Inorganic Chemistry
including bioinorganic chemistry
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Table 1. Crystal data and structure refinement for ~~MART26.~~ Cpd 1

Identification code	MART26
Empirical formula	$C_{37}H_{25}Br_2F_8In_2N_5$
Formula weight	1081.08
Temperature	195(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 17.632(2) Å α = 90° b = 15.010(1) Å β = 101.72(1)° c = 14.562(1) Å γ = 90°
Volume	3773.6(6) Å^3
Z	4
Density (calculated)	1.903 Mg/m^3
Absorption coefficient	3.414 mm^{-1}
F(000)	2088
Crystal size	0.55 x 0.40 x 0.15 mm
θ range for data collection	3.07 to 26.98°
Index ranges	$0 \le h \le 22$, $0 \le k \le 19$, $-18 \le \ell \le 18$
Reflections collected	8448
Independent reflections	8193 (R_{int} = 0.0261)
Absorption correction	DIFABS
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7233 / 0 / 481
Goodness-of-fit on F^2	1.031
Final R indices [I>2σ(I)]	R1 = 0.0324, wR2 = 0.0726
R indices (all data)	R1 = 0.0687, wR2 = 0.0913
Largest diff. peak and hole	0.576 and -0.636 eÅ^{-3}

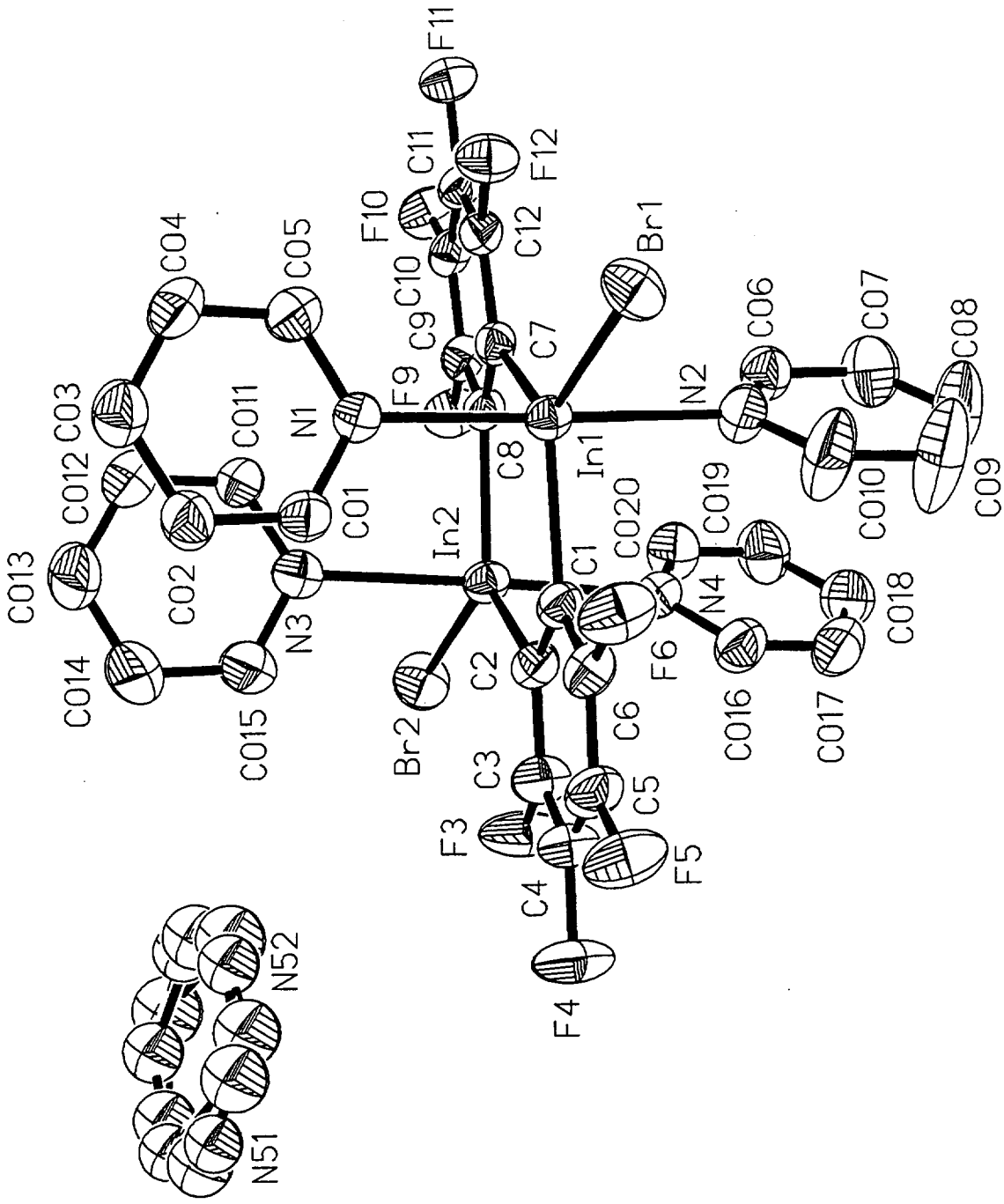

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [Å^2] for MART26. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In(1)	0.764081(14)	0.58070(2)	0.18301(2)	0.02987(7)
In(2)	0.72837(2)	0.38926(2)	0.32426(2)	0.03239(8)
Br(1)	0.80609(3)	0.69829(3)	0.07782(3)	0.04706(12)
Br(2)	0.68783(3)	0.27060(3)	0.42841(3)	0.05476(13)
F(3)	0.8482(2)	0.4107(2)	0.5233(2)	0.0731(9)
F(4)	0.9507(2)	0.5361(2)	0.6006(2)	0.0697(8)
F(5)	0.9764(2)	0.6792(2)	0.4973(2)	0.0645(8)
F(6)	0.89870(14)	0.6987(2)	0.3201(2)	0.0539(7)
F(9)	0.60453(13)	0.2640(2)	0.1818(2)	0.0475(6)
F(10)	0.51744(13)	0.2898(2)	0.0104(2)	0.0497(6)
F(11)	0.53325(13)	0.4394(2)	-0.0875(2)	0.0478(6)
F(12)	0.63217(14)	0.5677(2)	-0.0105(2)	0.0444(6)
N(1)	0.6784(2)	0.6849(2)	0.2324(2)	0.0321(7)
C(01)	0.6889(2)	0.7136(3)	0.3204(3)	0.0393(9)
C(02)	0.6406(2)	0.7740(3)	0.3508(3)	0.0458(10)
C(03)	0.5786(2)	0.8075(3)	0.2875(3)	0.0481(11)
C(04)	0.5656(3)	0.7772(3)	0.1964(3)	0.0500(11)
C(05)	0.6165(2)	0.7165(3)	0.1713(3)	0.0459(10)
N(2)	0.8569(2)	0.4771(2)	0.1266(2)	0.0437(8)
C(06)	0.8399(2)	0.4008(3)	0.0809(3)	0.0435(10)
C(07)	0.8948(3)	0.3500(3)	0.0493(4)	0.0597(13)
C(08)	0.9689(3)	0.3790(4)	0.0643(5)	0.085(2)
C(09)	0.9872(3)	0.4564(5)	0.1132(6)	0.106(3)
C(010)	0.9293(3)	0.5033(4)	0.1415(5)	0.080(2)
N(3)	0.6289(2)	0.4857(2)	0.3672(2)	0.0423(8)
C(011)	0.5682(2)	0.5177(3)	0.3066(3)	0.0431(10)
C(012)	0.5138(3)	0.5719(3)	0.3321(3)	0.0524(11)
C(013)	0.5217(3)	0.5958(3)	0.4239(4)	0.0596(13)
C(014)	0.5835(3)	0.5653(4)	0.4868(4)	0.077(2)
C(015)	0.6367(3)	0.5106(4)	0.4557(3)	0.067(2)
N(4)	0.8237(2)	0.2898(2)	0.2885(2)	0.0402(8)
C(016)	0.8996(2)	0.3059(3)	0.3091(3)	0.0505(11)
C(017)	0.9531(3)	0.2482(4)	0.2835(4)	0.0653(14)
C(018)	0.9278(3)	0.1713(4)	0.2370(3)	0.0615(14)
C(019)	0.8499(3)	0.1535(3)	0.2175(4)	0.0618(13)
C(020)	0.8008(3)	0.2144(3)	0.2435(3)	0.0543(12)
C(1)	0.8296(2)	0.5637(2)	0.3259(2)	0.0316(8)
C(2)	0.8158(2)	0.4890(2)	0.3793(3)	0.0341(8)
C(3)	0.8575(2)	0.4819(3)	0.4700(3)	0.0435(10)
C(4)	0.9107(2)	0.5450(3)	0.5106(3)	0.0482(11)
C(5)	0.9239(2)	0.6172(3)	0.4590(3)	0.0449(10)
C(6)	0.8833(2)	0.6250(3)	0.3682(3)	0.0377(9)
C(7)	0.6755(2)	0.4828(2)	0.1280(2)	0.0293(8)
C(8)	0.6674(2)	0.4036(2)	0.1790(2)	0.0310(8)
C(9)	0.6149(2)	0.3409(2)	0.1364(3)	0.0325(8)
C(10)	0.5694(2)	0.3520(3)	0.0483(3)	0.0341(8)
C(11)	0.5769(2)	0.4280(3)	-0.0005(3)	0.0345(8)
C(12)	0.6290(2)	0.4922(2)	0.0405(3)	0.0313(8)
N(51)	0.8063(5)	0.5910(7)	0.8334(8)	0.059(2)
C(021)	0.7613(8)	0.5244(9)	0.8669(7)	0.051(3)
C(022)	0.7050(9)	0.4806(9)	0.8004(12)	0.061(4)
C(023)	0.6984(11)	0.4946(13)	0.704(2)	0.075(6)
C(024)	0.7313(10)	0.5429(13)	0.6747(11)	0.085(5)
C(025)	0.7928(9)	0.6060(10)	0.7346(12)	0.069(4)

N(52)	0.7492(6)	0.5779(7)	0.6887(7)	0.054(2)
C(026)	0.6953(9)	0.5169(11)	0.6967(11)	0.054(4)
C(027)	0.6962(9)	0.4717(11)	0.7674(13)	0.078(5)
C(028)	0.7395(8)	0.4874(9)	0.8503(10)	0.062(3)
C(029)	0.7937(9)	0.5532(11)	0.8629(9)	0.066(3)
C(030)	0.8013(8)	0.6073(9)	0.7712(13)	0.063(4)

Table 3. Selected bond lengths [Å] and angles [°] for MART26.

