1)	88.0(3)
F(12)-Sb(2)-F(11)	94.1(4)	F(12)-Sb(2)-F(9)	91.4(4)
F(11)-Sb(2)-F(9)	91.2(4)	F(12)-Sb(2)-F(8)	174.1(4)
F(11)-Sb(2)-F(8)	90.6(4)	F(9)-Sb(2)-F(8)	92.1(3)
F(12)-Sb(2)-F(7)	86.4(4)	F(11)-Sb(2)-F(7)	177.8(4)
F(9)-Sb(2)-F(7)	90.9(4)	F(8)-Sb(2)-F(7)	88.7(4)
F(12)-Sb(2)-F(10)	89.3(3)	F(11)-Sb(2)-F(10)	89.0(3)
F(9)-Sb(2)-F(10)	179.3(4)	F(8)-Sb(2)-F(10)	87.3(3)
F(7)-Sb(2)-F(10)	89.0(3)	Cl(2)-C(1S)-Cl(1)	111.4(8)
Cl(1B)-C(1SB)-Cl(2B)	115(3)		

Table 41. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.[a]

atom	U11	U22	U33	U23	U13	U12
Cu(1)	38(1)	28(1)	31(1)	1(1)	12(1)	0(1)
O(1)	34(3)	76(4)	67(4)	10(4)	6(3)	5(3)
O(2)	60(4)	47(3)	27(3)	3(3)	1(3)	2(3)
O(3)	81(5)	49(4)	51(4)	-2(3)	23(3)	-31(3)
O(4)	64(4)	39(3)	48(4)	-17(3)	15(3)	-2(3)
N(1)	37(4)	44(4)	41(4)	8(3)	6(3)	7(3)
N(2)	38(3)	28(3)	36(3)	-7(3)	12(3)	-8(3)
N(3)	47(4)	30(3)	29(3)	3(3)	12(3)	2(3)
N(4)	48(4)	28(3)	34(4)	5(3)	7(3)	-4(3)
N(5)	35(3)	37(3)	23(3)	4(3)	9(2)	3(3)
N(6)	49(4)	31(3)	30(4)	-5(3)	2(3)	3(3)
C(1)	27(4)	34(4)	61(6)	-2(4)	6(4)	3(3)
C(2)	57(6)	51(5)	44(5)	-3(4)	3(4)	-11(4)
C(3)	52(6)	96(8)	66(7)	13(7)	-1(5)	-3(6)

