Supporting Information

Table S1. Complete Crystallographic Details for $[Fe(TEtP^{\bullet})(Cl)]SbCl_6$

formula	$C_{28}H_{28}Cl_7FeN_4Sb{\cdot}CH_2Cl_2$
FW, amu	931.22
a, Å	9.768(2)
b, Å	13.585(3)
c, Å	14.508(3)
α, deg	76.90(3)
β, deg	87.32(3)
γ, deg	71.77(3)
V, Å^3	1780.2(6)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.737
F(000)	924
μ, mm^{-1}	1.870
power and current settings	50kV, 30mA
detector distance, mm	40
detector tilt angle, deg	−25
image time, sec	10
increment, deg	0.20
crystal dimensions, mm	0.30 × 0.20 × 0.11
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	Enraf Nonius FAST
θ range for collected data, deg	2.20–29.95
index range	$-13 \le h \le 12$
	$-13 \le k \le 18$
	$-17 \le l \le 20$
total data collected	17182
unique data	9071 (R_{int} = 0.0753)
unique observed data [I > 2σ(I)]	7801
refinement method	Full-matrix least-squares
data/restraints/parameters	9071 / 0 / 434
goodness-of-fit (based on F^2)	1.045
max($\Delta\rho$), e/Å^3	1.46
min($\Delta\rho$), e/Å^3	−1.71
final R indices [I > 2σ(I)]	R_1 = 0.0516, wR_2 = 0.1213
final R indices (all data)	R_1 = 0.0632, wR_2 = 0.1286

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TEtP$^{\bullet}$)(Cl)]$SbCl_6$[a]

atom	x	y	z	U(eq)
Fe(1)	−0.23871(5)	0.02041(4)	0.09616(3)	0.0130(1)
Cl(1)	−0.47021(9)	0.08480(8)	0.07469(7)	0.0272(2)
N(1)	−0.1937(3)	0.1134(2)	0.17896(19)	0.0165(5)
N(2)	−0.1675(3)	0.1119(2)	−0.01806(18)	0.0142(5)
N(3)	−0.1858(3)	−0.0986(2)	0.02224(18)	0.0137(5)
N(4)	−0.2095(3)	−0.0978(2)	0.21820(19)	0.0189(5)
C(a1)	−0.2106(4)	0.1005(3)	0.2756(2)	0.0212(7)
C(a2)	−0.1818(4)	0.2133(3)	0.1472(2)	0.0203(6)
C(a3)	−0.1617(3)	0.2135(3)	−0.0234(2)	0.0176(6)
C(a4)	−0.1603(3)	0.0991(3)	−0.1092(2)	0.0152(6)
C(a5)	−0.1732(3)	−0.0850(3)	−0.0749(2)	0.0153(6)
C(a6)	−0.1995(3)	−0.1986(3)	0.0534(2)	0.0179(6)
C(a7)	−0.2118(4)	−0.2005(3)	0.2249(3)	0.0234(7)
C(a8)	−0.2147(4)	−0.0852(3)	0.3098(2)	0.0241(7)
C(b1)	−0.2076(5)	0.1943(3)	0.3036(3)	0.0297(8)
C(b2)	−0.1893(5)	0.2631(3)	0.2253(3)	0.0297(8)
C(b3)	−0.1503(4)	0.2642(3)	−0.1213(3)	0.0237(7)
C(b4)	−0.1496(4)	0.1942(3)	−0.1733(2)	0.0217(7)
C(b5)	−0.1762(4)	−0.1790(3)	−0.1032(2)	0.0195(6)
C(b6)	−0.1940(4)	−0.2481(3)	−0.0243(3)	0.0216(7)
C(b7)	−0.2143(6)	−0.2525(4)	0.3222(3)	0.0377(10)
C(b8)	−0.2163(5)	−0.1817(4)	0.3744(3)	0.0359(9)
C(m1)	−0.2226(4)	0.0092(3)	0.3375(2)	0.0239(7)
C(m2)	−0.1665(4)	0.2615(3)	0.0526(2)	0.0190(6)
C(m3)	−0.1630(3)	0.0068(3)	−0.1376(2)	0.0164(6)
C(m4)	−0.2143(4)	−0.2468(3)	0.1485(3)	0.0223(7)
C(11a)	−0.2665(15)	0.0083(17)	0.4393(14)	0.029(2)
C(12a)	−0.4260(9)	0.0118(7)	0.4565(6)	0.0305(16)
C(11b)	−0.2221(14)	0.0139(17)	0.4413(14)	0.029(2)
C(12b)	−0.0707(9)	−0.0140(7)	0.4837(5)	0.0321(17)
C(21)	−0.1659(4)	0.3754(3)	0.0310(3)	0.0248(7)
C(22)	−0.3193(5)	0.4519(3)	0.0144(4)	0.0372(10)
C(31)	−0.1633(4)	0.0099(3)	−0.2424(2)	0.0224(7)
C(32)	−0.3170(5)	0.0491(4)	−0.2832(3)	0.0358(9)

Table S2. Continued

atom	x	y	z	U(eq)
C(41)	−0.2435(5)	−0.3529(3)	0.1684(3)	0.0325(9)
C(42)	−0.4053(6)	−0.3360(4)	0.1656(5)	0.0528(14)
Sb(1)	−0.26385(3)	0.63664(2)	−0.31326(2)	0.0231(1)
Cl(2a)	−0.0985(5)	0.5718(9)	−0.4274(6)	0.0389(19)
Cl(2b)	−0.0935(4)	0.5255(9)	−0.3948(7)	0.065(2)
Cl(3)	−0.42624(17)	0.71309(12)	−0.44384(8)	0.0546(4)
Cl(4)	−0.16025(16)	0.77650(11)	−0.35534(7)	0.0492(3)
Cl(5)	−0.42506(12)	0.73222(13)	−0.21739(9)	0.0513(3)
Cl(6)	−0.09793(12)	0.55930(8)	−0.18202(9)	0.0405(3)
Cl(7)	−0.36235(18)	0.49597(11)	−0.27085(13)	0.0702(5)
C(5a)	0.8221(14)	0.3643(9)	0.5024(8)	0.050(3)
C(5b)	0.6721(14)	0.4096(9)	0.5058(8)	0.052(3)
Cl(8)	0.7095(2)	0.44892(15)	0.39777(13)	0.0718(5)
Cl(9)	0.7751(3)	0.2652(2)	0.55309(12)	0.1013(8)