Symmetry transformations used to generate equivalent atoms:

LITERATURSTELLEN FUER DIE VERWENDETEN PROGRAMME:
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SHELXTL-PC: Siemens Analytical X-Ray Instruments (1990)

SHELXS-86: G.M. Sheldrick, University of Göttingen
G.M. Sheldrick, C. Krüger, R. Goddard, Oxford Univ. Press, 1985,pp.175-189.

SHELXL-93: G.M Sheldrick, Progr. for the Refinement of Structures University of Göttingen, 1993.

DIFABS: N. Walker and D. Stuart, Acta Cryst. A39,158 (1983)

CADSHEL: J. Kopf,H.-Chr. Rübcke, Progr. CADHKL4 (CADSHEL.FOR, V3.10), Universität Hamburg (1993). E

Table 4. Bond lengths [Å] and angles [°] for MART26.

In(1)-C(7)	2.176(3)	In(1)-C(1)	2.181(3)
In(1)-N(1)	2.385(3)	In(1)-N(2)	2.514(3)
In(1)-Br(1)	2.5438(5)	In(2)-C(8)	2.180(4)
In(2)-C(2)	2.181(4)	In(2)-N(4)	2.384(3)
In(2)-N(3)	2.451(3)	In(2)-Br(2)	2.5346(5)
F(3)-C(3)	1.351(5)	F(4)-C(4)	1.363(4)
F(5)-C(5)	1.349(5)	F(6)-C(6)	1.366(4)
F(9)-C(9)	1.361(4)	F(10)-C(10)	1.345(4)
F(11)-C(11)	1.353(4)	F(12)-C(12)	1.363(4)
N(1)-C(01)	1.330(5)	N(1)-C(05)	1.346(5)
C(01)-C(02)	1.376(5)	C(01)-H(01A)	0.96
C(02)-C(03)	1.375(6)	C(02)-H(02A)	0.96
C(03)-C(04)	1.378(6)	C(03)-H(03A)	0.96
C(04)-C(05)	1.379(6)	C(04)-H(04A)	0.96
C(05)-H(05A)	0.96	N(2)-C(010)	1.311(6)
N(2)-C(06)	1.327(5)	C(06)-C(07)	1.382(6)
C(06)-H(06A)	0.96	C(07)-C(08)	1.351(7)
C(07)-H(07A)	0.96	C(08)-C(09)	1.368(8)
C(08)-H(08A)	0.96	C(09)-C(010)	1.370(7)
C(09)-H(09A)	0.96	C(010)-H(01B)	0.96
N(3)-C(015)	1.323(6)	N(3)-C(011)	1.331(5)
C(011)-C(012)	1.365(6)	C(011)-H(01C)	0.96
C(012)-C(013)	1.364(6)	C(012)-H(01D)	0.96
C(013)-C(014)	1.353(7)	C(013)-H(01E)	0.96
C(014)-C(015)	1.391(7)	C(014)-H(01F)	0.96
C(015)-H(01G)	0.96	N(4)-C(020)	1.329(5)
N(4)-C(016)	1.333(5)	C(016)-C(017)	1.386(6)
C(016)-H(01H)	0.96	C(017)-C(018)	1.366(7)
C(017)-H(01I)	0.96	C(018)-C(019)	1.371(7)
C(018)-H(01J)	0.96	C(019)-C(020)	1.364(6)
C(019)-H(01K)	0.96	C(020)-H(02B)	0.96
C(1)-C(6)	1.374(5)	C(1)-C(2)	1.413(5)
C(2)-C(3)	1.378(5)	C(3)-C(4)	1.379(6)
C(4)-C(5)	1.366(6)	C(5)-C(6)	1.375(6)
C(7)-C(12)	1.375(5)	C(7)-C(8)	1.423(5)
C(8)-C(9)	1.376(5)	C(9)-C(10)	1.377(5)
C(10)-C(11)	1.365(5)	C(11)-C(12)	1.380(5)
N(51)-C(029)	0.771(14)	N(51)-C(030)	0.926(14)
N(51)-C(021)	1.42(2)	N(51)-C(025)	1.43(2)
C(021)-C(028)	0.690(14)	C(021)-C(029)	0.730(14)
C(021)-C(022)	1.40(2)	C(021)-C(027)	1.83(2)
C(022)-C(028)	0.85(2)	C(022)-C(023)	1.40(3)
C(022)-C(026)	1.58(2)	C(022)-C(029)	1.97(2)
C(023)-C(027)	0.99(2)	C(023)-C(024)	1.07(3)
C(023)-N(52)	1.58(2)	C(024)-N(52)	0.62(2)
C(024)-C(026)	0.86(2)	C(024)-C(025)	1.56(2)
C(024)-C(030)	1.93(2)	C(024)-C(027)	1.92(2)
C(025)-C(030)	0.52(2)	C(025)-N(52)	1.00(2)
C(025)-C(029)	2.03(2)	N(52)-C(026)	1.34(2)
N(52)-C(030)	1.43(2)	C(026)-C(027)	1.23(3)
C(027)-C(028)	1.31(2)	C(028)-C(029)	1.36(2)
C(029)-C(030)	1.59(2)		

C(7)-In(1)-C(1)	118.27(14)	C(7)-In(1)-N(1)	95.86(12)
C(1)-In(1)-N(1)	91.97(12)	C(7)-In(1)-N(2)	85.89(12)
C(1)-In(1)-N(2)	89.17(12)	N(1)-In(1)-N(2)	177.15(11)
C(7)-In(1)-Br(1)	121.49(9)	C(1)-In(1)-Br(1)	119.56(10)
N(1)-In(1)-Br(1)	90.37(7)	N(2)-In(1)-Br(1)	86.79(9)
C(8)-In(2)-C(2)	117.45(14)	C(8)-In(2)-N(4)	94.61(12)
C(2)-In(2)-N(4)	91.91(13)	C(8)-In(2)-N(3)	87.23(12)

C(2)-In(2)-N(3)	89.39(13)	N(4)-In(2)-N(3)	176.95(11)
C(8)-In(2)-Br(2)	120.46(10)	C(2)-In(2)-Br(2)	121.76(10)
N(4)-In(2)-Br(2)	89.31(8)	N(3)-In(2)-Br(2)	87.66(8)
C(01)-N(1)-C(05)	117.3(3)	C(01)-N(1)-In(1)	122.0(3)
C(05)-N(1)-In(1)	120.7(3)	N(1)-C(01)-C(02)	123.4(4)
N(1)-C(01)-H(01A)	118.1(2)	C(02)-C(01)-H(01A)	118.6(2)
C(03)-C(02)-C(01)	119.0(4)	C(03)-C(02)-H(02A)	120.5(3)
C(01)-C(02)-H(02A)	120.5(2)	C(02)-C(03)-C(04)	118.6(4)
C(02)-C(03)-H(03A)	120.7(3)	C(04)-C(03)-H(03A)	120.7(3)
C(03)-C(04)-C(05)	119.0(4)	C(03)-C(04)-H(04A)	120.4(3)
C(05)-C(04)-H(04A)	120.6(3)	N(1)-C(05)-C(04)	122.7(4)
N(1)-C(05)-H(05A)	118.4(2)	C(04)-C(05)-H(05A)	118.8(3)
C(010)-N(2)-C(06)	117.2(4)	C(010)-N(2)-In(1)	115.9(3)
C(06)-N(2)-In(1)	126.9(3)	N(2)-C(06)-C(07)	122.7(4)
N(2)-C(06)-H(06A)	118.2(2)	C(07)-C(06)-H(06A)	119.1(3)
C(08)-C(07)-C(06)	119.2(5)	C(08)-C(07)-H(07A)	120.4(3)
C(06)-C(07)-H(07A)	120.4(3)	C(07)-C(08)-C(09)	118.4(5)
C(07)-C(08)-H(08A)	120.6(3)	C(09)-C(08)-H(08A)	121.0(3)
C(08)-C(09)-C(010)	118.8(5)	C(08)-C(09)-H(09A)	120.3(3)
C(010)-C(09)-H(09A)	120.9(4)	N(2)-C(010)-C(09)	123.7(5)
N(2)-C(010)-H(01B)	117.7(3)	C(09)-C(010)-H(01B)	118.6(4)
C(015)-N(3)-C(011)	117.0(4)	C(015)-N(3)-In(2)	118.5(3)
C(011)-N(3)-In(2)	124.4(3)	N(3)-C(011)-C(012)	123.4(4)
N(3)-C(011)-H(01C)	118.0(2)	C(012)-C(011)-H(01C)	118.6(3)
C(013)-C(012)-C(011)	119.0(4)	C(013)-C(012)-H(01D)	120.4(3)
C(011)-C(012)-H(01D)	120.6(3)	C(014)-C(013)-C(012)	118.9(4)
C(014)-C(013)-H(01E)	120.5(3)	C(012)-C(013)-H(01E)	120.6(3)
C(013)-C(014)-C(015)	118.9(5)	C(013)-C(014)-H(01F)	120.6(3)
C(015)-C(014)-H(01F)	120.5(3)	N(3)-C(015)-C(014)	122.7(5)
N(3)-C(015)-H(01G)	118.1(3)	C(014)-C(015)-H(01G)	119.2(3)
C(020)-N(4)-C(016)	117.2(4)	C(020)-N(4)-In(2)	118.9(3)
C(016)-N(4)-In(2)	123.9(3)	N(4)-C(016)-C(017)	122.1(4)
N(4)-C(016)-H(01H)	118.4(3)	C(017)-C(016)-H(01H)	119.5(3)
C(018)-C(017)-C(016)	119.4(5)	C(018)-C(017)-H(01I)	120.4(3)
C(016)-C(017)-H(01I)	120.2(3)	C(017)-C(018)-C(019)	118.7(5)
C(017)-C(018)-H(01J)	120.6(3)	C(019)-C(018)-H(01J)	120.8(3)
C(020)-C(019)-C(018)	118.5(5)	C(020)-C(019)-H(01K)	121.1(3)
C(018)-C(019)-H(01K)	120.4(3)	N(4)-C(020)-C(019)	124.2(5)
N(4)-C(020)-H(02B)	117.6(3)	C(019)-C(020)-H(02B)	118.2(3)
C(6)-C(1)-C(2)	117.7(3)	C(6)-C(1)-In(1)	122.2(3)
C(2)-C(1)-In(1)	120.1(3)	C(3)-C(2)-C(1)	118.1(3)
C(3)-C(2)-In(2)	119.9(3)	C(1)-C(2)-In(2)	122.0(3)
F(3)-C(3)-C(2)	120.6(4)	F(3)-C(3)-C(4)	116.6(4)
C(2)-C(3)-C(4)	122.8(4)	C(5)-C(4)-F(4)	119.6(4)
C(5)-C(4)-C(3)	119.1(4)	F(4)-C(4)-C(3)	121.3(4)
F(5)-C(5)-C(4)	120.0(4)	F(5)-C(5)-C(6)	121.2(4)
C(4)-C(5)-C(6)	118.9(4)	F(6)-C(6)-C(1)	120.3(3)
F(6)-C(6)-C(5)	116.3(3)	C(1)-C(6)-C(5)	123.4(4)
C(12)-C(7)-C(8)	117.7(3)	C(12)-C(7)-In(1)	121.3(3)
C(8)-C(7)-In(1)	120.8(2)	C(9)-C(8)-C(7)	117.7(3)
C(9)-C(8)-In(2)	121.6(3)	C(7)-C(8)-In(2)	120.5(2)
F(9)-C(9)-C(10)	116.3(3)	F(9)-C(9)-C(8)	120.4(3)
C(10)-C(9)-C(8)	123.3(3)	F(10)-C(10)-C(11)	119.7(3)
F(10)-C(10)-C(9)	121.3(3)	C(11)-C(10)-C(9)	119.1(3)
F(11)-C(11)-C(10)	119.8(3)	F(11)-C(11)-C(12)	121.3(3)
C(10)-C(11)-C(12)	118.9(3)	F(12)-C(12)-C(7)	120.5(3)
F(12)-C(12)-C(11)	116.2(3)	C(7)-C(12)-C(11)	123.3(3)
C(029)-N(51)-C(030)	139(2)	C(029)-N(51)-C(021)	17.8(12)
C(030)-N(51)-C(021)	124.9(13)	C(029)-N(51)-C(025)	132(2)
C(030)-N(51)-C(025)	7.4(13)	C(021)-N(51)-C(025)	117.8(9)
C(028)-C(021)-C(029)	147(3)	C(028)-C(021)-C(022)	27.8(14)
C(029)-C(021)-C(022)	133(2)	C(028)-C(021)-N(51)	139(2)
C(029)-C(021)-N(51)	18.9(13)	C(022)-C(021)-N(51)	117.3(10)

