Electronic Supplementary Material (ESI) for MedChemComm.
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Supplementary Information for: "Transition Metal Piano-Stool Complexes with Activity Against S. Aureus and MRSA: It is past time to truly think outside of the box."

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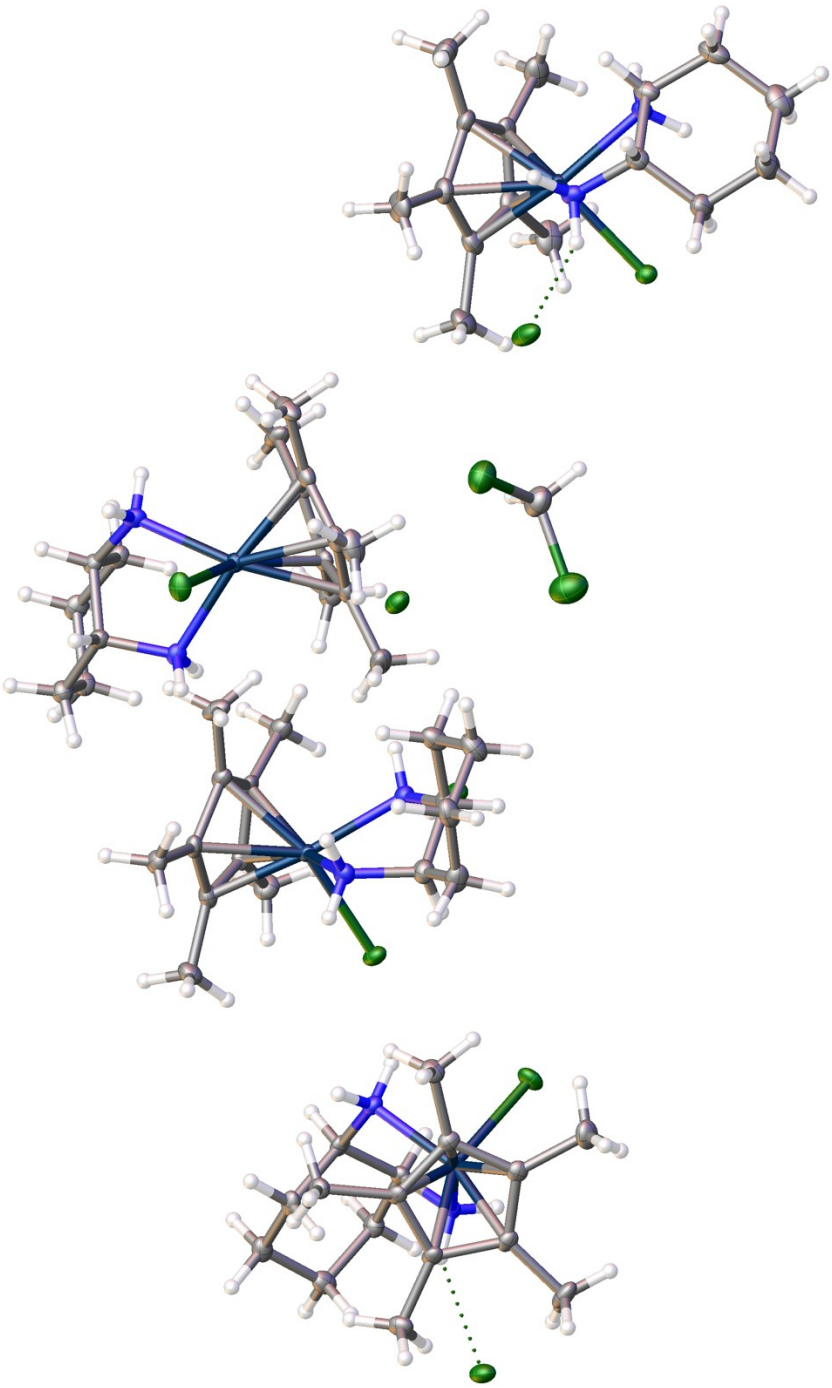
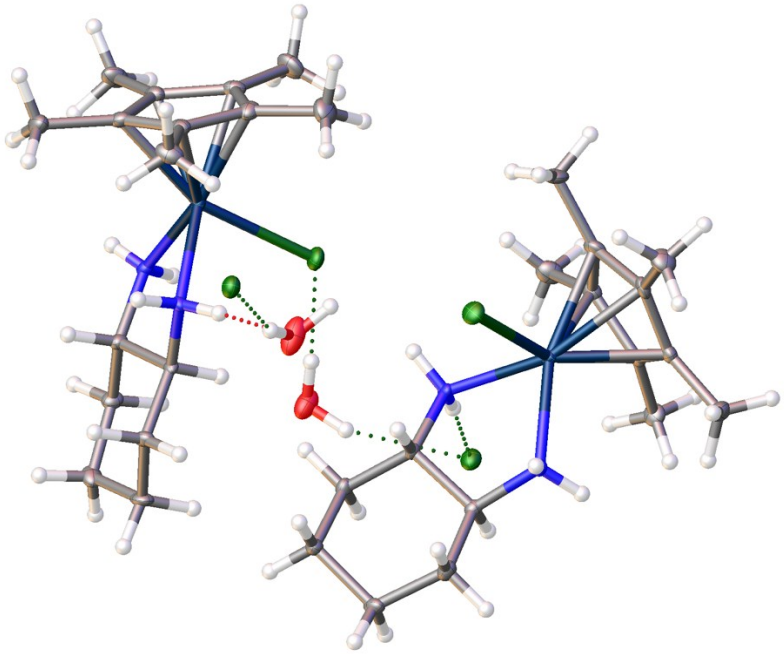


Entry 2S. Asymmetric Unit for [Cp*IrCl(trans(+)-1,2-diaminocyclohexane)]Cl CCDC1901125



Entry 3S. SAFETY STUDY IN MICE OF AN AGENT WITH POTENTIAL AS AN ANTIINFECTIVE

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ABSTRACT

In vitro experiments resulted in the discovery that a series of iridium (Ir) ethylene diamine l complexes exhibited antimicrobial activity against *Staphylococcus aureus* and methicillin-resistant *S. aureus* at 1-10 µg/ml. For the initial toxicity screening, we examined one of the most active compounds; 3-Ir. The safety study was conducted in groups of adult male mice given a single dose of 5 mg/kg by intravenous (IV) administration. Mice were examined for a series of behavioral indices using a modified functional observational battery at 1, 4 and 6 hr, and 1, 2, 7, 9, 12 and 14 days post-dosing (Tegeria and Balster, Tox Sci 22:240). Body weight was measured and recorded at the time of each assessment. Blood and tissue samples were collected at 24 hr, 4 days and 14 days for clinical pathology and histopathological assessment. Of the animals receiving 3-Ir, 5/19 animals showed immediate signs of distress following dosing. Signs of distress ceased within one minute and animals appeared to have normal appearance, activity and locomotion within 5 minutes. No subsequent evidence of neurobehavioral, clinical or histopathological detriments was noted. The doses tested in this IV safety study are within the mg/kg range of currently used drugs. In circumstances such as used here, neurobehavioral or pathological detriments after single administration would be unlikely. These compounds, therefore, have potential to be a useful new class of antimicrobial agents. (Supported by the Virginia Tech Foundation)

PURPOSE:

- Merola/Falkinham discovered a series of metal complexes of amino acids with antimicrobial activity at very low concentrations (1-10 µg/ml) against G^+, G^- and mycobacteria.
- Further development as potential therapeutic agents requires safety be comprehensively assessed.

METHODS:

- *Test Compound Characterization:* analytically pure as evidenced by NMR spectroscopy, mass spectroscopy and other laboratory techniques. Soluble in saline, pH 6.5-7. Not cytotoxic to Vero cells at a concentration of 250 µg/ml.
- *Animal Dosing*: Outbred mice were given one IV dose of 2.5 or 5 mg/kg test compound.
- *Neurobehavioral Assessment:* 1-3 day before, 1, 4, 6 hr, 1, 2, 7, 9, 12 and 14 days after dosing.
  Body weights were evaluated as present/absent or normal/abnormal locomotor activity, posture, coat and tail condition, respiration, excretion and secretions, reflexes.
- *Pathology:* Blood samples collected for standard clinical pathology panel that included blood chemistry; histopathological examination of heart, kidney, liver, and other organs assessed.

