Supplementary Material (ESI) for Dalton Transactions

The Role of Halogenated Carborane Monoanions in Olefin Hydrogenation Catalysed by Cationic Iridium Phosphine Complexes.

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Electronic Supporting Information.

X-ray structure of $[\{Ir(PPh_3)_2H\}_2(\mu\text{-}H)_3][BAr^F{}_4]$, 4d

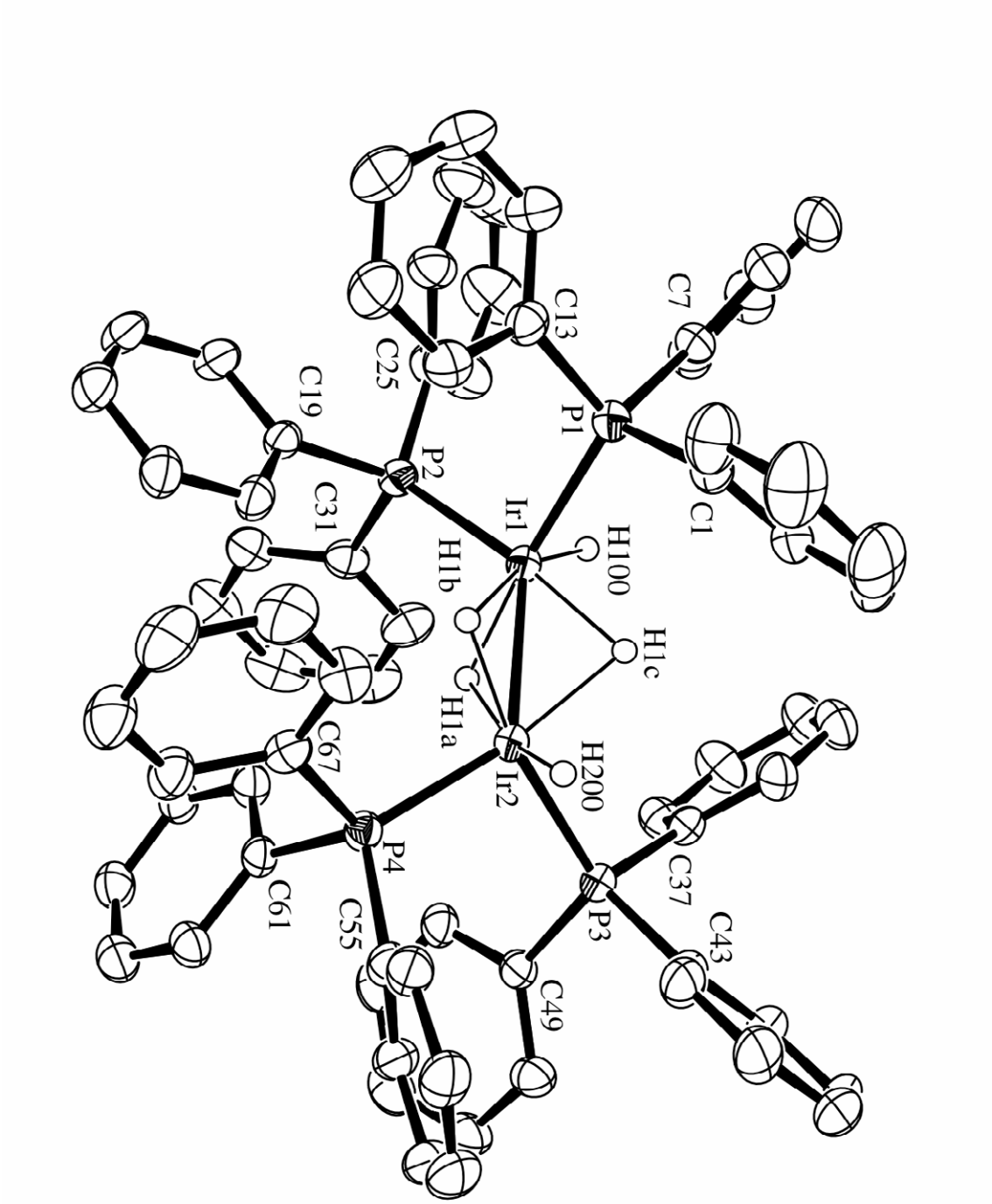

Figure S1. Solid state structure of the cationic portion of **4d**.