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S3. Bond Lengths for [Fe(TEtP$^{\bullet}$)(Cl)]$SbCl_6$[a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(3)	2.060(3)	C(a8)–C(b8)	1.433(5)
Fe(1)–N(4)	2.066(3)	C(b1)–C(b2)	1.342(6)
Fe(1)–N(2)	2.067(3)	C(b3)–C(b4)	1.339(5)
Fe(1)–N(1)	2.078(3)	C(b5)–C(b6)	1.348(5)
Fe(1)–Cl(1)	2.1634(11)	C(b7)–C(b8)	1.348(7)
N(1)–C(a2)	1.370(4)	C(m1)–C(11a)	1.52(2)
N(1)–C(a1)	1.381(4)	C(m1)–C(11b)	1.523(19)
N(2)–C(a4)	1.369(4)	C(m2)–C(21)	1.510(5)
N(2)–C(a3)	1.384(4)	C(m3)–C(31)	1.513(4)
N(3)–C(a6)	1.377(4)	C(m4)–C(41)	1.517(5)
N(3)–C(a5)	1.383(4)	C(11a)–C(12a)	1.554(14)
N(4)–C(a8)	1.374(4)	C(11b)–C(12b)	1.529(14)
N(4)–C(a7)	1.383(5)	C(21)–C(22)	1.527(6)
C(a1)–C(m1)	1.390(5)	C(31)–C(32)	1.526(5)
C(a1)–C(b1)	1.431(5)	C(41)–C(42)	1.525(7)
C(a2)–C(m2)	1.403(5)	Sb(1)–Cl(5)	2.3311(14)
C(a2)–C(b2)	1.433(5)	Sb(1)–Cl(2b)	2.346(3)
C(a3)–C(m2)	1.395(5)	Sb(1)–Cl(7)	2.3490(13)
C(a3)–C(b3)	1.446(5)	Sb(1)–Cl(3)	2.3542(15)
C(a4)–C(m3)	1.412(5)	Sb(1)–Cl(4)	2.3719(12)
C(a4)–C(b4)	1.440(4)	Sb(1)–Cl(2a)	2.377(5)
C(a5)–C(m3)	1.395(4)	Sb(1)–Cl(6)	2.3815(14)
C(a5)–C(b5)	1.437(4)	Cl(2a)–Cl(2b)	0.686(4)
C(a6)–C(m4)	1.409(5)	C(5a)–Cl(9)	1.571(10)
C(a6)–C(b6)	1.428(5)	C(5a)–Cl(8)	1.846(12)
C(a7)–C(m4)	1.398(5)	C(5b)–Cl(8)	1.602(11)
C(a7)–C(b7)	1.430(5)	C(5b)–Cl(9)	1.884(12)
C(a8)–C(m1)	1.408(6)		

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

Table S4. Bond Angles for [Fe(TEtP$^{\bullet}$)(Cl)]$SbCl_6$[a]

angle	degree	angle	degree
N(3)–Fe(1)–N(4)	87.15(11)	C(b5)–C(b6)–C(a6)	107.2(3)
N(3)–Fe(1)–N(2)	87.20(11)	C(b8)–C(b7)–C(a7)	107.3(4)
N(4)–Fe(1)–N(2)	153.83(11)	C(b7)–C(b8)–C(a8)	107.1(3)
N(3)–Fe(1)–N(1)	154.48(10)	C(a1)–C(m1)–C(a8)	124.0(3)
N(4)–Fe(1)–N(1)	86.84(12)	C(a1)–C(m1)–C(11a)	121.9(8)
N(2)–Fe(1)–N(1)	87.34(11)	C(a8)–C(m1)–C(11a)	113.6(8)
N(3)–Fe(1)–Cl(1)	102.39(8)	C(a1)–C(m1)–C(11b)	113.7(8)
N(4)–Fe(1)–Cl(1)	104.44(9)	C(a8)–C(m1)–C(11b)	121.7(8)
N(2)–Fe(1)–Cl(1)	101.73(8)	C(11a)–C(m1)–C(11b)	17.7(6)
N(1)–Fe(1)–Cl(1)	103.13(8)	C(a3)–C(m2)–C(a2)	124.3(3)
C(a2)–N(1)–C(a1)	106.0(3)	C(a3)–C(m2)–C(21)	117.9(3)
C(a2)–N(1)–Fe(1)	126.1(2)	C(a2)–C(m2)–C(21)	117.7(3)
C(a1)–N(1)–Fe(1)	125.6(2)	C(a5)–C(m3)–C(a4)	123.9(3)
C(a4)–N(2)–C(a3)	105.9(3)	C(a5)–C(m3)–C(31)	117.9(3)
C(a4)–N(2)–Fe(1)	125.9(2)	C(a4)–C(m3)–C(31)	118.0(3)
C(a3)–N(2)–Fe(1)	125.5(2)	C(a7)–C(m4)–C(a6)	124.2(3)
C(a6)–N(3)–C(a5)	105.2(3)	C(a7)–C(m4)–C(41)	118.0(3)
C(a6)–N(3)–Fe(1)	126.1(2)	C(a6)–C(m4)–C(41)	117.7(3)
C(a5)–N(3)–Fe(1)	126.0(2)	C(m1)–C(11a)–C(12a)	113.5(10)
C(a8)–N(4)–C(a7)	105.4(3)	C(m1)–C(11b)–C(12b)	113.3(11)
C(a8)–N(4)–Fe(1)	126.8(2)	C(m2)–C(21)–C(22)	110.7(3)
C(a7)–N(4)–Fe(1)	126.5(2)	C(m3)–C(31)–C(32)	110.9(3)
N(1)–C(a1)–C(m1)	125.8(3)	C(m4)–C(41)–C(42)	110.4(4)
N(1)–C(a1)–C(b1)	109.5(3)	Cl(5)–Sb(1)–Cl(2b)	173.7(3)
C(m1)–C(a1)–C(b1)	124.7(3)	Cl(5)–Sb(1)–Cl(7)	90.93(7)
N(1)–C(a2)–C(m2)	125.8(3)	Cl(2b)–Sb(1)–Cl(7)	85.6(3)
N(1)–C(a2)–C(b2)	109.8(3)	Cl(5)–Sb(1)–Cl(3)	91.44(6)
C(m2)–C(a2)–C(b2)	124.4(3)	Cl(2b)–Sb(1)–Cl(3)	93.8(2)
N(2)–C(a3)–C(m2)	126.2(3)	Cl(7)–Sb(1)–Cl(3)	89.82(5)
N(2)–C(a3)–C(b3)	109.5(3)	Cl(5)–Sb(1)–Cl(4)	89.69(6)
C(m2)–C(a3)–C(b3)	124.3(3)	Cl(2b)–Sb(1)–Cl(4)	93.7(3)
N(2)–C(a4)–C(m3)	125.6(3)	Cl(7)–Sb(1)–Cl(4)	178.98(5)
N(2)–C(a4)–C(b4)	110.0(3)	Cl(3)–Sb(1)–Cl(4)	90.96(5)
C(m3)–C(a4)–C(b4)	124.4(3)	Cl(5)–Sb(1)–Cl(2a)	169.0(3)