RESULTS:

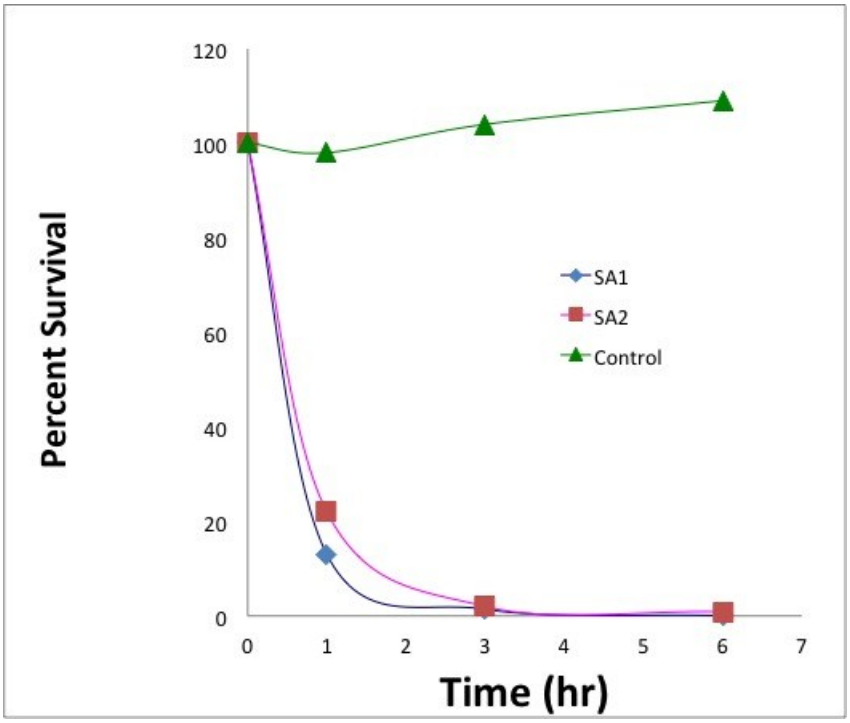
- *At Dosing*: 5/19 dosed mice showed abnormal respirations, tremors, jumping, or crouched posture immediately following dosing. These ceased within one minute, and all had normal appearance, activity and locomotion in < 5 min.
- *Behavioral Assessment*: No significant differences between groups for all variables except coat condition, which occurred at 12 and 14 days post-dosing. In the absence of significant differences of other variables, the statistician (Dr. S. Werre) suggested that this was a chance occurrence.

- *Clinical Pathology*: No effect on erythrocytes and indices, white blood cell or platelet concentrations noted. Most parameters of clinical pathology were not affected by treatment. Non-adverse effects of treatment included minimal increases in sodium and chloride and decreases in potassium at 4 and 14 days after IV administration of the compound at 2.5 mg/kg and 5.0 mg/kg concentrations. These non-adverse effects are biologically insignificant, so do not have toxicologic significance.
- *Histopathology*: No significant treatment-related lesions were noted at any of the sacrifice intervals (post-dosing days 1, 4 or 14). There were a few background lesions noted in controls or in both controls and high-dose rats. Given the focal nature and low incidence of these, they are considered background lesions, and not of toxicologic significance.

CONCLUSIONS:

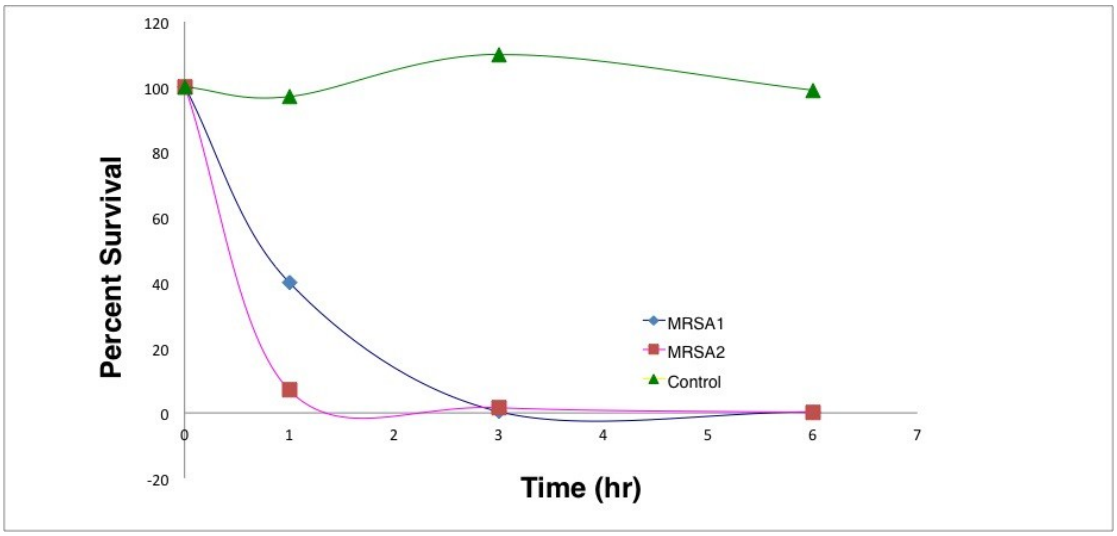
- IV administration of drugs results in immediate high blood concentrations. Signs that appeared immediately did not appear in all mice, and disappeared rapidly. No longer-term toxic effects were evident.
- The iridium compound administered to mice as a single IV injection was generally nontoxic, as long as the dose was below 5.0 mg/kg, with neurobehavioral or pathological detriments after a single administration unlikely.

Figure : Time-related effect of <10 µg/ml iridium-containing agent on survival of *Staphlococcus aureus*



This one is for S. aureus.

Figure 2: Time-related effect of <10 µg/ml iridium-containing agent on survival of methicillin resistant *Staphlococcus aureus* (MRSA)