C(028)-C(021)-C(027)	33.1(14)	C(029)-C(021)-C(027)	125(2)
C(022)-C(021)-C(027)	8.4(9)	N(51)-C(021)-C(027)	109.6(9)
C(028)-C(022)-C(023)	137(2)	C(028)-C(022)-C(021)	22.1(11)
C(023)-C(022)-C(021)	121.7(13)	C(028)-C(022)-C(026)	134(2)
C(023)-C(022)-C(026)	11.6(11)	C(021)-C(022)-C(026)	115.0(12)
C(028)-C(022)-C(029)	34.9(12)	C(023)-C(022)-C(029)	106.0(12)
C(021)-C(022)-C(029)	15.8(6)	C(026)-C(022)-C(029)	99.9(10)
C(027)-C(023)-C(024)	137(3)	C(027)-C(023)-C(022)	13.5(14)
C(024)-C(023)-C(022)	124(2)	C(027)-C(023)-N(52)	122(2)
C(024)-C(023)-N(52)	16.0(10)	C(022)-C(023)-N(52)	109.0(13)
N(52)-C(024)-C(026)	128(3)	N(52)-C(024)-C(023)	136(3)
C(026)-C(024)-C(023)	17(2)	N(52)-C(024)-C(025)	21(2)
C(026)-C(024)-C(025)	123(2)	C(023)-C(024)-C(025)	124(2)
N(52)-C(024)-C(030)	30(2)	C(026)-C(024)-C(030)	112(2)
C(023)-C(024)-C(030)	112(2)	C(025)-C(024)-C(030)	12.4(7)
N(52)-C(024)-C(027)	117(2)	C(026)-C(024)-C(027)	28.1(14)
C(023)-C(024)-C(027)	20.7(12)	C(025)-C(024)-C(027)	103.3(10)
C(030)-C(024)-C(027)	91.0(9)	C(030)-C(025)-N(52)	136(3)
C(030)-C(025)-N(51)	13(2)	N(52)-C(025)-N(51)	123.5(14)
C(030)-C(025)-C(024)	128(3)	N(52)-C(025)-C(024)	12.6(10)
N(51)-C(025)-C(024)	114.9(11)	C(030)-C(025)-C(029)	30(2)
N(52)-C(025)-C(029)	108.1(13)	N(51)-C(025)-C(029)	16.4(6)
C(024)-C(025)-C(029)	98.8(10)	C(024)-N(52)-C(025)	147(3)
C(024)-N(52)-C(026)	30(2)	C(025)-N(52)-C(026)	133.6(14)
C(024)-N(52)-C(030)	137(2)	C(025)-N(52)-C(030)	14.9(11)
C(026)-N(52)-C(030)	119.0(11)	C(024)-N(52)-C(023)	28(2)
C(025)-N(52)-C(023)	128.2(14)	C(026)-N(52)-C(023)	10.2(12)
C(030)-N(52)-C(023)	114.4(11)	C(024)-C(026)-C(027)	133(2)
C(024)-C(026)-N(52)	21.4(14)	C(027)-C(026)-N(52)	124.1(14)
C(024)-C(026)-C(022)	125(2)	C(027)-C(026)-C(022)	14.2(10)
N(52)-C(026)-C(022)	112.2(12)	C(023)-C(027)-C(026)	14(2)
C(023)-C(027)-C(028)	132(2)	C(026)-C(027)-C(028)	125(2)
C(023)-C(027)-C(021)	117(2)	C(026)-C(027)-C(021)	108.8(13)
C(028)-C(027)-C(021)	16.7(7)	C(023)-C(027)-C(024)	22.3(14)
C(026)-C(027)-C(024)	19.3(9)	C(028)-C(027)-C(024)	109.7(12)
C(021)-C(027)-C(024)	94.4(9)	C(021)-C(028)-C(022)	130(3)
C(021)-C(028)-C(027)	130(2)	C(022)-C(028)-C(027)	10(2)
C(021)-C(028)-C(029)	17.0(13)	C(022)-C(028)-C(029)	124(2)
C(027)-C(028)-C(029)	121.0(12)	C(021)-C(029)-N(51)	143(3)
C(021)-C(029)-C(028)	16.0(13)	N(51)-C(029)-C(028)	137(2)
C(021)-C(029)-C(030)	125(2)	N(51)-C(029)-C(030)	22.3(11)
C(028)-C(029)-C(030)	115.8(11)	C(021)-C(029)-C(022)	31.5(13)
N(51)-C(029)-C(022)	116(2)	C(028)-C(029)-C(022)	21.0(6)
C(030)-C(029)-C(022)	95.1(9)	C(021)-C(029)-C(025)	117(2)
N(51)-C(029)-C(025)	31.6(11)	C(028)-C(029)-C(025)	106.7(9)
C(030)-C(029)-C(025)	9.3(8)	C(022)-C(029)-C(025)	86.2(8)
C(025)-C(030)-N(51)	160(4)	C(025)-C(030)-N(52)	30(2)
N(51)-C(030)-N(52)	131(2)	C(025)-C(030)-C(029)	141(3)
N(51)-C(030)-C(029)	18.4(9)	N(52)-C(030)-C(029)	113.5(10)
C(025)-C(030)-C(024)	40(3)	N(51)-C(030)-C(024)	120.0(14)
N(52)-C(030)-C(024)	12.7(7)	C(029)-C(030)-C(024)	101.8(10)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [Å^2] for MART26.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
In(1)	0.02806(13	0.0301(2)	0.03067(14)	-0.00031(10)	0.00399(10)	-0.00307(1
In(2)	0.03148(14	0.0332(2)	0.03117(14)	0.00393(11)	0.00333(11)	-0.00296(1
Br(1)	0.0562(3)	0.0447(3)	0.0433(2)	0.0038(2)	0.0172(2)	-0.0106(2)
Br(2)	0.0587(3)	0.0513(3)	0.0582(3)	0.0201(2)	0.0213(2)	-0.0013(2)
F(3)	0.092(2)	0.074(2)	0.042(2)	0.0214(14)	-0.0138(14)	-0.026(2)
F(4)	0.071(2)	0.085(2)	0.0396(14)	0.0017(14)	-0.0189(13)	-0.011(2)
F(5)	0.052(2)	0.067(2)	0.062(2)	-0.0079(14)	-0.0179(13)	-0.0215(14
F(6)	0.0483(14)	0.047(2)	0.059(2)	0.0076(12)	-0.0062(12)	-0.0184(12
F(9)	0.0442(13)	0.0398(14)	0.054(2)	0.0084(11)	-0.0002(11)	-0.0138(11
F(10)	0.0417(13)	0.047(2)	0.055(2)	-0.0070(11)	-0.0042(11)	-0.0158(11
F(11)	0.0419(13)	0.058(2)	0.0371(13)	-0.0008(11)	-0.0070(10)	-0.0004(11
F(12)	0.0518(14)	0.0409(14)	0.0377(12)	0.0084(10)	0.0027(11)	-0.0050(11
N(1)	0.031(2)	0.031(2)	0.034(2)	-0.0030(13)	0.0061(13)	-0.0005(13
C(01)	0.033(2)	0.047(3)	0.035(2)	-0.010(2)	0.000(2)	0.001(2)
C(02)	0.041(2)	0.052(3)	0.044(2)	-0.015(2)	0.008(2)	0.002(2)
C(03)	0.042(2)	0.047(3)	0.057(3)	-0.008(2)	0.015(2)	0.004(2)
C(04)	0.041(2)	0.052(3)	0.055(3)	0.003(2)	0.006(2)	0.014(2)
C(05)	0.041(2)	0.055(3)	0.040(2)	-0.003(2)	0.002(2)	0.007(2)
N(2)	0.034(2)	0.044(2)	0.052(2)	-0.012(2)	0.006(2)	0.001(2)
C(06)	0.043(2)	0.041(3)	0.046(2)	-0.003(2)	0.009(2)	0.002(2)
C(07)	0.065(3)	0.045(3)	0.073(3)	-0.009(2)	0.023(3)	0.007(2)
C(08)	0.051(3)	0.064(4)	0.150(6)	-0.026(4)	0.042(4)	0.009(3)
C(09)	0.040(3)	0.091(5)	0.193(8)	-0.047(5)	0.039(4)	-0.003(3)
C(010)	0.036(3)	0.078(4)	0.125(5)	-0.045(4)	0.015(3)	-0.005(3)
N(3)	0.043(2)	0.046(2)	0.037(2)	0.001(2)	0.007(2)	0.004(2)
C(011)	0.034(2)	0.054(3)	0.041(2)	-0.001(2)	0.006(2)	0.001(2)
C(012)	0.040(2)	0.060(3)	0.056(3)	0.003(2)	0.006(2)	0.009(2)
C(013)	0.059(3)	0.054(3)	0.069(3)	-0.001(2)	0.020(3)	0.020(2)
C(014)	0.088(4)	0.090(4)	0.051(3)	-0.017(3)	0.014(3)	0.030(3)
C(015)	0.070(3)	0.087(4)	0.040(3)	-0.006(3)	0.004(2)	0.032(3)
N(4)	0.036(2)	0.044(2)	0.039(2)	0.000(2)	0.004(2)	0.001(2)
C(016)	0.038(2)	0.060(3)	0.051(3)	-0.010(2)	0.002(2)	0.000(2)
C(017)	0.043(3)	0.087(4)	0.062(3)	-0.012(3)	0.003(2)	0.015(3)
C(018)	0.062(3)	0.066(3)	0.058(3)	-0.006(3)	0.015(3)	0.024(3)
C(019)	0.065(3)	0.055(3)	0.070(3)	-0.012(3)	0.024(3)	0.003(3)
C(020)	0.051(3)	0.049(3)	0.064(3)	-0.010(2)	0.014(2)	-0.009(2)
C(1)	0.027(2)	0.034(2)	0.032(2)	-0.003(2)	0.002(2)	0.000(2)
C(2)	0.033(2)	0.032(2)	0.036(2)	-0.002(2)	0.002(2)	0.002(2)
C(3)	0.043(2)	0.047(3)	0.037(2)	0.005(2)	0.001(2)	-0.006(2)
C(4)	0.044(2)	0.061(3)	0.034(2)	-0.002(2)	-0.007(2)	-0.001(2)
C(5)	0.035(2)	0.050(3)	0.044(2)	-0.011(2)	-0.004(2)	-0.005(2)
C(6)	0.029(2)	0.037(2)	0.046(2)	0.002(2)	0.005(2)	-0.002(2)
C(7)	0.026(2)	0.031(2)	0.031(2)	-0.001(2)	0.007(2)	-0.002(2)
C(8)	0.026(2)	0.034(2)	0.032(2)	-0.003(2)	0.003(2)	-0.001(2)
C(9)	0.029(2)	0.031(2)	0.039(2)	0.002(2)	0.008(2)	-0.002(2)
C(10)	0.026(2)	0.034(2)	0.041(2)	-0.008(2)	0.002(2)	-0.005(2)
C(11)	0.028(2)	0.041(2)	0.032(2)	-0.005(2)	0.001(2)	0.003(2)
C(12)	0.031(2)	0.031(2)	0.032(2)	0.002(2)	0.008(2)	0.003(2)