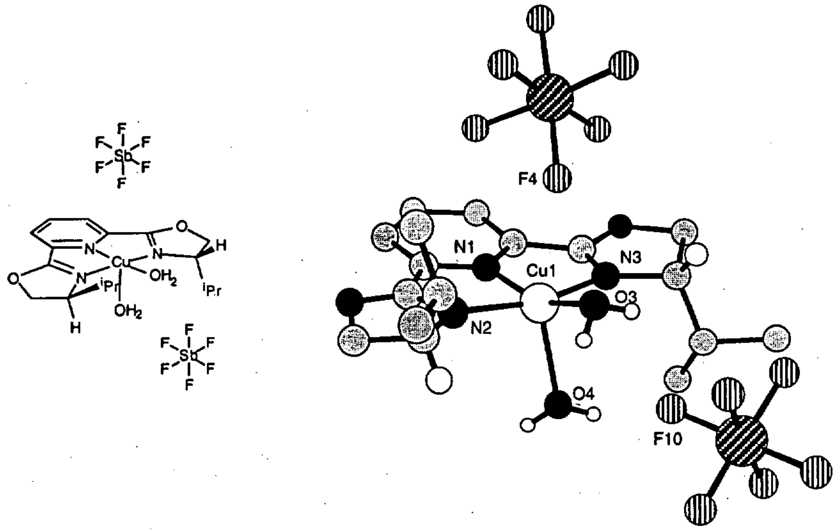
C(4)	37(4)	32(4)	51(5)	-9(4)	14(4)	-4(3)
C(5)	52(5)	34(4)	63(6)	-9(4)	36(5)	-6(4)
C(6)	65(6)	57(6)	52(5)	3(5)	44(5)	1(4)
C(7)	64(6)	41(5)	36(4)	1(4)	19(4)	-8(4)
C(8)	51(5)	31(4)	34(4)	-1(3)	13(4)	-14(3)
C(9)	44(4)	23(3)	27(4)	0(3)	10(3)	3(3)
C(10)	33(4)	37(4)	44(5)	0(4)	-1(4)	7(3)
C(11)	66(6)	65(6)	35(5)	-5(4)	-14(4)	24(5)
C(12)	55(6)	38(5)	34(5)	3(4)	-5(4)	2(4)
C(13)	62(6)	40(5)	45(5)	6(4)	1(5)	5(4)
C(14)	64(7)	102(9)	51(6)	16(6)	13(5)	4(6)
C(15)	96(9)	69(8)	60(7)	24(6)	-11(6)	-25(7)
C(16)	136(13)	39(6)	93(10)	-9(6)	-3(9)	-17(7)
C(17)	106(9)	49(6)	70(7)	-10(5)	16(6)	-4(5)
C(18)	34(4)	46(5)	54(6)	-9(4)	-6(4)	9(4)
C(19)	65(7)	58(6)	89(8)	-2(6)	35(6)	4(5)
C(20)	93(9)	59(7)	126(11)	-23(8)	49(8)	12(6)
C(21)	68(7)	79(8)	95(9)	-44(7)	16(7)	24(6)
C(22)	69(7)	107(10)	49(6)	-2(6)	17(5)	34(6)
C(23)	61(6)	62(6)	43(5)	11(5)	11(5)	22(5)
C(24)	50(5)	32(4)	46(5)	9(4)	10(4)	-10(3)
C(25)	69(6)	38(4)	36(4)	-8(4)	12(4)	-11(4)
C(26)	107(9)	63(7)	57(7)	-8(6)	21(7)	-35(6)
C(27)	34(4)	46(4)	30(4)	0(3)	8(3)	-5(3)
C(28)	42(5)	56(5)	44(5)	9(4)	18(4)	1(4)
C(29)	49(5)	82(7)	44(5)	8(6)	25(4)	8(5)
C(30)	63(6)	56(5)	32(4)	-10(4)	17(4)	7(4)
C(31)	34(4)	43(4)	36(4)	0(4)	13(4)	7(3)
C(32)	37(4)	38(4)	33(4)	-3(3)	2(3)	8(3)
C(33)	47(5)	37(5)	38(4)	3(4)	4(4)	-3(3)
C(34)	81(7)	31(4)	50(5)	0(4)	22(5)	-9(4)
C(35)	71(6)	34(4)	40(5)	0(4)	13(4)	9(4)
C(36)	126(10)	70(7)	37(5)	11(5)	13(6)	49(7)
C(37)	128(11)	106(10)	54(7)	13(7)	1(7)	63(9)
C(38)	91(8)	61(6)	75(7)	-9(6)	7(6)	38(6)
C(39)	74(7)	39(5)	57(6)	0(4)	8(5)	-1(4)
C(40)	59(5)	33(4)	39(5)	6(4)	-2(4)	2(4)
C(41)	62(6)	29(4)	49(5)	-6(4)	19(4)	-6(4)
C(42)	57(6)	42(5)	66(6)	-3(4)	23(5)	-12(4)
C(43)	89(8)	51(6)	85(8)	0(6)	55(7)	-10(5)
C(44)	119(10)	48(6)	66(7)	7(5)	41(8)	-19(6)
C(45)	105(9)	52(6)	64(7)	13(6)	-16(7)	-7(6)
C(46)	60(6)	44(5)	61(6)	5(4)	15(5)	4(4)
Sb(1)	53(1)	48(1)	42(1)	-3(1)	10(1)	-10(1)
Sb(2)	46(1)	47(1)	43(1)	3(1)	11(1)	4(1)
F(1)	119(5)	85(4)	50(3)	-18(3)	17(3)	-22(4)
F(2)	97(5)	91(5)	83(5)	-7(4)	33(4)	-45(4)
F(3)	119(5)	85(5)	96(5)	3(4)	34(4)	-47(4)
F(4)	82(5)	75(5)	199(10)	4(5)	-42(6)	7(4)
F(5)	101(6)	88(5)	124(6)	0(5)	-41(5)	14(4)
F(6)	145(7)	98(5)	98(5)	-55(5)	65(5)	-40(5)
F(7)	96(5)	80(5)	187(9)	-19(5)	-14(6)	-34(4)
F(8)	112(5)	156(8)	66(4)	39(5)	35(4)	15(5)
F(9)	72(4)	132(6)	106(6)	-17(5)	-1(4)	47(4)
F(10)	61(4)	68(4)	112(5)	-1(4)	7(3)	25(3)
F(11)	103(6)	52(4)	149(7)	-27(4)	12(5)	-11(3)
F(12)	136(6)	187(9)	50(4)	15(5)	34(4)	40(6)
Cl(2)	60(2)	73(3)	93(3)	-7(2)	1(2)	3(2)

Cl(1)	77(4)	63(2)	123(4)	11(2)	42(4)	12(3)
C(1S)	60(8)	48(7)	71(9)	4(6)	23(7)	-3(6)
Cl(1B)	77(4)	63(2)	123(4)	11(2)	42(4)	12(3)
Cl(2B)	60(2)	73(3)	93(3)	-7(2)	1(2)	3(2)
C(1SB)	60(8)	48(7)	71(9)	4(6)	23(7)	-3(6)

[a]The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11} + ... + 2hka^*b^*U_{12}]$.