Table S2. Crystal data and structure refinement for 4d.

	4d
Empirical formula	$C_{108}H_{85.5}BCl_3F_{24}P_4Ir_2$
M/g mol^{-1}	2464.70
Crystal colour	Pale yellow
Crystal size /mm	0.38 × 0.2 × 0.13
Crystal system	triclinic
Space group	P -1 (no.2)
a /Å	14.0950(1)
b /Å	18.4279(2)
c /Å	22.3514(2)
α /°	67.904(1)
ß /°	81.927(1)
γ/°	80.160(1)
V/Å^3	5281.51(8)
Z	2
D_c /g cm^{-3}	1.549
μ(Mo-K$_\alpha$) /mm^{-1}	2.742
F (000)	2435
2Θ range/°	9-60
Collected data	92810
Unique Data (I>2σI)	30494 (R(int) = 0.0416)
Refined parameter	1384
min./max density /e Å^{-3}	-1.986 / 2.132
R_1 [a] (I>2σI)	0.0442
wR_2 [b] (I>2σI)	0.1158
GOF [cd]	1.053

Table S2. Bond lengths [A] for 4d.

Ir(1)-P(2)	2.2639(11)
Ir(1)-P(1)	2.2827(11)
Ir(1)-Ir(2)	2.5132(2)
Ir(1)-H(1A)	1.71(4)
Ir(1)-H(1B)	1.91(5)
Ir(1)-H(1C)	1.81(6)
Ir(1)-H(100)	1.65(5)
Ir(2)-P(4)	2.2665(10)
Ir(2)-P(3)	2.2873(10)
Ir(2)-H(1A)	1.84(4)
Ir(2)-H(1B)	1.71(5)
Ir(2)-H(1C)	1.88(6)
Ir(2)-H(200)	1.59(6)
P(2)-C(25)	1.823(5)
P(2)-C(19)	1.833(4)
P(2)-C(31)	1.844(5)
P(1)-C(7)	1.822(4)
P(1)-C(13)	1.828(4)
P(1)-C(1)	1.839(5)
P(4)-C(55)	1.814(4)
P(4)-C(61)	1.828(4)
P(4)-C(67)	1.833(4)
P(3)-C(43)	1.824(4)
P(3)-C(37)	1.828(4)
P(3)-C(49)	1.831(4)
C(1)-C(2)	1.387(7)
C(1)-C(6)	1.395(8)
C(2)-C(3)	1.389(7)
C(3)-C(4)	1.380(10)
C(4)-C(5)	1.386(10)
C(5)-C(6)	1.391(8)
C(7)-C(12)	1.378(7)
C(7)-C(8)	1.412(7)
C(8)-C(9)	1.397(7)
C(10)-C(9)	1.373(9)
C(10)-C(11)	1.398(9)
C(11)-C(12)	1.396(7)
C(13)-C(18)	1.390(7)
C(13)-C(14)	1.397(6)
C(14)-C(15)	1.388(7)
C(15)-C(16)	1.391(8)
C(16)-C(17)	1.370(8)
C(17)-C(18)	1.392(7)
C(19)-C(24)	1.395(6)
C(19)-C(20)	1.400(6)
C(20)-C(21)	1.394(6)
C(21)-C(22)	1.393(7)
C(22)-C(23)	1.378(8)
C(23)-C(24)	1.391(7)
C(25)-C(30)	1.392(7)
C(25)-C(26)	1.394(7)
C(26)-C(27)	1.398(7)
C(27)-C(28)	1.370(10)