Complex structure

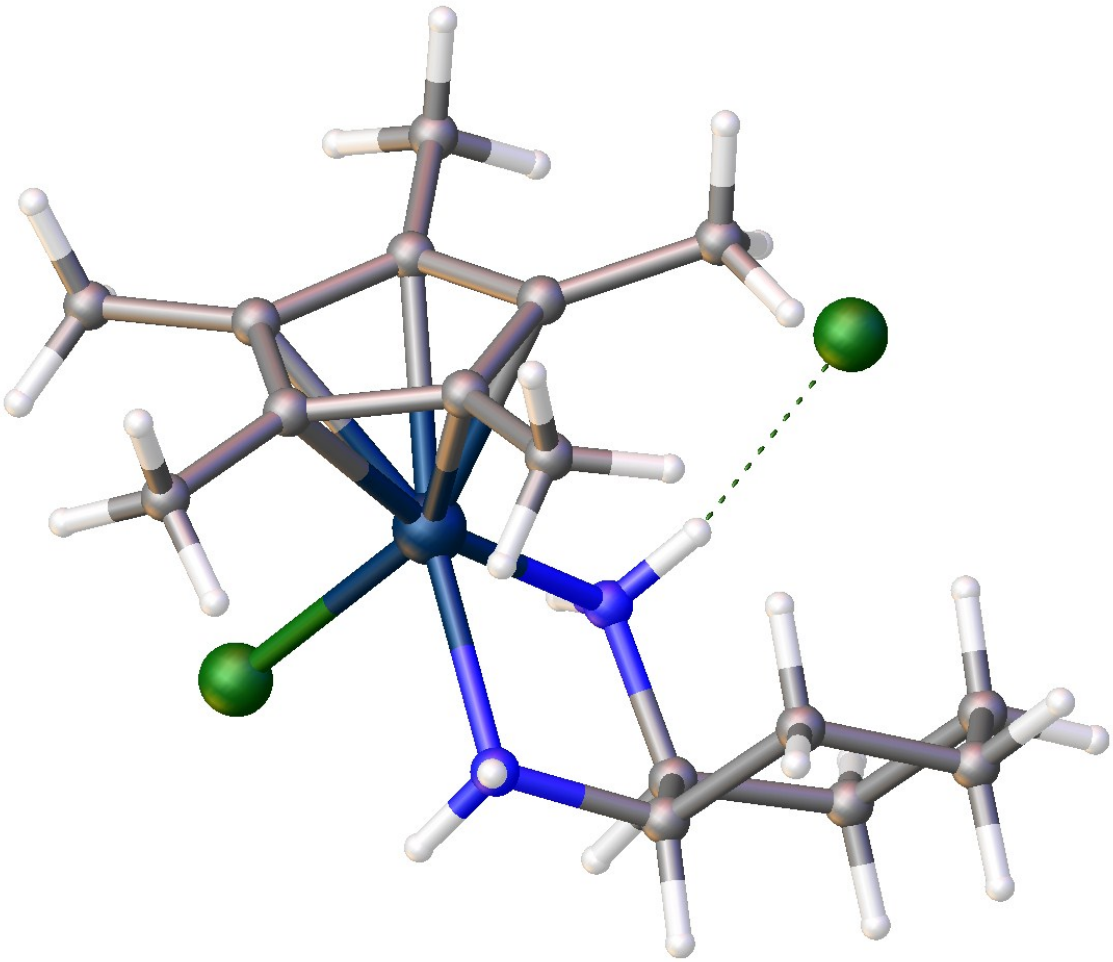
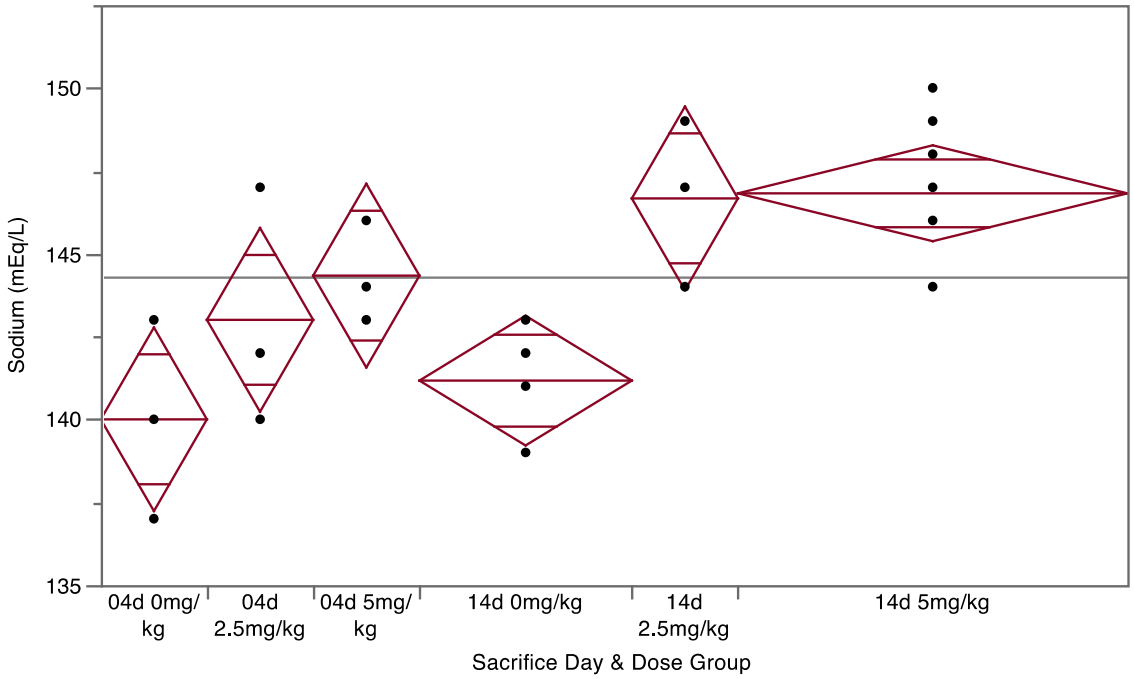
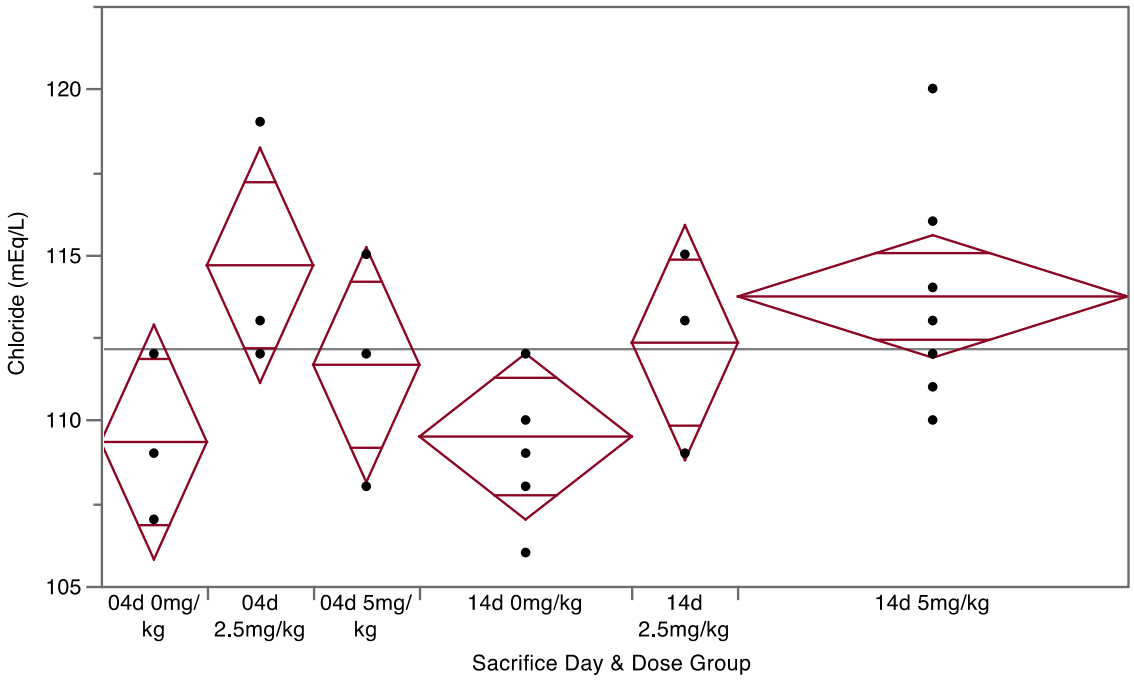
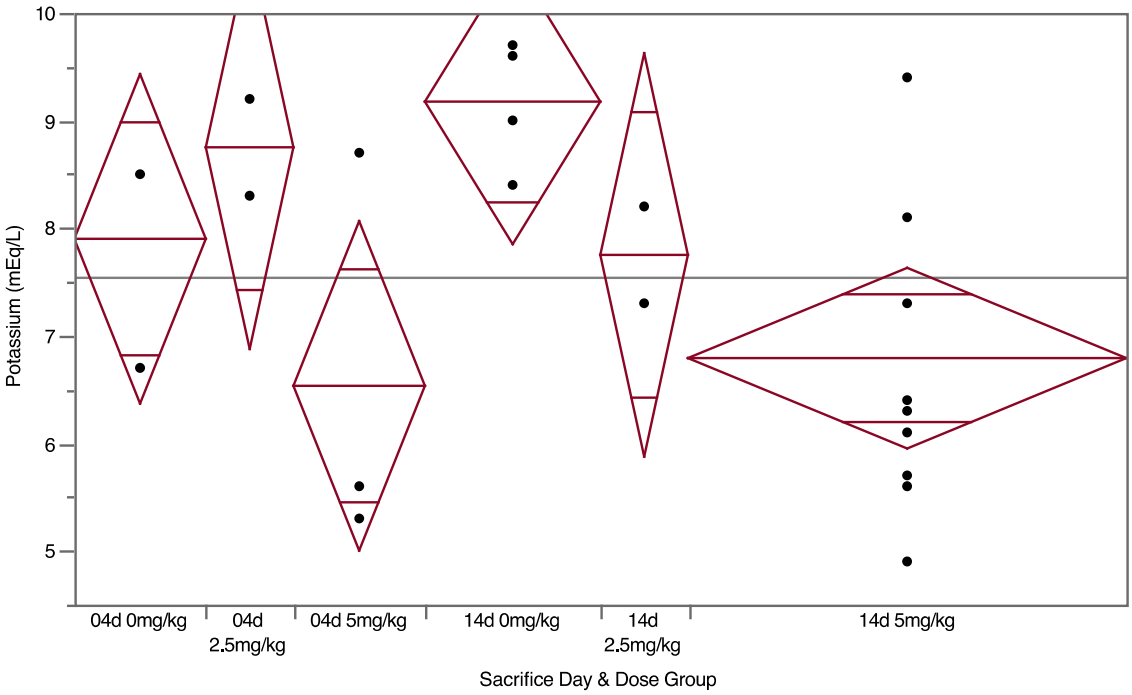