Table 42. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal Parameters (Å^2 x 10^3) for $C_{47}H_{40}Cl_2CuF_{12}N_6O_4Sb_2$.

atom	x	y	z	U(eq)
H(2A)	20175	6232	14710	62
H(3A)	22119	5890	14366	87
H(3B)	21511	5250	14058	87
H(5A)	21269	5916	10255	56
H(6A)	20365	6206	8294	65
H(7A)	18136	6544	7845	55
H(10A)	13692	6433	9745	46
H(11A)	13652	6766	7888	70
H(11B)	14203	7399	8354	70
H(13A)	18554	6073	15872	60
H(14A)	17222	5468	16833	87
H(15A)	17148	4477	16457	93
H(16A)	18395	4082	15062	110
H(17A)	19775	4692	14132	90
H(19A)	13790	7981	9629	82
H(20A)	13084	8617	10968	107
H(21A)	12665	8282	12776	96
H(22A)	12799	7297	13244	89
H(23A)	13462	6627	11862	66
H(25A)	15473	5164	10294	57
H(26A)	14315	4505	11189	90
H(26B)	15673	4240	11950	90
H(28A)	14498	5527	14881	56
H(29A)	14536	6369	16055	68
H(30A)	15626	7213	15527	59
H(33A)	19378	7645	12815	49
H(34A)	18650	8404	13749	63
H(34B)	17313	8477	12762	63
H(36A)	17917	4352	12347	93
H(37A)	20009	4054	11931	117
H(38A)	20643	4237	10054	92
H(39A)	19139	4758	8643	68
H(40A)	17101	5080	9074	54
H(42A)	20226	7639	11063	64
H(43A)	20089	7767	8992	84
H(44A)	18105	8094	7870	90
H(45A)	16252	8296	8757	93
H(46A)	16380	8158	10838	66
H(1SA)	4248	3874	5646	70
H(1SB)	4708	4382	4837	70
H(1SC)	3400	4104	4943	70
H(1SD)	2534	3561	4377	70



[Cu{(*S*,*S*)-*i*-propyl-bis(oxazolinyl)pyridine}$(H_2O)_2$]$(SbF_6)_2$. The single crystal X-ray structure[41] was determined for the dark blue crystals obtained by slow evaporation of a CH_2Cl_2 solution of [Cu(*i*-Pr-pybox)]$(SbF_6)_2$ (method C) in a septum-sealed flask after brief exposure to the atmosphere.

Table 43. Crystal and Data Collection Parameters for $C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$.

Empirical formula	$C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$
Formula weight	957.38
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P*2(1)
a, alpha	12.1435(1) Å, 90 deg.
b, beta	8.5940(2) Å, 90.322(1) deg.
c, gamma	15.6652(3) Å, 90 deg.
Volume, Z	1630.19(5) $Å^3$, 2
Density (calculated)	1.950 mg/mm^3
Absorption coefficient	2.553 mm^{-1}
F(000)	926
Crystal size	0.05 x 0.15 x 0.3 mm
θ range for data collection	1.30 to 24.74 deg.
Limiting indices	$-14 \le h \le 13$, $-10 \le k \le 6$, $-18 \le l \le 15$
Reflections collected	6613
Independent reflections	3945 [R_{int} = 0.0244]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.962234 and 0.748891
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3945 / 1 / 379
Goodness-of-fit on F^2	1.055
Final R indices [$I>2\sigma(I)$]	R1 = 0.0398, wR2 = 0.0921
R indices (all data)	R1 = 0.0507, wR2 = 0.0995
Absolute structure parameter	0.04(3)
Largest diff. peak and hole	0.746 and -0.856 eA^{-3}

Table 44. Atomic Coordinates (x 10^4) and Isotropic Thermal Parameters ($Å^2$ x 10^3) for $C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$.

