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C(63)-C(62)-F(62)	120.5(7)
C(63)-C(62)-C(61)	120.4(7)
F(62)-C(62)-C(61)	119.1(7)
F(63)-C(63)-C(62)	120.0(8)
F(63)-C(63)-C(64)	120.7(7)
C(62)-C(63)-C(64)	119.3(7)
F(65)-C(64)-C(65)	122.6(7)
F(65)-C(64)-C(63)	119.6(7)
C(65)-C(64)-C(63)	117.8(7)
F(65)-C(65)-C(64)	114.8(6)
F(65)-C(65)-C(66)	117.8(6)
C(64)-C(65)-C(66)	127.4(6)
C(65)-C(66)-C(61)	111.9(6)
C(65)-C(66)-B	120.9(5)
C(61)-C(66)-B	127.1(6)
C(76)-C(71)-C(72)	123.6(8)
C(73)-C(72)-C(71)	118.3(8)
C(72)-C(73)-C(74)	120.3(8)
C(75)-C(74)-C(73)	120.0(8)
C(74)-C(75)-C(76)	121.7(8)
C(71)-C(76)-C(75)	116.1(7)
C(71)-C(76)-Zr	94.5(5)
C(75)-C(76)-Zr	149.3(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.0-3b
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr	64(1)	47(1)	61(1)	-3(1)	-1(1)	0(1)
B	49(4)	51(4)	54(4)	5(3)	1(3)	1(3)
F(41)	79(3)	68(3)	118(3)	0(2)	30(3)	10(2)
F(42)	107(4)	85(3)	137(4)	1(3)	30(3)	42(3)
F(43)	169(5)	53(3)	103(3)	-5(2)	5(3)	23(3)
F(44)	137(4)	55(2)	110(3)	2(2)	-2(3)	-28(3)
F(45)	82(3)	65(2)	80(3)	3(2)	2(2)	-11(2)
F(51)	97(3)	56(2)	69(3)	9(2)	-5(2)	9(2)
F(52)	100(3)	72(3)	107(3)	-19(2)	-7(3)	30(2)
F(53)	119(4)	132(4)	87(3)	-24(3)	28(3)	36(3)
F(54)	132(4)	119(4)	59(3)	15(3)	23(3)	13(3)
F(55)	101(3)	63(2)	60(2)	10(2)	4(2)	15(2)
F(61)	101(3)	74(3)	71(3)	21(2)	-11(2)	-17(2)
F(62)	129(4)	79(3)	96(3)	8(3)	19(3)	-41(3)
F(63)	103(4)	125(4)	122(4)	-26(3)	9(3)	-55(3)
F(65)	89(3)	76(3)	82(3)	11(2)	-17(2)	-4(2)
F(65)	89(3)	123(4)	109(4)	-5(3)	-32(3)	-12(3)
C(1)	67(5)	66(4)	56(4)	-1(3)	1(3)	-4(4)
C(2)	72(5)	55(4)	63(4)	0(3)	11(4)	-13(4)
C(3)	94(6)	40(3)	60(4)	4(3)	-3(4)	-9(4)
C(4)	70(5)	50(4)	53(4)	5(3)	-7(3)	5(3)
C(5)	56(4)	60(4)	47(4)	-1(3)	-1(3)	1(3)
C(6)	63(4)	57(4)	49(4)	4(3)	0(3)	3(3)
C(11)	68(5)	106(6)	62(4)	-3(4)	10(4)	8(4)
C(12)	72(5)	93(6)	92(6)	-2(5)	7(4)	-22(4)
C(13)	115(6)	55(4)	79(5)	-15(4)	-4(5)	-12(4)
C(14)	84(5)	65(5)	79(5)	-5(4)	7(4)	22(4)
C(21)	84(5)	62(4)	74(5)	13(4)	0(4)	15(4)
C(22)	72(5)	58(4)	71(5)	-5(4)	-11(4)	12(4)
C(23)	75(5)	68(5)	70(5)	-6(4)	-10(4)	23(4)
C(24)	95(6)	53(4)	82(5)	-17(4)	-19(5)	20(4)
C(25)	87(6)	41(4)	115(7)	9(4)	-24(5)	2(4)
C(31)	132(8)	118(7)	105(7)	51(6)	6(6)	18(6)
C(32)	96(6)	93(6)	92(6)	-24(5)	-29(5)	5(5)
C(33)	81(6)	127(8)	110(7)	1(6)	21(5)	36(5)
C(34)	157(9)	98(6)	109(7)	-54(6)	-50(6)	55(6)
C(35)	125(8)	57(5)	218(12)	15(6)	-47(8)	-30(5)
C(41)	65(5)	60(4)	67(5)	3(3)	5(4)	3(4)
C(42)	96(6)	54(5)	71(5)	-2(4)	6(4)	20(5)
C(43)	128(8)	38(4)	75(5)	-6(3)	-4(5)	20(5)
C(44)	112(7)	48(4)	59(4)	-6(3)	-4(4)	-10(5)
C(45)	72(5)	61(5)	53(4)	-7(3)	4(3)	5(4)
C(46)	60(4)	53(4)	51(4)	1(3)	-1(3)	3(4)
C(51)	65(4)	55(4)	59(4)	0(4)	-4(3)	2(3)
C(52)	73(5)	58(4)	70(5)	-15(4)	-5(4)	19(4)
C(53)	70(5)	90(6)	64(5)	-23(5)	4(4)	11(4)
C(54)	79(5)	84(5)	49(4)	2(4)	12(4)	9(4)
C(55)	65(4)	56(4)	58(4)	-2(3)	-5(3)	6(3)
C(56)	51(4)	48(4)	49(4)	2(3)	-4(3)	3(3)
C(61)	66(4)	59(4)	59(4)	0(4)	8(4)	-5(4)

C(62)	91(6)	58(4)	72(5)	-7(4)	18(4)	-16(4)
C(63)	72(5)	83(5)	76(5)	-25(5)	13(4)	-27(5)
C(64)	67(5)	82(5)	72(5)	-12(4)	-6(4)	-7(4)
C(65)	72(5)	53(4)	68(5)	8(4)	6(4)	0(4)
C(66)	59(4)	48(4)	51(4)	-6(3)	-1(3)	5(3)
C(71)	91(6)	75(5)	62(4)	9(4)	5(4)	-1(5)
C(72)	81(6)	116(7)	91(6)	16(6)	-5(5)	-20(5)
C(73)	93(7)	154(9)	83(7)	14(6)	24(5)	-1(7)
C(74)	122(8)	110(7)	77(6)	-18(5)	23(6)	9(6)
C(75)	88(6)	79(5)	79(5)	-9(4)	8(5)	2(4)
C(76)	75(5)	59(4)	79(5)	10(4)	2(4)	5(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ~~1~~. O-3b

	x	y	z	U(eq)
H(6A)	9503(6)	8967(3)	2765(3)	68
H(6B)	10643(6)	8578(3)	2458(3)	68
H(11A)	7630(7)	8580(4)	3405(3)	118
H(11B)	6597(7)	7973(4)	3392(3)	118
H(11C)	6286(7)	8636(4)	2977(3)	118
H(12A)	5065(7)	7611(4)	2331(4)	129
H(12B)	5517(7)	6865(4)	2151(4)	129
H(12C)	5202(7)	7421(4)	1618(4)	129
H(13A)	8574(8)	6642(3)	1069(3)	126
H(13B)	7141(8)	6942(3)	904(3)	126
H(13C)	7365(8)	6347(3)	1407(3)	126
H(14A)	11289(7)	7527(4)	2078(3)	114
H(14B)	10653(7)	7395(4)	1386(3)	114
H(14C)	10686(7)	6800(4)	1891(3)	114
H(31A)	8522(10)	9884(5)	175(4)	178
H(31B)	7043(10)	9801(5)	-109(4)	178
H(31C)	7961(10)	9148(5)	-10(4)	178
H(32A)	4647(8)	8457(4)	729(4)	143
H(32B)	5861(8)	8331(4)	324(4)	143
H(32C)	4927(8)	8971(4)	180(4)	143
H(33A)	4193(8)	8742(5)	1652(4)	158
H(33B)	4172(8)	9480(5)	1960(4)	158
H(33C)	4916(8)	8870(5)	2328(4)	158
H(34A)	6326(10)	9905(4)	2741(4)	187
H(34B)	6793(10)	10579(4)	2409(4)	187
H(34C)	7850(10)	10052(4)	2709(4)	187
H(35A)	9330(9)	10392(4)	1018(5)	205
H(35B)	9573(9)	10268(4)	1752(5)	205
H(35C)	8580(9)	10846(4)	1490(5)	205
H(71A)	10313(8)	8984(4)	1337(3)	91
H(72A)	12186(9)	8945(5)	782(4)	116
H(73A)	12149(10)	8280(6)	-133(4)	131
H(74A)	10275(11)	7646(5)	-461(4)	122
H(75A)	8404(8)	7713(4)	92(4)	98