Figure 4 (sodium), Figure 5 (chloride), Figure 6 (potassium): One-way analysis of select plasma biochemical results by sacrifice day and/or test group. Solid dots represent each test result. Mean diamonds display the group means (center horizontal line of each diamond) and 95% confidence intervals for the group mean (vertical span of each diamond). The grey horizontal line that spans the length of the graph represents the grand mean for all mice.






10
9
8
7
6
5
Potassium (mEq/L)
04d 0mg/kg
04d 2.5mg/kg
04d 5mg/kg
14d 0mg/kg
14d 2.5mg/kg
14d 5mg/kg
Sacrifice Day & Dose Group

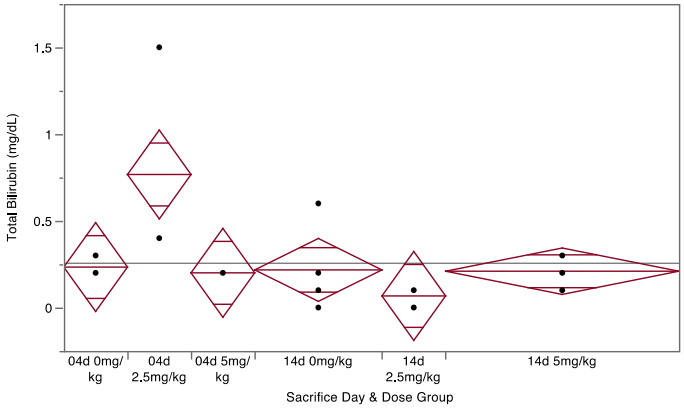
Have decided to leave the table below out for the present time as the poster should not become too crowded. (SOT always warns about not having a poster become a manuscript on a board.) Need to see what the first design looks like before considering putting this in.

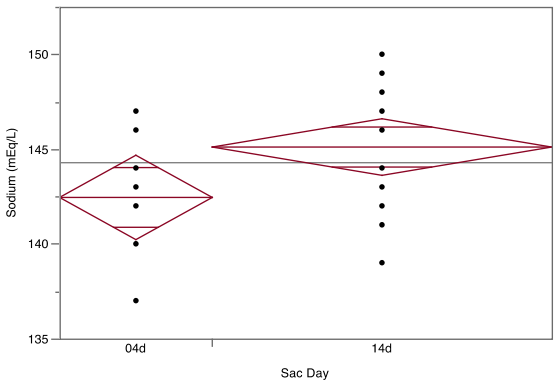
Table 1. Summary of statistically significant changes between means of results grouped by dose group and sacrifice day.

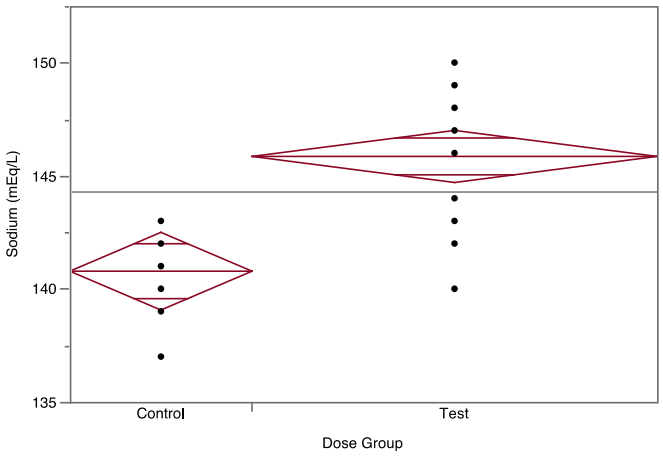
Group	Parameter	Group Means	Units	p-Value	Harlan RI
$High_{4d}$ v. $Control_{4d}$	BUN	24.0 v. 36.7	mg/dL	0.0110	17.2 – 27.2
	Creatinine	0.07 v. 0.17	mg/dL	0.0391	0.1 – 0.5
$High_{4d}$ v. Low_{4d}	Creatinine	0.07 v. 0.17	mg/dL	0.0391	0.1 – 0.5
	T. Bilirubin	0.2 v. 0.8	mg/dL	0.0375	0.1 – 0.5
Low_{14d} v. $Control_{14d}$	Sodium	147 v. 141	mEq/L	0.0291	158 – 170
$High_{14d}$ v. $Control_{14d}$	Basophils	3 v. 20	/uL	0.0174	0 – 0
	Sodium	147 v. 141	mEq/L	0.0010	158 – 170
	Potassium	6.8 v. 9.2	mEq/L	0.0485	8.8 – 10.4

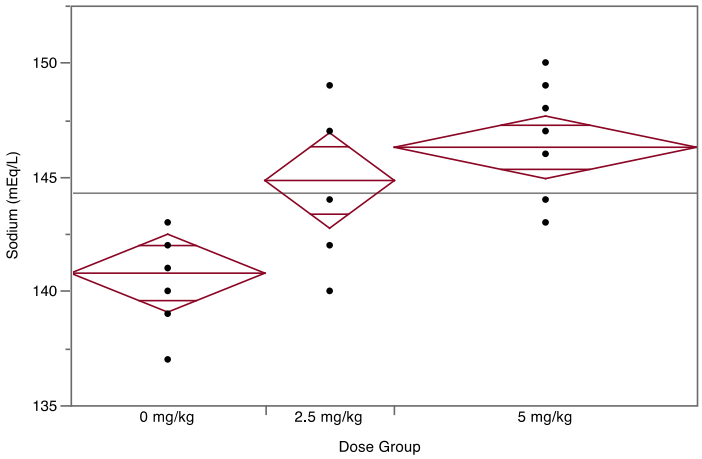
Abbreviations: BUN, blood urea nitrogen; RI, reference interval; T. Bilirubin, total bilirubin.

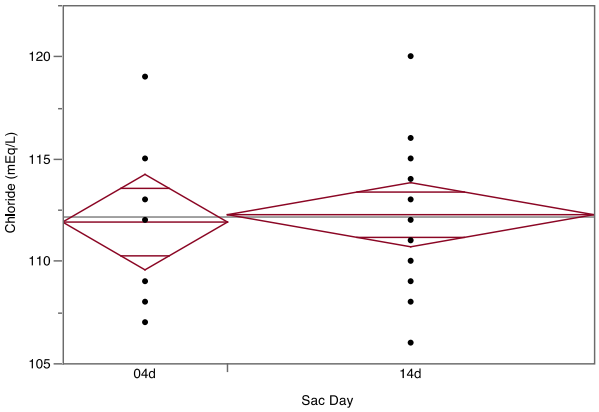
Figures below are to be left in reserve, just in case poster has room and/or needs more….

