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Table S1. Experimental details for the structure determination of **2a**.

Empirical formula	C ₃₃ H ₄₉ Cl Ir ₂ N ₈ · 0.3 (C ₆ H ₆)
Formula weight	1001.08
Temperature	150.0(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	<i>P</i> 1 21/ <i>c</i> 1
Unit cell dimensions	<i>a</i> = 21.862(6) Å α = 90 deg. <i>b</i> = 9.383(2) Å β = 117.302(2) deg. <i>c</i> = 23.552(7) Å γ = 90 deg.
Volume	4293(2) Å ³
<i>Z</i>	4
Density (calculated)	1.549 Mg/m ³
Absorption coefficient	6.286 mm ⁻¹
<i>F</i> (000)	1946
Crystal size	0.5 x 0.4 x 0.1 mm
Theta range data collection	2.11 to 25.00 deg.
Index ranges	0 ≤ <i>h</i> ≤ 25, -1 ≤ <i>k</i> ≤ 11, -28 ≤ <i>l</i> ≤ 24
Reflections collected	8637
Independent reflections	7437 [<i>R</i> _(int) = 0.0270]
Absorption correction	Gaussian
Max. and min. transmission	0.5793 and 0.1418
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	7437 / 168 / 400
Goodness-of-fit on <i>F</i> ²	1.649
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0455, <i>wR</i> ₂ = 0.0659
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0862, <i>wR</i> ₂ = 0.0676
Largest diff. peak and hole	1.027 and -0.892 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2a**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U_{(eq)}$
Ir(1)	7778(1)	2326(1)	6209(1)	40(1)
Ir(2)	6871(1)	2164(1)	4950(1)	44(1)
Cl	8442(1)	1381(3)	7336(1)	68(1)
N(1)	6886(3)	1282(8)	6103(4)	37(2)
N(2)	6434(4)	1229(7)	5476(3)	34(2)
C(1)	6609(5)	699(10)	6456(4)	41(3)
C(2)	5954(5)	258(11)	6039(5)	50(3)
C(3)	5861(4)	599(11)	5438(5)	54(4)
N(3)	7945(4)	464(8)	5831(4)	46(3)
N(4)	7501(4)	401(9)	5196(4)	57(3)
C(4A) ^a	8268(9)	-802(15)	6058(9)	78(8)
C(5A) ^a	8017(11)	-1710(3)	5536(9)	86(9)
C(6A) ^a	7538(8)	-966(15)	5011(9)	68(7)
C(4B) ^a	8463(9)	-470(2)	5959(13)	46(10)
C(5B) ^a	8294(15)	-1070(3)	5372(12)	69(12)
C(6B) ^a	7699(12)	-550(2)	4875(10)	64(11)
C(7)	7531(5)	3992(11)	6468(5)	49(3)
N(5)	7407(4)	5039(10)	6667(4)	66(3)
C(8A) ^b	7461(8)	6255(15)	7099(6)	106(12)
C(9A) ^b	7954(9)	5726(19)	7765(7)	101(8)
C(10A) ^b	6758(7)	6530(2)	7063(8)	99(8)
C(11A) ^b	7741(9)	7540(2)	6901(8)	110(8)
C(8B) ^b	7408(11)	6070(2)	7153(9)	17(12)
C(9B) ^b	6859(14)	7240(4)	6849(16)	74(15)
C(10B) ^b	8112(12)	6800(4)	7435(17)	78(17)
C(11B) ^b	7320(2)	5320(4)	7683(17)	100(2)
C(12)	8538(5)	3285(11)	6225(5)	59(4)
N(6)	9027(4)	3897(10)	6266(4)	67(3)
C(13)	9721(4)	4545(10)	6646(4)	70(4)
C(14A) ^b	9914(10)	4500(2)	7357(6)	73(8)
C(15A) ^b	10184(9)	3570(18)	6497(10)	76(8)
C(16A) ^b	9700(9)	6055(15)	6410(9)	64(7)
C(14B) ^b	10271(12)	3390(2)	6899(16)	58(12)
C(15B) ^b	9818(16)	5520(4)	6176(12)	76(14)
C(16B) ^b	9749(16)	5340(4)	7225(12)	77(14)
C(17)	6321(6)	3842(11)	4783(5)	66(4)
N(7A) ^b	6151(12)	5016(14)	4612(10)	73(7)
C(18A) ^b	5937(10)	6520(15)	4410(9)	100(11)
C(19A) ^b	6204(9)	6660(2)	3927(8)	56(7)
C(20A) ^b	6335(12)	7340(3)	5018(9)	130(11)
C(21A) ^b	5168(9)	6550(3)	4134(11)	113(11)
N(7B) ^b	5902(8)	4741(18)	4712(9)	45(6)
C(18B) ^b	5497(8)	6109(16)	4579(8)	71(8)
C(19B) ^b	5708(15)	7060(3)	4175(11)	123(12)
C(20B) ^b	4738(8)	5720(2)	4178(9)	60(7)
C(21B) ^b	5602(11)	6840(2)	5193(8)	92(10)