Table 1. Crystal data and structure refinement for 1. y-3b

Identification code	wp003
Empirical formula	C47 H41 B F15 Zr
Formula weight	992.83
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.3399(2) A alpha = 95.604(1) deg b = 13.7300(2) A beta = 102.559(1) de c = 16.6497(2) A gamma = 101.829(1) de
Volume, Z	2448.95(6) A^3, 2
Density (calculated)	1.346 Mg/m^3
Absorption coefficient	0.312 mm^-1
F(000)	1006
Crystal size	0.10 x 0.10 x 0.10 mm
Theta range for data collection	1.27 to 22.50 deg.
Limiting indices	-14<=h<=14, -18<=k<=13, -21<=l<=18
Reflections collected	10032
Independent reflections	6142 [R(int) = 0.0321]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5978 / 4 / 562
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0577, wR2 = 0.1642
R indices (all data)	R1 = 0.0824, wR2 = 0.1899
Largest diff. peak and hole	0.765 and -0.356 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr	2189(1)	2176(1)	-1278(1)	42(1)
B	2601(6)	-835(5)	-2407(4)	43(2)
C(1)	2598(5)	947(4)	-289(3)	44(1)
C(2)	1611(5)	1348(4)	-70(3)	45(1)
C(3)	551(5)	1017(4)	-744(4)	45(1)
C(4)	877(5)	463(4)	-1400(3)	41(1)
C(5)	2157(5)	409(4)	-1119(3)	38(1)
C(6)	3033(5)	7(4)	-1555(3)	47(1)
C(11)	3777(6)	883(5)	320(4)	59(2)
C(12)	1613(7)	1876(5)	765(4)	63(2)
C(13)	-754(6)	1090(5)	-718(4)	61(2)
C(14)	-45(5)	-10(4)	-2210(4)	50(2)
C(21)	3200(6)	3984(5)	-574(4)	61(2)
C(22)	3108(6)	3989(5)	-1445(5)	65(2)
C(23)	3880(7)	3395(5)	-1684(4)	66(2)
C(24)	4461(6)	3016(5)	-966(4)	59(2)
C(25)	4059(6)	3394(4)	-281(4)	56(2)
C(31)	2677(8)	4651(5)	-22(5)	91(3)
C(32)	2427(8)	4619(6)	-1998(6)	103(3)
C(33)	4157(8)	3281(7)	-2528(5)	108(3)
C(34)	5519(6)	2478(6)	-921(5)	86(2)
C(35)	4652(7)	3413(5)	624(4)	79(2)
C(41)	393(6)	-2252(4)	-2795(4)	58(2)
C(42)	-456(7)	-3052(5)	-2619(6)	79(2)
C(43)	-152(10)	-3419(6)	-1883(8)	90(3)
C(44)	992(10)	-3019(6)	-1336(6)	85(2)
C(45)	1794(7)	-2224(5)	-1540(5)	64(2)
C(46)	1551(5)	-1808(4)	-2276(4)	48(1)
C(51)	4109(6)	-2141(5)	-2599(4)	59(2)
C(52)	5195(8)	-2381(6)	-2726(5)	71(2)
C(53)	6122(7)	-1654(7)	-2797(4)	76(2)
C(54)	6004(6)	-663(6)	-2742(4)	71(2)
C(55)	4909(5)	-460(5)	-2616(4)	56(2)
C(56)	3911(5)	-1179(5)	-2535(3)	48(2)
C(61)	1972(6)	-902(5)	-4056(4)	57(2)
C(62)	1669(7)	-564(6)	-4803(4)	70(2)
C(63)	1568(6)	418(6)	-4813(4)	70(2)
C(64)	1754(6)	1038(5)	-4061(4)	61(2)
C(65)	2055(5)	634(4)	-3332(4)	49(2)
C(66)	2154(5)	-348(4)	-3275(3)	45(1)
C(71)	64(7)	2595(5)	-2413(6)	78(2)
C(72)	-995(9)	2873(6)	-2825(6)	104(3)
C(73)	-1615(8)	3379(7)	-2362(8)	105(3)
C(74)	-1202(8)	3603(6)	-1538(7)	86(2)
C(75)	-173(7)	3316(5)	-1133(5)	77(2)
C(76)	504(6)	2798(5)	-1568(5)	65(2)
F(41)	-25(3)	-1933(3)	-3520(3)	75(1)
F(42)	-1571(4)	-3434(3)	-3159(4)	123(2)
F(43)	-991(6)	-4165(3)	-1695(4)	141(2)
F(44)	1306(6)	-3384(4)	-617(3)	125(2)

F(45)	2914(4)	-1918(3)	-983(3)	89(1)
F(51)	3210(4)	-2951(3)	-2561(3)	82(1)
F(52)	5319(5)	-3330(4)	-2766(3)	108(2)
F(53)	7201(4)	-1847(4)	-2928(3)	113(2)
F(54)	6929(4)	101(4)	-2827(3)	102(2)
F(55)	4851(3)	527(3)	-2593(3)	73(1)
F(61)	2062(4)	-1876(3)	-4103(2)	76(1)
F(62)	1479(5)	-1159(4)	-5531(2)	106(2)
F(63)	1290(5)	780(4)	-5534(3)	106(2)
F(64)	1645(4)	1996(3)	-4044(3)	84(1)
F(65)	2230(3)	1337(2)	-2611(2)	59(1)
C(91)	4948(25)	-2643(22)	-5284(17)	321(13)
C(92)	4792(23)	-1612(16)	-5308(15)	280(10)
C(93)	5028(21)	-523(8)	-5028(14)	234(8)

Table 3. Bond lengths [A] and angles [deg] for 4-36

Zr-C(76)	2.227(6)
Zr-F(65)	2.414(3)
Zr-C(5)	2.461(5)
Zr-C(4)	2.476(5)
Zr-C(1)	2.511(5)
Zr-C(24)	2.514(6)
Zr-C(23)	2.531(6)
Zr-C(2)	2.546(5)
Zr-C(25)	2.554(6)
Zr-C(21)	2.555(6)
Zr-C(3)	2.560(5)
Zr-C(22)	2.560(6)
B-C(6)	1.654(8)
B-C(46)	1.664(9)
B-C(66)	1.674(8)
B-C(56)	1.698(8)
C(1)-C(5)	1.433(8)
C(1)-C(2)	1.441(8)
C(1)-C(11)	1.517(8)
C(2)-C(3)	1.415(8)
C(2)-C(12)	1.503(8)
C(3)-C(4)	1.428(8)
C(3)-C(13)	1.513(8)
C(4)-C(5)	1.445(7)
C(4)-C(14)	1.506(7)
C(5)-C(6)	1.508(8)
C(21)-C(25)	1.426(9)
C(21)-C(22)	1.432(9)
C(21)-C(31)	1.527(10)
C(22)-C(23)	1.404(10)
C(22)-C(32)	1.521(10)
C(23)-C(24)	1.434(9)
C(23)-C(33)	1.505(10)
C(24)-C(25)	1.409(9)
C(24)-C(34)	1.525(9)
C(25)-C(35)	1.506(9)
C(41)-F(41)	1.347(7)
C(41)-C(46)	1.385(8)
C(41)-C(42)	1.403(10)
C(42)-F(42)	1.350(9)
C(42)-C(43)	1.373(12)
C(43)-F(43)	1.358(9)
C(43)-C(44)	1.382(12)
C(44)-F(44)	1.347(9)
C(44)-C(45)	1.391(11)
C(45)-F(45)	1.358(8)
C(45)-C(46)	1.399(9)
C(51)-F(51)	1.362(8)
C(51)-C(56)	1.382(8)
C(51)-C(52)	1.391(9)
C(52)-C(53)	1.328(11)
C(52)-F(52)	1.336(8)
C(53)-F(53)	1.361(8)
C(53)-C(54)	1.390(10)
C(54)-F(54)	1.365(8)
C(54)-C(55)	1.380(9)

