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Supplementary Material

Experimental procedure for the X-ray diffraction study of **2a**.

The crystals of **2a** are always grown polysynthetically twined. A prismatic crystal was coated with epoxi resin and mounted in a SMART diffractometer. No absorption corrections have been applied. The intensities were corrected for Lorentz and polarization effects. The structure was resolved by Direct and Fourier methods. The hydride H atom has been located from a difference map. The refinement was based on F^2 for all reflections. The refinement involved anisotropic thermal parameters for the non-hydrogen atoms except the CF_3 groups which have been considered as rigid-body. The H(1) atom has been refined isotropically and the other hydrogen atoms were included at their calculated positions. Wheighted R-factors w$R2$ and all goodnesses of fit S are based on F^2, conventional R-factors $R1$ are based on F. The calculations were carried out with the Shelxs-92 and Shelxs-93 programs.

Table S1. Crystal data and structure refinement for **2a**.

Empirical formula	$C_{53.25}H_{46}B_2Cl_{0.50}F_{24}IrN_7$
Formula weight	1471.52
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 13.5390(2) Å alpha = 96.5403(13)°
	b = 15.4865(4) Å beta = 108.6817(12)°
	c = 16.4806(5) Å gamma = 92.7549(14)°
Volume, Z	3239.00(14) Å^3, 2
Density (calculated)	1.509 Mg/m^3
Absorption coefficient	2.190 mm^{-1}
F(000)	1452
Crystal size	0.15 x 0.10 x 0.10 mm
Θ range for data collection	1.70 to 23.32°
Limiting indices	$-15 \le h \le 14$, $-17 \le k \le 13$, $-17 \le l \le 18$
Reflections collected	12239
Independent reflections	8742 (R_{int} = 0.0391)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8740 / 0 / 507
Goodness-of-fit on F^2	0.638
Final R indices [I>2σ(I)]	R1 = 0.1025, wR2 = 0.2700
R indices (all data)	R1 = 0.1709, wR2 = 0.3092
Largest diff. peak and hole	1.930 and -1.022 eÅ^{-3}

Table S2. Selected bond distances and angles for **2a**.

Ir(1)-C(6)	1.80(3)	Ir(1)-N(1)	2.01(2)
Ir(1)-N(11)	2.05(2)	Ir(1)-N(31)	2.13(2)
Ir(1)-N(21)	2.15(2)	Ir(1)-H(1)	2.03(14)
N(1)-C(2)	1.28(2)	C(2)-C(3)	1.45
C(2)-C(4)	1.46(3)	C(4)-C(5)	1.49(4)
C(4)-C(6)	1.67(4)	C(6)-C(7)	1.54(4)

C(6)-Ir(1)-N(1)	77.2(13)	C(6)-Ir(1)-N(11)	101.7(12)
N(1)-Ir(1)-N(11)	178.1(7)	C(6)-Ir(1)-N(31)	169.7(12)
N(1)-Ir(1)-N(31)	94.7(7)	N(11)-Ir(1)-N(31)	86.2(6)
C(6)-Ir(1)-N(21)	101.8(12)	N(1)-Ir(1)-N(21)	94.9(8)
N(11)-Ir(1)-N(21)	86.9(7)	N(31)-Ir(1)-N(21)	85.1(7)
C(6)-Ir(1)-H(1)	78(4)	N(1)-Ir(1)-H(1)	83(4)
N(11)-Ir(1)-H(1)	95(4)	N(31)-Ir(1)-H(1)	94(4)
N(21)-Ir(1)-H(1)	178(4)	C(2)-N(1)-Ir(1)	123.0(13)
N(1)-C(2)-C(3)	125.9(9)	N(1)-C(2)-C(4)	110(2)
C(3)-C(2)-C(4)	124.1(14)	C(5)-C(4)-C(2)	115(3)
C(5)-C(4)-C(6)	98(3)	C(2)-C(4)-C(6)	104(2)
C(7)-C(6)-C(4)	118(3)	C(7)-C(6)-Ir(1)	128(3)
C(4)-C(6)-Ir(1)	113(2)		

Symmetry transformations used to generate equivalent atoms:

Table S3. Atomic coordinates for **2a**.