Table 6. Hydrogen coordinates and isotropic displacement parameters [Å^2] for MART26.

	x/a	y/b	z/c	U(eq)
H(01A)	0.7325(2)	0.6911(3)	0.3648(3)	0.059
H(02A)	0.6502(2)	0.7923(3)	0.4153(3)	0.069
H(03A)	0.5451(2)	0.8512(3)	0.3064(3)	0.072
H(04A)	0.5213(3)	0.7973(3)	0.1514(3)	0.075
H(05A)	0.6081(2)	0.6967(3)	0.1073(3)	0.069
H(06A)	0.7871(2)	0.3807(3)	0.0691(3)	0.065
H(07A)	0.8806(3)	0.2946(3)	0.0175(4)	0.090
H(08A)	1.0076(3)	0.3455(4)	0.0415(5)	0.128
H(09A)	1.0396(3)	0.4778(5)	0.1265(6)	0.158
H(01B)	0.9422(3)	0.5583(4)	0.1747(5)	0.120
H(01C)	0.5624(2)	0.5015(3)	0.2418(3)	0.065
H(01D)	0.4705(3)	0.5929(3)	0.2862(3)	0.079
H(01E)	0.4842(3)	0.6338(3)	0.4436(4)	0.089
H(01F)	0.5902(3)	0.5806(4)	0.5520(4)	0.115
H(01G)	0.6815(3)	0.4903(4)	0.4998(3)	0.100
H(01H)	0.9173(2)	0.3598(3)	0.3421(3)	0.076
H(01I)	1.0073(3)	0.2621(4)	0.2984(4)	0.098
H(01J)	0.9639(3)	0.1308(4)	0.2181(3)	0.092
H(01K)	0.8306(3)	0.0991(3)	0.1866(4)	0.093
H(02B)	0.7463(3)	0.2021(3)	0.2288(3)	0.081

Table 1. Crystal data and structure refinement for MART24. Cpd 6

Identification code	MART24
Empirical formula	$C_{28}H_{32}Br_2F_8In_2O_4$
Formula weight	974.00
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.636(1) Å α = 90° b = 11.129(1) Å β = 104.40(1)° c = 16.029(1) Å γ = 90°
Volume	1664.9(3) $Å^3$
Z	2
Density (calculated)	1.943 Mg/m^3
Absorption coefficient	3.861 mm^{-1}
F(000)	944
Crystal size	0.40 x 0.40 x 0.25 mm
θ range for data collection	3.20 to 27.98°
Index ranges	$-12 \le h \le 12$, $0 \le k \le 14$, $0 \le \ell \le 21$
Reflections collected	4129
Independent reflections	4000 (R_{int} = 0.0206)
Absorption correction	DIFABS
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3542 / 0 / 195
Goodness-of-fit on F^2	1.073
Final R indices [$I>2\sigma(I)$]	R1 = 0.0411, wR2 = 0.1001
R indices (all data)	R1 = 0.0768, wR2 = 0.1150
Largest diff. peak and hole	1.057 and -1.227 $eÅ^{-3}$

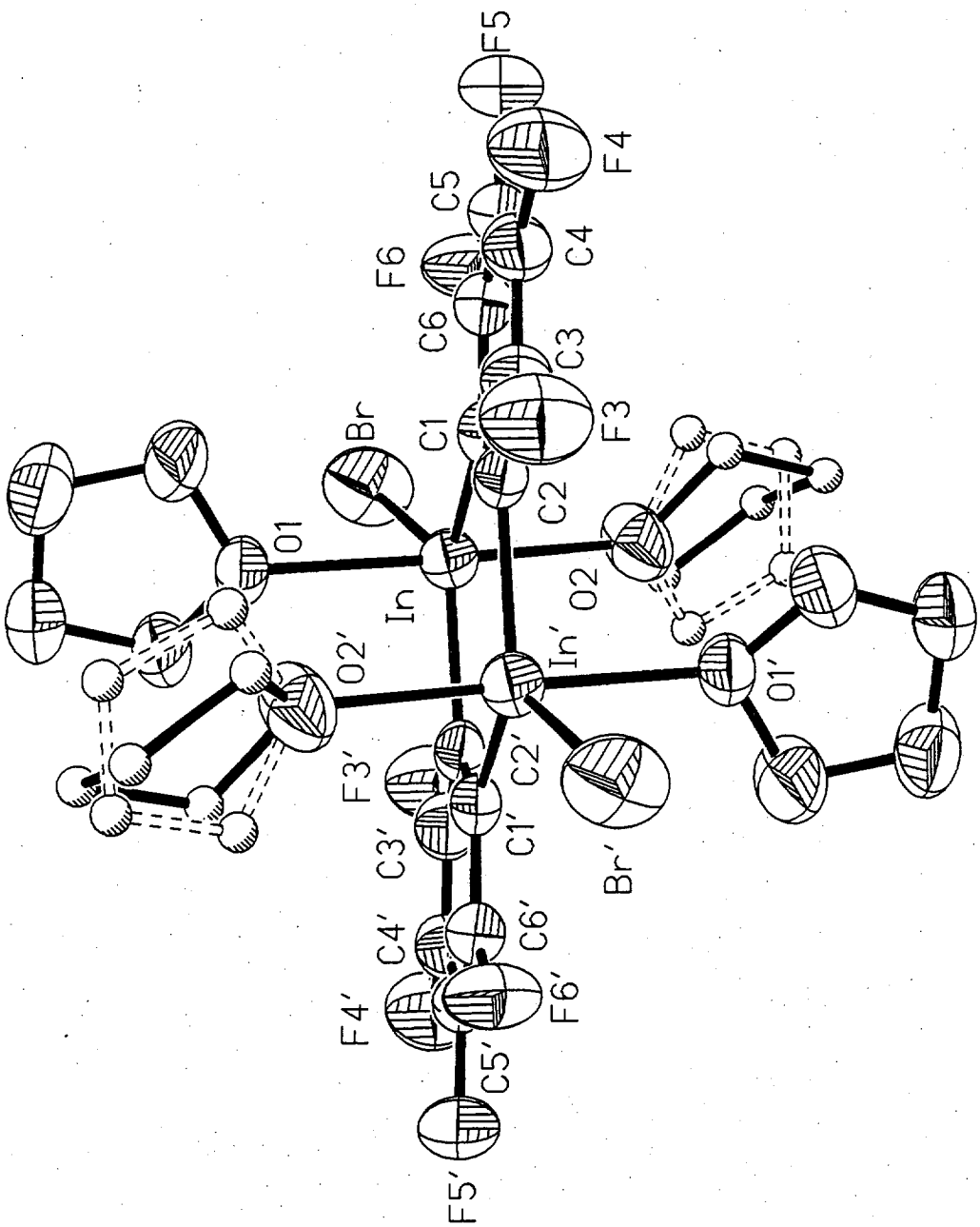
F5
F4
C5
C4
F6
C6
C3
F3
C1
Br
C2
O1
In
O2
In'
O2'
O1'
F3'
C2'
C3'
C1'
Br'
C4'
C6'
F4'
F6'
C5'
F5'