atom	x	y	z	U(eq)
Cu(1)	13214(1)	7628(1)	7344(1)	36(1)
Sb(1)	12230(1)	12096(1)	6341(1)	46(1)
F(1)	11296(8)	10459(11)	5997(7)	126(4)
F(2)	11780(7)	13205(12)	5360(5)	112(3)
F(3)	13134(9)	13745(12)	6638(9)	165(5)
F(4)	12652(8)	10905(13)	7293(5)	114(3)
F(5)	11086(8)	12991(14)	6840(5)	122(4)
F(6)	13371(7)	11214(11)	5798(6)	113(3)
Sb(2)	16823(1)	7800(1)	9933(1)	58(1)
F(7)	17251(20)	9259(19)	9196(10)	267(10)
F(8)	18085(9)	8176(20)	10649(9)	181(6)
F(9)	16422(10)	6370(15)	10696(8)	169(6)
F(10)	15633(8)	7506(22)	9234(6)	197(7)
F(11)	17631(10)	6389(16)	9346(8)	165(5)
F(12)	16129(12)	9344(16)	10478(6)	170(6)
O(1)	10051(5)	6149(9)	7345(4)	50(2)
O(2)	14605(5)	8337(8)	5100(4)	47(2)
O(3)	13870(6)	8827(10)	8340(4)	60(2)
O(4)	14088(6)	5620(9)	7910(4)	53(2)
N(1)	12372(5)	7210(11)	6254(4)	35(2)
N(2)	11740(5)	7060(11)	7761(4)	38(2)
N(3)	14339(6)	8131(9)	6509(4)	39(2)
C(1)	11322(7)	6782(10)	6263(5)	37(2)
C(2)	10678(8)	6561(13)	5492(6)	51(3)
C(3)	11164(8)	6816(14)	4745(6)	57(3)
C(4)	12238(7)	7254(13)	4735(5)	42(2)
C(5)	12839(7)	7430(11)	5517(5)	41(2)
C(6)	11022(7)	6656(10)	7154(6)	39(2)
C(7)	10132(9)	5997(15)	8291(7)	57(3)
C(8)	11203(7)	6878(15)	8578(5)	49(3)
C(9)	11069(9)	8445(17)	8995(7)	66(4)
C(10)	10344(12)	9554(16)	8470(9)	82(4)
C(11)	10653(11)	8234(22)	9897(7)	100(6)
C(12)	13971(7)	7967(12)	5712(5)	39(2)
C(13)	15585(8)	9043(14)	5527(7)	58(3)
C(14)	15499(7)	8673(12)	6498(6)	46(2)
C(15)	16306(7)	7498(14)	6878(6)	53(3)
C(16)	17471(8)	8204(22)	6940(8)	97(6)
C(17)	16273(11)	5945(14)	6413(7)	69(3)
C(1S)	16895(16)	2827(27)	8368(10)	132(7)
Cl(1S)	18049(4)	2820(7)	7782(3)	117(1)
Cl(2S)	15703(4)	2360(6)	7732(4)	143(2)

[a]U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 45. Interatomic Distances (Å) for $C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$.

Cu(1)-N(1)	1.957(6)	Cu(1)-O(3)	1.985(7)
Cu(1)-N(3)	2.009(7)	Cu(1)-N(2)	2.011(7)
Cu(1)-O(4)	2.179(7)	Cu(1)-F(4)	2.897(10)
Cu(1)-F(10)	4.011(7)	Sb(1)-F(5)	1.816(7)
Sb(1)-F(3)	1.831(9)	Sb(1)-F(6)	1.842(7)
Sb(1)-F(4)	1.850(7)	Sb(1)-F(2)	1.854(7)

Sb(1)-F(1)	1.861(9)	Sb(2)-F(10)	1.764(8)
Sb(2)-F(9)	1.806(9)	Sb(2)-F(7)	1.807(12)
Sb(2)-F(12)	1.819(9)	Sb(2)-F(11)	1.848(10)
Sb(2)-F(8)	1.859(10)	O(1)-C(6)	1.312(10)
O(1)-C(7)	1.483(13)	O(2)-C(12)	1.314(10)
O(2)-C(13)	1.453(11)	N(1)-C(1)	1.327(11)
N(1)-C(5)	1.337(10)	N(2)-C(6)	1.288(11)
N(2)-C(8)	1.489(10)	N(3)-C(12)	1.301(11)
N(3)-C(14)	1.484(11)	C(1)-C(2)	1.402(12)
C(1)-C(6)	1.473(12)	C(2)-C(3)	1.367(14)
C(3)-C(4)	1.358(14)	C(4)-C(5)	1.386(11)
C(5)-C(12)	1.461(12)	C(7)-C(8)	1.543(14)
C(8)-C(9)	1.51(2)	C(9)-C(10)	1.50(2)
C(9)-C(11)	1.55(2)	C(13)-C(14)	1.565(14)
C(14)-C(15)	1.499(14)	C(15)-C(17)	1.52(2)
C(15)-C(16)	1.536(14)	C(1S)-Cl(1S)	1.73(2)
C(1S)-Cl(2S)	1.74(2)		

Table 46. Bond Angles (deg) for $C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$.