C(22)	7379(6)	3053(15)	4552(5)	83(5)
N(8A) ^b	7710(2)	3680(4)	4350(2)	72(6)
C(23A) ^b	8145(10)	4010(3)	4031(9)	97(7)
C(24A) ^b	7774(16)	5190(3)	3548(13)	95(5)
C(25A) ^b	8132(14)	2690(3)	3660(12)	95(5)
C(26A) ^b	8858(13)	4400(3)	4552(12)	95(5)
N(8B) ^b	7767(18)	3190(4)	4330(2)	72(6)
C(23B) ^b	8061(13)	4260(3)	4051(13)	97(7)
C(24B) ^b	7600(2)	4590(4)	3344(15)	95(5)
C(25B) ^b	8400(2)	5630(4)	4413(19)	95(5)
C(26B) ^b	8627(18)	3230(4)	4113(17)	95(5)
N(8C) ^b	7560(3)	3960(4)	4310(3)	72(6)
C(23C) ^b	7837(18)	4740(4)	3922(14)	97(7)
C(24C) ^b	7860(2)	3890(5)	3376(19)	95(5)
C(25C) ^b	8550(2)	5200(6)	4420(2)	95(5)
C(26C) ^b	7360(2)	6010(4)	3640(19)	95(5)
C(27)	6119(5)	1138(11)	4067(4)	59(4)
C(28A) ^c	5832(11)	2030(3)	3531(9)	36(8)
C(29A) ^c	5196(12)	2730(3)	3369(10)	73(8)
C(30A) ^c	4939(14)	3690(3)	2802(12)	94(11)
C(31A) ^c	5260(15)	3870(3)	2404(12)	78(9)
C(32A) ^c	5853(14)	3060(3)	2513(10)	66(9)
C(33A) ^c	6116(11)	2160(3)	3100(7)	37(6)
C(28B) ^c	5925(16)	2030(4)	3452(16)	30(11)
C(29B) ^c	5368(17)	3000(3)	3276(13)	48(10)
C(30B) ^c	5150(2)	3830(5)	2673(17)	77(14)
C(31B) ^c	5590(2)	3560(4)	2388(18)	80(15)
C(32B) ^c	6110(2)	2500(4)	2579(13)	81(12)
C(33B) ^c	6354(19)	1630(4)	3174(13)	72(12)
C(40) ^d	9495(6)	-285(19)	4364(3)	149(10)
C(41) ^d	9329(3)	-440(18)	4878(7)	131(10)
C(42) ^d	9834(7)	-160(2)	5513(5)	138(10)

^a Disordered carbon atoms for a bridging pyrazolate ligand; refined with complementary occupancy factors (0.61 and 0.39(4), respectively). ^b Disordered carbon and nitrogen atoms of the *tert*-butylisocyanide ligands; complementary occupancy factors as follows: C(8A)-C(11A) 0.72(2), C(14A)-C(16A) 0.65(3), N(7A)-C(21A) 0.51(2), and N(8A)-C(26A) 0.43(2), N(8B)-C(26B) 0.31(2). ^c Disordered atoms for the phenyl groups; refined with complementary occupancy factors (0.59 and 0.41(5)). ^d A solvent molecule (benzene) was located around a symmetry center; atoms included with a 0.30 occupancy factor.