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [Å^2] for MART24. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In	0.00751(3)	0.14287(3)	0.94710(2)	0.04752(12)
Br	0.05840(9)	0.31961(7)	0.86259(5)	0.0904(2)
F(3)	-0.2377(4)	-0.3064(3)	0.9140(3)	0.0905(12)
F(4)	-0.4174(4)	-0.2585(4)	0.7606(3)	0.0945(12)
F(5)	-0.4175(4)	-0.0427(4)	0.6867(2)	0.0858(11)
F(6)	-0.2391(4)	0.1309(3)	0.7670(2)	0.0840(11)
C(1)	-0.1419(5)	0.0048(4)	0.8864(3)	0.0457(10)
C(2)	-0.1417(5)	-0.1092(4)	0.9252(3)	0.0463(10)
C(3)	-0.2335(6)	-0.1954(5)	0.8801(4)	0.0589(13)
C(4)	-0.3256(6)	-0.1748(5)	0.8012(4)	0.0613(14)
C(5)	-0.3253(5)	-0.0651(6)	0.7640(3)	0.063(2)
C(6)	-0.2356(5)	0.0225(5)	0.8065(3)	0.0543(12)
O(1)	0.1837(3)	0.0344(4)	0.8935(2)	0.0615(9)
C(11)	0.1513(7)	-0.0076(9)	0.8072(5)	0.119(4)
C(12)	0.2866(7)	-0.0384(7)	0.7840(5)	0.085(2)
C(13)	0.4023(7)	-0.0049(7)	0.8619(4)	0.086(2)
C(14)	0.3291(6)	0.0717(8)	0.9152(4)	0.084(2)
O(2)	-0.1644(4)	0.2524(4)	0.9942(3)	0.0782(12)
C(21)	-0.3194(11)	0.2336(10)	0.9643(7)	0.049(2)
C(22)	-0.3851(12)	0.3231(11)	1.0098(8)	0.061(3)
C(23)	-0.2910(13)	0.4330(11)	1.0032(9)	0.065(3)
C(24)	-0.146(2)	0.379(2)	1.0223(11)	0.096(5)
C(25)	-0.133(2)	0.3319(13)	1.0667(10)	0.081(4)
C(26)	-0.267(2)	0.397(2)	1.0584(12)	0.106(5)
C(27)	-0.359(2)	0.375(2)	0.9825(14)	0.124(7)
C(28)	-0.296(2)	0.278(2)	0.9387(13)	0.114(6)

Table 3. Bond lengths [Å] and angles [°] for MART24.

In-C(2)#1	2.164(5)	In-C(1)	2.164(5)
In-O(2)	2.328(4)	In-O(1)	2.408(3)
In-Br	2.5050(7)	F(3)-C(3)	1.354(7)
F(4)-C(4)	1.337(6)	F(5)-C(5)	1.356(6)
F(6)-C(6)	1.358(6)	C(1)-C(6)	1.385(7)
C(1)-C(2)	1.413(7)	C(2)-C(3)	1.382(7)
C(2)-In#1	2.164(5)	C(3)-C(4)	1.372(8)
C(4)-C(5)	1.359(9)	C(5)-C(6)	1.367(8)
O(1)-C(11)	1.420(7)	O(1)-C(14)	1.420(6)
C(11)-C(12)	1.481(9)	C(11)-H(111)	0.96
C(11)-H(112)	0.96	C(12)-C(13)	1.500(9)
C(12)-H(121)	0.96	C(12)-H(122)	0.96
C(13)-C(14)	1.501(8)	C(13)-H(131)	0.96
C(13)-H(132)	0.96	C(14)-H(141)	0.96
C(14)-H(142)	0.96	O(2)-C(28)	1.38(2)
O(2)-C(25)	1.43(2)	O(2)-C(21)	1.466(11)
O(2)-C(24)	1.48(2)	C(21)-C(28)	0.71(2)
C(21)-C(22)	1.47(2)	C(21)-C(27)	1.66(2)
C(21)-H(211)	0.96	C(21)-H(212)	0.96
C(21)-H(281)	0.60(2)	C(22)-C(27)	0.80(2)
C(22)-C(26)	1.46(2)	C(22)-C(23)	1.54(2)
C(22)-C(28)	1.67(2)	C(22)-H(221)	0.96
C(22)-H(222)	0.96	C(22)-H(262)	1.57(2)
C(22)-H(272)	0.75(3)	C(23)-C(27)	0.92(2)
C(23)-C(26)	0.94(2)	C(23)-C(24)	1.48(2)
C(23)-C(25)	1.96(2)	C(23)-C(28)	2.01(2)
C(23)-H(231)	0.96	C(23)-H(232)	0.96
C(23)-H(261)	1.13(2)	C(23)-H(271)	1.01(3)
C(24)-C(25)	0.87(2)	C(24)-C(26)	1.44(2)
C(24)-C(27)	1.99(3)	C(24)-H(241)	0.96
C(24)-H(242)	0.96	C(24)-H(251)	0.90(2)
C(25)-C(26)	1.46(2)	C(25)-H(251)	0.96
C(25)-H(252)	0.96	C(26)-C(27)	1.34(2)
C(26)-H(261)	0.96	C(26)-H(262)	0.96
C(27)-C(28)	1.50(3)	C(27)-H(271)	0.96
C(27)-H(272)	0.96	C(28)-H(281)	0.96
C(28)-H(282)	0.96		

C(2)#1-In-C(1)	118.4(2)	C(2)#1-In-O(2)	95.2(2)
C(1)-In-O(2)	94.0(2)	C(2)#1-In-O(1)	86.69(14)
C(1)-In-O(1)	86.15(14)	O(2)-In-O(1)	177.8(2)
C(2)#1-In-Br	119.75(13)	C(1)-In-Br	120.80(13)
O(2)-In-Br	90.85(12)	O(1)-In-Br	87.16(10)
C(6)-C(1)-C(2)	117.7(4)	C(6)-C(1)-In	121.5(4)
C(2)-C(1)-In	120.7(3)	C(3)-C(2)-C(1)	117.5(4)
C(3)-C(2)-In#1	121.9(4)	C(1)-C(2)-In#1	120.5(3)
F(3)-C(3)-C(4)	116.5(5)	F(3)-C(3)-C(2)	120.2(5)
C(4)-C(3)-C(2)	123.4(6)	F(4)-C(4)-C(5)	119.1(5)
F(4)-C(4)-C(3)	122.0(6)	C(5)-C(4)-C(3)	118.9(5)
F(5)-C(5)-C(4)	119.6(5)	F(5)-C(5)-C(6)	120.9(6)
C(4)-C(5)-C(6)	119.5(5)	F(6)-C(6)-C(5)	117.5(5)
F(6)-C(6)-C(1)	119.4(5)	C(5)-C(6)-C(1)	123.1(5)
C(11)-O(1)-C(14)	107.4(4)	C(11)-O(1)-In	120.6(4)
C(14)-O(1)-In	120.5(3)	O(1)-C(11)-C(12)	109.1(5)
O(1)-C(11)-H(111)	109.0(5)	C(12)-C(11)-H(111)	109.7(5)
O(1)-C(11)-H(112)	110.4(4)	C(12)-C(11)-H(112)	110.2(5)
H(111)-C(11)-H(112)	108.4	C(11)-C(12)-C(13)	104.6(5)
C(11)-C(12)-H(121)	111.2(5)	C(13)-C(12)-H(121)	110.5(4)
C(11)-C(12)-H(122)	110.6(5)	C(13)-C(12)-H(122)	111.0(4)
H(121)-C(12)-H(122)	108.9	C(14)-C(13)-C(12)	104.9(5)