N(1)-Cu(1)-O(3)	159.0(4)	N(1)-Cu(1)-N(3)	78.9(3)
O(3)-Cu(1)-N(3)	98.5(3)	N(1)-Cu(1)-N(2)	79.6(3)
O(3)-Cu(1)-N(2)	100.7(3)	N(3)-Cu(1)-N(2)	158.3(3)
N(1)-Cu(1)-O(4)	114.6(3)	O(3)-Cu(1)-O(4)	86.4(3)
N(3)-Cu(1)-O(4)	95.8(3)	N(2)-Cu(1)-O(4)	95.4(3)
N(1)-Cu(1)-F(4)	92.7(3)	O(3)-Cu(1)-F(4)	66.2(3)
N(3)-Cu(1)-F(4)	86.8(3)	N(2)-Cu(1)-F(4)	91.8(3)
O(4)-Cu(1)-F(4)	152.5(3)	N(1)-Cu(1)-F(10)	160.9(3)
O(3)-Cu(1)-F(10)	37.4(3)	N(3)-Cu(1)-F(10)	89.4(3)
N(2)-Cu(1)-F(10)	112.0(3)	O(4)-Cu(1)-F(10)	51.1(3)
F(4)-Cu(1)-F(10)	101.7(3)	F(5)-Sb(1)-F(3)	91.5(6)
F(5)-Sb(1)-F(6)	178.1(4)	F(3)-Sb(1)-F(6)	88.8(5)
F(5)-Sb(1)-F(4)	93.5(4)	F(3)-Sb(1)-F(4)	95.7(5)
F(6)-Sb(1)-F(4)	88.4(4)	F(5)-Sb(1)-F(2)	87.3(4)
F(3)-Sb(1)-F(2)	86.9(5)	F(6)-Sb(1)-F(2)	90.8(4)
F(4)-Sb(1)-F(2)	177.2(5)	F(5)-Sb(1)-F(1)	88.6(5)
F(3)-Sb(1)-F(1)	177.7(6)	F(6)-Sb(1)-F(1)	91.0(5)
F(4)-Sb(1)-F(1)	86.6(5)	F(2)-Sb(1)-F(1)	90.8(5)
Sb(1)-F(4)-Cu(1)	127.6(4)	F(10)-Sb(2)-F(9)	93.7(7)
F(10)-Sb(2)-F(7)	88.0(9)	F(9)-Sb(2)-F(7)	178.2(9)
F(10)-Sb(2)-F(12)	90.5(6)	F(9)-Sb(2)-F(12)	91.6(6)
F(7)-Sb(2)-F(12)	87.6(8)	F(10)-Sb(2)-F(11)	92.2(6)
F(9)-Sb(2)-F(11)	93.6(7)	F(7)-Sb(2)-F(11)	87.0(7)
F(12)-Sb(2)-F(11)	173.9(8)	F(10)-Sb(2)-F(8)	177.9(8)
F(9)-Sb(2)-F(8)	88.3(6)	F(7)-Sb(2)-F(8)	90.0(10)
F(12)-Sb(2)-F(8)	88.8(6)	F(11)-Sb(2)-F(8)	88.2(6)
Sb(2)-F(10)-Cu(1)	167.0(8)	C(6)-O(1)-C(7)	105.3(7)
C(12)-O(2)-C(13)	105.7(7)	C(1)-N(1)-C(5)	121.2(7)
C(1)-N(1)-Cu(1)	118.7(5)	C(5)-N(1)-Cu(1)	120.0(5)
C(6)-N(2)-C(8)	106.9(7)	C(6)-N(2)-Cu(1)	113.3(5)
C(8)-N(2)-Cu(1)	139.7(5)	C(12)-N(3)-C(14)	106.3(7)
C(12)-N(3)-Cu(1)	113.5(6)	C(14)-N(3)-Cu(1)	140.1(6)
N(1)-C(1)-C(2)	120.1(8)	N(1)-C(1)-C(6)	109.7(7)
C(2)-C(1)-C(6)	130.1(8)	C(3)-C(2)-C(1)	117.8(9)
C(4)-C(3)-C(2)	122.1(8)	C(3)-C(4)-C(5)	117.5(8)
N(1)-C(5)-C(4)	121.2(8)	N(1)-C(5)-C(12)	108.5(7)
C(4)-C(5)-C(12)	130.1(8)	N(2)-C(6)-O(1)	119.4(8)
N(2)-C(6)-C(1)	118.5(7)	O(1)-C(6)-C(1)	122.1(8)

O(1)-C(7)-C(8)	103.9(8)	N(2)-C(8)-C(9)	110.3(9)
N(2)-C(8)-C(7)	102.4(7)	C(9)-C(8)-C(7)	116.6(9)
C(10)-C(9)-C(8)	114.1(9)	C(10)-C(9)-C(11)	110.9(11)
C(8)-C(9)-C(11)	110.1(11)	N(3)-C(12)-O(2)	119.7(8)
N(3)-C(12)-C(5)	119.1(7)	O(2)-C(12)-C(5)	121.2(7)
O(2)-C(13)-C(14)	104.4(7)	N(3)-C(14)-C(15)	112.1(8)
N(3)-C(14)-C(13)	102.0(7)	C(15)-C(14)-C(13)	115.7(8)
C(14)-C(15)-C(17)	114.1(8)	C(14)-C(15)-C(16)	109.4(11)
C(17)-C(15)-C(16)	111.7(10)	Cl(1S)-C(1S)-Cl(2S)	111.6(9)