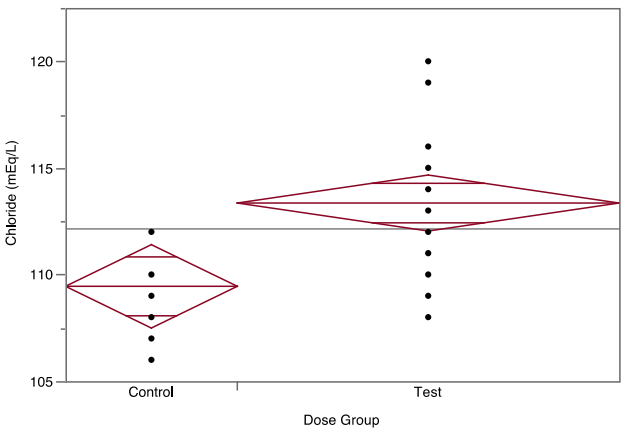


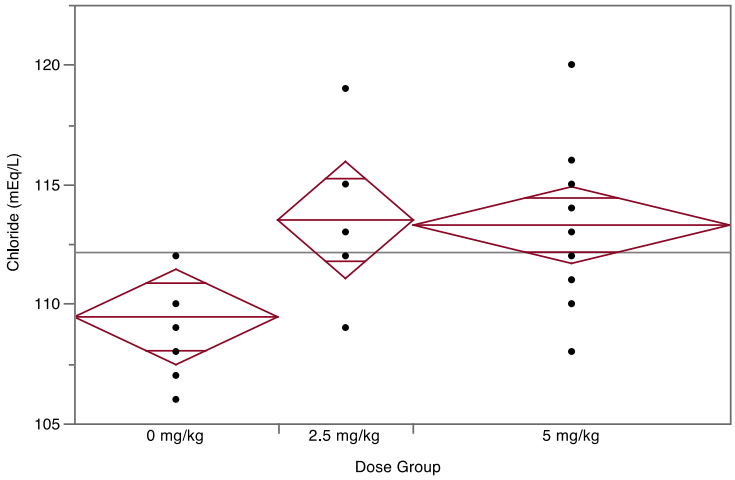


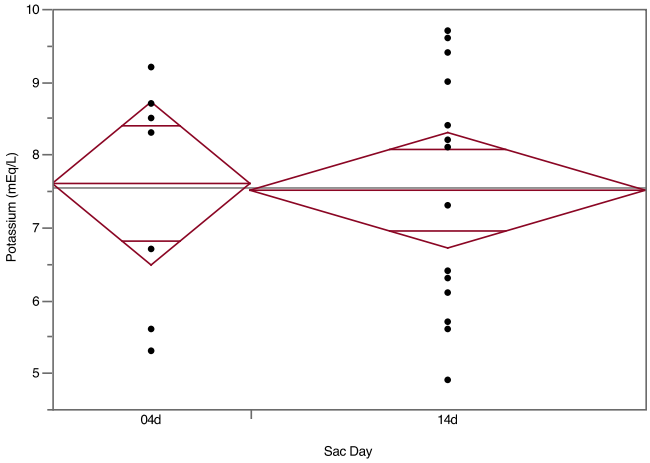

Sodium (mEq/L)
150
145
140
135
Control
Test
Dose Group

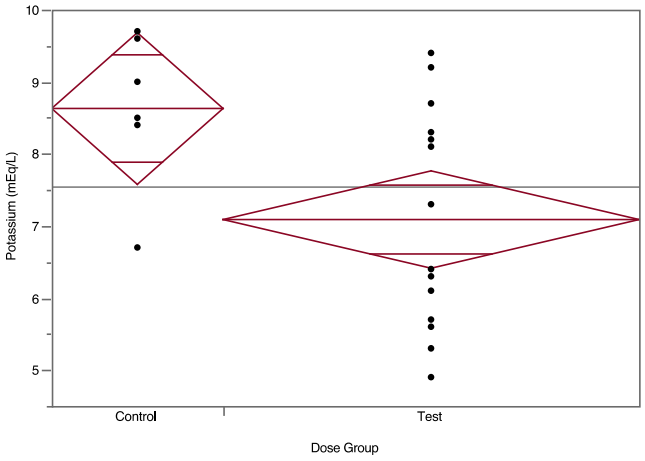

Sodium (mEq/L)
150
145
140
135
0 mg/kg
2.5 mg/kg
5 mg/kg
Dose Group

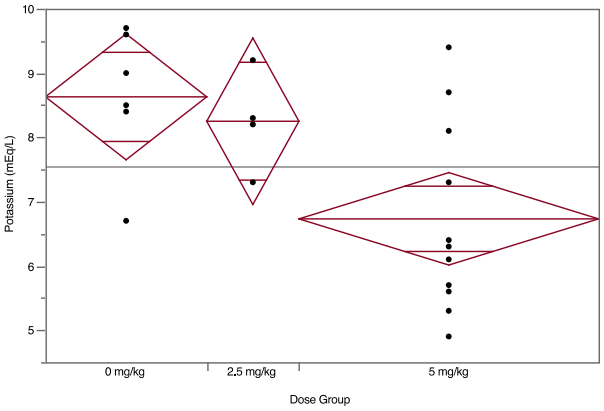

Chloride (mEq/L)
120
115
110
105
04d
14d
Sac Day


Chloride (mEq/L)
120
115
110
105
Control
Test
Dose Group


Chloride (mEq/L)
120
115
110
105
0 mg/kg
2.5 mg/kg
5 mg/kg
Dose Group


Potassium (mEq/L)
10
9
8
7
6
5
04d
14d
Sac Day


Potassium (mEq/L)
10
9
8
7
6
5
Control
Test
Dose Group


Potassium (mEq/L)
10
9
8
7
6
5
0 mg/kg
2.5 mg/kg
5 mg/kg
Dose Group

Entry 4S. PDF of Excel Spreadsheet of data behind Figure 8.

ICP concentration (ppm) for Blood and Organs in VT Mouse Toxicity Study

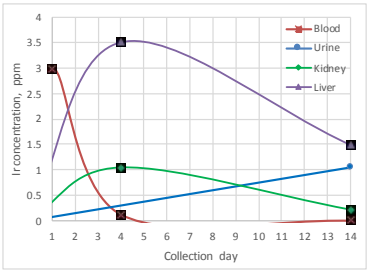
Numbers are not corrected for dilutions.

Day	Urine
0	0
14	1.05

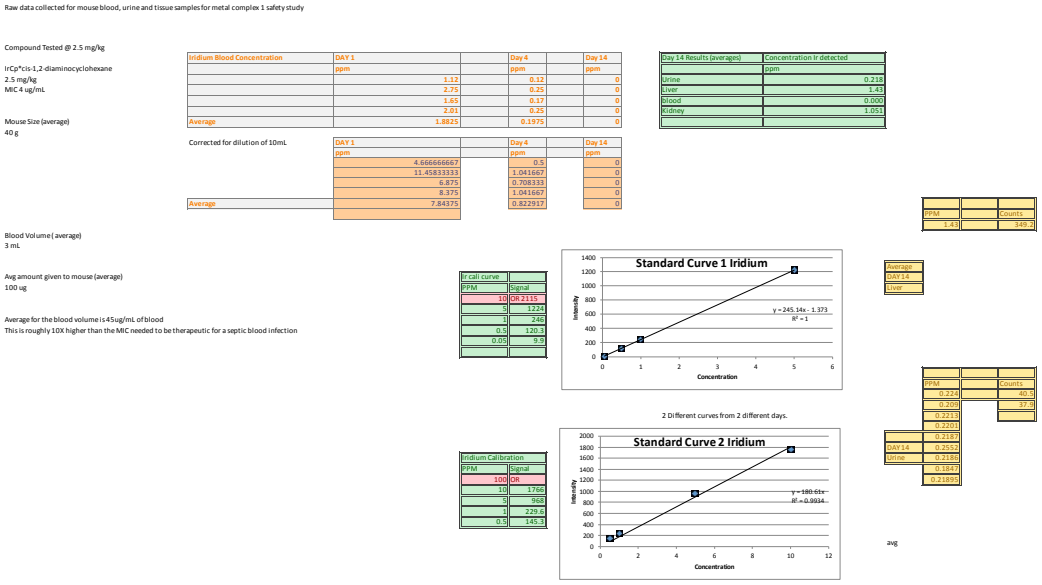
Day	Kidney
0	0
4	1.05
14	0.22

Day	Liver
0	0
4	3.51
14	1.49

Day	Blood
0	0
1	3
4	0.12
14	0



Entry 5S. PDF of Excel Spreadsheet of raw ICP data.