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2} U_{11} + \dots + 2hka^*b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir(1)	28(1)	52(1)	38(1)	-2(1)	12(1)	-5(1)
Ir(2)	41(1)	49(1)	37(1)	1(1)	14(1)	-13(1)
Cl	45(2)	103(3)	44(2)	7(2)	10(1)	9(2)
N(1)	24(4)	41(6)	41(5)	8(4)	10(4)	-1(4)
N(2)	38(5)	20(5)	37(5)	3(4)	11(4)	6(4)
C(1)	59(7)	24(7)	56(7)	9(5)	39(6)	11(6)
C(2)	45(7)	52(8)	73(8)	21(7)	44(7)	0(6)
C(3)	26(6)	54(8)	75(9)	-1(7)	17(6)	-11(6)
N(3)	32(5)	37(6)	60(6)	-8(5)	13(5)	6(4)
N(4)	40(5)	68(7)	49(6)	-11(5)	8(5)	-4(5)
C(7)	51(7)	47(8)	47(7)	-7(6)	20(6)	-6(7)
N(5)	56(6)	60(8)	58(7)	7(6)	7(5)	3(6)
C(12)	73(8)	52(9)	43(6)	-8(6)	20(6)	-21(7)
N(6)	62(7)	76(8)	65(6)	-15(6)	29(6)	-33(6)
C(13)	43(7)	76(10)	83(9)	-4(8)	21(7)	-33(7)
C(17)	69(8)	39(8)	54(7)	6(6)	-3(7)	-14(7)
C(22)	75(8)	101(12)	47(7)	-26(8)	6(7)	-31(9)
C(27)	76(8)	58(8)	17(5)	-1(5)	0(5)	-25(7)

Table S4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2a**.

	x	y	z	U_{eq}
H(1)	6825	609	6908	50
H(2)	5632	-192	6146	60
H(3)	5454	418	5053	64

Table S5. Full list of Bond lengths [Å] and angles [deg] for **2a**.

Ir(1)-C(7)	1.848(10)
Ir(1)-C(12)	1.874(10)
Ir(1)-N(3)	2.066(8)
Ir(1)-N(1)	2.092(7)
Ir(1)-Cl	2.532(3)
Ir(1)-Ir(2)	2.7112(8)
Ir(2)-C(17)	1.909(11)
Ir(2)-C(22)	1.940(13)
Ir(2)-N(4)	2.059(9)
Ir(2)-N(2)	2.074(8)
Ir(2)-C(27)	2.195(8)
N(1)-C(1)	1.348(8)
N(1)-N(2)	1.350(8)
N(2)-C(3)	1.350(8)
C(1)-C(2)	1.376(8)
C(2)-C(3)	1.372(9)
N(3)-C(4B)	1.350(9)
N(3)-C(4A)	1.360(9)
N(3)-N(4)	1.362(9)
N(4)-C(6B)	1.359(9)
N(4)-C(6A)	1.368(9)
C(4A)-C(5A)	1.383(10)
C(5A)-C(6A)	1.385(10)
C(4B)-C(5B)	1.381(10)
C(5B)-C(6B)	1.382(10)
C(7)-N(5)	1.172(8)
N(5)-C(8A)	1.498(9)
N(5)-C(8B)	1.500(10)
C(8A)-C(11A)	1.519(10)
C(8A)-C(9A)	1.522(10)
C(8A)-C(10A)	1.523(10)
C(8B)-C(11B)	1.524(11)
C(8B)-C(10B)	1.531(11)
C(8B)-C(9B)	1.534(11)
C(12)-N(6)	1.180(8)
N(6)-C(13)	1.491(8)
C(13)-C(16A)	1.515(9)
C(13)-C(15A)	1.521(9)
C(13)-C(15B)	1.521(10)
C(13)-C(14B)	1.526(10)
C(13)-C(14A)	1.528(9)
C(13)-C(16B)	1.533(10)
C(17)-N(7A)	1.173(9)
C(17)-N(7B)	1.199(9)
N(7A)-C(18A)	1.494(10)
C(18A)-C(21A)	1.498(10)
C(18A)-C(20A)	1.501(10)
C(18A)-C(19A)	1.505(10)
N(7B)-C(18B)	1.508(9)
C(18B)-C(19B)	1.520(10)
C(18B)-C(21B)	1.521(10)
C(18B)-C(20B)	1.531(10)
C(22)-N(8A)	1.183(10)
C(22)-N(8C)	1.185(10)
C(22)-N(8B)	1.189(10)
N(8A)-C(23A)	1.497(10)
C(23A)-C(25A)	1.516(10)

