Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9b**.

	x	y	z	U(eq)
H(1A)	508	469	9224	35
H(1B)	1894	600	9861	35
H(2A)	1140	788	11500	73
H(3A)	-763	359	10827	108
H(3B)	-287	538	12171	108
H(4A)	52	1691	7918	71
H(4B)	1056	1573	7169	71
H(5A)	-727	1395	5558	130
H(6A)	-1755	1885	6909	282
H(6B)	-2455	1773	5485	282
H(7A)	-943	1119	10414	27
H(7B)	-899	1474	9854	27
H(8A)	-2075	1284	7764	67
H(9A)	-1650	810	7087	60
H(9B)	-1458	676	8522	60
H(7'A)	-804	1307	10196	72
H(7'B)	-1437	1464	8820	72
H(8'A)	-1559	817	9374	42
H(9'A)	-2034	1065	6846	27
H(9'B)	-1621	699	7197	27
H(11A)	5658	1448	9052	68
H(12A)	7081	1862	9125	93
H(13A)	6442	2368	9243	98
H(14A)	4156	2480	9021	118
H(15A)	2756	2066	8947	77
H(17A)	2143	1368	12515	53
H(18A)	762	1459	13900	62
H(19A)	-619	1867	13618	79
H(20A)	-882	2174	11793	75
H(21A)	385	2065	10339	60
H(23A)	5031	787	10496	49
H(24A)	7228	851	11224	56
H(25A)	8008	1290	12421	57
H(26A)	6620	1669	12854	73
H(27A)	4360	1588	12182	70
H(29A)	2663	173	8591	61
H(30A)	3987	-262	8668	80
H(31A)	5936	-220	8213	88
H(32A)	6652	266	7650	93
H(33A)	5360	710	7581	65
H(35A)	-12	62	7210	60
H(36A)	-2083	-114	6235	71
H(37A)	-3267	139	4426	80
H(38A)	-2380	573	3662	74
H(39A)	-280	749	4634	66
H(41A)	2213	649	4532	86
H(42A)	3937	602	3552	117
H(43A)	5703	928	4063	105
H(44A)	5694	1327	5531	77
H(45A)	3928	1395	6420	65
H(47A)	2644	2235	13154	125
H(48A)	3736	2363	11835	131

H(49A)	6176	2436	12295	234
H(50A)	6901	2362	14448	208
H(51A)	5978	2179	15871	173
H(52A)	2436	2099	14842	337
H(52B)	3343	2268	16016	337
H(52C)	3511	1906	15792	337

Table 1. Crystal data and structure refinement for **12**.

