Table 1. Crystal data and structure refinement for C16 H21 Cl3 Ir N O5.

Identification code	irohpym	
Empirical formula	C16 H21 Cl3 Ir N O5	
Formula weight	605.89	
Temperature	128(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.7108(5) Å	α= 90°.
	b = 18.4718(12) Å	β= 93.3430(10)°.
	c = 14.8523(10) Å	γ = 90°.
Volume	2111.8(2) $Å^3$	
Z	4	
Density (calculated)	1.906 Mg/m^3	
Absorption coefficient	6.726 mm^{-1}	
F(000)	1168	
Crystal size	0.24 x 0.18 x 0.10 mm^3	
Theta range for data collection	1.76 to 27.50°.	
Index ranges	-9<=h<=9, -24<=k<=19, -17<=l<=19	
Reflections collected	12793	
Independent reflections	4724 [R(int) = 0.0305]	
Completeness to theta = 27.50°	97.6 %	
Transmission factors	min/max ratio: 0.736	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4724 / 0 / 240	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0207, wR2 = 0.0502	
R indices (all data)	R1 = 0.0242, wR2 = 0.0512	
Largest diff. peak and hole	1.116 and -0.537 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C16 H21 Cl3 Ir N O5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	2892(1)	1584(1)	1029(1)	16(1)
Cl(1)	1963(2)	10421(1)	4320(1)	61(1)
Cl(2)	4766(1)	9618(1)	3605(1)	53(1)
Cl(3)	1214(1)	9248(1)	3084(1)	55(1)
O(1)	4781(2)	2320(1)	1262(1)	19(1)
O(2)	4085(2)	1045(1)	60(1)	20(1)
O(3)	1784(2)	2107(1)	2032(1)	20(1)
O(4)	987(2)	844(1)	841(1)	19(1)
O(5)	3978(2)	938(1)	1999(1)	23(1)
N(1)	1754(3)	2238(1)	51(1)	17(1)
C(1)	7420(4)	2907(2)	1090(2)	31(1)
C(2)	6183(3)	2306(2)	845(2)	21(1)
C(3)	6597(4)	1807(2)	185(2)	25(1)
C(4)	5594(4)	1234(2)	-172(2)	23(1)
C(5)	6286(4)	774(2)	-909(2)	31(1)
C(6)	500(4)	1833(2)	2420(2)	23(1)
C(7)	-201(3)	780(2)	1401(2)	22(1)
C(8)	-432(4)	1218(2)	2154(2)	26(1)
C(9)	1024(4)	3409(2)	-525(2)	28(1)
C(10)	1034(3)	1947(2)	-718(2)	22(1)
C(11)	293(4)	3115(2)	-1316(2)	29(1)
C(12)	1738(3)	2961(2)	138(2)	22(1)
C(13)	286(3)	2369(2)	-1401(2)	26(1)
C(14)	2663(4)	9961(2)	3370(2)	38(1)
C(15)	-1427(4)	161(2)	1208(2)	30(1)
C(16)	36(4)	2240(2)	3246(2)	34(1)

Table 3. Bond lengths [Å] and angles [°] for C16 H21 Cl3 Ir N O5.

Ir(1)-O(1)	2.0075(17)
Ir(1)-O(3)	2.0081(18)
Ir(1)-O(4)	2.0138(18)
Ir(1)-O(5)	2.0148(18)
Ir(1)-O(2)	2.0153(18)
Ir(1)-N(1)	2.047(2)
Cl(1)-C(14)	1.759(4)
Cl(2)-C(14)	1.757(4)
Cl(3)-C(14)	1.763(3)
O(1)-C(2)	1.277(3)
O(2)-C(4)	1.281(3)
O(3)-C(6)	1.278(3)
O(4)-C(7)	1.278(3)
N(1)-C(12)	1.341(3)
N(1)-C(10)	1.352(3)
C(1)-C(2)	1.495(4)
C(2)-C(3)	1.397(4)
C(3)-C(4)	1.397(4)
C(4)-C(5)	1.506(4)
C(6)-C(8)	1.390(4)
C(6)-C(16)	1.500(4)
C(7)-C(8)	1.400(4)
C(7)-C(15)	1.500(4)
C(9)-C(12)	1.377(4)
C(9)-C(11)	1.384(4)
C(10)-C(13)	1.377(4)
C(11)-C(13)	1.385(4)

O(1)-Ir(1)-O(3)	83.24(8)
O(1)-Ir(1)-O(4)	178.05(7)
O(3)-Ir(1)-O(4)	95.21(7)
O(1)-Ir(1)-O(5)	90.64(7)
O(3)-Ir(1)-O(5)	86.09(8)
O(4)-Ir(1)-O(5)	88.07(7)