C(23A)-C(26A)	1.520(10)
C(23A)-C(24A)	1.527(10)
N(8B)-C(23B)	1.501(10)
C(23B)-C(26B)	1.526(11)
C(23B)-C(25B)	1.532(11)
C(23B)-C(24B)	1.533(11)
N(8C)-C(23C)	1.500(10)
C(23C)-C(26C)	1.524(11)
C(23C)-C(24C)	1.525(11)
C(23C)-C(25C)	1.526(11)
C(27)-C(28A)	1.40(2)
C(27)-C(28B)	1.55(4)
C(28A)-C(33A)	1.419(11)
C(28A)-C(29A)	1.425(11)
C(29A)-C(30A)	1.49(2)
C(30A)-C(31A)	1.41(2)
C(31A)-C(32A)	1.42(2)
C(32A)-C(33A)	1.50(2)
C(28B)-C(33B)	1.418(11)
C(28B)-C(29B)	1.421(11)
C(29B)-C(30B)	1.49(2)
C(30B)-C(31B)	1.42(2)
C(31B)-C(32B)	1.42(2)
C(32B)-C(33B)	1.50(2)
C(40)-C(42) #1	1.4198(8)
C(40)-C(41)	1.4199(9)
C(41)-C(42)	1.4200(9)

C(7)-Ir(1)-C(12)	88.7(5)
C(7)-Ir(1)-N(3)	173.5(3)
C(12)-Ir(1)-N(3)	94.9(4)
C(7)-Ir(1)-N(1)	92.1(4)
C(12)-Ir(1)-N(1)	175.0(4)
N(3)-Ir(1)-N(1)	83.8(3)
C(7)-Ir(1)-Cl	93.6(3)
C(12)-Ir(1)-Cl	94.0(3)
N(3)-Ir(1)-Cl	91.5(2)
N(1)-Ir(1)-Cl	90.9(2)
C(7)-Ir(1)-Ir(2)	103.3(3)
C(12)-Ir(1)-Ir(2)	104.3(3)
N(3)-Ir(1)-Ir(2)	70.6(2)
N(1)-Ir(1)-Ir(2)	70.7(2)
Cl-Ir(1)-Ir(2)	155.14(8)
C(17)-Ir(2)-C(22)	89.5(6)
C(17)-Ir(2)-N(4)	176.0(4)
C(22)-Ir(2)-N(4)	91.4(5)
C(17)-Ir(2)-N(2)	93.0(4)
C(22)-Ir(2)-N(2)	173.2(3)
N(4)-Ir(2)-N(2)	85.6(3)
C(17)-Ir(2)-C(27)	92.3(4)
C(22)-Ir(2)-C(27)	94.4(4)
N(4)-Ir(2)-C(27)	91.6(4)
N(2)-Ir(2)-C(27)	91.8(3)
C(17)-Ir(2)-Ir(1)	104.8(3)
C(22)-Ir(2)-Ir(1)	102.1(3)
N(4)-Ir(2)-Ir(1)	71.2(2)
N(2)-Ir(2)-Ir(1)	71.2(2)
C(27)-Ir(2)-Ir(1)	156.2(3)
C(1)-N(1)-N(2)	110.4(7)