	x	y	z	U(eq)
Ir(1)	1702(1)	3865(1)	6787(1)	72(1)
H(1)	1832(109)	3562(91)	5597(89)	50
N(1)	1039(16)	2635(13)	6554(13)	100(6)
C(2)	1501	1974	6374	86
C(3)	1041	1082	6130	90
C(4)	2562(27)	2255(23)	6415(23)	146(11)
C(5)	3406(28)	1807(24)	6986(23)	170(13)
C(6)	2814(27)	3234(22)	7022(22)	151(11)
C(7)	3966(32)	3559(27)	7537(27)	200(16)
B(1)	1003(20)	5571(15)	7574(16)	73(7)
N(11)	2407(12)	5113(10)	6997(10)	70(4)
N(12)	1970(13)	5767(11)	7309(11)	73(5)
C(13)	2474(18)	6521(14)	7340(13)	80(6)
C(14)	3219(15)	6370(14)	7008(13)	76(6)
C(15)	3189(16)	5489(14)	6792(15)	82(6)
C(16)	2198(22)	7369(17)	7689(18)	109(9)
C(17)	3839(21)	5025(17)	6380(17)	118(8)
N(21)	1519(13)	4143(13)	8037(11)	78(5)
N(22)	1215(14)	4936(11)	8247(12)	72(5)
C(23)	1162(21)	4976(16)	9055(15)	91(7)
C(24)	1441(22)	4222(20)	9346(18)	105(9)
C(25)	1671(18)	3710(16)	8699(17)	85(6)
C(26)	880(23)	5760(19)	9469(19)	122(9)
C(27)	2063(23)	2845(18)	8714(18)	115(9)
N(31)	259(13)	4430(11)	6320(11)	71(4)
N(32)	101(14)	5169(12)	6779(12)	71(5)
C(33)	-892(19)	5384(18)	6396(19)	93(8)
C(34)	-1357(20)	4814(24)	5692(19)	118(10)
C(35)	-650(24)	4232(20)	5626(16)	101(9)
C(36)	-1252(23)	6165(18)	6747(18)	118(9)
C(37)	-748(29)	3507(24)	4916(24)	147(12)
B(2)	3614(16)	1754(13)	1977(13)	57(5)
C(41)	4551(15)	1824(12)	2921(11)	59(5)
C(42)	5464(15)	1404(12)	3090(12)	61(5)
C(43)	6252(17)	1553(14)	3874(13)	67(6)
C(44)	6165(19)	2118(16)	4534(15)	82(7)
C(45)	5288(18)	2574(15)	4402(14)	74(6)
C(46)	4464(15)	2446(12)	3599(12)	66(5)
C(47)	7218(9)	1050(9)	4081(8)	123(11)
F(471)	7194(9)	462(10)	4583(8)	309(22)
F(472)	8032(9)	1612(8)	4457(8)	325(24)
F(473)	7280(9)	672(9)	3351(10)	232(16)
C(48)	5221(11)	3232(9)	5163(7)	155(16)
F(481)	5181(11)	2857(8)	5823(7)	303(23)
F(482)	4394(12)	3656(9)	4891(7)	344(24)
F(483)	6060(9)	3775(9)	5396(7)	289(21)
C(51)	2426(17)	1648(13)	2032(13)	65(6)
C(52)	2182(16)	1414(14)	2739(14)	79(6)
C(53)	1145(22)	1266(16)	2699(19)	91(7)
C(54)	358(20)	1311(15)	1972(19)	88(7)
C(55)	576(16)	1556(15)	1285(17)	80(7)

Table S4. Anisotropic displacement parameters for **2a**.