Raw data collected for mouse blood, urine and tissue samples for metal complex 1 safety study

Compound Tested @ 2.5 mg/kg

IrCp*cis-1,2-diaminocyclohexane
2.5 mg/kg
MIC 4 ug/mL

Mouse Size (average)
40 g

Iridium Blood Concentration	DAY 1		Day 4		Day 14
	ppm		ppm		ppm
	1.12		0.12		0
	2.75		0.25		0
	1.65		0.17		0
	2.01		0.25		0
Average	1.8825		0.1975		0

Day 14 Results (averages)	Concentration Ir detected
	ppm
Urine	0.218
Liver	1.43
Blood	0.000
Kidney	1.051

Corrected for dilution of 10mL

	DAY 1		Day 4		Day 14
	ppm		ppm		ppm
	4.666666667		0.5		0
	11.45833333		1.041667		0
	6.875		0.708333		0
	8.375		1.041667		0
Average	7.84375		0.822917		0

PPM		Counts
1.43		349.2

Blood Volume (average)
3 mL

Avg amount given to mouse (average)
100 ug

Average for the blood volume is 45ug/mL of blood
This is roughly 10X higher than the MIC needed to be therapeutic for a septic blood infection

Ir call curve	
PPM	Signal
10	OR 2115
5	1224
1	246
0.5	120.7
0.05	9.9

Average
DAY14
Liver

PPM		Counts
0.224		40.5
0.209		37.9
0.2213		
0.2201		
	0.2187	
DAY14	0.2552	
Urine	0.2186	
	0.1847	
	0.21895	

2 Different curves from 2 different days.

Iridium Calibration	
PPM	Signal
100	OR
10	1766
5	968
1	229.6
0.5	145.3

avg

Entry 6S. Activation Energy Calculations for Conformation Change of

[Cp*Ir(cis-1,2-diaminocyclohexane)Cl]$^+$

Supplementary Information for

"Iridium Piano Stool Complexes with Activity Against S. aureus and MRSA: It is past time to truly think outside of the box."

All calculations were performed using the WebMO interface, Version 17.0.012e.

The coordinates for the two conformers found in the crystal were input separately into WebMO[1] using the "Create New Job" command followed by the "Import Molecule" command. For each conformer, the geometry was optimized by the "Geometry Optimization & Vibrational Frequencies" command. These calculations were performed using Gaussian[2] at the B3LYP[3] level of theory with the lanl2dz basis set that covers many heavy elements, including iridium. These optimizations required from between 3 and 5 hrs of computation time on the server available.

In order to calculate possible transition states between the two conformers, the crystal-based structures were manipulated to provide multiple possible conformations along the ring-flip coordinate. This was done by taking a crystal conformer and deleting the cyclohexane ring. Then, different cyclohexane fragments (chair, boat, half-chair, twist-boat) that were available in the WebMO fragment library were added, and these various compounds with different conformations were subject to Transition State Optimization (TSO) followed by Vibrational Frequencies. The TSO calculations required from between 8 and 18 hrs to complete. For each TSO calculation, the different energies calculated were noted and shown in Table 1 below. For some starting points, the same possible transition state was obtained and are only entered once in the table. Because of the complexity of the system, the "perturbed" conformations for the TSO calculations had to be entered by hand – attempts at performing a "Saddle Calculation" failed.

The table lists the energy of the complex as a function of the Ir-N-C-H dihedral angle highlighted in the figure below. (This was arbitrarily chosen as an indicator of the conformer). Because there was no systematic way of varying and calculating that dihedral, the number of data points for possible transition states was limited by random generation of the optimized states and limited computational time. Nevertheless, samples of the computational space have no values greater than 10 kcal/mol in keeping with the similarities to decalin and cyclohexane.

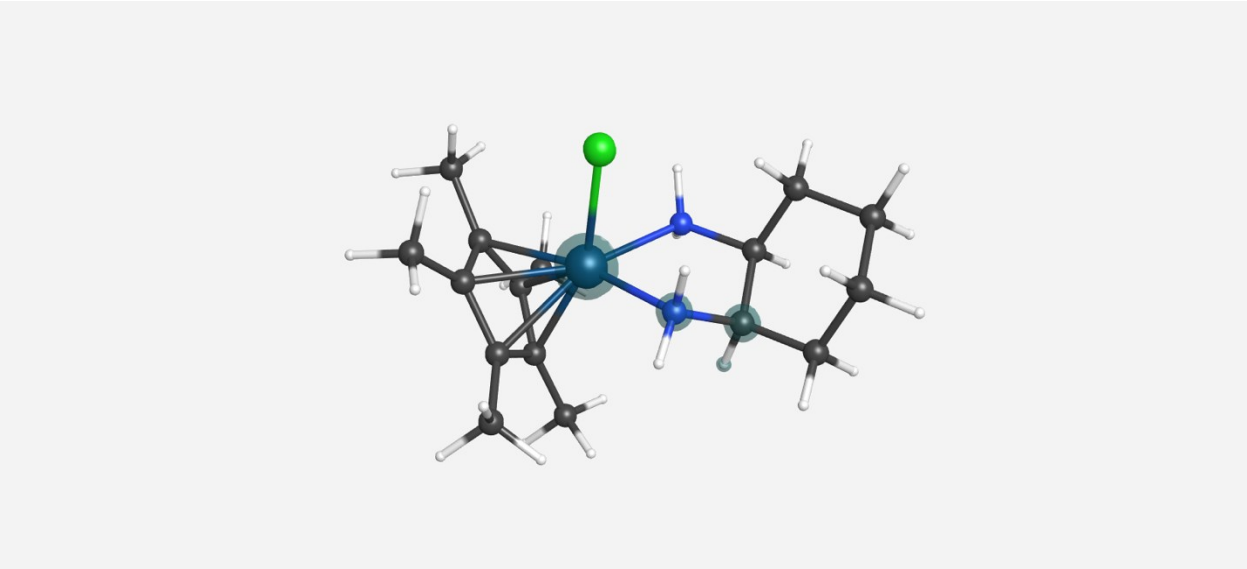


Table 1. Energy of conformer at various M-N-C-H dihedral angles

The conformer with the lowest energy corresponds to one from the crystal structure and shown in the paper as Figure 5. This was set as the 0 energy level. The other conformer showin in the paper as Figure 6 is only slightly higher in energy at +0.48 kcal/mol.

M-N-C-H Dihedral Angle	Energy (kcal/mol)
-135	5.08
-75.1	9.48
-64.9	5.10
79.8	0.48
81.7	9.90
157.4	8.85
158.1	0

1. Schmidt, J.R.; Polik, W.F. WebMO Enterprise, version 17.0.012e; WebMO LLC: Holland, MI, USA, 2016; https://www.webmo.net (accessed April, 2019)
2. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
3. a. A.D. Becke, J.Chem.Phys. 98 (1993) 5648-5652; b. C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785-789
4. P. J. Hay and W. R. Wadt, “Ab initio effective core potentials for molecular calculations – potentials for K to Au including the outermost core orbitals,” J. Chem. Phys., 82(1985) 299-310. DOI: 10.1063/1.448975

Entry 7S. Tables of Experimental Data and Bond Lengths and Angles form Compound 1. CCDC1901126

Table 1 Crystal data and structure refinement for DMMXI044A_ABS.