C(1)-N(1)-Ir(1)	140.8(6)
N(2)-N(1)-Ir(1)	108.8(6)
N(1)-N(2)-C(3)	106.2(7)
N(1)-N(2)-Ir(2)	109.4(5)
C(3)-N(2)-Ir(2)	144.4(7)
N(1)-C(1)-C(2)	107.3(8)
C(3)-C(2)-C(1)	106.2(9)
N(2)-C(3)-C(2)	109.9(8)
C(4B)-N(3)-N(4)	108.6(12)
C(4A)-N(3)-N(4)	111.9(10)
C(4B)-N(3)-Ir(1)	138.3(11)
C(4A)-N(3)-Ir(1)	137.1(10)
N(4)-N(3)-Ir(1)	109.4(6)
C(6B)-N(4)-N(3)	113.0(12)
N(3)-N(4)-C(6A)	105.9(10)
C(6B)-N(4)-Ir(2)	135.4(12)
N(3)-N(4)-Ir(2)	108.8(6)
C(6A)-N(4)-Ir(2)	142.5(9)
N(3)-C(4A)-C(5A)	105(2)
C(4A)-C(5A)-C(6A)	108(2)
N(4)-C(6A)-C(5A)	109(2)
N(3)-C(4B)-C(5B)	103(2)
C(4B)-C(5B)-C(6B)	115(2)
N(4)-C(6B)-C(5B)	100(2)
N(5)-C(7)-Ir(1)	176.0(9)
C(7)-N(5)-C(8A)	161.8(11)
C(7)-N(5)-C(8B)	158.0(13)
N(5)-C(8A)-C(11A)	108.1(12)
N(5)-C(8A)-C(9A)	104.5(12)
C(11A)-C(8A)-C(9A)	112.4(11)
N(5)-C(8A)-C(10A)	109.3(13)
C(11A)-C(8A)-C(10A)	112.7(11)
C(9A)-C(8A)-C(10A)	109.5(11)
N(5)-C(8B)-C(11B)	112(2)
N(5)-C(8B)-C(10B)	106(2)
C(11B)-C(8B)-C(10B)	109.5(13)
N(5)-C(8B)-C(9B)	112(2)
C(11B)-C(8B)-C(9B)	110.2(13)
C(10B)-C(8B)-C(9B)	107.4(13)
N(6)-C(12)-Ir(1)	176.8(10)
C(12)-N(6)-C(13)	152.0(11)
N(6)-C(13)-C(16A)	108.1(10)
N(6)-C(13)-C(15A)	102.6(10)
C(16A)-C(13)-C(15A)	112.9(10)
N(6)-C(13)-C(15B)	104.5(13)
N(6)-C(13)-C(14B)	110.2(13)
C(15B)-C(13)-C(14B)	111.3(12)
N(6)-C(13)-C(14A)	109.9(10)
C(16A)-C(13)-C(14A)	112.0(9)
C(15A)-C(13)-C(14A)	111.0(9)
N(6)-C(13)-C(16B)	110.4(14)
C(15B)-C(13)-C(16B)	113.1(12)
C(14B)-C(13)-C(16B)	107.4(11)
N(7A)-C(17)-Ir(2)	156(2)
N(7B)-C(17)-Ir(2)	168(2)
C(17)-N(7A)-C(18A)	179(2)
N(7A)-C(18A)-C(21A)	107(2)
N(7A)-C(18A)-C(20A)	103(2)
C(21A)-C(18A)-C(20A)	116.6(13)