Identification code	ccd179	
Empirical formula	C36 H42 Ir N3	
Formula weight	708.93	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.9408(5) Å	α= 90°.
	b = 14.6602(7) Å	β= 98.0250(10)°.
	c = 20.4426(9) Å	γ = 90°.
Volume	3246.8(3) Å^3	
Z	4	
Density (calculated)	1.450 Mg/m^3	
Absorption coefficient	4.139 mm^{-1}	
F(000)	1424	
Crystal size	0.12 x 0.17 x 0.17 mm^3	
Theta range for data collection	1.72 to 26.57°.	
Index ranges	-12<=h<=13, -18<=k<=17, -25<=l<=24	
Reflections collected	15979	
Independent reflections	6434 [R(int) = 0.0374]	
Completeness to theta = 26.57°	94.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6434 / 0 / 361	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0689	
R indices (all data)	R1 = 0.0554, wR2 = 0.0749	
Largest diff. peak and hole	0.862 and -0.789 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir	3007(1)	329(1)	2474(1)	37(1)
N(1)	1431(4)	-569(2)	1245(2)	44(1)
C(1)	4590(6)	-361(5)	2204(4)	84(2)
N(2)	793(4)	1103(2)	3118(2)	41(1)
C(2)	5372(10)	44(8)	1889(7)	202(7)
N(3)	3423(4)	2091(3)	1659(2)	42(1)
C(3)	5873(11)	106(7)	1413(7)	204(8)
C(4)	2887(6)	-922(3)	3029(3)	61(2)
C(5)	1705(7)	-1114(4)	3247(3)	71(2)
C(6)	1434(9)	-1166(4)	3851(4)	102(3)
C(7)	4169(5)	840(4)	3341(3)	68(2)
C(8)	4291(5)	1833(5)	3406(3)	72(2)
C(9)	3899(6)	2381(5)	3802(4)	84(2)
C(10)	2005(5)	-245(3)	1704(2)	41(1)
C(11)	779(5)	-914(3)	660(2)	40(1)
C(12)	-447(5)	-1177(3)	656(3)	57(2)
C(13)	-1037(6)	-1503(4)	47(4)	82(2)
C(14)	-418(9)	-1581(5)	-487(4)	92(3)
C(15)	782(8)	-1327(4)	-448(3)	80(2)
C(16)	1423(5)	-994(3)	118(2)	50(1)
C(17)	-1053(6)	-1112(5)	1258(4)	98(3)
C(18)	2741(6)	-715(4)	176(3)	77(2)
C(19)	1600(4)	840(3)	2862(2)	35(1)
C(20)	-260(4)	1400(3)	3380(2)	36(1)
C(21)	-234(4)	1425(3)	4059(2)	39(1)
C(22)	-1300(5)	1723(3)	4288(2)	43(1)
C(23)	-2326(5)	1974(3)	3865(3)	46(1)
C(24)	-2322(5)	1944(3)	3193(3)	47(1)
C(25)	-1284(4)	1647(3)	2931(2)	40(1)
C(26)	-1263(6)	1581(4)	2195(3)	71(2)
C(27)	868(5)	1135(4)	4521(3)	60(2)
C(28)	3296(4)	1448(3)	1970(2)	39(1)
C(29)	3409(4)	2933(3)	1327(2)	37(1)
C(30)	4121(5)	3035(3)	818(3)	47(1)
C(31)	4055(5)	3868(4)	494(3)	50(1)
C(32)	3328(5)	4564(3)	676(3)	54(1)
C(33)	2650(5)	4447(3)	1187(3)	51(1)
C(34)	2668(4)	3631(3)	1531(2)	43(1)
C(35)	4928(6)	2287(4)	636(3)	72(2)
C(36)	1976(5)	3495(4)	2103(3)	65(2)

Table 3. Bond lengths [Å] and angles [°] for **12**.

Ir-C(19)	1.975(5)
Ir-C(10)	1.976(5)
Ir-C(28)	1.986(5)
Ir-C(1)	2.144(6)
Ir-C(7)	2.166(5)
Ir-C(4)	2.171(5)
N(1)-C(10)	1.156(6)
N(1)-C(11)	1.399(6)
C(1)-C(2)	1.286(11)
N(2)-C(19)	1.154(5)
N(2)-C(20)	1.406(6)
C(2)-C(3)	1.185(13)
N(3)-C(28)	1.156(6)
N(3)-C(29)	1.407(6)
C(4)-C(5)	1.453(8)
C(5)-C(6)	1.312(8)
C(7)-C(8)	1.466(8)
C(8)-C(9)	1.258(8)
C(11)-C(12)	1.395(7)
C(11)-C(16)	1.397(6)
C(12)-C(13)	1.403(9)
C(12)-C(17)	1.481(8)
C(13)-C(14)	1.368(10)
C(14)-C(15)	1.356(10)
C(15)-C(16)	1.357(8)
C(16)-C(18)	1.488(8)
C(20)-C(21)	1.384(6)
C(20)-C(25)	1.393(6)
C(21)-C(22)	1.386(6)
C(21)-C(27)	1.486(7)
C(22)-C(23)	1.368(7)
C(23)-C(24)	1.376(7)
C(24)-C(25)	1.390(6)
C(25)-C(26)	1.511(7)
C(29)-C(30)	1.393(6)
C(29)-C(34)	1.404(6)
C(30)-C(31)	1.385(7)
C(30)-C(35)	1.487(7)
C(31)-C(32)	1.377(7)
C(32)-C(33)	1.374(8)
C(33)-C(34)	1.387(7)
C(34)-C(36)	1.493(7)
C(19)-Ir-C(10)	96.03(18)
C(19)-Ir-C(28)	94.85(18)
C(10)-Ir-C(28)	92.82(18)
C(19)-Ir-C(1)	170.2(2)
C(10)-Ir-C(1)	88.4(3)
C(28)-Ir-C(1)	93.7(2)
C(19)-Ir-C(7)	86.7(2)
C(10)-Ir-C(7)	174.95(19)
C(28)-Ir-C(7)	91.2(2)
C(1)-Ir-C(7)	88.3(3)
C(19)-Ir-C(4)	90.2(2)
C(10)-Ir-C(4)	89.4(2)
C(28)-Ir-C(4)	174.2(2)