Table S4. Continued

angle	degree	angle	degree
N(3)–C(a5)–C(m3)	125.8(3)	Cl(2b)–Sb(1)–Cl(2a)	16.68(11)
N(3)–C(a5)–C(b5)	110.0(3)	Cl(7)–Sb(1)–Cl(2a)	99.0(3)
C(m3)–C(a5)–C(b5)	124.2(3)	Cl(3)–Sb(1)–Cl(2a)	83.94(18)
N(3)–C(a6)–C(m4)	125.1(3)	Cl(4)–Sb(1)–Cl(2a)	80.4(3)
N(3)–C(a6)–C(b6)	110.5(3)	Cl(5)–Sb(1)–Cl(6)	88.95(5)
C(m4)–C(a6)–C(b6)	124.3(3)	Cl(2b)–Sb(1)–Cl(6)	85.8(2)
N(4)–C(a7)–C(m4)	125.5(3)	Cl(7)–Sb(1)–Cl(6)	90.44(5)
N(4)–C(a7)–C(b7)	110.0(3)	Cl(3)–Sb(1)–Cl(6)	179.52(5)
C(m4)–C(a7)–C(b7)	124.5(3)	Cl(4)–Sb(1)–Cl(6)	88.77(5)
N(4)–C(a8)–C(m1)	125.7(3)	Cl(2a)–Sb(1)–Cl(6)	95.63(18)
N(4)–C(a8)–C(b8)	110.2(3)	Cl(2b)–Cl(2a)–Sb(1	79.1(5)
C(m1)–C(a8)–C(b8)	124.0(3)	Cl(2a)–Cl(2b)–Sb(1	84.3(6)
C(b2)–C(b1)–C(a1)	107.4(3)	Cl(9)–C(5a)–Cl(8)	114.7(7)
C(b1)–C(b2)–C(a2)	107.3(3)	Cl(8)–C(5b)–Cl(9)	111.3(6)
C(b4)–C(b3)–C(a3)	107.1(3)	C(5b)–Cl(8)–C(5a)	47.4(6)
C(b3)–C(b4)–C(a4)	107.5(3)	C(5a)–Cl(9)–C(5b)	46.9(6)
C(b6)–C(b5)–C(a5)	107.1(3)		