C(55)-F(55)	1.368(7)
C(55)-C(56)	1.381(8)
C(61)-F(61)	1.358(7)
C(61)-C(62)	1.368(9)
C(61)-C(66)	1.392(8)
C(62)-F(62)	1.343(8)
C(62)-C(63)	1.378(10)
C(63)-F(63)	1.344(8)
C(63)-C(64)	1.393(10)
C(64)-F(64)	1.344(7)
C(64)-C(65)	1.388(8)
C(65)-C(66)	1.387(8)
C(65)-F(65)	1.415(7)
C(71)-C(76)	1.367(10)
C(71)-C(72)	1.393(11)
C(72)-C(73)	1.380(13)
C(73)-C(74)	1.332(12)
C(74)-C(75)	1.367(11)
C(75)-C(76)	1.409(10)
C(91)-C(92)	1.47(2)
C(92)-C(93)	1.47(2)
C(93)-C(93)#1	1.45(2)

C(76)-Zr-F(65)	103.4(2)
C(76)-Zr-C(5)	124.5(2)
F(65)-Zr-C(5)	73.28(14)
C(76)-Zr-C(4)	90.7(2)
F(65)-Zr-C(4)	75.3(2)
C(5)-Zr-C(4)	34.0(2)
C(76)-Zr-C(1)	126.8(2)
F(65)-Zr-C(1)	104.7(2)
C(5)-Zr-C(1)	33.5(2)
C(4)-Zr-C(1)	55.1(2)
C(76)-Zr-C(24)	131.3(2)
F(65)-Zr-C(24)	92.1(2)
C(5)-Zr-C(24)	104.1(2)
C(4)-Zr-C(24)	138.1(2)
C(1)-Zr-C(24)	91.7(2)
C(76)-Zr-C(23)	105.8(2)
F(65)-Zr-C(23)	77.5(2)
C(5)-Zr-C(23)	126.0(2)
C(4)-Zr-C(23)	150.8(2)
C(1)-Zr-C(23)	123.9(2)
C(24)-Zr-C(23)	33.0(2)
C(76)-Zr-C(2)	94.8(2)
F(65)-Zr-C(2)	126.82(14)
C(5)-Zr-C(2)	55.6(2)
C(4)-Zr-C(2)	54.7(2)
C(1)-Zr-C(2)	33.1(2)
C(24)-Zr-C(2)	112.2(2)
C(23)-Zr-C(2)	143.6(2)
C(76)-Zr-C(25)	113.7(2)
F(65)-Zr-C(25)	124.3(2)
C(5)-Zr-C(25)	112.3(2)
C(4)-Zr-C(25)	140.1(2)
C(1)-Zr-C(25)	85.1(2)
C(24)-Zr-C(25)	32.3(2)
C(23)-Zr-C(25)	53.8(2)
C(2)-Zr-C(25)	90.6(2)
C(76)-Zr-C(21)	82.4(2)

F(65)-Zr-C(21)	129.8(2)
C(5)-Zr-C(21)	142.8(2)
C(4)-Zr-C(21)	154.9(2)
C(1)-Zr-C(21)	111.0(2)
C(24)-Zr-C(21)	53.7(2)
C(23)-Zr-C(21)	53.6(2)
C(2)-Zr-C(21)	101.6(2)
C(25)-Zr-C(21)	32.4(2)
C(76)-Zr-C(3)	74.9(2)
F(65)-Zr-C(3)	106.9(2)
C(5)-Zr-C(3)	55.2(2)
C(4)-Zr-C(3)	32.9(2)
C(1)-Zr-C(3)	54.1(2)
C(24)-Zr-C(3)	143.7(2)
C(23)-Zr-C(3)	175.3(2)
C(2)-Zr-C(3)	32.2(2)
C(25)-Zr-C(3)	121.6(2)
C(21)-Zr-C(3)	122.4(2)
C(76)-Zr-C(22)	77.9(2)
F(65)-Zr-C(22)	99.0(2)
C(5)-Zr-C(22)	157.1(2)
C(4)-Zr-C(22)	165.8(2)
C(1)-Zr-C(22)	138.9(2)
C(24)-Zr-C(22)	53.9(2)
C(23)-Zr-C(22)	32.0(2)
C(2)-Zr-C(22)	133.8(2)
C(25)-Zr-C(22)	53.8(2)
C(21)-Zr-C(22)	32.5(2)
C(3)-Zr-C(22)	145.9(2)
C(6)-B-C(46)	109.0(5)
C(6)-B-C(66)	113.2(5)
C(46)-B-C(66)	114.0(4)
C(6)-B-C(56)	106.0(4)
C(46)-B-C(56)	111.5(4)
C(66)-B-C(56)	102.7(4)
C(5)-C(1)-C(2)	108.7(5)
C(5)-C(1)-C(11)	124.7(5)
C(2)-C(1)-C(11)	125.1(5)
C(5)-C(1)-Zr	71.3(3)
C(2)-C(1)-Zr	74.8(3)
C(11)-C(1)-Zr	131.2(4)
C(3)-C(2)-C(1)	107.6(5)
C(3)-C(2)-C(12)	124.6(5)
C(1)-C(2)-C(12)	127.1(5)
C(3)-C(2)-Zr	74.4(3)
C(1)-C(2)-Zr	72.1(3)
C(12)-C(2)-Zr	126.5(4)
C(2)-C(3)-C(4)	108.7(5)
C(2)-C(3)-C(13)	125.3(5)
C(4)-C(3)-C(13)	125.3(5)
C(2)-C(3)-Zr	73.4(3)
C(4)-C(3)-Zr	70.3(3)
C(13)-C(3)-Zr	129.9(4)
C(3)-C(4)-C(5)	108.3(5)
C(3)-C(4)-C(14)	122.5(5)
C(5)-C(4)-C(14)	129.1(5)
C(3)-C(4)-Zr	76.8(3)
C(5)-C(4)-Zr	72.4(3)
C(14)-C(4)-Zr	119.8(4)
C(1)-C(5)-C(4)	106.7(5)

C(1)-C(5)-C(6)	120.6(5)
C(4)-C(5)-C(6)	132.4(5)
C(1)-C(5)-Zr	75.2(3)
C(4)-C(5)-Zr	73.6(3)
C(6)-C(5)-Zr	111.9(3)
C(5)-C(6)-B	125.0(5)
C(25)-C(21)-C(22)	108.0(6)
C(25)-C(21)-C(31)	125.1(7)
C(22)-C(21)-C(31)	125.9(7)
C(25)-C(21)-Zr	73.7(3)
C(22)-C(21)-Zr	73.9(3)
C(31)-C(21)-Zr	127.0(5)
C(23)-C(22)-C(21)	107.8(6)
C(23)-C(22)-C(32)	125.1(7)
C(21)-C(22)-C(32)	126.7(7)
C(23)-C(22)-Zr	72.8(4)
C(21)-C(22)-Zr	73.5(3)
C(32)-C(22)-Zr	124.8(4)
C(22)-C(23)-C(24)	108.3(6)
C(22)-C(23)-C(33)	125.3(7)
C(24)-C(23)-C(33)	126.1(8)
C(22)-C(23)-Zr	75.1(4)
C(24)-C(23)-Zr	72.8(3)
C(33)-C(23)-Zr	123.4(5)
C(25)-C(24)-C(23)	108.1(6)
C(25)-C(24)-C(34)	125.7(6)
C(23)-C(24)-C(34)	125.1(7)
C(25)-C(24)-Zr	75.4(3)
C(23)-C(24)-Zr	74.1(4)
C(34)-C(24)-Zr	125.7(4)
C(24)-C(25)-C(21)	107.8(6)
C(24)-C(25)-C(35)	126.4(6)
C(21)-C(25)-C(35)	124.1(6)
C(24)-C(25)-Zr	72.3(3)
C(21)-C(25)-Zr	73.8(3)
C(35)-C(25)-Zr	131.3(4)
F(41)-C(41)-C(46)	122.0(6)
F(41)-C(41)-C(42)	113.7(6)
C(46)-C(41)-C(42)	124.2(7)
F(42)-C(42)-C(43)	120.6(8)
F(42)-C(42)-C(41)	120.2(8)
C(43)-C(42)-C(41)	119.1(7)
F(43)-C(43)-C(42)	119.4(10)
F(43)-C(43)-C(44)	120.7(10)
C(42)-C(43)-C(44)	119.9(7)
F(44)-C(44)-C(43)	120.4(9)
F(44)-C(44)-C(45)	121.2(9)
C(43)-C(44)-C(45)	118.4(8)
F(45)-C(45)-C(44)	113.8(7)
F(45)-C(45)-C(46)	121.0(6)
C(44)-C(45)-C(46)	125.0(8)
C(41)-C(46)-C(45)	113.3(6)
C(41)-C(46)-B	128.1(5)
C(45)-C(46)-B	118.6(5)
F(51)-C(51)-C(56)	121.3(6)
F(51)-C(51)-C(52)	114.1(6)
C(56)-C(51)-C(52)	124.5(7)
C(53)-C(52)-F(52)	119.9(7)
C(53)-C(52)-C(51)	119.4(7)
F(52)-C(52)-C(51)	120.7(8)