C(1)-Ir-C(4)	81.1(2)
C(7)-Ir-C(4)	86.3(2)
C(10)-N(1)-C(11)	175.6(5)
C(2)-C(1)-Ir	121.9(6)
C(19)-N(2)-C(20)	175.0(5)
C(3)-C(2)-C(1)	149.6(18)
C(28)-N(3)-C(29)	170.4(5)
C(5)-C(4)-Ir	116.4(4)
C(6)-C(5)-C(4)	128.9(7)
C(8)-C(7)-Ir	117.0(4)
C(9)-C(8)-C(7)	131.1(7)
N(1)-C(10)-Ir	178.6(4)
C(12)-C(11)-C(16)	124.3(5)
C(12)-C(11)-N(1)	118.7(5)
C(16)-C(11)-N(1)	117.0(5)
C(11)-C(12)-C(13)	115.0(6)
C(11)-C(12)-C(17)	121.3(6)
C(13)-C(12)-C(17)	123.7(6)
C(14)-C(13)-C(12)	121.3(7)
C(15)-C(14)-C(13)	120.8(7)
C(16)-C(15)-C(14)	122.0(7)
C(15)-C(16)-C(11)	116.6(6)
C(15)-C(16)-C(18)	123.1(6)
C(11)-C(16)-C(18)	120.3(5)
N(2)-C(19)-Ir	176.1(4)
C(21)-C(20)-C(25)	123.7(4)
C(21)-C(20)-N(2)	119.2(4)
C(25)-C(20)-N(2)	117.1(4)
C(20)-C(21)-C(22)	116.5(4)
C(20)-C(21)-C(27)	122.0(4)
C(22)-C(21)-C(27)	121.5(4)
C(23)-C(22)-C(21)	121.8(5)
C(22)-C(23)-C(24)	120.3(5)
C(23)-C(24)-C(25)	120.7(5)
C(24)-C(25)-C(20)	117.0(4)
C(24)-C(25)-C(26)	122.0(5)
C(20)-C(25)-C(26)	121.1(4)
N(3)-C(28)-Ir	177.3(4)
C(30)-C(29)-C(34)	123.3(4)
C(30)-C(29)-N(3)	119.0(4)
C(34)-C(29)-N(3)	117.6(4)
C(31)-C(30)-C(29)	117.1(5)
C(31)-C(30)-C(35)	121.6(5)
C(29)-C(30)-C(35)	121.4(4)
C(32)-C(31)-C(30)	121.2(5)
C(33)-C(32)-C(31)	120.4(5)
C(32)-C(33)-C(34)	121.4(5)
C(33)-C(34)-C(29)	116.5(5)
C(33)-C(34)-C(36)	122.6(5)
C(29)-C(34)-C(36)	120.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir	38(1)	40(1)	34(1)	3(1)	6(1)	11(1)
N(1)	62(3)	38(2)	33(2)	2(2)	11(2)	11(2)
C(1)	66(4)	112(6)	81(5)	31(4)	30(4)	47(4)
N(2)	45(2)	37(2)	43(2)	2(2)	16(2)	6(2)
C(2)	148(9)	194(11)	302(17)	162(11)	160(11)	135(9)
N(3)	41(2)	44(2)	39(2)	2(2)	6(2)	-1(2)
C(3)	183(11)	135(8)	342(18)	143(10)	204(13)	111(8)
C(4)	94(5)	42(3)	44(3)	5(3)	9(3)	21(3)
C(5)	119(6)	43(3)	54(4)	10(3)	22(4)	-1(3)
C(6)	175(8)	63(4)	74(5)	12(4)	42(5)	-11(5)
C(7)	58(4)	69(4)	66(4)	13(3)	-24(3)	6(3)
C(8)	47(4)	105(5)	60(4)	-8(4)	-9(3)	-2(3)
C(9)	74(5)	89(5)	85(5)	-16(4)	-4(4)	-17(4)
C(10)	55(3)	36(3)	34(3)	2(2)	16(2)	13(2)
C(11)	53(3)	34(2)	33(3)	0(2)	4(2)	6(2)
C(12)	49(3)	35(3)	87(5)	6(3)	8(3)	7(2)
C(13)	62(4)	40(3)	133(7)	-3(4)	-27(4)	-1(3)
C(14)	124(7)	58(4)	76(5)	-6(4)	-46(5)	12(4)
C(15)	144(7)	58(4)	34(3)	0(3)	-2(4)	17(4)
C(16)	67(4)	48(3)	35(3)	8(2)	10(3)	11(3)
C(17)	85(5)	76(5)	148(7)	2(5)	70(5)	3(4)
C(18)	86(5)	84(4)	69(4)	6(4)	41(4)	10(4)
C(19)	46(3)	31(2)	29(2)	-1(2)	2(2)	-3(2)
C(20)	40(3)	29(2)	43(3)	0(2)	16(2)	3(2)
C(21)	45(3)	36(2)	37(3)	-5(2)	10(2)	-3(2)
C(22)	55(3)	41(3)	36(3)	-8(2)	18(2)	-6(2)
C(23)	45(3)	40(3)	56(4)	-6(2)	21(3)	2(2)
C(24)	45(3)	47(3)	49(3)	1(2)	7(2)	5(2)
C(25)	53(3)	32(2)	36(3)	4(2)	12(2)	5(2)
C(26)	94(5)	81(4)	39(3)	13(3)	13(3)	33(4)
C(27)	60(4)	69(4)	50(3)	-2(3)	0(3)	3(3)
C(28)	30(2)	47(3)	41(3)	-4(2)	5(2)	5(2)
C(29)	33(2)	39(2)	37(3)	-1(2)	-1(2)	-1(2)
C(30)	44(3)	48(3)	48(3)	3(2)	5(2)	6(2)
C(31)	49(3)	57(3)	44(3)	10(3)	5(2)	-9(3)
C(32)	60(3)	42(3)	53(3)	6(3)	-9(3)	-7(3)
C(33)	53(3)	38(3)	58(4)	-8(2)	-6(3)	1(2)
C(34)	40(3)	47(3)	41(3)	-7(2)	-1(2)	-4(2)
C(35)	79(4)	76(4)	68(4)	14(3)	33(3)	24(4)
C(36)	67(4)	65(4)	67(4)	-2(3)	22(3)	8(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **12**.