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

Table S5. Anisotropic Displacement Parameters (Å^2) for [Fe(TEtP$^{\bullet}$)(Cl)]$SbCl_6$[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0121(2)	0.0168(2)	0.0111(2)	−0.0035(2)	0.0006(2)	−0.0057(2)
Cl(1)	0.0126(3)	0.0370(5)	0.0339(5)	−0.0157(4)	0.0005(3)	−0.0048(3)
N(1)	0.0156(12)	0.0223(13)	0.0132(12)	−0.0069(10)	−0.0002(9)	−0.0062(10)
N(2)	0.0134(11)	0.0165(12)	0.0143(12)	−0.0028(9)	0.0007(9)	−0.0071(9)
N(3)	0.0128(11)	0.0152(12)	0.0151(12)	−0.0047(9)	0.0023(9)	−0.0067(9)
N(4)	0.0191(13)	0.0228(14)	0.0136(12)	−0.0012(10)	0.0005(10)	−0.0070(11)
C(a1)	0.0196(15)	0.0302(18)	0.0143(14)	−0.0078(13)	−0.0013(11)	−0.0064(13)
C(a2)	0.0189(15)	0.0255(16)	0.0207(15)	−0.0089(13)	−0.0010(12)	−0.0097(13)
C(a3)	0.0147(13)	0.0173(14)	0.0199(15)	−0.0015(12)	−0.0006(11)	−0.0055(11)
C(a4)	0.0143(13)	0.0217(15)	0.0101(12)	−0.0042(11)	0.0025(10)	−0.0062(11)
C(a5)	0.0125(13)	0.0195(14)	0.0159(14)	−0.0069(11)	0.0010(10)	−0.0057(11)
C(a6)	0.0160(14)	0.0163(14)	0.0221(15)	−0.0048(12)	0.0018(11)	−0.0059(11)
C(a7)	0.0295(18)	0.0211(16)	0.0220(16)	−0.0030(13)	0.0036(13)	−0.0131(14)
C(a8)	0.0253(17)	0.0345(19)	0.0134(14)	−0.0018(13)	0.0002(12)	−0.0128(14)
C(b1)	0.037(2)	0.034(2)	0.0192(16)	−0.0126(15)	−0.0033(15)	−0.0071(16)
C(b2)	0.038(2)	0.0278(19)	0.0269(18)	−0.0123(15)	−0.0022(16)	−0.0106(16)
C(b3)	0.0242(16)	0.0239(17)	0.0203(16)	0.0017(13)	−0.0012(13)	−0.0082(13)
C(b4)	0.0277(17)	0.0226(16)	0.0159(14)	−0.0001(12)	0.0003(12)	−0.0122(13)
C(b5)	0.0184(14)	0.0246(16)	0.0200(15)	−0.0116(13)	0.0009(12)	−0.0083(12)
C(b6)	0.0200(15)	0.0190(15)	0.0290(17)	−0.0089(13)	0.0005(13)	−0.0079(12)
C(b7)	0.057(3)	0.035(2)	0.0232(19)	0.0035(16)	0.0038(18)	−0.024(2)
C(b8)	0.053(3)	0.039(2)	0.0160(16)	0.0033(15)	0.0030(16)	−0.020(2)
C(m1)	0.0229(16)	0.0336(19)	0.0142(14)	−0.0065(13)	−0.0007(12)	−0.0061(14)
C(m2)	0.0173(14)	0.0178(14)	0.0242(16)	−0.0041(12)	−0.0023(12)	−0.0084(12)
C(m3)	0.0150(13)	0.0220(15)	0.0119(13)	−0.0049(11)	0.0017(10)	−0.0050(11)
C(m4)	0.0217(16)	0.0202(15)	0.0248(17)	−0.0033(13)	0.0024(13)	−0.0077(13)
C(11a)	0.033(8)	0.040(3)	0.0129(18)	−0.0071(19)	−0.002(5)	−0.010(6)
C(12a)	0.033(4)	0.042(4)	0.027(4)	−0.015(3)	0.013(3)	−0.023(3)
C(11b)	0.033(8)	0.040(3)	0.0129(18)	−0.0071(19)	−0.002(5)	−0.010(6)
C(12b)	0.039(4)	0.044(5)	0.015(3)	−0.005(3)	−0.001(3)	−0.017(4)
C(21)	0.0274(17)	0.0198(16)	0.0294(18)	−0.0070(13)	−0.0013(14)	−0.0093(13)
C(22)	0.035(2)	0.0205(18)	0.053(3)	−0.0107(17)	−0.0048(19)	−0.0013(16)
C(31)	0.0289(17)	0.0298(18)	0.0114(14)	−0.0049(12)	0.0019(12)	−0.0130(14)
C(32)	0.037(2)	0.053(3)	0.0192(17)	−0.0050(17)	−0.0083(15)	−0.0169(19)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	0.046(2)	0.0217(18)	0.033(2)	−0.0025(15)	0.0057(17)	−0.0182(17)
C(42)	0.053(3)	0.047(3)	0.075(4)	−0.019(3)	0.020(3)	−0.037(3)
Sb(1)	0.0283(1)	0.0253(1)	0.0222(1)	−0.0082(1)	0.0028(1)	−0.0155(1)
Cl(2a)	0.055(2)	0.034(4)	0.037(3)	−0.020(3)	0.0190(16)	−0.0208(18)
Cl(2b)	0.0687(16)	0.075(5)	0.075(4)	−0.059(4)	0.0317(16)	−0.0299(17)
Cl(3)	0.0755(9)	0.0761(9)	0.0274(5)	0.0073(5)	−0.0175(5)	−0.0555(8)
Cl(4)	0.0818(9)	0.0620(7)	0.0238(5)	0.0043(5)	−0.0093(5)	−0.0588(7)
Cl(5)	0.0282(5)	0.0797(9)	0.0445(6)	−0.0329(6)	0.0022(4)	−0.0015(5)
Cl(6)	0.0334(5)	0.0295(5)	0.0548(7)	0.0040(4)	−0.0164(5)	−0.0115(4)
Cl(7)	0.0742(10)	0.0443(7)	0.0964(12)	0.0219(7)	−0.0423(9)	−0.0447(7)
C(5a)	0.067(8)	0.042(6)	0.050(6)	−0.002(5)	0.004(5)	−0.036(5)
C(5b)	0.073(8)	0.051(6)	0.048(6)	−0.023(5)	0.011(5)	−0.036(6)
Cl(8)	0.0916(13)	0.0636(10)	0.0631(9)	−0.0134(8)	−0.0095(9)	−0.0273(9)
Cl(9)	0.173(2)	0.1059(16)	0.0367(8)	0.0016(9)	−0.0313(11)	−0.0681(16)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2\ \pi\ [h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$.

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TEtP$^{\bullet}$)(Cl)]$SbCl_6$[a]

atom	x	y	z	U(eq)
H(b1)	−0.2168	0.2057	0.3661	0.036
H(b2)	−0.1825	0.3320	0.2221	0.036
H(b3)	−0.1445	0.3340	−0.1443	0.028
H(b4)	−0.1431	0.2052	−0.2401	0.026
H(b5)	−0.1673	−0.1904	−0.1657	0.023
H(b6)	−0.2015	−0.3169	−0.0209	0.026
H(b7)	−0.2146	−0.3236	0.3456	0.045
H(b8)	−0.2183	−0.1936	0.4415	0.043
H(11a)	−0.2516	0.0703	0.4573	0.034
H(11b)	−0.2030	−0.0567	0.4809	0.034
H(12a)	−0.4887	0.0693	0.4088	0.046
H(12b)	−0.4528	0.0243	0.5198	0.046
H(12c)	−0.4371	−0.0562	0.4519	0.046
H(11c)	−0.2707	−0.0359	0.4780	0.034
H(11d)	−0.2785	0.0865	0.4476	0.034
H(12d)	−0.0126	−0.0843	0.4748	0.048
H(12e)	−0.0771	−0.0149	0.5515	0.048
H(12f)	−0.0255	0.0392	0.4520	0.048
H(2a)	−0.1088	0.3886	−0.0261	0.030
H(2b)	−0.1197	0.3881	0.0846	0.030
H(2c)	−0.3683	0.4345	−0.0342	0.056
H(2d)	−0.3161	0.5250	−0.0068	0.056
H(2e)	−0.3719	0.4454	0.0735	0.056
H(3a)	−0.1141	−0.0623	−0.2529	0.027
H(3b)	−0.1094	0.0577	−0.2757	0.027
H(3c)	−0.3698	0.0008	−0.2513	0.054
H(3d)	−0.3146	0.0509	−0.3512	0.054
H(3e)	−0.3655	0.1207	−0.2733	0.054
H(4a)	−0.2024	−0.3951	0.2315	0.039
H(4b)	−0.1961	−0.3931	0.1205	0.039
H(4c)	−0.4504	−0.3035	0.2178	0.079
H(4d)	−0.4222	−0.4046	0.1721	0.079
H(4e)	−0.4472	−0.2889	0.1052	0.079
H(5a)	0.9231	0.3389	0.4826	0.059

Table S6. Continued

atom	x	y	z	U(eq)
H(5b)	0.8197	0.4083	0.5486	0.059
H(5c)	0.5674	0.4196	0.5104	0.062
H(5d)	0.6964	0.4532	0.5448	0.062