Identification code	DMMXI044A_ABS
Empirical formula	$C_{32.5}H_{59}N_4Cl_5Ir_2$
Formula weight	1067.48
Temperature/K	99.9
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	25.3023(2)
b/Å	14.75173(12)
c/Å	20.32938(18)
α/°	90
β/°	93.8630(8)
γ/°	90
Volume/Å^3	7570.75(11)
Z	8
ρ_{calc}g/cm^3	1.873
μ/mm ^{1}	7.405
F(000)	4168.0
Crystal size/mm^3	0.3461 × 0.0947 × 0.0664
Radiation	MoKα (λ = 0.71073) 2Θ
range for data collection/°	6.956 to 64.946
Index ranges	$-38 \le h \le 38$, $-21 \le k \le 22$, $-30 \le l \le 29$
Reflections collected	161024
Independent reflections	25813 [R_{int} = 0.0659, R_{sigma} = 0.0486]
Data/restraints/parameters	25813/0/804
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0338, wR_2 = 0.0586
Final R indexes [all data]	R_1 = 0.0581, wR_2 = 0.0669
Largest diff. peak/hole / e Å^{-3}	2.31/-1.25

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for DMMXI044A_ABS. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ir1	9468.0(2)	4694.2(2)	6806.8(2)	13.43(3)
Cl1	8614.6(4)	4485.6(6)	7246.6(5)	16.93(18)
N1	9803.7(14)	3898(2)	7606.5(17)	17.9(7)
N2	9633.4(13)	5707(2)	7531.2(17)	18.3(7)
C1	9724.6(18)	3899(3)	5994(2)	21.7(9)
C2	9187.7(18)	4156(3)	5863(2)	22.8(9)
C3	9161.6(18)	5142(3)	5851(2)	23.5(9)
C4	9688.8(17)	5475(3)	5971(2)	21.6(9)
C5	10041.3(17)	4715(3)	6080(2)	20.4(8)
C6	9934(2)	2947(3)	6036(2)	31.0(11)
C7	8724(2)	3531(3)	5758(2)	32.3(11)
C8	8663.2(19)	5684(4)	5712(2)	31.5(11)
C9	9844(2)	6455(3)	5990(3)	30.9(11)
C10	10629.3(19)	4764(4)	6195(3)	33.3(11)
C11	9795.6(16)	5354(3)	8201(2)	19.5(8)
C12	9331.0(18)	5218(3)	8619(2)	23.9(9)
C13	9507(2)	4776(3)	9276(2)	30.0(10)
C14	9789(2)	3876(3)	9168(2)	33.4(11)
C15	10263.6(18)	4017(3)	8747(2)	28.2(10)
C16	10114.3(16)	4492(3)	8102(2)	20.7(9)
Ir2	7579.2(2)	8504.7(2)	3731.8(2)	13.79(3)
Cl2	7825.1(4)	10048.5(6)	3937.6(5)	22.3(2)
N3	7020.4(13)	9088(2)	3009.4(16)	15.8(7)
N4	8048.0(13)	8647(2)	2908.0(17)	17.1(7)
C17	7620.5(18)	8178(3)	4779(2)	21.7(9)
C18	7115.7(16)	7906(3)	4486(2)	17.7(8)
C19	7205.9(16)	7239(3)	3980(2)	16.4(8)
C20	7771.2(16)	7111(3)	3971(2)	17.9(8)
C21	8033.3(17)	7713(3)	4452(2)	20.9(9)
C22	7722(2)	8843(3)	5329(2)	30.1(11)
C23	6585.3(18)	8163(3)	4701(2)	25.2(9)
C24	6779.7(16)	6728(3)	3588(2)	20.1(8)
C25	8037.2(17)	6446(3)	3553(2)	24.0(9)
C26	8619.3(17)	7796(3)	4611(3)	29.2(11)
C27	7273.7(15)	9384(3)	2399(2)	15.7(8)
C28	6885.2(17)	9464(3)	1792(2)	19.4(8)
C29	6696.4(16)	8542(3)	1522(2)	19.8(8)
C30	7159.5(17)	7914(3)	1407(2)	20.3(8)
C31	7516.8(16)	7799(3)	2043(2)	17.7(8)
C32	7719.3(15)	8719(3)	2277(2)	15.0(7)
Ir3	4585.5(2)	6335.5(2)	1898.6(2)	12.55(3)
Cl3	3648.1(4)	6147.3(7)	2067.2(5)	20.0(2)
N5	4734.8(13)	5375(2)	2675.9(16)	17.2(7)
N6	4617.7(14)	7199(2)	2738.7(17)	18.2(7)