	x	y	z	U(eq)
H(1A)	5049	-598	2609	101
H(1B)	4286	-886	1941	101
H(2A)	5702	511	2168	243
H(3A)	5681	-301	1065	245
H(3B)	6458	560	1388	245
H(4A)	3091	-1428	2758	73
H(4B)	3511	-901	3416	73
H(5A)	1051	-1214	2912	85
H(6A)	2046	-1074	4209	122
H(6B)	631	-1296	3922	122
H(7A)	3849	610	3728	81
H(7B)	4988	585	3345	81
H(8A)	4735	2105	3102	87
H(9A)	3446	2166	4122	101
H(9B)	4062	3002	3774	101
H(13A)	-1864	-1670	7	99
H(14A)	-826	-1811	-882	110
H(15A)	1178	-1382	-820	96
H(17A)	-479	-869	1614	147
H(17B)	-1315	-1707	1376	147
H(17C)	-1756	-716	1175	147
H(18A)	3041	-818	-238	115
H(18B)	3220	-1067	515	115
H(18C)	2814	-79	286	115
H(22A)	-1318	1752	4741	52
H(23A)	-3030	2167	4033	55
H(24A)	-3021	2123	2910	57
H(26A)	-465	1374	2114	107
H(26B)	-1428	2170	1997	107
H(26C)	-1881	1156	2007	107
H(27A)	702	1196	4967	90
H(27B)	1559	1513	4457	90
H(27C)	1056	510	4436	90
H(31A)	4510	3958	148	60
H(32A)	3295	5117	451	64
H(33A)	2168	4926	1305	61
H(35A)	5342	2481	276	109
H(35B)	4434	1759	506	109
H(35C)	5528	2138	1009	109
H(36A)	1529	4041	2175	98
H(36B)	2547	3359	2491	98
H(36C)	1408	2998	2011	98