C(28)-C(29)	1.410(10)
C(29)-C(30)	1.377(8)
C(31)-C(36)	1.383(7)
C(31)-C(32)	1.390(7)
C(32)-C(33)	1.388(7)
C(33)-C(34)	1.392(9)
C(34)-C(35)	1.373(9)
C(35)-C(36)	1.405(8)
C(37)-C(38)	1.385(6)
C(37)-C(42)	1.408(6)
C(38)-C(39)	1.398(7)
C(39)-C(40)	1.386(7)
C(40)-C(41)	1.387(7)
C(41)-C(42)	1.382(6)
C(43)-C(48)	1.387(7)
C(43)-C(44)	1.401(6)
C(44)-C(45)	1.400(7)
C(45)-C(46)	1.388(9)
C(46)-C(47)	1.370(9)
C(47)-C(48)	1.383(6)
C(49)-C(54)	1.391(6)
C(49)-C(50)	1.399(6)
C(50)-C(51)	1.393(7)
C(51)-C(52)	1.366(8)
C(52)-C(53)	1.387(8)
C(53)-C(54)	1.397(6)
C(55)-C(56)	1.393(6)
C(55)-C(60)	1.394(6)
C(56)-C(57)	1.398(6)
C(57)-C(58)	1.372(8)
C(58)-C(59)	1.373(8)
C(59)-C(60)	1.405(6)
C(61)-C(66)	1.389(6)
C(61)-C(62)	1.398(6)
C(62)-C(63)	1.395(6)
C(63)-C(64)	1.395(7)
C(64)-C(65)	1.382(6)
C(65)-C(66)	1.391(6)
C(67)-C(72)	1.384(6)
C(67)-C(68)	1.407(6)
C(68)-C(69)	1.403(7)
C(69)-C(70)	1.378(8)
C(70)-C(71)	1.376(8)
C(71)-C(72)	1.399(7)
B-C(101)	1.611(10)
B-C(111)	1.620(10)
B-C(81)	1.667(8)
B-C(91)	1.667(10)
C(81)-C(82)	1.403(8)
C(81)-C(88)	1.427(8)
C(82)-C(83)	1.386(7)
C(83)-C(85)	1.388(8)
C(83)-C(84)	1.503(8)
C(84)-F(1)	1.331(7)
C(84)-F(3)	1.349(6)
C(84)-F(2)	1.351(7)
C(85)-C(86)	1.391(8)

C(86)-C(88)	1.384(7)
C(86)-C(87)	1.490(8)
C(87)-F(5A)	1.230(15)
C(87)-F(6)	1.255(10)
C(87)-F(4A)	1.315(13)
C(87)-F(4)	1.318(11)
C(87)-F(5)	1.345(10)
C(87)-F(6A)	1.349(13)
C(91)-C(92)	1.387(8)
C(91)-C(98)	1.390(8)
C(92)-C(93)	1.427(9)
C(93)-C(95)	1.372(9)
C(93)-C(94)	1.438(11)
C(94)-F(9)	1.290(12)
C(94)-F(8)	1.315(12)
C(94)-F(7)	1.340(11)
C(95)-C(96)	1.388(9)
C(96)-C(98)	1.403(8)
C(96)-C(97)	1.486(8)
C(97)-F(12)	1.326(8)
C(97)-F(10)	1.359(8)
C(97)-F(11)	1.365(8)
C(101)-C(102)	1.378(10)
C(101)-C(108)	1.459(11)
C(102)-C(103)	1.362(9)
C(103)-C(105)	1.372(12)
C(103)-C(104)	1.512(13)
C(104)-F(13)	1.197(10)
C(104)-F(15)	1.265(14)
C(104)-F(14)	1.270(12)
C(105)-C(106)	1.415(14)
C(106)-C(108)	1.369(11)
C(106)-C(107)	1.414(15)
C(107)-F(17)	1.239(14)
C(107)-F(18)	1.299(17)
C(107)-F(16)	1.39(2)
C(111)-C(118)	1.372(8)
C(111)-C(112)	1.447(9)
C(112)-C(113)	1.399(11)
C(113)-C(115)	1.380(11)
C(113)-C(114)	1.463(11)
C(114)-F(19)	1.224(14)
C(114)-F(20)	1.288(14)
C(114)-F(21)	1.333(16)
C(115)-C(116)	1.389(9)
C(116)-C(118)	1.407(8)
C(116)-C(117)	1.485(9)
C(117)-F(23)	1.327(8)
C(117)-F(24)	1.334(7)
C(117)-F(22)	1.352(9)
C(80)-Cl(2)	1.73(2)
C(80)-Cl(1)	1.82(2)
C(90)-Cl(4)	1.710(16)
C(90)-Cl(3)	1.742(17)
C(100)-Cl(6)	1.769(10)
C(100)-Cl(5)	1.784(10)
C(110)-Cl(7)#1	1.57(3)

C(110)-Cl(7)	1.750(10)
Cl(7)-C(110)#1	1.57(3)
C(120)-C(121)	1.29(13)
C(121)-C(122)	1.41(4)
C(122)-C(122)#2	1.21(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z #2 -x,-y,-z+2

Table S3. Bond angles [deg] for 4d.