C(52)-C(53)-F(53)	121.9(8)
C(52)-C(53)-C(54)	120.0(6)
F(53)-C(53)-C(54)	118.2(8)
F(54)-C(54)-C(55)	119.8(7)
F(54)-C(54)-C(53)	121.5(6)
C(55)-C(54)-C(53)	118.6(7)
F(55)-C(55)-C(54)	115.1(6)
F(55)-C(55)-C(56)	120.6(5)
C(54)-C(55)-C(56)	124.4(7)
C(55)-C(56)-C(51)	113.1(6)
C(55)-C(56)-B	119.7(5)
C(51)-C(56)-B	127.1(5)
F(61)-C(61)-C(62)	115.4(6)
F(61)-C(61)-C(66)	118.7(5)
C(62)-C(61)-C(66)	125.8(6)
F(62)-C(62)-C(61)	122.0(7)
F(62)-C(62)-C(63)	118.7(6)
C(61)-C(62)-C(63)	119.4(6)
F(63)-C(63)-C(62)	121.0(7)
F(63)-C(63)-C(64)	119.9(7)
C(62)-C(63)-C(64)	119.1(6)
F(64)-C(64)-C(65)	121.2(6)
F(64)-C(64)-C(63)	121.0(6)
C(65)-C(64)-C(63)	117.9(6)
C(66)-C(65)-C(64)	126.1(6)
C(66)-C(65)-F(65)	121.2(5)
C(64)-C(65)-F(65)	112.6(5)
C(65)-C(66)-C(61)	111.7(5)
C(65)-C(66)-B	127.1(5)
C(61)-C(66)-B	120.8(5)
C(76)-C(71)-C(72)	122.4(8)
C(73)-C(72)-C(71)	118.6(9)
C(74)-C(73)-C(72)	120.6(8)
C(73)-C(74)-C(75)	120.7(8)
C(74)-C(75)-C(76)	121.6(8)
C(71)-C(76)-C(75)	116.0(7)
C(71)-C(76)-Zr	106.0(5)
C(75)-C(76)-Zr	138.0(6)
C(65)-F(65)-Zr	165.2(3)
C(93)-C(92)-C(91)	157(3)
C(93)#1-C(93)-C(92)	163(3)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.4-3b
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr	39(1)	40(1)	45(1)	6(1)	9(1)	4(1)
B	34(3)	53(4)	45(4)	7(3)	8(3)	19(3)
C(1)	44(3)	45(3)	45(3)	11(3)	12(3)	10(3)
C(2)	53(4)	38(3)	47(3)	10(3)	19(3)	11(3)
C(3)	42(3)	37(3)	62(4)	18(3)	21(3)	12(3)
C(4)	37(3)	37(3)	47(3)	6(2)	8(3)	6(2)
C(5)	37(3)	37(3)	41(3)	7(2)	11(3)	9(2)
C(6)	39(3)	54(4)	47(3)	5(3)	6(3)	13(3)
C(11)	57(4)	67(4)	51(4)	7(3)	4(3)	22(3)
C(12)	84(5)	57(4)	61(4)	10(3)	35(4)	24(3)
C(13)	54(4)	49(4)	89(5)	13(3)	37(4)	12(3)
C(14)	37(3)	47(3)	62(4)	6(3)	7(3)	10(3)
C(21)	60(4)	44(4)	69(5)	2(3)	12(4)	-5(3)
C(22)	58(4)	46(4)	80(5)	18(3)	7(4)	-6(3)
C(23)	62(4)	65(4)	57(4)	8(3)	14(4)	-17(4)
C(24)	44(4)	53(4)	72(5)	3(3)	14(3)	-6(3)
C(25)	55(4)	43(4)	56(4)	0(3)	4(3)	-6(3)
C(31)	92(6)	55(5)	111(7)	-22(4)	26(5)	2(4)
C(32)	104(7)	66(5)	115(7)	43(5)	-8(5)	-11(5)
C(33)	94(6)	130(8)	79(6)	7(5)	37(5)	-31(5)
C(34)	47(4)	87(6)	112(7)	1(5)	18(4)	0(4)
C(35)	82(5)	69(5)	62(5)	-1(3)	-5(4)	-5(4)
C(41)	55(4)	43(4)	78(5)	7(3)	17(4)	18(3)
C(42)	62(5)	42(4)	132(8)	-9(5)	31(5)	12(4)
C(43)	101(7)	47(5)	154(9)	22(5)	84(7)	26(5)
C(44)	121(8)	63(5)	107(7)	24(5)	66(6)	50(5)
C(45)	71(5)	58(4)	83(5)	24(4)	39(4)	32(4)
C(46)	51(4)	45(3)	54(4)	4(3)	17(3)	22(3)
C(51)	65(4)	63(4)	55(4)	8(3)	15(3)	30(4)
C(52)	76(5)	79(5)	71(5)	5(4)	20(4)	46(5)
C(53)	58(5)	116(7)	60(5)	-4(4)	10(4)	46(5)
C(54)	48(4)	102(6)	59(4)	-2(4)	11(3)	20(4)
C(55)	42(4)	73(5)	54(4)	3(3)	9(3)	19(3)
C(56)	47(4)	61(4)	40(3)	5(3)	10(3)	24(3)
C(61)	49(4)	64(4)	55(4)	0(3)	4(3)	21(3)
C(62)	69(5)	93(6)	43(4)	1(4)	0(3)	29(4)
C(63)	56(4)	107(6)	51(4)	26(4)	9(3)	23(4)
C(64)	56(4)	69(5)	67(5)	27(4)	21(3)	23(3)
C(65)	44(3)	56(4)	49(4)	7(3)	13(3)	13(3)
C(66)	35(3)	54(4)	46(4)	4(3)	7(3)	13(3)
C(71)	75(5)	64(5)	107(7)	18(4)	32(5)	34(4)
C(72)	109(7)	79(6)	105(7)	-9(5)	-10(6)	24(5)
C(73)	84(6)	80(6)	147(10)	2(6)	-2(6)	47(5)
C(74)	74(6)	64(5)	130(8)	9(5)	33(5)	30(4)
C(75)	78(5)	59(4)	96(6)	19(4)	29(5)	13(4)
C(76)	49(4)	52(4)	102(6)	31(4)	23(4)	16(3)
F(41)	54(2)	67(2)	87(3)	2(2)	-9(2)	6(2)
F(42)	71(3)	69(3)	209(6)	-20(3)	26(4)	-5(2)
F(43)	166(5)	61(3)	236(7)	39(4)	133(5)	16(3)
F(44)	201(6)	108(4)	123(4)	73(3)	96(4)	73(4)