Table 47. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$.[a]

atom	U11	U22	U33	U23	U13	U12
Cu(1)	32(1)	45(1)	32(1)	-1(1)	0(1)	3(1)
Sb(1)	52(1)	38(1)	49(1)	-1(1)	0(1)	10(1)
F(1)	115(7)	66(6)	190(10)	-9(6)	-43(7)	-5(5)
F(2)	132(7)	116(8)	87(5)	55(5)	6(5)	49(6)
F(3)	133(8)	84(8)	264(14)	-59(8)	-80(9)	-19(6)
F(4)	137(8)	151(9)	54(4)	30(5)	10(4)	60(7)
F(5)	136(7)	124(9)	113(6)	18(6)	59(6)	75(7)
F(6)	129(7)	89(7)	128(7)	40(6)	67(6)	60(6)
Sb(2)	78(1)	51(1)	45(1)	2(1)	7(1)	2(1)
F(7)	478(30)	152(13)	192(14)	83(12)	153(17)	-37(17)
F(8)	110(7)	220(15)	205(11)	-25(11)	-45(7)	-21(9)
F(9)	171(10)	161(12)	171(10)	118(9)	-10(8)	-43(9)
F(10)	144(8)	284(20)	146(8)	-74(12)	-106(7)	63(12)
F(11)	160(9)	163(13)	174(10)	-61(9)	23(8)	73(9)
F(12)	238(13)	172(12)	99(7)	-61(8)	5(8)	105(10)
O(1)	38(4)	58(5)	56(4)	-4(4)	8(3)	-5(3)
O(2)	41(4)	53(4)	49(4)	4(3)	14(3)	5(3)
O(3)	51(4)	72(6)	57(5)	-21(4)	1(3)	3(4)
O(4)	49(4)	49(4)	61(4)	9(4)	1(3)	6(3)
N(1)	28(3)	35(4)	40(4)	8(3)	-3(3)	1(3)
N(2)	33(3)	47(4)	32(3)	10(4)	-2(3)	5(4)
N(3)	35(4)	39(5)	42(4)	-1(3)	1(3)	4(3)
C(1)	41(5)	28(6)	39(5)	-1(4)	-7(4)	11(4)
C(2)	32(5)	67(8)	52(6)	-4(5)	-11(4)	-1(5)
C(3)	66(7)	69(9)	33(5)	-14(5)	-19(4)	13(6)
C(4)	47(5)	50(6)	30(4)	1(4)	-3(3)	11(5)
C(5)	40(5)	38(7)	45(5)	-2(4)	2(4)	10(4)
C(6)	24(4)	37(6)	56(5)	2(4)	8(4)	3(4)
C(7)	54(7)	66(8)	50(6)	9(5)	6(5)	-11(6)
C(8)	35(5)	80(8)	33(5)	7(5)	2(4)	5(5)
C(9)	48(6)	97(10)	56(6)	-29(7)	19(5)	-24(6)
C(10)	84(9)	59(9)	105(11)	-10(8)	25(8)	9(8)
C(11)	96(10)	155(17)	52(7)	-25(9)	26(7)	-25(10)
C(12)	43(5)	37(6)	36(4)	3(4)	11(4)	8(4)
C(13)	43(6)	48(7)	83(8)	13(6)	14(5)	-6(5)
C(14)	31(5)	52(7)	55(6)	-10(5)	8(4)	0(4)
C(15)	43(5)	73(9)	42(5)	-4(5)	0(4)	1(5)
C(16)	31(6)	169(19)	90(9)	-33(10)	2(6)	-5(8)
C(17)	84(9)	58(8)	68(8)	17(6)	15(7)	25(7)
C(1S)	206(20)	89(13)	98(11)	-6(12)	-9(13)	29(16)
Cl(1S)	125(3)	116(4)	104(3)	-1(3)	-37(2)	5(3)
Cl(2S)	118(3)	73(3)	232(6)	-46(4)	-19(3)	13(3)

[a]The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11} + ... + 2hka^*b^*U_{12}]$.

Table 48. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal Parameters (Å^2 x 10^3) for $C_{18}H_{29}Cl_2CuF_{12}N_3O_4Sb_2$.

atom	x	y	z	U(eq)
H(3B)	14550(6)	8879(10)	8249(4)	72
H(3C)	13836(6)	8196(10)	8755(4)	72
H(4B)	14763(6)	5573(9)	7801(4)	64
H(4C)	13762(6)	4762(9)	7795(4)	64
H(2A)	9936(8)	6248(13)	5488(6)	61
H(3A)	10742(8)	6685(14)	4222(6)	69
H(4A)	12561(7)	7430(13)	4217(5)	51
H(7A)	10181(9)	4902(15)	8463(7)	68
H(7B)	9492(9)	6471(15)	8535(7)	68
H(8A)	11671(7)	6207(15)	8971(5)	59
H(9A)	11812(9)	8922(17)	9071(7)	80
H(10A)	10296(12)	10530(16)	8776(9)	123
H(10B)	9611(12)	9110(16)	8367(9)	123
H(10C)	10655(12)	9740(16)	7927(9)	123
H(11A)	11133(11)	7514(22)	10225(7)	150
H(11B)	9907(11)	7825(22)	9846(7)	150
H(11C)	10659(11)	9232(22)	10187(7)	150
H(13A)	15592(8)	10169(14)	5428(7)	69
H(13B)	16257(8)	8590(14)	5322(7)	69
H(14A)	15585(7)	9652(12)	6829(6)	55
H(15A)	16111(7)	7295(14)	7470(6)	63
H(16A)	17995(8)	7446(22)	7186(8)	145
H(16B)	17485(8)	9122(22)	7302(8)	145
H(16C)	17670(8)	8491(22)	6373(8)	145
H(17A)	16815(11)	5248(14)	6693(7)	104
H(17B)	16441(11)	6103(14)	5824(7)	104
H(17C)	15543(11)	5493(14)	6426(7)	104
H(1SB)	16810(16)	3860(27)	8619(10)	159
H(1SC)	16999(16)	2074(27)	8836(10)	159