P(2)-Ir(1)-P(1)	98.77(4)
P(2)-Ir(1)-Ir(2)	127.95(3)
P(1)-Ir(1)-Ir(2)	122.65(3)
P(2)-Ir(1)-H(1A)	89.9(15)
P(1)-Ir(1)-H(1A)	169.8(15)
Ir(2)-Ir(1)-H(1A)	47.2(15)
P(2)-Ir(1)-H(1B)	109.0(16)
P(1)-Ir(1)-H(1B)	96.5(16)
Ir(2)-Ir(1)-H(1B)	42.8(16)
H(1A)-Ir(1)-H(1B)	76(2)
P(2)-Ir(1)-H(1C)	171.1(18)
P(1)-Ir(1)-H(1C)	89.3(18)
Ir(2)-Ir(1)-H(1C)	48.1(18)
H(1A)-Ir(1)-H(1C)	82(2)
H(1B)-Ir(1)-H(1C)	74(2)
P(2)-Ir(1)-H(100)	84.0(18)
P(1)-Ir(1)-H(100)	90.3(18)
Ir(2)-Ir(1)-H(100)	121.9(18)
H(1A)-Ir(1)-H(100)	96(2)
H(1B)-Ir(1)-H(100)	164(2)
H(1C)-Ir(1)-H(100)	92(3)
P(4)-Ir(2)-P(3)	99.50(4)
P(4)-Ir(2)-Ir(1)	129.25(3)
P(3)-Ir(2)-Ir(1)	120.77(3)
P(4)-Ir(2)-H(1A)	105.8(14)
P(3)-Ir(2)-H(1A)	99.1(14)
Ir(1)-Ir(2)-H(1A)	43.0(14)
P(4)-Ir(2)-H(1B)	92.5(18)
P(3)-Ir(2)-H(1B)	168.0(18)
Ir(1)-Ir(2)-H(1B)	49.3(18)
H(1A)-Ir(2)-H(1B)	77(2)
P(4)-Ir(2)-H(1C)	167.8(17)
P(3)-Ir(2)-H(1C)	91.6(17)
Ir(1)-Ir(2)-H(1C)	45.8(17)
H(1A)-Ir(2)-H(1C)	77(2)
H(1B)-Ir(2)-H(1C)	76(2)
P(4)-Ir(2)-H(200)	83(2)
P(3)-Ir(2)-H(200)	90(2)
Ir(1)-Ir(2)-H(200)	124(2)
H(1A)-Ir(2)-H(200)	167(2)
H(1B)-Ir(2)-H(200)	92(3)
H(1C)-Ir(2)-H(200)	92(3)
C(25)-P(2)-C(19)	104.7(2)
C(25)-P(2)-C(31)	102.9(2)
C(19)-P(2)-C(31)	103.8(2)
C(25)-P(2)-Ir(1)	118.81(16)
C(19)-P(2)-Ir(1)	114.76(14)
C(31)-P(2)-Ir(1)	110.34(15)
C(7)-P(1)-C(13)	106.0(2)
C(7)-P(1)-C(1)	101.5(2)
C(13)-P(1)-C(1)	103.9(2)
C(7)-P(1)-Ir(1)	120.33(16)
C(13)-P(1)-Ir(1)	114.93(14)