O(1)-Ir(1)-O(2)	95.79(7)
O(3)-Ir(1)-O(2)	177.58(7)
O(4)-Ir(1)-O(2)	85.71(7)
O(5)-Ir(1)-O(2)	91.71(7)
O(1)-Ir(1)-N(1)	89.95(8)
O(3)-Ir(1)-N(1)	93.39(8)
O(4)-Ir(1)-N(1)	91.32(8)
O(5)-Ir(1)-N(1)	179.16(8)
O(2)-Ir(1)-N(1)	88.82(8)
C(2)-O(1)-Ir(1)	121.92(18)
C(4)-O(2)-Ir(1)	121.19(18)
C(6)-O(3)-Ir(1)	121.20(18)
C(7)-O(4)-Ir(1)	121.20(17)
C(12)-N(1)-C(10)	118.1(2)
C(12)-N(1)-Ir(1)	121.65(18)
C(10)-N(1)-Ir(1)	120.22(18)
O(1)-C(2)-C(3)	126.1(3)
O(1)-C(2)-C(1)	114.4(3)
C(3)-C(2)-C(1)	119.5(3)
C(2)-C(3)-C(4)	128.5(3)
O(2)-C(4)-C(3)	126.5(3)
O(2)-C(4)-C(5)	114.1(3)
C(3)-C(4)-C(5)	119.4(3)
O(3)-C(6)-C(8)	126.6(3)
O(3)-C(6)-C(16)	113.5(3)
C(8)-C(6)-C(16)	119.9(3)
O(4)-C(7)-C(8)	126.5(3)
O(4)-C(7)-C(15)	114.5(2)
C(8)-C(7)-C(15)	119.0(3)
C(6)-C(8)-C(7)	127.8(3)
C(12)-C(9)-C(11)	119.9(3)
N(1)-C(10)-C(13)	122.1(3)
C(9)-C(11)-C(13)	117.8(3)
N(1)-C(12)-C(9)	122.3(3)
C(10)-C(13)-C(11)	119.8(3)
Cl(2)-C(14)-Cl(1)	109.77(18)

Cl(2)-C(14)-Cl(3)	110.0(2)
Cl(1)-C(14)-Cl(3)	109.55(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C16 H21 Cl3 Ir N O5. 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(1)	18(1)	15(1)	14(1)	-1(1)	1(1)	-1(1)
Cl(1)	71(1)	68(1)	44(1)	-7(1)	6(1)	-9(1)
Cl(2)	50(1)	54(1)	55(1)	22(1)	-7(1)	-1(1)
Cl(3)	66(1)	45(1)	51(1)	11(1)	-18(1)	-23(1)
O(1)	20(1)	19(1)	19(1)	0(1)	3(1)	-2(1)
O(2)	23(1)	20(1)	18(1)	-2(1)	4(1)	1(1)
O(3)	21(1)	22(1)	18(1)	-3(1)	3(1)	-2(1)
O(4)	22(1)	18(1)	19(1)	-1(1)	3(1)	-3(1)
O(5)	27(1)	21(1)	20(1)	2(1)	0(1)	3(1)
N(1)	17(1)	19(1)	16(1)	-1(1)	4(1)	0(1)
C(1)	25(1)	30(2)	39(2)	-2(1)	1(1)	-7(1)
C(2)	19(1)	21(1)	23(2)	7(1)	1(1)	0(1)
C(3)	21(1)	25(2)	28(2)	1(1)	5(1)	1(1)
C(4)	28(2)	24(2)	16(1)	6(1)	2(1)	7(1)
C(5)	34(2)	30(2)	30(2)	-6(1)	11(1)	4(1)
C(6)	20(1)	28(2)	22(2)	-3(1)	2(1)	4(1)
C(7)	21(1)	22(2)	21(1)	4(1)	-2(1)	-2(1)
C(8)	25(1)	30(2)	24(2)	-3(1)	6(1)	-6(1)
C(9)	36(2)	18(2)	30(2)	3(1)	1(1)	7(1)
C(10)	22(1)	22(2)	22(2)	-1(1)	3(1)	-5(1)
C(11)	30(2)	32(2)	26(2)	8(1)	1(1)	5(1)
C(12)	26(1)	19(1)	21(1)	-3(1)	3(1)	0(1)
C(13)	25(1)	36(2)	18(2)	-1(1)	-2(1)	-3(1)
C(14)	46(2)	35(2)	33(2)	10(2)	-3(2)	-9(2)
C(15)	29(2)	29(2)	31(2)	-1(1)	1(1)	-8(1)
C(16)	31(2)	44(2)	30(2)	-16(2)	12(1)	-8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C16 H21 Cl3 Ir N O5.

	x	y	z	U(eq)
H(5)	4818	713	1796	34
H(1A)	7149	3327	703	47
H(1B)	8611	2746	1004	47
H(1C)	7312	3042	1722	47
H(3)	7706	1865	-53	30
H(5A)	6373	270	-706	46
H(5B)	7438	950	-1050	46
H(5C)	5496	804	-1449	46
H(8)	-1334	1078	2527	31
H(9)	1032	3919	-440	33
H(10)	1044	1436	-791	26
H(11)	-188	3416	-1786	35
H(12)	2238	3171	676	26
H(13)	-232	2148	-1928	32
H(14)	2682	10306	2852	46
H(15A)	-1165	-67	636	45
H(15B)	-2624	341	1167	45
H(15C)	-1292	-196	1696	45
H(16A)	955	2176	3723	52
H(16B)	-1064	2055	3453	52
H(16C)	-88	2756	3102	52