(1) (a) Inoue, T.; Mukaiyama, T. *Bull. Chem. Soc. Jpn.* **1980**, *53*, 174. (b) Evans, D. A.; Vogel, E.; Nelson, J. V. *J. Am. Chem. Soc.* **1979**, *101*, 6120-6123.

(2) Prepared following the procedure of: Corey, E. J.; Imai, N.; Zhang, H.-Y. *J. Am. Chem. Soc.* **1991**, *113*, 728-729.

(3) Prepared using a modified method of: (a) Evans, D. A.; Woerpel, K. A.; Hinman, M. M.; Faul, M. M. *J. Am. Chem. Soc.* **1991**, *113*, 1726-1728. (b) Evans, D. A.; Peterson, G. S.; Johnson, J. S.; Barnes, D. M.; Campos, K. R.; Woerpel, K. A. *J. Org. Chem.*, *in press*.

(4) For the preparation of (*S*,*S*)-bis(phenyloxazolinyl)pyridine and (*S*,*S*)-bis(isopropyl-oxazolinyl)pyridine see: Nishiyama, H.; Kondo, M.; Nakamura, T.; Itoh, K. *Organometallics*, **1991**, *10*, 500-508.

(5) Benzyloxyacetaldehyde is commercially available from Aldrich Chemical Company. Alternatively, an inexpensive two-step synthesis from 2-butene-1,4-diol is amenable to large scale preparations via bis-benzylation (Garner, P.; Park, J. M. *Synthesis Commun.* **1987**, *17*, 189-193) followed by ozonolysis (Danishefsky, S. J.; DeNinno, M. P. *J. Org. Chem.* **1986**, *51*, 2615-2617).

(6) For a general review of this reagent see: Casiraghi, G.; Rassu, G. *Synthesis* **1995**, 607-626.

(7) (a) Unless otherwise specified the procedure of Kuwajima was used, employing the appropriate thioester and the appropriate silyl chloride: Kuwajima, I.; Kato, M.; Sato, T. *J. Chem. Soc., Chem. Commun.* **1978**, 478-479. (b) For the silylketene acetal of ethyl acetate: Kita, Y.; Segawa, J.; Yasuda, J. H.; Tamura, Y. *J. Chem. Soc., Perkin I* **1982**, 1099-1104. (c) For the silylketene acetal of 2,2,6 trimethyl-1,3-dioxene-4-one: Sato, M.; Sunami, S.; Sugita, Y.; Kaneko, C. *Chem. Pharm. Bull.* **1994**, 42, 839-845. (d) For the silylketene acetal of methyl acetoacetate: Brownbridge, P.; Chan, T. H.; Brook, M. A.; Kang, G. J. *Can. J. Chem.* **1983**, *61*, 688-693. (e) The *E* and *Z* silylketene acetals of *tert*-butyl thiopropionate were prepared following the method of Gennari, *et al.* This procedure was also applied to the preparation of all other thioester derived silylketene acetals containing alkyl substitution. Gennari, C.; Beretta, M. G.; Bernardi, A.; Moro, G.; Solastico, C.; Todeschini, R. *Tetrahedron* **1986**, *42*, 893-909. (f) For the *E* and *Z* silylketene acetals of ethyl propionate: Otera, J.; Fujita, Y.; Fukusumi, S. *Synthesis Lett.* **1994**, 213-214. Chan, T. H.; Aida, T.; Lau, P. W. K.; Gorys, V.; Harpp, D. N. *Tetrahedron Lett.* **1979**, 4029-4032. (g) For the *Z* silylketene acetal of ethyl benzyloxythioacetate: Kobayashi, S; Horibe, M.; Saito, Y. *Tetrahedron* **1994**, *50*, 9629-9642. (h) For the silylketene acetal of γ-butyrolactone and the *Z* and *E* enolsilanes of 2-methyl-3-pentanone: : Heathcock, C. H.; Davidsen, S. K.; Hug, K. T.; Flippin, L. A. *J. Org. Chem.* **1986**, *51*, 3027-3037.