F(45)	96(3)	114(3)	66(3)	36(2)	13(2)	45(3)
F(51)	99(3)	61(2)	105(3)	11(2)	46(3)	39(2)
F(52)	124(4)	109(4)	121(4)	12(3)	41(3)	82(3)
F(53)	60(3)	167(5)	118(4)	-17(3)	20(3)	61(3)
F(54)	46(2)	131(4)	122(4)	-1(3)	28(2)	8(3)
F(55)	55(2)	72(3)	93(3)	6(2)	28(2)	7(2)
F(61)	86(3)	72(3)	63(2)	-11(2)	3(2)	32(2)
F(62)	132(4)	136(4)	43(2)	-10(2)	4(2)	47(3)
F(63)	114(4)	155(4)	59(3)	46(3)	9(3)	54(3)
F(64)	98(3)	77(3)	90(3)	42(2)	23(2)	34(2)
F(65)	75(2)	48(2)	58(2)	10(2)	22(2)	19(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for X.Y-3b

	x	y	z	U(eq)
H(6A)	3560(5)	-270(4)	-1141(3)	56
H(6B)	3565(5)	589(4)	-1682(3)	56
H(11A)	3878(6)	1310(5)	834(4)	88
H(11B)	4477(6)	1097(5)	90(4)	88
H(11C)	3722(6)	200(5)	421(4)	88
H(12A)	2436(7)	2025(5)	1121(4)	95
H(12B)	1052(7)	1451(5)	1011(4)	95
H(12C)	1351(7)	2492(5)	697(4)	95
H(13A)	-1308(6)	817(5)	-1252(4)	91
H(13B)	-768(6)	1782(5)	-582(4)	91
H(13C)	-1013(6)	716(5)	-304(4)	91
H(14A)	357(5)	-347(4)	-2564(4)	74
H(14B)	-363(5)	503(4)	-2478(4)	74
H(14C)	-718(5)	-488(4)	-2102(4)	74
H(31A)	2120(8)	4970(5)	-364(5)	136
H(31B)	3346(8)	5156(5)	339(5)	136
H(31C)	2237(8)	4247(5)	307(5)	136
H(32A)	1961(8)	4956(6)	-1694(6)	154
H(32B)	1871(8)	4189(6)	-2479(6)	154
H(32C)	3019(8)	5108(6)	-2171(6)	154
H(33A)	4707(8)	2835(7)	-2538(5)	161
H(33B)	4544(8)	3927(7)	-2639(5)	161
H(33C)	3397(8)	3007(7)	-2945(5)	161
H(34A)	5606(6)	2293(6)	-1473(5)	129
H(34B)	5339(6)	1883(6)	-668(5)	129
H(34C)	6279(6)	2918(6)	-595(5)	129
H(35A)	4196(7)	3712(5)	962(4)	118
H(35B)	5494(7)	3801(5)	755(4)	118
H(35C)	4644(7)	2738(5)	732(4)	118
H(71A)	488(7)	2259(5)	-2725(6)	93
H(72A)	-1279(9)	2721(6)	-3401(6)	125
H(73A)	-2328(8)	3565(7)	-2627(8)	126
H(74A)	-1618(8)	3958(6)	-1235(7)	103
H(75A)	86(7)	3467(5)	-556(5)	92

EXPERIMENTAL DETAILS

A. Crystal Data for 4

Empirical Formula	$C_{38}H_{30}F_{15}BZr$
Formula Weight	873.66
Crystal Color, Habit	yellow, prism
Crystal Dimensions	0.60 X 0.32 X 0.19 mm
Crystal System	monoclinic
No. of Reflections Used for Unit	
Cell Determination (2θ range)	23 (18.3 - 21.4°)
Omega Scan Peak Width	
at Half-height	0.39°
Lattice Parameters	a = 11.802(3)Å b = 18.438(2) Å c = 16.524(3) Å β = 97.98(2)°
	V = 3560(1) $Å^3$
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.630 g/cm^3
F_{000}	1752.00
μ(MoKα)	4.16 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Temperature	-103.0°C
Scan Type	ω-2θ
Scan Rate	4.0°/min (in ω) (up to 4 scans)
Scan Width	$(1.52 + 0.34 \tan \theta)°$
$2\theta_{max}$	50.1°
No. of Reflections Measured	Total: 6847 Unique: 6514 (R_{int} = 0.124)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9234 - 1.0000) Decay (2.52%)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SAPI91)
Refinement	Full-matrix least-squares
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	2747
No. Variables	496
Reflection/Parameter Ratio	5.54
Residuals: R; Rw	0.044 ; 0.033
Goodness of Fit Indicator	1.89
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.39 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.47 $e^-/\AA^3$

Table 1. Atomic coordinates and B_{eq} 4

atom	x	y	z	B_{eq}
Zr(1)	0.29645(7)	0.09824(4)	0.63944(5)	2.83(2)
F(1)	0.2633(3)	0.1853(2)	0.5449(2)	3.3(1)
F(2)	0.4079(4)	0.1585(2)	0.4394(3)	5.0(1)
F(3)	0.5618(4)	0.2602(3)	0.4044(3)	5.2(1)
F(4)	0.5640(4)	0.3909(3)	0.4797(3)	5.4(1)
F(5)	0.4164(4)	0.4228(2)	0.5791(3)	4.7(1)
F(6)	0.1581(4)	0.4146(2)	0.4919(2)	3.9(1)
F(7)	0.1035(4)	0.5535(2)	0.4901(3)	5.7(2)
F(8)	0.1108(4)	0.6292(2)	0.6330(3)	6.2(2)
F(9)	0.1871(4)	0.5618(2)	0.7761(3)	5.5(1)
F(10)	0.2542(4)	0.4262(2)	0.7801(3)	4.4(1)
F(11)	0.1085(4)	0.2653(2)	0.4634(3)	4.2(1)
F(12)	-0.1077(4)	0.2294(3)	0.4322(3)	6.3(2)
F(13)	-0.2491(4)	0.2424(3)	0.5485(4)	7.8(2)
F(14)	-0.1621(4)	0.2902(3)	0.6997(3)	6.7(2)
F(15)	0.0560(4)	0.3255(2)	0.7341(3)	4.3(1)
C(1)	0.3332(6)	0.2092(4)	0.7310(4)	2.7(2)
C(2)	0.2720(6)	0.1553(4)	0.7707(4)	2.5(2)
C(3)	0.3451(6)	0.0954(4)	0.7892(4)	3.0(2)
C(4)	0.4475(6)	0.1087(4)	0.7587(4)	3.4(2)
C(5)	0.4404(6)	0.1780(4)	0.7216(4)	3.0(2)
C(6)	0.2975(6)	0.2880(4)	0.7174(4)	3.0(2)
C(7)	0.1580(7)	0.1670(4)	0.8005(5)	4.0(2)
C(8)	0.3300(7)	0.0339(4)	0.8486(4)	4.1(2)

Table 1. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
C(9)	0.5525(7)	0.0623(5)	0.7715(5)	5.4(3)
C(10)	0.5404(6)	0.2163(4)	0.6913(5)	4.2(2)
C(11)	0.1066(7)	0.0452(4)	0.5944(5)	3.1(2)
C(12)	0.1673(7)	0.0412(4)	0.5262(5)	3.3(2)
C(13)	0.2583(7)	-0.0086(4)	0.5461(5)	3.4(2)
C(14)	0.2519(7)	-0.0351(4)	0.6262(5)	3.7(2)
C(15)	0.1582(6)	-0.0027(4)	0.6556(4)	2.9(2)
C(16)	0.0011(6)	0.0905(4)	0.5985(5)	4.0(2)
C(17)	0.1337(7)	0.0787(4)	0.4455(5)	4.2(2)
C(18)	0.3362(8)	-0.0358(5)	0.4865(5)	5.5(3)
C(19)	0.3278(7)	-0.0956(5)	0.6670(5)	5.8(3)
C(20)	0.1042(7)	-0.0258(4)	0.7289(5)	4.6(3)
C(21)	0.3240(6)	0.3082(4)	0.5626(4)	2.5(2)
C(22)	0.3358(6)	0.2420(4)	0.5259(4)	2.7(2)
C(23)	0.4095(7)	0.2235(4)	0.4731(5)	3.5(2)
C(24)	0.4855(7)	0.2740(5)	0.4558(5)	3.7(2)
C(25)	0.4862(7)	0.3405(5)	0.4927(5)	3.6(2)
C(26)	0.4079(7)	0.3556(4)	0.5456(5)	3.4(2)
C(27)	0.2091(5)	0.4111(4)	0.6354(4)	2.5(2)
C(28)	0.1686(6)	0.4494(4)	0.5655(5)	2.8(2)
C(29)	0.1359(7)	0.5210(5)	0.5619(5)	3.6(2)
C(30)	0.1413(7)	0.5583(5)	0.6320(6)	4.2(3)
C(31)	0.1794(7)	0.5256(5)	0.7043(5)	3.6(2)
C(32)	0.2140(6)	0.4535(4)	0.7054(5)	3.0(2)