C(1)-P(1)-Ir(1)	108.13(15)
C(55)-P(4)-C(61)	105.8(2)
C(55)-P(4)-C(67)	101.72(19)
C(61)-P(4)-C(67)	103.11(19)
C(55)-P(4)-Ir(2)	116.07(14)
C(61)-P(4)-Ir(2)	116.31(13)
C(67)-P(4)-Ir(2)	112.05(14)
C(43)-P(3)-C(37)	101.85(19)
C(43)-P(3)-C(49)	105.6(2)
C(37)-P(3)-C(49)	103.93(19)
C(43)-P(3)-Ir(2)	120.12(16)
C(37)-P(3)-Ir(2)	106.62(13)
C(49)-P(3)-Ir(2)	116.54(13)
C(2)-C(1)-C(6)	118.9(5)
C(2)-C(1)-P(1)	117.6(4)
C(6)-C(1)-P(1)	123.5(4)
C(1)-C(2)-C(3)	120.8(5)
C(4)-C(3)-C(2)	119.9(6)
C(3)-C(4)-C(5)	120.0(5)
C(4)-C(5)-C(6)	120.1(6)
C(5)-C(6)-C(1)	120.2(6)
C(12)-C(7)-C(8)	119.3(4)
C(12)-C(7)-P(1)	122.4(3)
C(8)-C(7)-P(1)	118.2(4)
C(9)-C(8)-C(7)	119.1(5)
C(9)-C(10)-C(11)	119.6(5)
C(12)-C(11)-C(10)	119.7(5)
C(7)-C(12)-C(11)	121.0(5)
C(18)-C(13)-C(14)	118.8(4)
C(18)-C(13)-P(1)	117.7(3)
C(14)-C(13)-P(1)	123.6(4)
C(15)-C(14)-C(13)	120.2(5)
C(14)-C(15)-C(16)	120.3(5)
C(17)-C(16)-C(15)	119.7(5)
C(16)-C(17)-C(18)	120.5(5)
C(13)-C(18)-C(17)	120.5(5)
C(24)-C(19)-C(20)	118.8(4)
C(24)-C(19)-P(2)	122.7(4)
C(20)-C(19)-P(2)	118.5(3)
C(21)-C(20)-C(19)	120.7(4)
C(22)-C(21)-C(20)	119.7(5)
C(23)-C(22)-C(21)	119.8(5)
C(22)-C(23)-C(24)	120.8(5)
C(23)-C(24)-C(19)	120.2(5)
C(30)-C(25)-C(26)	118.6(5)
C(30)-C(25)-P(2)	120.5(4)
C(26)-C(25)-P(2)	120.8(4)
C(25)-C(26)-C(27)	120.8(5)
C(28)-C(27)-C(26)	119.6(6)
C(27)-C(28)-C(29)	120.4(5)
C(30)-C(29)-C(28)	119.2(6)
C(29)-C(30)-C(25)	121.3(6)
C(36)-C(31)-C(32)	119.4(5)
C(36)-C(31)-P(2)	119.7(4)
C(32)-C(31)-P(2)	120.8(4)
C(33)-C(32)-C(31)	120.8(5)
C(32)-C(33)-C(34)	119.4(5)

C(35)-C(34)-C(33)	120.3(5)
C(34)-C(35)-C(36)	120.1(5)
C(31)-C(36)-C(35)	119.9(5)
C(38)-C(37)-C(42)	119.4(4)
C(38)-C(37)-P(3)	122.7(3)
C(42)-C(37)-P(3)	117.4(3)
C(37)-C(38)-C(39)	120.2(4)
C(40)-C(39)-C(38)	120.1(5)
C(39)-C(40)-C(41)	119.9(5)
C(42)-C(41)-C(40)	120.4(5)
C(41)-C(42)-C(37)	120.0(4)
C(48)-C(43)-C(44)	119.2(4)
C(48)-C(43)-P(3)	121.5(3)
C(44)-C(43)-P(3)	119.3(4)
C(45)-C(44)-C(43)	120.1(5)
C(46)-C(45)-C(44)	119.4(5)
C(47)-C(46)-C(45)	120.1(5)
C(46)-C(47)-C(48)	121.1(6)
C(46)-C(47)-H(47)	119.5
C(48)-C(47)-H(47)	119.5
C(47)-C(48)-C(43)	120.1(5)
C(47)-C(48)-H(48)	120.0
C(43)-C(48)-H(48)	120.0
C(54)-C(49)-C(50)	119.7(4)
C(54)-C(49)-P(3)	117.6(3)
C(50)-C(49)-P(3)	122.6(3)
C(51)-C(50)-C(49)	119.1(5)
C(51)-C(50)-H(50)	120.4
C(49)-C(50)-H(50)	120.4
C(52)-C(51)-C(50)	121.1(5)
C(52)-C(51)-H(51)	119.5
C(50)-C(51)-H(51)	119.5
C(51)-C(52)-C(53)	120.4(5)
C(51)-C(52)-H(52)	119.8
C(53)-C(52)-H(52)	119.8
C(52)-C(53)-C(54)	119.5(5)
C(52)-C(53)-H(53)	120.3
C(54)-C(53)-H(53)	120.3
C(49)-C(54)-C(53)	120.2(4)
C(49)-C(54)-H(54)	119.9
C(53)-C(54)-H(54)	119.9
C(56)-C(55)-C(60)	119.4(4)
C(56)-C(55)-P(4)	120.7(3)
C(60)-C(55)-P(4)	119.6(3)
C(55)-C(56)-C(57)	119.8(5)
C(58)-C(57)-C(56)	120.4(5)
C(57)-C(58)-C(59)	120.6(5)
C(58)-C(59)-C(60)	119.9(5)
C(55)-C(60)-C(59)	119.9(5)
C(66)-C(61)-C(62)	118.9(4)
C(66)-C(61)-P(4)	118.3(3)
C(62)-C(61)-P(4)	122.8(3)
C(63)-C(62)-C(61)	120.5(4)
C(64)-C(63)-C(62)	119.6(4)
C(65)-C(64)-C(63)	120.1(4)
C(64)-C(65)-C(66)	120.1(4)
C(61)-C(66)-C(65)	120.7(4)