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S7. Complete Crystallographic Details for $[Fe(TPrP^{\bullet})(Cl)]SbCl_6$

formula	$C_{32}H_{36}Cl_7FeN_4Sb{\cdot}CH_2Cl_2$
FW, amu	987.32
a, Å	10.0407(1)
b, Å	14.4882(6)
c, Å	15.7601(9)
α, deg	111.079(5)
β, deg	103.848(7)
γ, deg	101.504(5)
V, Å^3	1971.21(14)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.663
F(000)	988
μ, mm^{-1}	1.694
power and current settings	50kV, 30mA
detector distance, mm	40
detector tilt angle, deg	−25
image time, sec	10
increment, deg	0.20
crystal dimensions, mm	0.37 × 0.23 × 0.20
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	Enraf Nonius FAST
θ range for collected data, deg	2.19–29.82
index range	$-13 \leq h \leq 10$
	$-19 \leq k \leq 19$
	$-15 \leq l \leq 21$
total data collected	19282
absorption correction	DIFABS
relative transmission coefficients (I)	1.0000 and 0.7870
unique data	9979 (R_{int} = 0.0701)
unique observed data [I > 2σ(I)]	8908
refinement method	Full-matrix least-sq
data/restraints/parameters	9979 / 0 / 452
goodness-of-fit (based on F^2)	1.078
max($\Delta\rho$), e/Å^3	1.726
min($\Delta\rho$), e/Å^3	−1.778
final R indices [I > 2σ(I)]	R_1 = 0.0497, wR_2 = 0.1227
final R indices (all data)	R_1 = 0.0571,wR_2 = 0.1338

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPrP$^{\bullet}$)(Cl)]$SbCl_6$[a]

atom	x	y	z	U(eq)
Fe(1)	0.23787(4)	0.02952(3)	0.06908(2)	0.0103(1)
Cl(1)	0.47041(7)	0.09086(6)	0.10837(5)	0.0212(2)
N(1)	0.1618(2)	0.10457(17)	−0.01262(15)	0.0125(4)
N(2)	0.1787(2)	−0.10056(17)	−0.05956(16)	0.0134(4)
N(3)	0.2116(2)	−0.07114(17)	0.13374(16)	0.0146(4)
N(4)	0.1985(2)	0.13490(17)	0.18165(15)	0.0124(4)
C(m1)	0.1719(3)	0.2668(2)	0.11903(19)	0.0155(5)
C(m2)	0.1466(3)	−0.0189(2)	−0.17372(18)	0.0147(5)
C(m3)	0.2072(3)	−0.2318(2)	0.0035(2)	0.0203(5)
C(m4)	0.2264(3)	0.0524(2)	0.29454(19)	0.0162(5)
C(a1)	0.1584(3)	0.2051(2)	0.02317(19)	0.0145(5)
C(a2)	0.1476(3)	0.0767(2)	−0.10887(18)	0.0136(4)
C(a3)	0.1609(3)	−0.1020(2)	−0.14869(18)	0.0148(5)
C(a4)	0.1919(3)	−0.1969(2)	−0.0689(2)	0.0176(5)
C(a5)	0.2127(3)	−0.1722(2)	0.0979(2)	0.0188(5)
C(a6)	0.2189(3)	−0.0446(2)	0.2285(2)	0.0166(5)
C(a7)	0.2205(3)	0.1370(2)	0.27171(18)	0.0151(5)
C(a8)	0.1927(3)	0.2326(2)	0.19257(18)	0.0137(4)
C(b1)	0.1427(3)	0.2417(2)	−0.0512(2)	0.0200(5)
C(b2)	0.1354(3)	0.1624(2)	−0.1324(2)	0.0190(5)
C(b3)	0.1607(3)	−0.2001(2)	−0.21541(19)	0.0196(5)
C(b4)	0.1819(3)	−0.2580(2)	−0.1661(2)	0.0219(6)
C(b5)	0.2194(3)	−0.2094(2)	0.1710(2)	0.0232(6)
C(b6)	0.2222(3)	−0.1323(2)	0.2508(2)	0.0227(6)
C(b7)	0.2318(3)	0.2378(2)	0.33990(19)	0.0191(5)
C(b8)	0.2127(3)	0.2966(2)	0.2910(2)	0.0189(5)
C(11)	0.1714(3)	0.3773(2)	0.1461(2)	0.0186(5)
C(12)	0.3237(3)	0.4535(2)	0.1837(2)	0.0236(6)
C(13)	0.3207(4)	0.5645(3)	0.2086(3)	0.0321(7)
C(21)	0.1330(3)	−0.0366(2)	−0.27652(19)	0.0188(5)
C(22)	0.2777(3)	−0.0296(3)	−0.2953(2)	0.0268(6)
C(23)	0.3915(4)	0.0757(3)	−0.2328(3)	0.0339(8)
C(31)	0.2218(5)	−0.3393(2)	−0.0194(3)	0.0342(8)
C(32a)	0.3592(11)	−0.3467(8)	0.0171(9)	0.0257(14)

Table S8. Continued

atom	x	y	z	U(eq)
C(33a)	0.4546(8)	−0.3119(7)	−0.0353(6)	0.0392(19)
C(32b)	0.3993(12)	−0.3265(9)	0.0095(9)	0.0257(14)
C(33b)	0.4256(9)	−0.4311(6)	−0.0100(6)	0.0357(19)
C(41)	0.2468(3)	0.0698(2)	0.3977(2)	0.0203(5)
C(42)	0.4070(3)	0.1088(3)	0.4593(2)	0.0231(6)
C(43)	0.4262(4)	0.1314(4)	0.5636(2)	0.0361(8)
Sb(1)	0.95613(2)	0.66319(1)	0.36357(1)	0.0177(1)
Cl(2)	0.70589(10)	0.58033(11)	0.30939(9)	0.0532(3)
Cl(3)	0.91839(12)	0.82530(8)	0.38609(8)	0.0429(2)
Cl(4)	0.96877(11)	0.69160(7)	0.52256(6)	0.0361(2)
Cl(5)	0.94337(11)	0.62697(8)	0.20241(6)	0.0377(2)
Cl(6)	0.99945(10)	0.50329(6)	0.34263(6)	0.0324(2)
Cl(7)	1.20642(8)	0.74833(6)	0.42024(6)	0.0291(2)
Cl(8)	1.42263(11)	0.58968(7)	0.46924(6)	0.0380(2)
Cl(9)	1.40350(11)	0.69185(8)	0.66159(7)	0.0444(2)
C(1)	1.3278(5)	0.5834(3)	0.5492(3)	0.0409(9)