C(14)-C(13)-H(131)	111.0(4)	C(12)-C(13)-H(131)	111.1(4)
C(14)-C(13)-H(132)	110.5(4)	C(12)-C(13)-H(132)	110.5(4)
H(131)-C(13)-H(132)	108.8	O(1)-C(14)-C(13)	105.7(5)
O(1)-C(14)-H(141)	110.6(3)	C(13)-C(14)-H(141)	111.0(4)
O(1)-C(14)-H(142)	110.2(4)	C(13)-C(14)-H(142)	110.4(4)
H(141)-C(14)-H(142)	108.8	C(28)-O(2)-C(25)	111.6(11)
C(28)-O(2)-C(21)	28.8(9)	C(25)-O(2)-C(21)	110.0(8)
C(28)-O(2)-C(24)	91.2(11)	C(25)-O(2)-C(24)	34.7(8)
C(21)-O(2)-C(24)	105.7(8)	C(28)-O(2)-In	120.7(9)
C(25)-O(2)-In	124.4(6)	C(21)-O(2)-In	124.7(5)
C(24)-O(2)-In	123.9(7)	C(28)-C(21)-O(2)	69(2)
C(28)-C(21)-C(22)	93(2)	O(2)-C(21)-C(22)	105.7(8)
C(28)-C(21)-C(27)	64(2)	O(2)-C(21)-C(27)	93.9(10)
C(22)-C(21)-C(27)	28.8(8)	C(28)-C(21)-H(211)	155(2)
O(2)-C(21)-H(211)	110.7(5)	C(22)-C(21)-H(211)	110.7(7)
C(27)-C(21)-H(211)	139.1(9)	C(28)-C(21)-H(212)	52(2)
O(2)-C(21)-H(212)	110.3(5)	C(22)-C(21)-H(212)	110.8(6)
C(27)-C(21)-H(212)	91.5(8)	H(211)-C(21)-H(212)	108.7
C(28)-C(21)-H(281)	93(3)	O(2)-C(21)-H(281)	134(3)
C(22)-C(21)-H(281)	118(3)	C(27)-C(21)-H(281)	117(3)
H(211)-C(21)-H(281)	68(2)	H(212)-C(21)-H(281)	42(2)
C(27)-C(22)-C(26)	65(2)	C(27)-C(22)-C(21)	89(2)
C(26)-C(22)-C(21)	106.0(11)	C(27)-C(22)-C(23)	29(2)
C(26)-C(22)-C(23)	36.5(8)	C(21)-C(22)-C(23)	99.9(9)
C(27)-C(22)-C(28)	64(2)	C(26)-C(22)-C(28)	94.1(12)
C(21)-C(22)-C(28)	25.3(8)	C(23)-C(22)-C(28)	77.4(10)
C(27)-C(22)-H(221)	140(2)	C(26)-C(22)-H(221)	76.5(10)
C(21)-C(22)-H(221)	112.0(7)	C(23)-C(22)-H(221)	111.9(7)
C(28)-C(22)-H(221)	131.9(8)	C(27)-C(22)-H(222)	92(2)
C(26)-C(22)-H(222)	135.3(9)	C(21)-C(22)-H(222)	111.5(6)
C(23)-C(22)-H(222)	111.7(7)	C(28)-C(22)-H(222)	109.7(8)
H(221)-C(22)-H(222)	109.6	C(27)-C(22)-H(262)	99(2)
C(26)-C(22)-H(262)	36.7(5)	C(21)-C(22)-H(262)	122.7(11)
C(23)-C(22)-H(262)	70.6(9)	C(28)-C(22)-H(262)	123.7(12)
H(221)-C(22)-H(262)	41.4(9)	H(222)-C(22)-H(262)	124.7(8)
C(27)-C(22)-H(272)	76(2)	C(26)-C(22)-H(272)	115(2)
C(21)-C(22)-H(272)	124(2)	C(23)-C(22)-H(272)	92(2)
C(28)-C(22)-H(272)	113(2)	H(221)-C(22)-H(272)	113(2)
H(222)-C(22)-H(272)	21(2)	H(262)-C(22)-H(272)	113(2)
C(27)-C(23)-C(26)	92(2)	C(27)-C(23)-C(24)	110(2)
C(26)-C(23)-C(24)	69(2)	C(27)-C(23)-C(22)	25(2)
C(26)-C(23)-C(22)	67.1(14)	C(24)-C(23)-C(22)	101.8(11)
C(27)-C(23)-C(25)	100(2)	C(26)-C(23)-C(25)	45.3(13)
C(24)-C(23)-C(25)	24.5(8)	C(22)-C(23)-C(25)	84.3(8)
C(27)-C(23)-C(28)	45(2)	C(26)-C(23)-C(28)	95(2)
C(24)-C(23)-C(28)	70.0(10)	C(22)-C(23)-C(28)	54.1(8)
C(25)-C(23)-C(28)	71.9(8)	C(27)-C(23)-H(231)	125(2)
C(26)-C(23)-H(231)	71.1(14)	C(24)-C(23)-H(231)	110.9(8)
C(22)-C(23)-H(231)	111.2(7)	C(25)-C(23)-H(231)	102.1(6)
C(28)-C(23)-H(231)	163.9(7)	C(27)-C(23)-H(232)	87(2)
C(26)-C(23)-H(232)	178(2)	C(24)-C(23)-H(232)	112.7(9)
C(22)-C(23)-H(232)	111.1(7)	C(25)-C(23)-H(232)	136.1(6)
C(28)-C(23)-H(232)	84.4(7)	H(231)-C(23)-H(232)	109.0
C(27)-C(23)-H(261)	136(2)	C(26)-C(23)-H(261)	54.1(10)
C(24)-C(23)-H(261)	85.2(13)	C(22)-C(23)-H(261)	113.4(13)
C(25)-C(23)-H(261)	76.3(11)	C(28)-C(23)-H(261)	146.7(13)
H(231)-C(23)-H(261)	26.3(11)	H(232)-C(23)-H(261)	126.7(11)
C(27)-C(23)-H(271)	59.6(14)	C(26)-C(23)-H(271)	147(2)
C(24)-C(23)-H(271)	133(2)	C(22)-C(23)-H(271)	82.6(13)
C(25)-C(23)-H(271)	147(2)	C(28)-C(23)-H(271)	75.8(14)
H(231)-C(23)-H(271)	110.9(14)	H(232)-C(23)-H(271)	31(2)
H(261)-C(23)-H(271)	137(2)	C(25)-C(24)-C(26)	74(2)
C(25)-C(24)-C(23)	110(2)	C(26)-C(24)-C(23)	37.7(9)

C(25)-C(24)-O(2)	70(2)	C(26)-C(24)-O(2)	102.2(13)
C(23)-C(24)-O(2)	106.8(11)	C(25)-C(24)-C(27)	100(2)
C(26)-C(24)-C(27)	42.2(10)	C(23)-C(24)-C(27)	25.7(8)
O(2)-C(24)-C(27)	81.2(10)	C(25)-C(24)-H(241)	139(2)
C(26)-C(24)-H(241)	141.1(11)	C(23)-C(24)-H(241)	108.8(9)
O(2)-C(24)-H(241)	108.7(7)	C(27)-C(24)-H(241)	120.4(8)
C(25)-C(24)-H(242)	45(2)	C(26)-C(24)-H(242)	79.8(10)
C(23)-C(24)-H(242)	111.6(9)	O(2)-C(24)-H(242)	112.1(7)
C(27)-C(24)-H(242)	121.5(8)	H(241)-C(24)-H(242)	108.8
C(25)-C(24)-H(251)	65.6(14)	C(26)-C(24)-H(251)	114(2)
C(23)-C(24)-H(251)	139(2)	O(2)-C(24)-H(251)	109(2)
C(27)-C(24)-H(251)	156(2)	H(241)-C(24)-H(251)	77.6(13)
H(242)-C(24)-H(251)	35.1(14)	C(24)-C(25)-O(2)	76(2)
C(24)-C(25)-C(26)	72(2)	O(2)-C(25)-C(26)	103.5(12)
C(24)-C(25)-C(23)	45(2)	O(2)-C(25)-C(23)	87.4(8)
C(26)-C(25)-C(23)	27.4(8)	C(24)-C(25)-H(242)	74(2)
O(2)-C(25)-H(242)	143(2)	C(26)-C(25)-H(242)	87(2)
C(23)-C(25)-H(242)	86(2)	C(24)-C(25)-H(251)	59(2)
O(2)-C(25)-H(251)	108.8(6)	C(26)-C(25)-H(251)	108.9(10)
C(23)-C(25)-H(251)	94.0(6)	H(242)-C(25)-H(251)	36(2)
C(24)-C(25)-H(252)	168(2)	O(2)-C(25)-H(252)	113.8(6)
C(26)-C(25)-H(252)	112.5(10)	C(23)-C(25)-H(252)	139.9(6)
H(242)-C(25)-H(252)	94(2)	H(251)-C(25)-H(252)	109.1
C(23)-C(26)-C(27)	43.5(13)	C(23)-C(26)-C(24)	73(2)
C(27)-C(26)-C(24)	92(2)	C(23)-C(26)-C(25)	107(2)
C(27)-C(26)-C(25)	111(2)	C(24)-C(26)-C(25)	34.8(9)
C(23)-C(26)-C(22)	76(2)	C(27)-C(26)-C(22)	32.9(11)
C(24)-C(26)-C(22)	107.8(14)	C(25)-C(26)-C(22)	108.5(14)
C(23)-C(26)-H(221)	112(2)	C(27)-C(26)-H(221)	69.6(14)
C(24)-C(26)-H(221)	126(2)	C(25)-C(26)-H(221)	105.0(14)
C(22)-C(26)-H(221)	37.0(5)	C(23)-C(26)-H(231)	55.1(11)
C(27)-C(26)-H(231)	86(2)	C(24)-C(26)-H(231)	105(2)
C(25)-C(26)-H(231)	133(2)	C(22)-C(26)-H(231)	108(2)
H(221)-C(26)-H(231)	122(2)	C(23)-C(26)-H(242)	105(2)
C(27)-C(26)-H(242)	128(2)	C(24)-C(26)-H(242)	36.6(5)
C(25)-C(26)-H(242)	26.5(9)	C(22)-C(26)-H(242)	134(2)
H(221)-C(26)-H(242)	128(2)	H(231)-C(26)-H(242)	109(2)
C(23)-C(26)-H(261)	73(2)	C(27)-C(26)-H(261)	110.8(14)
C(24)-C(26)-H(261)	94.0(11)	C(25)-C(26)-H(261)	111.4(9)
C(22)-C(26)-H(261)	135.1(9)	H(221)-C(26)-H(261)	139.7(8)
H(231)-C(26)-H(261)	27.1(11)	H(242)-C(26)-H(261)	85.3(10)
C(23)-C(26)-H(262)	141.5(14)	C(27)-C(26)-H(262)	107.6(14)
C(24)-C(26)-H(262)	142.5(11)	C(25)-C(26)-H(262)	107.7(10)
C(22)-C(26)-H(262)	77.8(9)	H(221)-C(26)-H(262)	42.3(8)
H(231)-C(26)-H(262)	108.4(11)	H(242)-C(26)-H(262)	113.8(10)
H(261)-C(26)-H(262)	108.0	C(22)-C(27)-C(23)	127(3)
C(22)-C(27)-C(26)	82(2)	C(23)-C(27)-C(26)	44.9(14)
C(22)-C(27)-C(28)	87(2)	C(23)-C(27)-C(28)	110(2)
C(26)-C(27)-C(28)	108(2)	C(22)-C(27)-C(21)	62(2)
C(23)-C(27)-C(21)	124(2)	C(26)-C(27)-C(21)	102(2)
C(28)-C(27)-C(21)	25.4(9)	C(22)-C(27)-C(24)	106(2)
C(23)-C(27)-C(24)	44.3(14)	C(26)-C(27)-C(24)	46.3(12)
C(28)-C(27)-C(24)	70.1(12)	C(21)-C(27)-C(24)	79.3(10)
C(22)-C(27)-H(222)	49.1(14)	C(23)-C(27)-H(222)	146(3)
C(26)-C(27)-H(222)	119(2)	C(28)-C(27)-H(222)	104(2)
C(21)-C(27)-H(222)	86(2)	C(24)-C(27)-H(222)	155(2)
C(22)-C(27)-H(232)	172(3)	C(23)-C(27)-H(232)	47.9(12)
C(26)-C(27)-H(232)	93(2)	C(28)-C(27)-H(232)	100(2)
C(21)-C(27)-H(232)	125(2)	C(24)-C(27)-H(232)	73.9(12)
H(222)-C(27)-H(232)	131(2)	C(22)-C(27)-H(271)	157(2)
C(23)-C(27)-H(271)	65(2)	C(26)-C(27)-H(271)	108(2)
C(28)-C(27)-H(271)	107.9(12)	C(21)-C(27)-H(271)	132.0(9)
C(24)-C(27)-H(271)	95.0(8)	H(222)-C(27)-H(271)	109.6(11)