N(7A)-C(18A)-C(19A)	99(2)
C(21A)-C(18A)-C(19A)	114.6(12)
C(20A)-C(18A)-C(19A)	114.8(12)
C(17)-N(7B)-C(18B)	165(2)
N(7B)-C(18B)-C(19B)	108(2)
N(7B)-C(18B)-C(21B)	112(2)
C(19B)-C(18B)-C(21B)	111.9(12)
N(7B)-C(18B)-C(20B)	107.0(14)
C(19B)-C(18B)-C(20B)	107.9(12)
C(21B)-C(18B)-C(20B)	110.0(11)
N(8A)-C(22)-Ir(2)	174(3)
N(8C)-C(22)-Ir(2)	158(3)
N(8B)-C(22)-Ir(2)	160(3)
C(22)-N(8A)-C(23A)	162(4)
N(8A)-C(23A)-C(25A)	106(3)
N(8A)-C(23A)-C(26A)	107(3)
C(25A)-C(23A)-C(26A)	113.6(13)
N(8A)-C(23A)-C(24A)	107(2)
C(25A)-C(23A)-C(24A)	107.7(12)
C(26A)-C(23A)-C(24A)	115.3(13)
C(22)-N(8B)-C(23B)	143(4)
N(8B)-C(23B)-C(26B)	91(2)
N(8B)-C(23B)-C(25B)	121(3)
C(26B)-C(23B)-C(25B)	108.2(14)
N(8B)-C(23B)-C(24B)	114(3)
C(26B)-C(23B)-C(24B)	109.6(14)
C(25B)-C(23B)-C(24B)	110.3(14)
C(22)-N(8C)-C(23C)	164(5)
N(8C)-C(23C)-C(26C)	105(3)
N(8C)-C(23C)-C(24C)	116(4)
C(26C)-C(23C)-C(24C)	108.5(14)
N(8C)-C(23C)-C(25C)	103(4)
C(26C)-C(23C)-C(25C)	111(2)
C(24C)-C(23C)-C(25C)	113(2)
C(28A)-C(27)-Ir(2)	115.1(13)
C(28B)-C(27)-Ir(2)	114(2)
C(27)-C(28A)-C(33A)	122(2)
C(27)-C(28A)-C(29A)	120(2)
C(33A)-C(28A)-C(29A)	118(2)
C(28A)-C(29A)-C(30A)	116(2)
C(31A)-C(30A)-C(29A)	125(2)
C(30A)-C(31A)-C(32A)	120(2)
C(31A)-C(32A)-C(33A)	114(2)
C(28A)-C(33A)-C(32A)	127(2)
C(33B)-C(28B)-C(29B)	134(3)
C(33B)-C(28B)-C(27)	109(2)
C(29B)-C(28B)-C(27)	117(2)
C(28B)-C(29B)-C(30B)	118(3)
C(31B)-C(30B)-C(29B)	112(3)
C(30B)-C(31B)-C(32B)	126(3)
C(31B)-C(32B)-C(33B)	125(3)
C(28B)-C(33B)-C(32B)	105(3)
C(42) ^{#1} -C(40)-C(41)	120.00(4)
C(40)-C(41)-C(42)	120.00(5)
C(40) ^{#1} -C(42)-C(41)	119.99(4)

^{#1} Symmetry transformation used to generate equivalent atoms $-x+2, -y, -z+1$.

Table S6. Elemental analyses for the new complexes

Complex	%C	%H	%N
[{Ir(μ-Pz)(CNBu^t)₂}₂(Cl)(CH₂Ph)] (2)			
Calcd. for C ₃₃ H ₄₉ N ₈ ClIr ₂ · 0.3 C ₆ H ₆	41.99	5.13	11.19
Found	42.23	5.11	11.13
[(CNBu^t)₂(Cl)Ir(μ-Pz)₂Ir{CH(Me)COOMe}(CNBu^t)₂] (3).			
Calcd. for C ₃₀ H ₄₉ N ₈ O ₂ ClIr ₂	37.01	5.07	11.51
Found	37.31	4.95	10.71
[{Ir(μ-Pz)(CH₂Ph)(CNBu^t)₂}₂(μ-Cl)]Cl (4)			
Calcd. for C ₄₀ H ₅₆ N ₈ Cl ₂ Ir ₂ · H ₂ O	42.80	5.21	9.98
Found	42.57	5.13	9.87
[(CNBu^t)₂(MeCO₂CH₂)Ir(μ-Pz)₂(μ-Cl)Ir(CH₂Ph)(CNBu^t)₂]Cl (5)			
Calcd. for C ₃₆ H ₅₄ N ₈ O ₂ Cl ₂ Ir ₂ · 2 H ₂ O	38.53	5.20	9.98
Found	38.00	5.30	9.75