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S9. Bond Lengths for [Fe(TPrP$^{\bullet}$)(Cl)]$SbCl_6$[a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(2)	2.060(2)	C(a4)–C(b4)	1.434(4)
Fe(1)–N(4)	2.064(2)	C(a5)–C(b5)	1.432(4)
Fe(1)–N(3)	2.069(2)	C(a6)–C(b6)	1.438(4)
Fe(1)–N(1)	2.071(2)	C(a7)–C(b7)	1.430(4)
Fe(1)–Cl(1)	2.1700(7)	C(a8)–C(b8)	1.431(4)
N(1)–C(a1)	1.370(3)	C(b1)–C(b2)	1.351(4)
N(1)–C(a2)	1.385(3)	C(b3)–C(b4)	1.347(4)
N(2)–C(a3)	1.365(3)	C(b5)–C(b6)	1.337(5)
N(2)–C(a4)	1.386(3)	C(b7)–C(b8)	1.351(4)
N(3)–C(a5)	1.370(3)	C(11)–C(12)	1.526(4)
N(3)–C(a6)	1.382(3)	C(12)–C(13)	1.521(4)
N(4)–C(a7)	1.371(3)	C(21)–C(22)	1.542(4)
N(4)–C(a8)	1.378(3)	C(22)–C(23)	1.512(5)
C(m1)–C(a8)	1.403(4)	C(31)–C(32a)	1.402(11)
C(m1)–C(a1)	1.408(4)	C(31)–C(32b)	1.684(12)
C(m1)–C(11)	1.504(4)	C(32a)–C(33a)	1.529(12)
C(m2)–C(a2)	1.391(4)	C(32b)–C(33b)	1.525(13)
C(m2)–C(a3)	1.417(4)	C(41)–C(42)	1.531(4)
C(m2)–C(21)	1.513(4)	C(42)–C(43)	1.511(4)
C(m3)–C(a4)	1.394(4)	Sb(1)–Cl(2)	2.3486(9)
C(m3)–C(a5)	1.407(4)	Sb(1)–Cl(7)	2.3519(8)
C(m3)–C(31)	1.513(4)	Sb(1)–Cl(4)	2.3557(8)
C(m4)–C(a6)	1.390(4)	Sb(1)–Cl(6)	2.3634(8)
C(m4)–C(a7)	1.404(4)	Sb(1)–Cl(5)	2.3668(8)
C(m4)–C(41)	1.508(4)	Sb(1)–Cl(3)	2.3677(9)
C(a1)–C(b1)	1.440(4)	Cl(8)–C(1)	1.768(4)
C(a2)–C(b2)	1.436(4)	Cl(9)–C(1)	1.749(4)
C(a3)–C(b3)	1.432(4)		

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

Table S10. Bond Angles for [Fe(TPrP$^{\bullet}$)(Cl)]$SbCl_6$[a]

angle	degree	angle	degree
N(2)–Fe(1)–N(4)	154.26(9)	N(3)–C(a5)–C(b5)	109.7(3)
N(2)–Fe(1)–N(3)	87.15(9)	C(m3)–C(a5)–C(b5)	124.4(3)
N(4)–Fe(1)–N(3)	86.91(9)	N(3)–C(a6)–C(m4)	126.0(2)
N(2)–Fe(1)–N(1)	87.00(9)	N(3)–C(a6)–C(b6)	109.7(2)
N(4)–Fe(1)–N(1)	87.16(8)	C(m4)–C(a6)–C(b6)	124.3(3)
N(3)–Fe(1)–N(1)	153.35(9)	N(4)–C(a7)–C(m4)	125.7(2)
N(2)–Fe(1)–Cl(1)	103.53(7)	N(4)–C(a7)–C(b7)	110.2(2)
N(4)–Fe(1)–Cl(1)	102.21(6)	C(m4)–C(a7)–C(b7)	124.1(2)
N(3)–Fe(1)–Cl(1)	104.01(7)	N(4)–C(a8)–C(m1)	125.7(2)
N(1)–Fe(1)–Cl(1)	102.64(6)	N(4)–C(a8)–C(b8)	110.4(2)
C(a1)–N(1)–C(a2)	105.8(2)	C(m1)–C(a8)–C(b8)	123.8(2)
C(a1)–N(1)–Fe(1)	125.75(17)	C(b2)–C(b1)–C(a1)	106.8(2)
C(a2)–N(1)–Fe(1)	125.79(17)	C(b1)–C(b2)–C(a2)	107.4(2)
C(a3)–N(2)–C(a4)	105.5(2)	C(b4)–C(b3)–C(a3)	107.2(2)
C(a3)–N(2)–Fe(1)	126.42(18)	C(b3)–C(b4)–C(a4)	107.0(2)
C(a4)–N(2)–Fe(1)	125.54(17)	C(b6)–C(b5)–C(a5)	107.9(3)
C(a5)–N(3)–C(a6)	105.8(2)	C(b5)–C(b6)–C(a6)	106.9(3)
C(a5)–N(3)–Fe(1)	126.44(19)	C(b8)–C(b7)–C(a7)	107.4(2)
C(a6)–N(3)–Fe(1)	126.60(18)	C(b7)–C(b8)–C(a8)	106.6(2)
C(a7)–N(4)–C(a8)	105.4(2)	C(m1)–C(11)–C(12)	112.0(2)
C(a7)–N(4)–Fe(1)	125.77(17)	C(13)–C(12)–C(11)	111.2(3)
C(a8)–N(4)–Fe(1)	125.75(17)	C(m2)–C(21)–C(22)	113.2(2)
C(a8)–C(m1)–C(a1)	123.7(2)	C(23)–C(22)–C(21)	113.3(3)
C(a8)–C(m1)–C(11)	117.6(2)	C(32a)–C(31)–C(m3)	118.1(5)
C(a1)–C(m1)–C(11)	118.6(2)	C(32a)–C(31)–C(32b)	16.0(5)
C(a2)–C(m2)–C(a3)	123.6(2)	C(m3)–C(31)–C(32b)	107.7(4)
C(a2)–C(m2)–C(21)	119.5(2)	C(31)–C(32a)–C(33a)	108.5(7)
C(a3)–C(m2)–C(21)	116.9(2)	C(33b)–C(32b)–C(31	111.7(7)
C(a4)–C(m3)–C(a5)	123.8(3)	C(m4)–C(41)–C(42)	111.7(2)
C(a4)–C(m3)–C(31)	118.6(3)	C(43)–C(42)–C(41)	111.2(3)
C(a5)–C(m3)–C(31)	117.5(3)	Cl(2)–Sb(1)–Cl(7)	179.00(4)
C(a6)–C(m4)–C(a7)	123.8(2)	Cl(2)–Sb(1)–Cl(4)	89.74(4)
C(a6)–C(m4)–C(41)	118.6(2)	Cl(7)–Sb(1)–Cl(4)	89.49(3)
C(a7)–C(m4)–C(41)	117.6(3)	Cl(2)–Sb(1)–Cl(6)	90.52(4)