C(72)-C(67)-C(68)	119.4(4)
C(72)-C(67)-P(4)	120.9(3)
C(68)-C(67)-P(4)	119.5(3)
C(69)-C(68)-C(67)	118.9(5)
C(70)-C(69)-C(68)	120.8(5)
C(71)-C(70)-C(69)	120.4(5)
C(70)-C(71)-C(72)	119.6(5)
C(67)-C(72)-C(71)	120.8(5)
C(101)-B-C(111)	107.6(5)
C(101)-B-C(81)	110.1(5)
C(111)-B-C(81)	114.5(5)
C(101)-B-C(91)	110.9(6)
C(111)-B-C(91)	108.3(5)
C(81)-B-C(91)	105.4(5)
C(82)-C(81)-C(88)	115.1(5)
C(82)-C(81)-B	122.7(5)
C(88)-C(81)-B	121.9(5)
C(83)-C(82)-C(81)	122.1(5)
C(82)-C(83)-C(85)	121.8(5)
C(82)-C(83)-C(84)	120.5(5)
C(85)-C(83)-C(84)	117.7(5)
F(1)-C(84)-F(3)	107.1(5)
F(1)-C(84)-F(2)	106.7(5)
F(3)-C(84)-F(2)	105.1(5)
F(1)-C(84)-C(83)	112.7(5)
F(3)-C(84)-C(83)	112.4(5)
F(2)-C(84)-C(83)	112.3(5)
C(83)-C(85)-C(86)	117.8(5)
C(88)-C(86)-C(85)	120.8(5)
C(88)-C(86)-C(87)	120.2(5)
C(85)-C(86)-C(87)	119.0(5)
F(5A)-C(87)-F(6)	125.3(11)
F(5A)-C(87)-F(4A)	100.8(17)
F(6)-C(87)-F(4A)	44.2(9)
F(5A)-C(87)-F(4)	37.8(17)
F(6)-C(87)-F(4)	106.4(10)
F(4A)-C(87)-F(4)	67.7(12)
F(5A)-C(87)-F(5)	67.6(17)
F(6)-C(87)-F(5)	106.4(10)
F(4A)-C(87)-F(5)	135.8(9)
F(4)-C(87)-F(5)	104.2(9)
F(5A)-C(87)-F(6A)	113.7(16)
F(6)-C(87)-F(6A)	53.1(12)
F(4A)-C(87)-F(6A)	95.5(15)
F(4)-C(87)-F(6A)	132.7(10)
F(5)-C(87)-F(6A)	56.8(12)
F(5A)-C(87)-C(86)	117.3(9)
F(6)-C(87)-C(86)	115.1(7)
F(4A)-C(87)-C(86)	111.9(7)
F(4)-C(87)-C(86)	112.9(8)
F(5)-C(87)-C(86)	111.1(6)
F(6A)-C(87)-C(86)	114.4(7)
C(86)-C(88)-C(81)	122.4(5)
C(10)-C(9)-C(8)	121.3(5)
C(92)-C(91)-C(98)	116.6(6)
C(92)-C(91)-B	121.5(5)
C(98)-C(91)-B	121.9(5)