Table 1. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
C(33)	0.1008(6)	0.2927(4)	0.6029(5)	2.7(2)
C(34)	0.0459(7)	0.2711(4)	0.5267(5)	3.4(2)
C(35)	-0.0681(8)	0.2538(5)	0.5073(6)	4.3(3)
C(36)	-0.1384(8)	0.2597(5)	0.5659(7)	4.9(3)
C(37)	-0.0922(8)	0.2828(5)	0.6420(6)	4.5(3)
C(38)	0.0221(7)	0.2984(4)	0.6580(5)	3.5(2)
B(1)	0.2336(7)	0.3232(4)	0.6307(5)	2.5(2)
H(1)	0.4424	0.0710	0.6209	7.0646
H(2)	0.2472	0.2975	0.7564	3.5708
H(3)	0.3657	0.3153	0.7308	3.5708
H(4)	0.1687	0.1684	0.8585	4.7946
H(5)	0.1258	0.2115	0.7795	4.7946
H(6)	0.1078	0.1282	0.7821	4.7946
H(7)	0.2540	0.0345	0.8615	4.9326
H(8)	0.3441	-0.0112	0.8241	4.9326
H(9)	0.3824	0.0402	0.8972	4.9326
H(10)	0.5346	0.0153	0.7499	6.4285
H(11)	0.6102	0.0834	0.7444	6.4285
H(12)	0.5792	0.0587	0.8283	6.4285
H(13)	0.5997	0.2234	0.7357	5.0558
H(14)	0.5681	0.1875	0.6506	5.0558
H(15)	0.5158	0.2620	0.6687	5.0558
H(16)	0.0185	0.1401	0.5913	4.7742
H(17)	-0.0578	0.0757	0.5566	4.7742

Table 1. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
H(18)	-0.0239	0.0840	0.6503	4.7742
H(19)	0.1320	0.1296	0.4538	5.0552
H(20)	0.1878	0.0675	0.4098	5.0552
H(21)	0.0600	0.0625	0.4219	5.0552
H(22)	0.3910	-0.0684	0.5138	6.6464
H(23)	0.2917	-0.0602	0.4423	6.6464
H(24)	0.3745	0.0041	0.4661	6.6464
H(25)	0.3086	-0.1044	0.7201	6.9449
H(26)	0.3161	-0.1385	0.6351	6.9449
H(27)	0.4057	-0.0814	0.6711	6.9449
H(28)	0.0903	0.0157	0.7602	5.5603
H(29)	0.0340	-0.0499	0.7113	5.5603
H(30)	0.1544	-0.0579	0.7616	5.5603

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos\gamma + 2U_{13}aa^*cc^* \cos\beta + 2U_{23}bb^*cc^* \cos\alpha)$$

Table 2. Anisotropic Displacement Parameters 4

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr(1)	0.0381(4)	0.0348(4)	0.0358(4)	0.0002(5)	0.0097(3)	0.0016(5)
F(1)	0.056(3)	0.034(3)	0.036(3)	-0.003(2)	0.006(2)	-0.005(2)
F(2)	0.085(4)	0.059(4)	0.051(3)	0.011(3)	0.024(3)	-0.010(3)
F(3)	0.061(4)	0.088(4)	0.056(3)	0.018(3)	0.031(3)	0.004(3)
F(4)	0.059(3)	0.066(4)	0.084(4)	-0.008(3)	0.028(3)	0.012(3)
F(5)	0.055(3)	0.046(3)	0.082(4)	-0.014(2)	0.027(3)	-0.013(3)
F(6)	0.070(3)	0.039(3)	0.039(3)	0.005(3)	0.001(2)	0.005(2)
F(7)	0.074(4)	0.048(3)	0.088(4)	0.007(3)	-0.013(3)	0.021(3)
F(8)	0.091(4)	0.032(3)	0.112(5)	0.017(3)	0.008(4)	-0.005(3)
F(9)	0.079(4)	0.048(3)	0.092(4)	-0.006(3)	0.042(3)	-0.027(3)
F(10)	0.083(4)	0.046(3)	0.041(3)	-0.005(3)	0.019(3)	-0.012(2)
F(11)	0.065(4)	0.057(3)	0.035(3)	-0.008(3)	-0.007(3)	0.005(3)
F(12)	0.074(4)	0.065(4)	0.085(4)	-0.015(3)	-0.045(3)	0.009(3)
F(13)	0.031(3)	0.093(5)	0.167(6)	-0.011(3)	-0.014(4)	0.014(4)
F(14)	0.050(3)	0.080(4)	0.134(5)	0.006(3)	0.046(4)	-0.001(4)
F(15)	0.052(3)	0.047(3)	0.068(4)	0.006(3)	0.027(3)	-0.006(3)
C(1)	0.030(5)	0.045(5)	0.024(5)	0.002(4)	-0.004(4)	-0.006(4)
C(2)	0.034(5)	0.035(5)	0.025(5)	0.001(4)	0.003(4)	0.002(4)
C(3)	0.044(5)	0.043(5)	0.028(4)	0.003(5)	0.003(4)	0.005(5)
C(4)	0.044(5)	0.048(6)	0.038(5)	0.014(5)	0.005(4)	0.005(5)
C(5)	0.031(5)	0.050(6)	0.033(5)	0.000(4)	0.001(4)	-0.001(4)
C(6)	0.034(5)	0.040(5)	0.040(5)	-0.003(4)	0.009(4)	-0.010(4)
C(7)	0.055(6)	0.056(6)	0.045(6)	0.011(5)	0.023(5)	0.006(5)
C(8)	0.063(6)	0.053(6)	0.040(5)	0.008(5)	0.005(5)	0.009(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(9)	0.055(6)	0.081(8)	0.068(7)	0.019(6)	0.007(5)	0.022(6)
C(10)	0.033(5)	0.069(7)	0.054(6)	-0.009(5)	-0.005(5)	0.006(5)
C(11)	0.038(6)	0.034(5)	0.047(6)	-0.008(4)	0.007(4)	-0.001(4)
C(12)	0.048(6)	0.035(5)	0.042(6)	-0.009(4)	0.013(5)	-0.006(4)
C(13)	0.043(6)	0.036(6)	0.054(6)	-0.003(4)	0.018(5)	-0.008(5)
C(14)	0.049(6)	0.026(5)	0.063(7)	0.003(4)	0.005(5)	-0.001(5)
C(15)	0.041(5)	0.031(5)	0.041(5)	-0.002(4)	0.011(4)	-0.001(4)
C(16)	0.041(5)	0.036(5)	0.076(6)	-0.005(5)	0.015(5)	0.006(5)
C(17)	0.071(7)	0.041(6)	0.045(6)	-0.018(5)	-0.003(5)	-0.008(5)
C(18)	0.082(8)	0.061(7)	0.073(7)	-0.001(6)	0.028(6)	-0.024(6)
C(19)	0.073(7)	0.043(6)	0.102(8)	0.014(6)	0.008(6)	0.002(6)
C(20)	0.057(6)	0.048(6)	0.073(7)	-0.017(5)	0.013(5)	0.015(5)
C(21)	0.039(5)	0.028(5)	0.029(5)	0.000(4)	0.008(4)	-0.001(4)
C(22)	0.039(5)	0.033(5)	0.032(5)	-0.005(4)	0.006(4)	0.004(4)
C(23)	0.065(7)	0.029(5)	0.041(6)	0.007(5)	0.011(5)	-0.002(4)
C(24)	0.045(6)	0.051(6)	0.046(6)	0.021(5)	0.019(5)	0.005(5)
C(25)	0.037(5)	0.054(6)	0.050(6)	-0.003(5)	0.013(5)	0.022(5)
C(26)	0.053(6)	0.027(5)	0.051(6)	-0.004(4)	0.013(5)	-0.004(4)
C(27)	0.023(4)	0.032(5)	0.042(5)	-0.005(4)	0.009(4)	-0.004(4)
C(28)	0.033(5)	0.030(5)	0.044(6)	-0.008(4)	0.003(4)	-0.006(4)
C(29)	0.046(6)	0.039(6)	0.050(6)	-0.002(5)	-0.003(5)	0.007(5)
C(30)	0.044(6)	0.039(6)	0.077(8)	0.007(5)	0.006(6)	-0.002(6)
C(31)	0.041(6)	0.043(6)	0.056(6)	-0.004(5)	0.021(5)	-0.022(5)
C(32)	0.033(5)	0.039(5)	0.041(6)	-0.008(4)	0.008(4)	0.001(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(33)	0.039(5)	0.026(5)	0.036(5)	-0.001(4)	0.007(4)	0.007(4)
C(34)	0.053(6)	0.038(5)	0.036(6)	0.005(5)	-0.003(5)	0.008(4)
C(35)	0.050(7)	0.040(6)	0.064(7)	-0.010(5)	-0.027(6)	0.016(5)
C(36)	0.031(6)	0.050(7)	0.104(9)	0.001(5)	0.005(6)	0.008(7)
C(37)	0.041(6)	0.055(6)	0.080(8)	0.003(5)	0.021(6)	0.001(6)
C(38)	0.051(6)	0.026(5)	0.056(6)	-0.003(4)	0.003(5)	-0.004(4)
B(1)	0.028(5)	0.025(5)	0.044(6)	0.000(4)	0.010(5)	-0.001(5)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å) 4