Table S10. Continued

angle	degree	angle	degree
N(1)–C(a1)–C(m1)	126.1(2)	Cl(7)–Sb(1)–Cl(6)	90.09(3)
N(1)–C(a1)–C(b1)	110.3(2)	Cl(4)–Sb(1)–Cl(6)	88.12(3)
C(m1)–C(a1)–C(b1)	123.6(2)	Cl(2)–Sb(1)–Cl(5)	89.84(4)
N(1)–C(a2)–C(m2)	125.9(2)	Cl(7)–Sb(1)–Cl(5)	90.95(3)
N(1)–C(a2)–C(b2)	109.7(2)	Cl(4)–Sb(1)–Cl(5)	177.46(3)
C(m2)–C(a2)–C(b2)	124.5(2)	Cl(6)–Sb(1)–Cl(5)	89.38(3)
N(2)–C(a3)–C(m2)	126.0(2)	Cl(2)–Sb(1)–Cl(3)	90.76(4)
N(2)–C(a3)–C(b3)	110.5(2)	Cl(7)–Sb(1)–Cl(3)	88.63(3)
C(m2)–C(a3)–C(b3)	123.5(2)	Cl(4)–Sb(1)–Cl(3)	91.78(4)
N(2)–C(a4)–C(m3)	125.8(2)	Cl(6)–Sb(1)–Cl(3)	178.72(4)
N(2)–C(a4)–C(b4)	109.8(2)	Cl(5)–Sb(1)–Cl(3)	90.73(4)
C(m3)–C(a4)–C(b4)	124.4(3)	Cl(9)–C(1)–Cl(8)	112.8(2)
N(3)–C(a5)–C(m3)	125.9(3)		

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

Table S11. Anisotropic Displacement Parameters (Å^2) for [Fe(TPrP$^{\bullet}$)(Cl)]$SbCl_6$[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0100(2)	0.0095(2)	0.0114(2)	0.0049(1)	0.0031(1)	0.0032(1)
Cl(1)	0.0105(3)	0.0235(3)	0.0232(3)	0.0059(3)	0.0040(2)	0.0022(2)
N(1)	0.0132(9)	0.0132(10)	0.0131(9)	0.0070(8)	0.0045(7)	0.0053(8)
N(2)	0.0115(9)	0.0124(10)	0.0143(9)	0.0052(8)	0.0029(7)	0.0026(8)
N(3)	0.0150(10)	0.0129(10)	0.0173(10)	0.0079(8)	0.0049(8)	0.0053(8)
N(4)	0.0125(9)	0.0141(10)	0.0123(9)	0.0057(8)	0.0049(7)	0.0063(8)
C(m1)	0.0148(11)	0.0151(11)	0.0168(11)	0.0067(9)	0.0037(9)	0.0071(9)
C(m2)	0.0110(10)	0.0175(12)	0.0143(11)	0.0063(9)	0.0033(9)	0.0037(9)
C(m3)	0.0220(13)	0.0126(12)	0.0245(13)	0.0086(10)	0.0046(10)	0.0047(10)
C(m4)	0.0111(11)	0.0252(13)	0.0172(11)	0.0136(10)	0.0058(9)	0.0060(10)
C(a1)	0.0147(11)	0.0141(11)	0.0166(11)	0.0075(9)	0.0058(9)	0.0058(9)
C(a2)	0.0111(10)	0.0180(12)	0.0144(11)	0.0095(9)	0.0048(9)	0.0046(9)
C(a3)	0.0101(10)	0.0155(11)	0.0134(10)	0.0028(9)	0.0014(8)	0.0026(9)
C(a4)	0.0161(12)	0.0116(11)	0.0189(12)	0.0035(9)	0.0021(9)	0.0024(9)
C(a5)	0.0188(12)	0.0145(12)	0.0249(13)	0.0114(10)	0.0057(10)	0.0053(10)
C(a6)	0.0142(11)	0.0189(12)	0.0208(12)	0.0143(10)	0.0050(9)	0.0041(9)
C(a7)	0.0139(11)	0.0195(12)	0.0135(11)	0.0085(9)	0.0050(9)	0.0052(9)
C(a8)	0.0124(11)	0.0145(11)	0.0150(11)	0.0062(9)	0.0050(9)	0.0057(9)
C(b1)	0.0269(14)	0.0175(12)	0.0209(12)	0.0131(11)	0.0069(11)	0.0103(11)
C(b2)	0.0233(13)	0.0199(12)	0.0161(11)	0.0108(10)	0.0058(10)	0.0068(10)
C(b3)	0.0195(12)	0.0157(12)	0.0143(11)	−0.0006(9)	0.0027(9)	0.0034(10)
C(b4)	0.0214(13)	0.0138(12)	0.0220(13)	0.0012(10)	0.0029(10)	0.0056(10)
C(b5)	0.0236(14)	0.0217(13)	0.0324(15)	0.0198(12)	0.0088(12)	0.0091(11)
C(b6)	0.0225(13)	0.0276(15)	0.0279(14)	0.0216(12)	0.0086(11)	0.0097(11)
C(b7)	0.0211(13)	0.0233(13)	0.0141(11)	0.0065(10)	0.0081(10)	0.0096(11)
C(b8)	0.0206(13)	0.0190(12)	0.0178(12)	0.0061(10)	0.0078(10)	0.0094(10)
C(11)	0.0211(13)	0.0150(12)	0.0216(12)	0.0075(10)	0.0065(10)	0.0110(10)
C(12)	0.0259(14)	0.0154(12)	0.0309(15)	0.0108(11)	0.0093(12)	0.0080(11)
C(13)	0.0398(19)	0.0166(14)	0.0410(18)	0.0127(13)	0.0140(15)	0.0099(13)
C(21)	0.0170(12)	0.0266(14)	0.0118(11)	0.0081(10)	0.0036(9)	0.0065(10)
C(22)	0.0248(14)	0.0387(17)	0.0195(13)	0.0128(13)	0.0120(11)	0.0095(13)
C(23)	0.0213(15)	0.048(2)	0.0288(16)	0.0183(15)	0.0079(12)	0.0001(14)
C(31)	0.056(2)	0.0138(13)	0.0327(16)	0.0101(12)	0.0111(16)	0.0150(14)
C(32a)	0.029(5)	0.020(4)	0.038(3)	0.019(2)	0.016(3)	0.012(3)