(8) Mikami, K.; Matsukawa, S. J. *J. Am. Chem. Soc.* **1994**, *116*, 4077-4078.

(9) Booth, P. M.; Fox, C. M. J.; Ley, S. V. *Tetrahedron Lett.* **1983**, *46*, 5143-5146.

(10) Sato, M.; Sunami, S.; Sugita, Y.; Kaneko, C. *Chem Pharm Bull.* **1994**, *42*, 839-845.

(11) Sato, M.; Sunami, S.; Sugita, Y.; Kaneko, C. *Heterocycles* **1995**, *41*, 1435-1444.

(12) Brownbridge, P.; Chan, T. H.; Brook, M. A.; Kang, G. J. *Can. J. Chem.* **1983**, *61*, 688-693.

(13) Evans, D. A.; Gauchet-Prunet, J. A.; Carreira, E. M.; Charette, A. B. *J. Org. Chem.* **1991**, *56*, 741-750.

(14) Molander, G. A.; Cameron, K. O. *J. Am. Chem. Soc.*, **1993**, *115*, 830-846. This material is a 10-15:1 mixture of desired substrate to the corresponding undesired C-silylated isomer. Careful distillation is required to minimize thermal isomerization to the undesired isomer (bp. 50 °C at 0.1 mm Hg, bath temp. ≤65 °C). See: Anderson, G.; Cameron, D. W.; Feutrill, G. I.; Read, R. W. *Tetrahedron Lett.*, **1981**, *22*, 4347-4348.

(15) The analytical data obtained from this material are consistent with those previously reported: Beck, G.; Jendralla, H.; Kesseler, K. *Synthesis*, **1995**, 1014-1018.

(16) Ward, D. E.; Rhee, C. K. *Tetrahedron Lett.*, **1991**, *32*, 7165-7166.

(17) This material was prepared as previously reported: Evans, D. A.; Ratz, A. M.; Huff, B. E.; Sheppard, G. S. *J. Am. Chem. Soc.* **1995**, *117*, 3448-3467.

(18) This material was prepared using a modified method of: Evans, D. A.; Bender, S. L.; Moris, J. *J. Am. Chem. Soc.* **1988**, *110*, 2506-2526.

(19) (a) Evans, D. A.; Kim, A. S. in *Encyclopedia of Reagents for Organic Synthesis*; Paquette, L. A., Ed.; Wiley, New York, NY 1995; Vol. 1, 345-356. (b) Evans, D. A.; Bartroli, J.; Shih, T. L. *J. Am. Chem. Soc.* **1981**, *103*, 2127-2129.

(20) Casiraghi, G.; Rassu, G. *Synthesis*, **1995**, 607-626.

(21) Silyl scrambling experiments have been reported previously for these substrates, see ref. 8.

(22) Prepared analogously to (benzyloxy)acetaldehyde.

(23) Takai, K; Heathcock, C. H. *J. Org. Chem.* **1985**, *50*, 3247-3251.

(24) Gennari, C. and Cozzi, P. G. *Tetrahedron* **1988**, *44*, 5965-5974.

(25) Graphite monochromated Mo K_{α} ($\lambda = 0.71073$ Å) radiation.

(26) SMART V 4.043 Software for the CCD Detector System, Siemens Analytical Instruments Division, Madison, WI (1995).

(27) SAINT V 4.035 Software for the CCD Detector System, Siemens Analytical Instruments Division, Madison, WI (1995).

(28) SADABS. Program for absorption corrections using Siemens CCD based on the method of Bob Blessing. *Acta Cryst.* **1995**, *A51*, 33-38.

(29) Sheldrick, G. M. SHELXL-90, Program for the Solution of Crystal Structure, University of Göttingen, Germany, 1986.

(30) Sheldrick, G. M. SHELXL-93, Program for the Refinement of Crystal Structure, University of Göttingen, Germany, 1993.

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(31) SHELXTL 5.03 (PC-Version), Program library for Structure Solution and Molecular Graphics, Siemens Analytical Instruments Division, Madison, WI (1995).

(32) Flack (absolute structure) parameter: Flack, H. D. *Acta Crystallogr.* **1983**, *A39*, 876.

(33) $R\ (R1) = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$, where $w = q/\sigma^2(F_o^2) + (aP)^2 + bP$. $R_w = \{\Sigma[w(|F_o| - |F_c|)^2]/\Sigma[w|F_o|^2]\}^{1/2}$.

(34) The X-Ray structure was determined by Kevin Campos.

(35) The X-Ray structure was determined by Dr. Richard Staples.

(36) The X-Ray structure was determined by Kevin Campos.

(37) The X-Ray structure was determined by Dr. Richard Staples.

(38) The X-Ray structure was determined by Dr. Richard Staples.

(39) The X-Ray structure was determined by Kevin Campos.

(40) The X-Ray structure was determined by Dr. Richard Staples.

(41) The X-Ray structure was determined by Dr. Richard Staples.