atom	atom	distance	atom	atom	distance
Zr(1)	F(1)	2.237(4)	Zr(1)	C(1)	2.546(7)
Zr(1)	C(2)	2.463(7)	Zr(1)	C(3)	2.463(7)
Zr(1)	C(4)	2.475(7)	Zr(1)	C(5)	2.501(7)
Zr(1)	C(11)	2.463(7)	Zr(1)	C(12)	2.477(8)
Zr(1)	C(13)	2.504(8)	Zr(1)	C(14)	2.517(8)
Zr(1)	C(15)	2.513(7)	F(1)	C(22)	1.414(7)
F(2)	C(23)	1.320(8)	F(3)	C(24)	1.345(8)
F(4)	C(25)	1.344(8)	F(5)	C(26)	1.355(8)
F(6)	C(28)	1.366(8)	F(7)	C(29)	1.336(8)
F(8)	C(30)	1.357(8)	F(9)	C(31)	1.354(8)
F(10)	C(32)	1.357(8)	F(11)	C(34)	1.365(8)
F(12)	C(35)	1.341(9)	F(13)	C(36)	1.337(9)
F(14)	C(37)	1.353(9)	F(15)	C(38)	1.361(8)
C(1)	C(2)	1.438(9)	C(1)	C(5)	1.418(9)
C(1)	C(6)	1.520(9)	C(2)	C(3)	1.409(9)
C(2)	C(7)	1.511(9)	C(3)	C(4)	1.395(9)
C(3)	C(8)	1.526(9)	C(4)	C(5)	1.415(9)
C(4)	C(9)	1.496(9)	C(5)	C(10)	1.518(9)
C(6)	B(1)	1.66(1)	C(11)	C(12)	1.418(9)
C(11)	C(15)	1.415(9)	C(11)	C(16)	1.509(9)
C(12)	C(13)	1.416(10)	C(12)	C(17)	1.506(10)
C(13)	C(14)	1.42(1)	C(13)	C(18)	1.523(10)
C(14)	C(15)	1.402(9)	C(14)	C(19)	1.526(10)
C(15)	C(20)	1.507(9)	C(21)	C(22)	1.379(9)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(21)	C(26)	1.379(9)	C(21)	B(1)	1.677(10)
C(22)	C(23)	1.358(9)	C(23)	C(24)	1.352(10)
C(24)	C(25)	1.37(1)	C(25)	C(26)	1.386(10)
C(27)	C(28)	1.380(9)	C(27)	C(32)	1.391(9)
C(27)	B(1)	1.65(1)	C(28)	C(29)	1.376(10)
C(29)	C(30)	1.34(1)	C(30)	C(31)	1.36(1)
C(31)	C(32)	1.389(10)	C(33)	C(34)	1.392(9)
C(33)	C(38)	1.391(10)	C(33)	B(1)	1.67(1)
C(34)	C(35)	1.38(1)	C(35)	C(36)	1.36(1)
C(36)	C(37)	1.37(1)	C(37)	C(38)	1.37(1)
Zr(1)	H(1)	1.86			