Table S11. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(33a)	0.029(4)	0.047(4)	0.044(4)	0.018(4)	0.009(3)	0.024(3)
C(32b)	0.029(5)	0.020(4)	0.038(3)	0.019(2)	0.016(3)	0.012(3)
C(33b)	0.046(4)	0.033(4)	0.038(4)	0.014(3)	0.017(3)	0.030(3)
C(41)	0.0178(12)	0.0298(14)	0.0171(12)	0.0143(11)	0.0062(10)	0.0072(11)
C(42)	0.0203(13)	0.0344(16)	0.0195(12)	0.0166(12)	0.0067(10)	0.0089(12)
C(43)	0.0265(16)	0.062(2)	0.0223(15)	0.0222(16)	0.0050(12)	0.0151(16)
Sb(1)	0.0174(1)	0.0183(1)	0.0171(1)	0.0078(1)	0.0060(1)	0.0043(1)
Cl(2)	0.0188(4)	0.0769(8)	0.0626(7)	0.0445(6)	0.0030(4)	−0.0025(4)
Cl(3)	0.0495(5)	0.0399(5)	0.0600(6)	0.0293(5)	0.0267(5)	0.0316(4)
Cl(4)	0.0481(5)	0.0397(4)	0.0207(3)	0.0088(3)	0.0189(3)	0.0135(4)
Cl(5)	0.0482(5)	0.0409(5)	0.0210(3)	0.0163(3)	0.0091(3)	0.0052(4)
Cl(6)	0.0485(5)	0.0150(3)	0.0267(4)	0.0047(3)	0.0092(3)	0.0081(3)
Cl(7)	0.0197(3)	0.0286(4)	0.0377(4)	0.0173(3)	0.0063(3)	0.0035(3)
Cl(8)	0.0480(5)	0.0323(4)	0.0322(4)	0.0117(3)	0.0086(4)	0.0195(4)
Cl(9)	0.0334(4)	0.0443(5)	0.0390(5)	0.0012(4)	0.0121(4)	0.0098(4)
C(1)	0.041(2)	0.0330(19)	0.0354(18)	0.0087(15)	0.0078(16)	0.0019(16)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2\,\pi\,[h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12}]$.

Table S12. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPrP$^{\bullet}$)(Cl)]SbCl$_6$[a]

atom	x	y	z	U(eq)
H(b1)	0.1384	0.3087	−0.0445	0.024
H(b2)	0.1241	0.1631	−0.1937	0.023
H(b3)	0.1480	−0.2205	−0.2820	0.023
H(b4)	0.1889	−0.3264	−0.1910	0.026
H(b5)	0.2215	−0.2770	0.1642	0.028
H(b6)	0.2258	−0.1349	0.3106	0.027
H(b7)	0.2495	0.2593	0.4072	0.023
H(b8)	0.2126	0.3668	0.3169	0.023
H(1a)	0.1262	0.3971	0.1966	0.022
H(1b)	0.1123	0.3822	0.0888	0.022
H(1c)	0.3823	0.4500	0.2421	0.028
H(1d)	0.3698	0.4331	0.1339	0.028
H(1e)	0.2611	0.5677	0.1512	0.048
H(1f)	0.4193	0.6113	0.2303	0.048
H(1g)	0.2797	0.5861	0.2603	0.048
H(2a)	0.0941	0.0158	−0.2908	0.023
H(2b)	0.0629	−0.1064	−0.3213	0.023
H(2c)	0.3148	−0.0838	−0.2832	0.032
H(2d)	0.2605	−0.0446	−0.3641	0.032
H(2e)	0.3562	0.1297	−0.2450	0.051
H(2f)	0.4802	0.0755	−0.2485	0.051
H(2g)	0.4118	0.0901	−0.1645	0.051
H(3a)	0.1559	−0.3751	0.0049	0.041
H(3b)	0.1869	−0.3788	−0.0906	0.041
H(32a)	0.3514	−0.4195	0.0064	0.031
H(32b)	0.4021	−0.3017	0.0875	0.031
H(33a)	0.4078	−0.3536	−0.1052	0.059
H(33b)	0.5486	−0.3218	−0.0143	0.059
H(33c)	0.4684	−0.2381	−0.0199	0.059
H(32c)	0.4406	−0.2953	−0.0287	0.031
H(32d)	0.4494	−0.2787	0.0788	0.031
H(33d)	0.3851	−0.4621	0.0278	0.054
H(33e)	0.5298	−0.4206	0.0085	0.054
H(33f)	0.3789	−0.4779	−0.0790	0.054

Table S12. Continued

atom	x	y	z	U(eq)
H(4a)	0.1990	0.0036	0.3987	0.024
H(4b)	0.2001	0.1215	0.4261	0.024
H(4c)	0.4526	0.0554	0.4332	0.028
H(4d)	0.4561	0.1729	0.4556	0.028
H(4e)	0.3948	0.1916	0.5925	0.054
H(4f)	0.5283	0.1467	0.5994	0.054
H(4g)	0.3679	0.0706	0.5667	0.054
H(1h)	1.2263	0.5782	0.5194	0.049
H(1i)	1.3273	0.5196	0.5591	0.049

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.