H(232)-C(27)-H(271)	21.1(11)	C(22)-C(27)-H(272)	50(2)
C(23)-C(27)-H(272)	136(2)	C(26)-C(27)-H(272)	111.1(14)
C(28)-C(27)-H(272)	113.8(12)	C(21)-C(27)-H(272)	94.7(9)
C(24)-C(27)-H(272)	153.0(8)	H(222)-C(27)-H(272)	10.4(12)
H(232)-C(27)-H(272)	128.5(11)	H(271)-C(27)-H(272)	108.1
C(21)-C(28)-O(2)	82(2)	C(21)-C(28)-C(27)	90(2)
O(2)-C(28)-C(27)	105(2)	C(21)-C(28)-C(22)	62(2)
O(2)-C(28)-C(22)	99.6(12)	C(27)-C(28)-C(22)	28.7(10)
C(21)-C(28)-C(23)	106(2)	O(2)-C(28)-C(23)	86.8(10)
C(27)-C(28)-C(23)	25.5(10)	C(22)-C(28)-C(23)	48.5(8)
C(21)-C(28)-H(212)	81(2)	O(2)-C(28)-H(212)	137(3)
C(27)-C(28)-H(212)	114(2)	C(22)-C(28)-H(212)	106(2)
C(23)-C(28)-H(212)	136(2)	C(21)-C(28)-H(281)	39(2)
O(2)-C(28)-H(281)	110.0(9)	C(27)-C(28)-H(281)	107.6(12)
C(22)-C(28)-H(281)	83.6(8)	C(23)-C(28)-H(281)	131.7(7)
H(212)-C(28)-H(281)	42(2)	C(21)-C(28)-H(282)	147(2)
O(2)-C(28)-H(282)	111.6(9)	C(27)-C(28)-H(282)	113.0(12)
C(22)-C(28)-H(282)	138.2(8)	C(23)-C(28)-H(282)	104.8(7)
H(212)-C(28)-H(282)	69(2)	H(281)-C(28)-H(282)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+2

Table 4. Anisotropic displacement parameters [Å^2] for MART24.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
In	0.0458(2)	0.0494(2)	0.0478(2)	-0.0010(2)	0.01229(13)	-0.0002(2)
Br	0.0966(5)	0.0743(4)	0.0949(5)	0.0339(4)	0.0135(4)	-0.0068(4)
F(3)	0.099(3)	0.070(2)	0.092(3)	-0.004(2)	0.003(2)	-0.028(2)
F(4)	0.079(2)	0.100(3)	0.094(3)	-0.033(2)	0.001(2)	-0.029(2)
F(5)	0.066(2)	0.129(3)	0.052(2)	-0.011(2)	-0.004(2)	-0.001(2)
F(6)	0.088(2)	0.091(3)	0.060(2)	0.015(2)	-0.005(2)	-0.002(2)
C(1)	0.038(2)	0.059(3)	0.043(2)	-0.005(2)	0.015(2)	0.002(2)
C(2)	0.039(2)	0.059(3)	0.044(2)	-0.011(2)	0.016(2)	-0.002(2)
C(3)	0.055(3)	0.061(3)	0.061(3)	-0.013(3)	0.015(2)	-0.008(2)
C(4)	0.047(3)	0.076(4)	0.059(3)	-0.026(3)	0.010(2)	-0.009(2)
C(5)	0.042(2)	0.101(5)	0.044(3)	-0.013(3)	0.009(2)	-0.001(3)
C(6)	0.046(2)	0.072(3)	0.046(3)	0.000(2)	0.014(2)	0.005(2)
O(1)	0.045(2)	0.086(3)	0.058(2)	-0.018(2)	0.021(2)	-0.002(2)
C(11)	0.068(4)	0.207(10)	0.084(5)	-0.079(6)	0.021(4)	0.005(5)
C(12)	0.076(4)	0.101(5)	0.090(5)	-0.035(4)	0.043(4)	-0.018(4)
C(13)	0.062(4)	0.120(6)	0.083(5)	-0.013(4)	0.035(3)	0.012(4)
C(14)	0.048(3)	0.132(6)	0.077(4)	-0.034(4)	0.020(3)	-0.005(3)
O(2)	0.061(2)	0.076(3)	0.095(3)	-0.030(2)	0.014(2)	0.012(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for MART24.

	x/a	y/b	z/c	U(eq)
H(111)	0.1024(7)	0.0547(9)	0.7697(5)	0.179
H(112)	0.0898(7)	-0.0766(9)	0.8008(5)	0.179
H(121)	0.2967(7)	0.0064(7)	0.7347(5)	0.127
H(122)	0.2898(7)	-0.1226(7)	0.7718(5)	0.127
H(131)	0.4777(7)	0.0388(7)	0.8459(4)	0.129
H(132)	0.4422(7)	-0.0754(7)	0.8933(4)	0.129
H(141)	0.3713(6)	0.0604(8)	0.9756(4)	0.127
H(142)	0.3359(6)	0.1551(8)	0.9014(4)	0.127
H(211)	-0.3446(11)	0.1537(10)	0.9777(7)	0.074
H(212)	-0.3504(11)	0.2450(10)	0.9031(7)	0.074
H(221)	-0.3777(12)	0.3006(11)	1.0686(8)	0.091
H(222)	-0.4837(12)	0.3369(11)	0.9811(8)	0.091
H(231)	-0.2972(13)	0.4928(11)	1.0453(9)	0.098
H(232)	-0.3184(13)	0.4684(11)	0.9469(9)	0.098
H(241)	-0.090(2)	0.420(2)	0.9890(11)	0.144
H(242)	-0.098(2)	0.386(2)	1.0823(11)	0.144
H(251)	-0.060(2)	0.3873(13)	1.0605(10)	0.121
H(252)	-0.103(2)	0.2915(13)	1.1211(10)	0.121
H(261)	-0.251(2)	0.482(2)	1.0666(12)	0.159
H(262)	-0.310(2)	0.369(2)	1.1027(12)	0.159
H(271)	-0.366(2)	0.447(2)	0.9481(14)	0.185
H(272)	-0.453(2)	0.357(2)	0.9896(14)	0.185
H(281)	-0.358(2)	0.209(2)	0.9334(13)	0.171
H(282)	-0.286(2)	0.301(2)	0.8827(13)	0.171

Table 1. Crystal data and structure refinement for ~~MART20~~. Cpd 5

Identification code	MART20
Empirical formula	$C_{28}H_{32}Cl_2F_8In_2O_4$
Formula weight	885.08
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.686(1) Å α = 90° b = 11.071(1) Å β = 105.55(1)° c = 15.725(2) Å γ = 90°
Volume	1624.5(3) $Å^3$
Z	2
Density (calculated)	1.809 Mg/m^3
Absorption coefficient	1.662 mm^{-1}
F(000)	872
Crystal size	0.55 x 0.40 x 0.22 mm
θ range for data collection	3.26 to 26.98°
Index ranges	$-12 \le h \le 11$, $0 \le k \le 14$, $0 \le \ell \le 20$
Reflections collected	3522
Independent reflections	3522 (R_{int} = 0.0000)
Absorption correction	DIFABS
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3333 / 0 / 199
Goodness-of-fit on F^2	1.032
Final R indices [$I>2\sigma(I)$]	R1 = 0.0275, wR2 = 0.0684
R indices (all data)	R1 = 0.0356, wR2 = 0.0747
Largest diff. peak and hole	0.500 and -0.549 $eÅ^{-3}$