Table 4. Bond Angles(°) 4

atom	atom	atom	angle	atom	atom	atom	angle
F(1)	Zr(1)	C(1)	80.6(2)	F(1)	Zr(1)	C(2)	106.1(2)
F(1)	Zr(1)	C(3)	135.3(2)	F(1)	Zr(1)	C(4)	122.5(2)
F(1)	Zr(1)	C(5)	89.8(2)	F(1)	Zr(1)	C(11)	90.6(2)
F(1)	Zr(1)	C(12)	75.4(2)	F(1)	Zr(1)	C(13)	97.8(2)
F(1)	Zr(1)	C(14)	128.8(2)	F(1)	Zr(1)	C(15)	123.5(2)
C(1)	Zr(1)	C(2)	33.3(2)	C(1)	Zr(1)	C(3)	54.7(2)
C(1)	Zr(1)	C(4)	54.5(2)	C(1)	Zr(1)	C(5)	32.6(2)
C(1)	Zr(1)	C(11)	124.9(2)	C(1)	Zr(1)	C(12)	145.7(3)
C(1)	Zr(1)	C(13)	178.4(3)	C(1)	Zr(1)	C(14)	148.5(3)
C(1)	Zr(1)	C(15)	126.2(2)	C(2)	Zr(1)	C(3)	33.2(2)
C(2)	Zr(1)	C(4)	54.9(2)	C(2)	Zr(1)	C(5)	54.9(2)
C(2)	Zr(1)	C(11)	102.9(2)	C(2)	Zr(1)	C(12)	135.3(2)
C(2)	Zr(1)	C(13)	147.7(2)	C(2)	Zr(1)	C(14)	116.4(3)
C(2)	Zr(1)	C(15)	93.8(2)	C(3)	Zr(1)	C(4)	32.8(2)
C(3)	Zr(1)	C(5)	54.6(2)	C(3)	Zr(1)	C(11)	111.7(2)
C(3)	Zr(1)	C(12)	141.6(2)	C(3)	Zr(1)	C(13)	126.8(3)
C(3)	Zr(1)	C(14)	94.8(3)	C(3)	Zr(1)	C(15)	86.6(2)
C(4)	Zr(1)	C(5)	33.0(2)	C(4)	Zr(1)	C(11)	142.8(3)
C(4)	Zr(1)	C(12)	159.1(3)	C(4)	Zr(1)	C(13)	126.9(3)
C(4)	Zr(1)	C(14)	105.3(3)	C(4)	Zr(1)	C(15)	112.3(3)
C(5)	Zr(1)	C(11)	156.7(2)	C(5)	Zr(1)	C(12)	163.7(2)
C(5)	Zr(1)	C(13)	148.0(2)	C(5)	Zr(1)	C(14)	137.7(3)
C(5)	Zr(1)	C(15)	141.3(2)	C(11)	Zr(1)	C(12)	33.4(2)
C(11)	Zr(1)	C(13)	54.8(2)	C(11)	Zr(1)	C(14)	54.2(2)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	Zr(1)	C(15)	33.0(2)	C(12)	Zr(1)	C(13)	33.0(2)
C(12)	Zr(1)	C(14)	54.6(3)	C(12)	Zr(1)	C(15)	55.0(2)
C(13)	Zr(1)	C(14)	32.9(2)	C(13)	Zr(1)	C(15)	54.5(2)
C(14)	Zr(1)	C(15)	32.4(2)	Zr(1)	F(1)	C(22)	129.3(4)
Zr(1)	C(1)	C(2)	70.2(4)	Zr(1)	C(1)	C(5)	71.9(4)
Zr(1)	C(1)	C(6)	131.2(5)	C(2)	C(1)	C(5)	106.4(7)
C(2)	C(1)	C(6)	125.5(7)	C(5)	C(1)	C(6)	127.2(7)
Zr(1)	C(2)	C(1)	76.5(4)	Zr(1)	C(2)	C(3)	73.4(4)
Zr(1)	C(2)	C(7)	124.5(5)	C(1)	C(2)	C(3)	108.1(6)
C(1)	C(2)	C(7)	125.2(7)	C(3)	C(2)	C(7)	125.9(7)
Zr(1)	C(3)	C(2)	73.4(4)	Zr(1)	C(3)	C(4)	74.1(4)
Zr(1)	C(3)	C(8)	129.1(5)	C(2)	C(3)	C(4)	108.6(7)
C(2)	C(3)	C(8)	126.9(7)	C(4)	C(3)	C(8)	123.2(7)
Zr(1)	C(4)	C(3)	73.1(4)	Zr(1)	C(4)	C(5)	74.5(4)
Zr(1)	C(4)	C(9)	123.9(6)	C(3)	C(4)	C(5)	108.3(7)
C(3)	C(4)	C(9)	126.2(8)	C(5)	C(4)	C(9)	125.1(7)
Zr(1)	C(5)	C(1)	75.4(4)	Zr(1)	C(5)	C(4)	72.5(4)
Zr(1)	C(5)	C(10)	126.5(5)	C(1)	C(5)	C(4)	108.5(7)
C(1)	C(5)	C(10)	126.5(7)	C(4)	C(5)	C(10)	124.1(7)
C(1)	C(6)	B(1)	125.9(6)	Zr(1)	C(11)	C(12)	73.9(5)
Zr(1)	C(11)	C(15)	75.4(4)	Zr(1)	C(11)	C(16)	119.3(5)
C(12)	C(11)	C(15)	108.8(7)	C(12)	C(11)	C(16)	125.1(8)
C(15)	C(11)	C(16)	126.1(7)	Zr(1)	C(12)	C(11)	72.8(5)
Zr(1)	C(12)	C(13)	74.5(5)	Zr(1)	C(12)	C(17)	122.2(5)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	C(12)	C(13)	107.4(7)	C(11)	C(12)	C(17)	125.5(8)
C(13)	C(12)	C(17)	126.9(7)	Zr(1)	C(13)	C(12)	72.5(5)
Zr(1)	C(13)	C(14)	74.0(5)	Zr(1)	C(13)	C(18)	125.8(5)
C(12)	C(13)	C(14)	107.6(7)	C(12)	C(13)	C(18)	124.8(8)
C(14)	C(13)	C(18)	127.1(8)	Zr(1)	C(14)	C(13)	73.0(5)
Zr(1)	C(14)	C(15)	73.7(4)	Zr(1)	C(14)	C(19)	124.9(5)
C(13)	C(14)	C(15)	108.8(7)	C(13)	C(14)	C(19)	123.9(8)
C(15)	C(14)	C(19)	127.0(8)	Zr(1)	C(15)	C(11)	71.5(4)
Zr(1)	C(15)	C(14)	74.0(4)	Zr(1)	C(15)	C(20)	130.5(5)
C(11)	C(15)	C(14)	107.5(7)	C(11)	C(15)	C(20)	124.3(7)
C(14)	C(15)	C(20)	126.8(8)	C(22)	C(21)	C(26)	110.6(7)
C(22)	C(21)	B(1)	123.7(7)	C(26)	C(21)	B(1)	125.0(7)
F(1)	C(22)	C(21)	117.0(6)	F(1)	C(22)	C(23)	114.7(7)
C(21)	C(22)	C(23)	128.3(8)	F(2)	C(23)	C(22)	121.8(8)
F(2)	C(23)	C(24)	120.6(8)	C(22)	C(23)	C(24)	117.7(8)
F(3)	C(24)	C(23)	121.6(8)	F(3)	C(24)	C(25)	119.2(8)
C(23)	C(24)	C(25)	119.2(7)	F(4)	C(25)	C(24)	120.6(8)
F(4)	C(25)	C(26)	119.5(8)	C(24)	C(25)	C(26)	119.9(8)
F(5)	C(26)	C(21)	120.8(7)	F(5)	C(26)	C(25)	115.0(7)
C(21)	C(26)	C(25)	124.2(8)	C(28)	C(27)	C(32)	112.2(7)
C(28)	C(27)	B(1)	120.4(7)	C(32)	C(27)	B(1)	127.2(7)
F(6)	C(28)	C(27)	118.9(7)	F(6)	C(28)	C(29)	115.0(8)
C(27)	C(28)	C(29)	126.1(8)	F(7)	C(29)	C(28)	120.8(8)
F(7)	C(29)	C(30)	120.8(8)	C(28)	C(29)	C(30)	118.4(9)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(8)	C(30)	C(29)	121.6(9)	F(8)	C(30)	C(31)	118.2(9)
C(29)	C(30)	C(31)	120.2(9)	F(9)	C(31)	C(30)	121.8(8)
F(9)	C(31)	C(32)	118.4(8)	C(30)	C(31)	C(32)	119.8(8)
F(10)	C(32)	C(27)	121.1(7)	F(10)	C(32)	C(31)	115.6(8)
C(27)	C(32)	C(31)	123.2(8)	C(34)	C(33)	C(38)	110.2(7)
C(34)	C(33)	B(1)	130.3(7)	C(38)	C(33)	B(1)	118.8(7)
F(11)	C(34)	C(33)	118.8(7)	F(11)	C(34)	C(35)	114.8(8)
C(33)	C(34)	C(35)	126.4(8)	F(12)	C(35)	C(34)	119.8(9)
F(12)	C(35)	C(36)	121.0(9)	C(34)	C(35)	C(36)	119.2(9)
F(13)	C(36)	C(35)	120(1)	F(13)	C(36)	C(37)	121.8(10)
C(35)	C(36)	C(37)	118.2(9)	F(14)	C(37)	C(36)	118.3(9)
F(14)	C(37)	C(38)	121.6(9)	C(36)	C(37)	C(38)	120.0(9)
F(15)	C(38)	C(33)	119.7(8)	F(15)	C(38)	C(37)	114.3(8)
C(33)	C(38)	C(37)	125.9(8)	C(6)	B(1)	C(21)	105.1(6)
C(6)	B(1)	C(27)	114.0(6)	C(6)	B(1)	C(33)	113.7(6)
C(21)	B(1)	C(27)	109.0(6)	C(21)	B(1)	C(33)	114.8(6)
C(27)	B(1)	C(33)	100.3(6)				
F(1)	Zr(1)	H(1)	98.9	C(1)	Zr(1)	H(1)	103.3
C(2)	Zr(1)	H(1)	119.0	C(3)	Zr(1)	H(1)	93.9
C(4)	Zr(1)	H(1)	64.6	C(5)	Zr(1)	H(1)	70.9
C(11)	Zr(1)	H(1)	131.9	C(12)	Zr(1)	H(1)	104.4
C(13)	Zr(1)	H(1)	77.2	C(14)	Zr(1)	H(1)	84.8
C(15)	Zr(1)	H(1)	116.6				

Table 5. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
F(2)	F(10)	3.365(7)	55404	F(3)	F(13)	3.046(7)	65501
F(3)	C(5)	3.358(8)	55404	F(3)	C(10)	3.522(9)	55404
F(3)	C(4)	3.543(9)	55404	F(3)	C(19)	3.568(10)	65603
F(4)	C(9)	3.531(10)	55404	F(4)	C(8)	3.547(9)	55404
F(4)	F(5)	3.586(6)	66603	F(4)	F(13)	3.600(7)	65501
F(5)	C(9)	3.549(9)	65602	F(6)	F(7)	3.197(6)	56603
F(6)	C(8)	3.457(8)	55404	F(6)	C(7)	3.501(8)	55404
F(7)	C(29)	3.152(9)	56603	F(7)	F(7)	3.191(9)	56603
F(7)	C(28)	3.215(9)	56603	F(7)	C(35)	3.579(10)	56603
F(8)	F(12)	2.820(7)	56603	F(8)	C(35)	3.155(10)	56603
F(8)	F(11)	3.446(6)	56603	F(8)	C(34)	3.523(9)	56603
F(8)	C(7)	3.568(9)	55602	F(9)	C(9)	3.277(9)	65602
F(9)	C(16)	3.283(8)	55602	F(10)	C(17)	3.252(8)	4
F(10)	C(9)	3.573(9)	65602	F(11)	C(7)	3.096(8)	55404
F(13)	C(24)	3.341(9)	45501	F(15)	C(20)	3.433(8)	55602
C(9)	C(31)	3.21(1)	64602	C(9)	C(32)	3.39(1)	64602
C(12)	C(16)	3.60(1)	55603	C(16)	C(17)	3.53(1)	55603

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ± 4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	X,	Y,	Z	(2)	-X,	1/2+Y,	1/2-Z
(3)	-X,	-Y,	-Z	(4)	X,	1/2-Y,	1/2+Z