C(91)-C(92)-C(93)	121.9(6)
C(95)-C(93)-C(92)	119.7(6)
C(95)-C(93)-C(94)	122.4(7)
C(92)-C(93)-C(94)	117.8(7)
F(9)-C(94)-F(8)	105.1(10)
F(9)-C(94)-F(7)	96.2(8)
F(8)-C(94)-F(7)	105.9(9)
F(9)-C(94)-C(93)	118.1(8)
F(8)-C(94)-C(93)	113.4(9)
F(7)-C(94)-C(93)	116.1(8)
C(93)-C(95)-C(96)	119.2(6)
C(95)-C(96)-C(98)	120.2(5)
C(95)-C(96)-C(97)	118.1(6)
C(98)-C(96)-C(97)	121.6(6)
F(12)-C(97)-F(10)	104.8(5)
F(12)-C(97)-F(11)	108.7(6)
F(10)-C(97)-F(11)	104.0(5)
F(12)-C(97)-C(96)	113.6(6)
F(10)-C(97)-C(96)	111.9(5)
F(11)-C(97)-C(96)	113.2(6)
C(91)-C(98)-C(96)	122.1(6)
C(102)-C(101)-C(108)	112.5(7)
C(102)-C(101)-B	128.6(6)
C(108)-C(101)-B	118.7(7)
C(103)-C(102)-C(101)	126.1(7)
C(102)-C(103)-C(105)	120.4(8)
C(102)-C(103)-C(104)	119.4(7)
C(105)-C(103)-C(104)	120.1(7)
F(13)-C(104)-F(15)	95.8(11)
F(13)-C(104)-F(14)	118.4(12)
F(15)-C(104)-F(14)	100.9(11)
F(13)-C(104)-C(103)	119.7(7)
F(15)-C(104)-C(103)	106.4(12)
F(14)-C(104)-C(103)	111.4(8)
C(103)-C(105)-C(106)	117.8(8)
C(108)-C(106)-C(107)	123.0(11)
C(108)-C(106)-C(105)	120.5(8)
C(107)-C(106)-C(105)	116.3(10)
F(17)-C(107)-F(18)	109.1(13)
F(17)-C(107)-F(16)	94.1(13)
F(18)-C(107)-F(16)	99.4(17)
F(17)-C(107)-C(106)	120.9(15)
F(18)-C(107)-C(106)	119.2(11)
F(16)-C(107)-C(106)	108.5(14)
C(106)-C(108)-C(101)	122.5(9)
C(118)-C(111)-C(112)	113.5(6)
C(118)-C(111)-B	121.4(6)
C(112)-C(111)-B	124.6(6)
C(113)-C(112)-C(111)	122.6(6)
C(115)-C(113)-C(112)	121.0(6)
C(115)-C(113)-C(114)	119.9(8)
C(112)-C(113)-C(114)	119.1(8)
F(19)-C(114)-F(20)	101.3(15)
F(19)-C(114)-F(21)	109.6(12)
F(20)-C(114)-F(21)	102.5(12)
F(19)-C(114)-C(113)	118.1(10)
F(20)-C(114)-C(113)	114.0(9)

F(21)-C(114)-C(113)	110.0(12)
C(113)-C(115)-C(116)	117.9(7)
C(115)-C(116)-C(118)	120.5(6)
C(115)-C(116)-C(117)	119.8(6)
C(118)-C(116)-C(117)	119.7(5)
F(23)-C(117)-F(24)	106.6(6)
F(23)-C(117)-F(22)	106.8(6)
F(24)-C(117)-F(22)	105.6(6)
F(23)-C(117)-C(116)	113.4(6)
F(24)-C(117)-C(116)	114.5(5)
F(22)-C(117)-C(116)	109.4(6)
C(111)-C(118)-C(116)	124.3(5)
Cl(2)-C(80)-Cl(1)	114.9(9)
Cl(4)-C(90)-Cl(3)	118.8(14)
Cl(6)-C(100)-Cl(5)	98.0(9)
Cl(7)#1-C(110)-Cl(7)	130.4(13)
C(110)#1-Cl(7)-C(110)	49.6(13)
C(120)-C(121)-C(122)	133(4)
C(122)#2-C(122)-C(121)	133(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z #2 -x,-y,-z+2