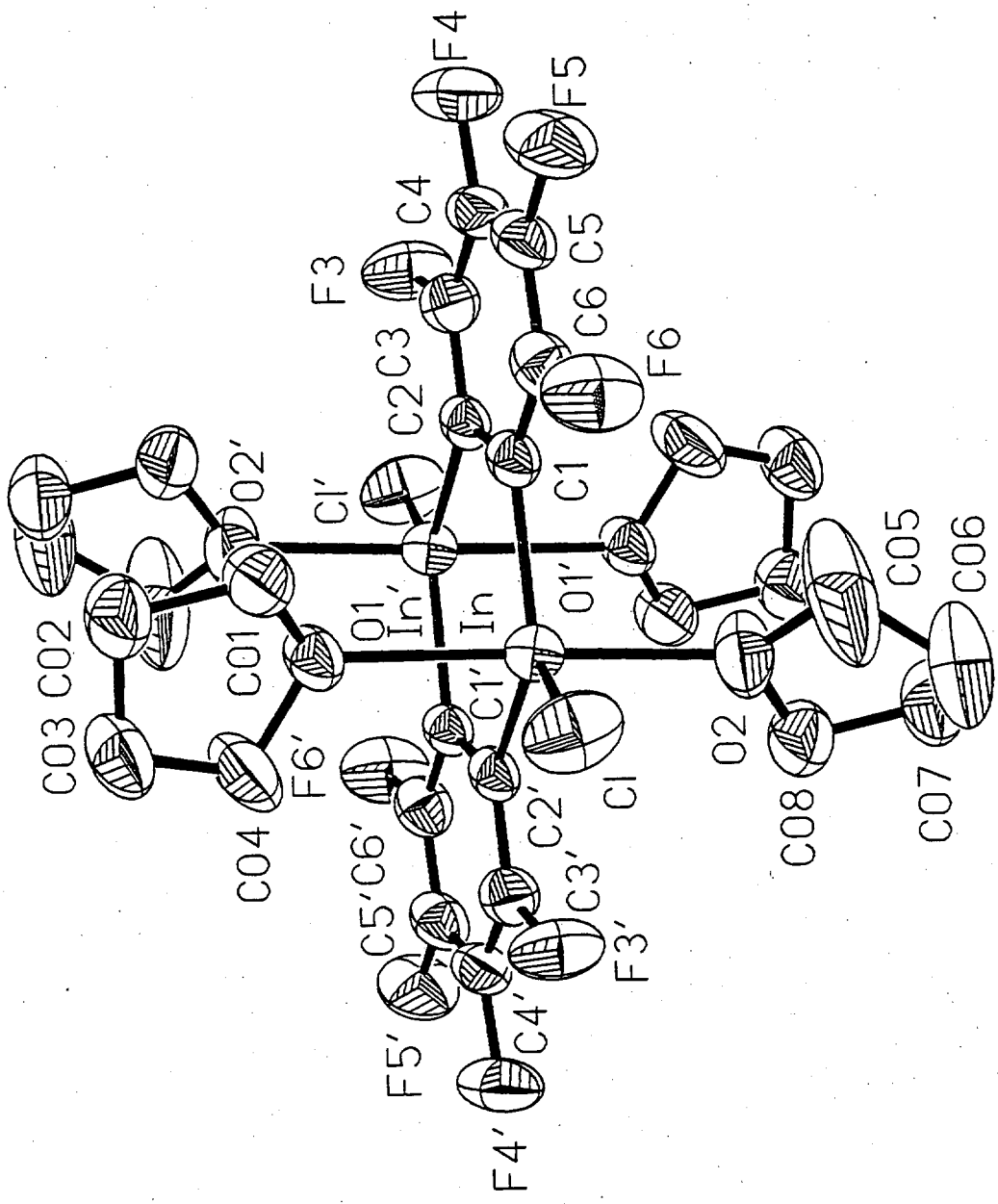

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [Å^2] for MART20. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In	0.00974(2)	0.14304(2)	0.944987(13)	0.04121(8)
Cl	0.05442(12)	0.31248(9)	0.86416(7)	0.0786(3)
C(1)	0.1459(3)	0.1087(3)	1.0764(2)	0.0397(6)
C(2)	0.1436(3)	-0.0054(3)	1.1170(2)	0.0387(6)
C(3)	0.2365(3)	-0.0240(3)	1.1989(2)	0.0477(7)
C(4)	0.3313(3)	0.0627(3)	1.2426(2)	0.0519(8)
C(5)	0.3346(3)	0.1717(3)	1.2031(2)	0.0518(8)
C(6)	0.2420(3)	0.1933(3)	1.1216(2)	0.0503(7)
F(3)	0.2380(3)	-0.1319(2)	1.2404(2)	0.0752(6)
F(4)	0.4235(2)	0.0398(2)	1.32174(13)	0.0762(6)
F(5)	0.4303(2)	0.2557(2)	1.2443(2)	0.0794(7)
F(6)	0.2501(3)	0.3032(2)	1.0857(2)	0.0814(7)
O(1)	0.1825(2)	0.0369(2)	0.88918(14)	0.0530(5)
C(01)	0.3273(4)	0.0788(4)	0.9093(3)	0.0680(10)
C(02)	0.3992(4)	-0.0021(4)	0.8577(3)	0.0701(10)
C(03)	0.2801(4)	-0.0347(4)	0.7766(3)	0.0714(11)
C(04)	0.1466(4)	-0.0100(6)	0.8018(3)	0.113(2)
O(2)	-0.1583(3)	0.2534(2)	0.9945(2)	0.0774(8)
C(05)	-0.1299(6)	0.3676(6)	1.0376(6)	0.176(4)
C(06)	-0.2738(6)	0.4304(4)	1.0185(4)	0.108(2)
C(07)	-0.3698(5)	0.3299(4)	1.0149(3)	0.0815(12)
C(08)	-0.3090(4)	0.2368(4)	0.9653(3)	0.0745(11)

Table 3. Bond lengths [Å] and angles [°] for MART20.

In-C(1)	2.166(3)	In-C(2)#1	2.168(3)
In-O(2)	2.330(2)	In-Cl	2.3699(9)
In-O(1)	2.395(2)	C(1)-C(6)	1.377(4)
C(1)-C(2)	1.418(4)	C(2)-C(3)	1.375(4)
C(2)-In#1	2.168(3)	C(3)-F(3)	1.359(4)
C(3)-C(4)	1.377(5)	C(4)-F(4)	1.348(3)
C(4)-C(5)	1.361(5)	C(5)-F(5)	1.350(4)
C(5)-C(6)	1.374(5)	C(6)-F(6)	1.353(4)
O(1)-C(04)	1.422(4)	O(1)-C(01)	1.429(4)
C(01)-C(02)	1.500(5)	C(01)-H(11)	0.96
C(01)-H(12)	0.96	C(02)-C(03)	1.516(5)
C(02)-H(21)	0.96	C(02)-H(22)	0.96
C(03)-C(04)	1.477(5)	C(03)-H(31)	0.96
C(03)-H(32)	0.96	C(04)-H(41)	0.96
C(04)-H(42)	0.96	O(2)-C(08)	1.420(5)
O(2)-C(05)	1.425(5)	C(05)-C(06)	1.514(8)
C(05)-H(51)	0.96	C(05)-H(52)	0.96
C(06)-C(07)	1.441(7)	C(06)-H(61)	0.96
C(06)-H(62)	0.96	C(07)-C(08)	1.505(5)
C(07)-H(71)	0.96	C(07)-H(72)	0.96
C(08)-H(81)	0.96	C(08)-H(82)	0.96

C(1)-In-C(2)#1	118.27(11)	C(1)-In-O(2)	94.26(10)
C(2)#1-In-O(2)	93.61(9)	C(1)-In-Cl	119.91(8)
C(2)#1-In-Cl	121.13(8)	O(2)-In-Cl	90.49(9)
C(1)-In-O(1)	87.53(9)	C(2)#1-In-O(1)	87.28(9)
O(2)-In-O(1)	177.33(10)	Cl-In-O(1)	86.90(7)
C(6)-C(1)-C(2)	117.6(3)	C(6)-C(1)-In	121.9(2)
C(2)-C(1)-In	120.5(2)	C(3)-C(2)-C(1)	118.0(3)
C(3)-C(2)-In#1	120.9(2)	C(1)-C(2)-In#1	121.0(2)
F(3)-C(3)-C(2)	120.1(3)	F(3)-C(3)-C(4)	116.9(3)
C(2)-C(3)-C(4)	122.9(3)	F(4)-C(4)-C(5)	119.8(3)
F(4)-C(4)-C(3)	121.2(3)	C(5)-C(4)-C(3)	119.0(3)
F(5)-C(5)-C(4)	119.3(3)	F(5)-C(5)-C(6)	121.3(3)
C(4)-C(5)-C(6)	119.4(3)	F(6)-C(6)-C(5)	116.8(3)
F(6)-C(6)-C(1)	120.2(3)	C(5)-C(6)-C(1)	123.0(3)
C(04)-O(1)-C(01)	107.7(3)	C(04)-O(1)-In	121.3(2)
C(01)-O(1)-In	120.0(2)	O(1)-C(01)-C(02)	104.9(3)
O(1)-C(01)-H(11)	110.7(2)	C(02)-C(01)-H(11)	110.7(2)
O(1)-C(01)-H(12)	110.7(2)	C(02)-C(01)-H(12)	111.0(2)
H(11)-C(01)-H(12)	108.9	C(01)-C(02)-C(03)	103.8(3)
C(01)-C(02)-H(21)	111.1(2)	C(03)-C(02)-H(21)	110.9(3)
C(01)-C(02)-H(22)	110.9(2)	C(03)-C(02)-H(22)	111.1(2)
H(21)-C(02)-H(22)	109.0	C(04)-C(03)-C(02)	104.6(3)
C(04)-C(03)-H(31)	111.3(3)	C(02)-C(03)-H(31)	110.9(2)
C(04)-C(03)-H(32)	110.4(3)	C(02)-C(03)-H(32)	110.7(2)
H(31)-C(03)-H(32)	108.8	O(1)-C(04)-C(03)	108.8(3)
O(1)-C(04)-H(41)	109.9(3)	C(03)-C(04)-H(41)	110.4(3)
O(1)-C(04)-H(42)	109.8(3)	C(03)-C(04)-H(42)	109.5(3)
H(41)-C(04)-H(42)	108.4	C(08)-O(2)-C(05)	108.6(3)
C(08)-O(2)-In	125.0(2)	C(05)-O(2)-In	124.1(3)
O(2)-C(05)-C(06)	105.3(4)	O(2)-C(05)-H(51)	109.3(3)
C(06)-C(05)-H(51)	110.0(4)	O(2)-C(05)-H(52)	112.4(4)
C(06)-C(05)-H(52)	111.0(4)	H(51)-C(05)-H(52)	108.8
C(07)-C(06)-C(05)	101.7(4)	C(07)-C(06)-H(61)	110.1(4)
C(05)-C(06)-H(61)	112.0(5)	C(07)-C(06)-H(62)	112.2(3)
C(05)-C(06)-H(62)	111.5(3)	H(61)-C(06)-H(62)	109.3
C(06)-C(07)-C(08)	102.2(4)	C(06)-C(07)-H(71)	112.4(3)
C(08)-C(07)-H(71)	111.5(2)	C(06)-C(07)-H(72)	110.1(3)
C(08)-C(07)-H(72)	111.3(3)	H(71)-C(07)-H(72)	109.3

O(2)-C(08)-C(07)	104.7(3)	O(2)-C(08)-H(81)	110.6(2)
C(07)-C(08)-H(81)	110.8(3)	O(2)-C(08)-H(82)	111.1(2)
C(07)-C(08)-H(82)	110.7(3)	H(81)-C(08)-H(82)	108.9

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+2

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for MART20.

	x/a	y/b	z/c	U(eq)
H(11)	0.3725(4)	0.0722(4)	0.9714(3)	0.102
H(12)	0.3306(4)	0.1616(4)	0.8918(3)	0.102
H(21)	0.4371(4)	-0.0730(4)	0.8909(3)	0.105
H(22)	0.4755(4)	0.0396(4)	0.8417(3)	0.105
H(31)	0.2863(4)	-0.1181(4)	0.7612(3)	0.107
H(32)	0.2851(4)	0.0145(4)	0.7272(3)	0.107
H(41)	0.0884(4)	0.0471(6)	0.7619(3)	0.169
H(42)	0.0931(4)	-0.0835(6)	0.7993(3)	0.169
H(51)	-0.0659(6)	0.4127(6)	1.0125(6)	0.263
H(52)	-0.0879(6)	0.3599(6)	1.1000(6)	0.263
H(61)	-0.2967(6)	0.4716(4)	0.9628(4)	0.162
H(62)	-0.2773(6)	0.4867(4)	1.0643(4)	0.162
H(71)	-0.4670(5)	0.3497(4)	0.9846(3)	0.122
H(72)	-0.3657(5)	0.3029(4)	1.0736(3)	0.122
H(81)	-0.3345(4)	0.1567(4)	0.9791(3)	0.112
H(82)	-0.3436(4)	0.2493(4)	0.9028(3)	0.112