	U11	U22	U33	U23	U13	U12
Ir(1)	72(1)	61(1)	83(1)	-3(1)	32(1)	-2(1)
B(1)	80(17)	55(14)	70(16)	-2(13)	6(13)	23(13)
N(11)	66(10)	59(10)	90(12)	-14(9)	42(9)	-2(8)
N(12)	60(11)	59(11)	98(12)	-9(9)	32(9)	-9(9)
C(13)	85(16)	65(15)	81(14)	-14(11)	26(12)	-2(12)
C(14)	63(13)	83(16)	70(13)	6(11)	9(11)	-10(11)
C(15)	85(14)	56(15)	98(17)	-20(12)	33(13)	-9(11)
N(21)	81(12)	98(14)	62(11)	29(11)	26(9)	9(10)
N(22)	70(12)	66(11)	76(14)	-7(10)	23(10)	9(9)
C(23)	111(21)	108(18)	68(15)	2(13)	50(15)	24(16)
C(24)	121(23)	110(25)	107(20)	53(19)	56(18)	33(19)
C(25)	94(16)	82(17)	81(17)	4(15)	36(13)	4(13)
N(31)	73(12)	65(11)	73(11)	2(9)	25(10)	0(9)
N(32)	67(14)	77(13)	87(13)	33(11)	41(11)	24(10)
C(33)	69(15)	91(20)	108(21)	15(17)	12(15)	6(14)
C(34)	47(15)	188(30)	112(21)	37(21)	9(15)	18(19)
C(35)	103(20)	95(23)	90(18)	-12(16)	22(16)	-17(18)
B(2)	61(12)	51(12)	58(13)	-2(10)	22(10)	5(10)
C(41)	61(13)	62(12)	49(11)	-6(9)	20(9)	-11(10)
C(42)	58(13)	59(11)	66(13)	2(9)	26(10)	-6(10)
C(43)	75(15)	65(14)	59(13)	-7(11)	26(12)	0(12)
C(44)	78(18)	87(17)	69(15)	16(13)	9(13)	-9(14)
C(45)	84(16)	78(15)	66(15)	3(12)	37(13)	1(13)
C(46)	66(12)	68(12)	61(12)	0(10)	22(10)	-3(9)
C(47)	118(23)	119(25)	107(21)	-26(18)	13(18)	41(20)
F(471)	284(38)	305(38)	456(53)	233(39)	198(37)	216(33)
F(472)	86(14)	235(28)	508(57)	-126(33)	-48(22)	43(16)
F(473)	203(25)	351(38)	157(17)	42(21)	51(17)	209(28)
C(48)	92(22)	258(45)	117(32)	-42(32)	58(23)	9(25)
F(481)	634(72)	188(23)	182(24)	-26(19)	286(38)	26(31)
F(482)	332(36)	466(50)	155(23)	-166(28)	14(23)	226(36)
F(483)	240(28)	304(40)	231(32)	-184(31)	32(24)	-40(27)
C(51)	80(15)	49(13)	71(13)	-20(10)	44(12)	-11(11)
C(52)	62(13)	92(16)	85(15)	14(12)	30(11)	-2(11)
C(53)	78(19)	81(17)	126(22)	16(15)	52(18)	-7(14)
C(54)	54(16)	81(17)	132(20)	17(15)	36(16)	-1(13)
C(55)	57(14)	82(15)	96(20)	18(14)	19(13)	9(11)
C(56)	48(13)	85(15)	71(16)	1(12)	6(12)	8(11)
C(57)	176(36)	100(21)	303(46)	85(26)	159(35)	17(22)
C(61)	46(11)	64(13)	69(12)	-4(9)	25(9)	-6(9)
C(62)	69(13)	66(13)	64(13)	6(11)	18(10)	-4(10)
C(63)	90(16)	56(14)	74(15)	4(11)	29(12)	-1(11)
C(64)	71(13)	68(13)	72(17)	-17(12)	14(12)	-8(10)
C(65)	59(13)	73(15)	55(12)	0(11)	18(10)	-14(11)
C(66)	67(13)	48(10)	59(12)	-12(9)	19(10)	0(9)
C(71)	61(12)	50(11)	55(11)	5(9)	20(9)	3(9)
C(72)	73(13)	70(15)	75(14)	-3(11)	28(11)	-4(11)
C(73)	82(14)	64(13)	85(17)	3(12)	30(13)	6(11)
C(74)	97(19)	55(13)	84(15)	19(11)	32(14)	3(13)
C(75)	63(13)	58(14)	54(11)	5(10)	22(10)	-22(11)
C(76)	65(13)	60(12)	53(13)	-11(10)	16(11)	2(10)

C(57)	897(7)	1065(6)	3557(7)	169(16)
F(571)	-61(7)	768(6)	3395(7)	175(2)
F(572)	1074(7)	1813(6)	4031(8)	175(2)
F(573)	1513(8)	529(6)	3960(8)	175(2)
C(58)	-400(7)	1617(6)	453(7)	140(10)
F(581)	-677(7)	863(6)	-10(7)	175(2)
F(582)	-141(7)	2165(6)	8(7)	175(2)
F(583)	-1170(7)	1882(6)	685(6)	175(2)
C(61)	3664(13)	888(12)	1351(11)	60(5)
C(62)	3675(9)	84(8)	1627(9)	68(5)
C(63)	3640(9)	-696(8)	1095(9)	73(6)
C(64)	3552(9)	-687(8)	233(9)	75(6)
C(65)	3407(15)	87(14)	-81(12)	64(6)
C(66)	3539(6)	874(5)	455(5)	60(5)
C(67)	3249(6)	53(5)	-1041(5)	120(8)
F(671)	2237(6)	-125(5)	-1423(5)	175(2)
F(672)	3750(6)	-562(5)	-1305(5)	175(2)
F(673)	3545(6)	806(5)	-1225(5)	175(2)
C(68)	3734(6)	-1590(5)	1438(5)	131(9)
F(681)	4542(6)	-1930(5)	1293(5)	175(2)
F(682)	2878(6)	-2099(5)	1007(5)	175(2)
F(683)	3866(6)	-1516(5)	2268(5)	175(2)
C(71)	3798(14)	2656(11)	1605(11)	55(5)
C(72)	3311(16)	3428(14)	1776(13)	73(6)
C(73)	3545(17)	4219(13)	1566(15)	77(6)
C(74)	4252(19)	4308(14)	1142(14)	78(6)
C(75)	4759(15)	3598(14)	962(11)	59(5)
C(76)	4549(6)	2826(5)	1199(5)	62(5)
C(77)	3014(6)	5031(5)	1810(5)	109(8)
F(771)	3187(6)	5679(5)	1436(5)	175(2)
F(772)	3364(6)	5238(5)	2637(5)	175(2)
F(773)	2021(6)	4798(5)	1560(5)	175(2)
C(78)	5559(6)	3714(5)	486(5)	124(8)
F(781)	5043(6)	3713(5)	-324(5)	175(2)
F(782)	6144(6)	3072(5)	574(5)	175(2)
F(783)	6139(6)	4442(5)	787(5)	175(2)
Cl(1)	1369	6773	2976	100(7)
Cl(2)	1003	8455	2525	142(7)
C(8)	1651	8003	3211	13(29)