C33	4986.6(16)	5635(3)	1149(2)	17.5(8)
C34	4468.0(16)	5904(3)	891(2)	18.1(8)
C35	4441.4(17)	6892(3)	930(2)	18.6(8)
C36	4942.1(16)	7218(3)	1199(2)	16.1(8)
C37	5281.1(16)	6448(3)	1366(2)	17.3(8)
C38	5176.7(17)	4679(3)	1185(2)	22.1(9)
C39	4047.5(17)	5257(3)	646(2)	23.8(9)
C40	3970.6(17)	7459(3)	716(2)	25.3(9)
C41	5096.3(17)	8185(3)	1291(2)	20.6(8)
C42	5848.5(16)	6465(3)	1628(2)	23.7(9)
C43	4447.4(17)	6681(3)	3324(2)	21.3(9)
C44	4508.1(19)	7203(3)	3971(2)	25.8(10)
C45	5077.2(19)	7303(3)	4247(2)	26.3(10)
C46	5356(2)	6389(3)	4283(2)	28.2(10)
C47	5329.7(18)	5932(3)	3606(2)	23.6(9)
C48	4759.1(17)	5786(3)	3353(2)	20.4(8)
Ir4	2449.0(2)	8289.9(2)	3268.6(2)	12.36(3)
Cl4	2709.0(4)	6789.6(7)	3618.2(5)	22.0(2)
N7	2914.5(13)	7998(2)	2462.0(17)	15.8(7)
N8	1898.2(13)	7589(2)	2617.1(17)	15.7(7)
C49	2061.8(15)	9590(3)	3387(2)	16.7(8)
C50	1989.7(16)	9035(3)	3959(2)	16.7(8)
C51	2498.5(16)	8825(3)	4266(2)	16.5(8)
C52	2897.2(15)	9233(3)	3886(2)	16.0(8)
C53	2620.1(15)	9722(2)	3350(2)	14.5(7)
C54	2878.8(16)	10305(3)	2867(2)	17.9(8)
C55	1626.2(16)	10028(3)	2967(2)	20.6(9)
C56	1460.9(18)	8848(3)	4232(2)	26.6(10)
C57	2609(2)	8269(3)	4875(2)	26.3(10)
C58	3480.1(16)	9230(3)	4024(2)	21.1(9)
C59	2575.4(16)	7882(3)	1842(2)	16.3(8)
C60	2374.9(17)	8796(3)	1575(2)	19.2(8)
C61	1986.7(17)	8677(3)	974(2)	21.4(9)
C62	1520.6(17)	8090(3)	1159(2)	21.5(9)
C63	1709.8(16)	7168(3)	1424(2)	19.4(8)
C64	2125.2(15)	7245(3)	1998(2)	15.3(7)
Cl5	9035.3(4)	7664.5(7)	7530.6(7)	29.2(3)
Cl6	4206.7(4)	3394.7(7)	2090.0(5)	19.57(19)
Cl7	5989.2(4)	4104.7(7)	2729.6(6)	23.1(2)
Cl8	690.8(4)	8158.8(7)	2545.9(6)	23.5(2)
Cl9	6173.8(6)	4788.8(10)	5112.4(8)	46.5(3)
Cl10	7276.1(5)	5300.9(9)	4970.7(6)	36.7(3)
C65	6804(2)	4411(3)	4946(3)	34.1(12)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for DMMXI044A_ABS. The Anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir1	14.57(7)	10.65(6)	15.13(7)	0.30(5)	1.52(5)	-1.09(5)
Cl1	13.8(4)	14.5(4)	22.5(5)	0.5(4)	1.3(4)	-0.7(3)
N1	19.7(17)	14.9(16)	19.2(18)	1.6(13)	2.0(14)	2.9(13)
N2	16.7(16)	13.3(16)	25.0(19)	-2.0(13)	2.1(14)	1.5(13)
C1	31(2)	18(2)	17(2)	-2.5(16)	9.0(18)	0.6(17)
C2	32(2)	24(2)	12.2(19)	-1.9(16)	-0.9(17)	-3.6(18)
C3	30(2)	23(2)	17(2)	3.8(17)	0.6(18)	3.5(18)
C4	26(2)	17(2)	22(2)	3.1(16)	4.3(18)	-3.8(17)
C5	21(2)	21(2)	20(2)	1.6(17)	7.8(16)	-1.4(16)
C6	45(3)	22(2)	26(2)	-2.2(19)	12(2)	4(2)
C7	42(3)	34(3)	20(2)	-6(2)	-4(2)	-12(2)
C8	32(3)	38(3)	24(2)	10(2)	-4(2)	7(2)
C9	37(3)	18(2)	38(3)	8(2)	7(2)	-8(2)
C10	30(3)	38(3)	33(3)	3(2)	14(2)	-1(2)
C11	20.4(19)	16.8(19)	21(2)	-0.7(16)	-2.4(16)	-2.0(16)
C12	26(2)	26(2)	20(2)	0.8(18)	3.1(18)	3.7(18)
C13	38(3)	34(3)	18(2)	2.2(19)	2(2)	4(2)
C14	40(3)	33(3)	26(3)	0(2)	-8(2)	-4(2)
C15	25(2)	19(2)	38(3)	1.8(19)	-11(2)	0.9(18)
C16	17.2(19)	16.0(19)	28(2)	0.3(17)	-3.0(17)	-0.6(15)
Ir2	15.93(7)	9.14(6)	16.45(7)	-0.93(5)	2.11(5)	-0.66(5)
Cl2	33.1(6)	11.7(4)	22.5(5)	-2.9(4)	4.1(4)	-5.7(4)
N3	18.9(16)	12.3(15)	16.5(16)	-3.1(13)	3.0(13)	-1.5(13)
N4	16.4(16)	11.9(15)	23.1(18)	-4.0(13)	0.9(14)	0.9(12)
C17	30(2)	14.6(19)	20(2)	3.7(16)	0.2(18)	-3.6(17)
C18	24(2)	12.3(18)	18(2)	3.5(15)	4.1(16)	0.2(15)
C19	19.2(19)	9.5(17)	21(2)	2.8(15)	2.9(16)	-1.5(14)
C20	18.4(19)	8.1(17)	27(2)	1.9(15)	2.3(17)	-0.9(14)
C21	22(2)	18(2)	23(2)	7.2(16)	-1.2(17)	-3.4(16)
C22	49(3)	24(2)	17(2)	-1.6(18)	1(2)	-7(2)
C23	30(2)	22(2)	25(2)	1.6(18)	12.1(19)	4.6(18)
C24	20(2)	16.3(19)	24(2)	-1.2(16)	1.9(17)	-0.9(16)
C25	22(2)	13.7(19)	38(3)	0.7(18)	12.2(19)	4.0(16)
C26	21(2)	26(2)	38(3)	13(2)	-12(2)	-5.5(18)
C27	16.9(18)	12.0(17)	19(2)	0.3(14)	2.7(15)	1.5(14)
C28	21(2)	17.7(19)	19(2)	0.2(16)	1.3(16)	-0.7(16)
C29	20(2)	20(2)	18(2)	-0.6(16)	-1.1(16)	-3.9(16)
C30	25(2)	14.0(19)	22(2)	-6.2(16)	5.5(17)	-2.2(16)
C31	19.8(19)	14.8(18)	19(2)	-3.6(15)	3.9(16)	-2.4(15)
C32	15.2(17)	11.4(17)	18.8(19)	-0.3(14)	3.8(15)	-1.7(14)
Ir3	11.74(6)	10.74(6)	15.39(7)	0.12(5)	2.55(5)	-0.47(5)
Cl3	14.2(4)	15.5(4)	31.0(6)	0.7(4)	6.7(4)	0.0(3)
N5	17.7(16)	15.1(16)	19.1(17)	0.3(13)	3.7(13)	-0.3(13)
N6	19.2(16)	12.8(16)	22.8(18)	0.5(13)	3.0(14)	-0.1(13)

C33	19.3(19)	16.5(19)	18(2)	-0.9(15)	8.7(16)	1.1(15)
C34	21(2)	20(2)	13.3(19)	-0.8(15)	0.9(16)	-1.3(16)
C35	25(2)	16.2(19)	14.9(19)	1.8(15)	2.2(16)	-0.6(16)
C36	22.3(19)	11.1(17)	15.6(19)	0.9(14)	6.0(16)	-1.0(15)
C37	17.7(18)	13.0(18)	22(2)	-0.2(15)	5.7(16)	0.2(15)
C38	22(2)	14.5(19)	31(2)	-0.5(17)	7.8(18)	0.7(16)
C39	21(2)	25(2)	25(2)	-2.9(18)	-1.4(18)	-6.2(17)
C40	24(2)	26(2)	26(2)	7.3(18)	-2.7(18)	4.1(18)
C41	22(2)	14.3(19)	26(2)	2.6(16)	5.9(17)	-1.6(16)
C42	14.9(18)	17(2)	40(3)	-3.3(18)	6.5(18)	-1.5(16)
C43	22(2)	19(2)	23(2)	1.2(17)	2.6(17)	-2.6(16)
C44	35(2)	18(2)	26(2)	-3.5(17)	11(2)	0.9(18)
C45	39(3)	21(2)	18(2)	1.2(17)	3.3(19)	1.5(19)
C46	37(3)	23(2)	24(2)	2.1(18)	-4(2)	2(2)
C47	28(2)	19(2)	23(2)	-1.7(17)	-2.4(18)	4.9(17)
C48	27(2)	13.3(19)	21(2)	1.8(16)	1.9(17)	-0.5(16)
Ir4	12.61(6)	9.00(6)	15.74(7)	-0.17(5)	2.93(5)	0.74(5)
Cl4	28.0(5)	12.8(4)	24.7(5)	2.4(4)	-1.7(4)	6.0(4)
N7	13.4(15)	13.8(15)	20.7(17)	-0.7(13)	4.4(13)	-1.5(12)
N8	16.0(15)	12.1(15)	19.8(17)	2.7(13)	6.1(13)	1.6(12)
C49	16.4(18)	11.1(17)	23(2)	-1.2(15)	6.3(16)	2.9(14)
C50	18.3(18)	12.8(18)	20(2)	-3.9(15)	6.8(16)	0.1(15)
C51	19.4(19)	13.5(18)	16.8(19)	-3.6(15)	2.9(15)	0.4(15)
C52	16.6(18)	14.1(18)	17.4(19)	-4.0(15)	1.8(15)	-0.5(14)
C53	16.1(17)	7.5(16)	20(2)	-1.4(14)	3.8(15)	0.7(14)
C54	18.8(19)	12.3(18)	23(2)	2.1(15)	1.7(16)	-0.8(15)
C55	19.4(19)	12.9(18)	29(2)	-0.5(16)	0.0(17)	1.9(15)
C56	24(2)	21(2)	37(3)	-3.6(19)	18(2)	-2.5(17)
C57	37(3)	25(2)	17(2)	-0.4(18)	6.7(19)	1(2)
C58	22(2)	23(2)	18(2)	-1.6(17)	-3.1(17)	-1.2(17)
C59	18.4(18)	13.9(18)	18(2)	-4.0(15)	7.8(16)	0.3(15)
C60	27(2)	10.0(17)	21(2)	-0.1(15)	7.5(17)	-2.1(15)
C61	29(2)	16.2(19)	19(2)	0.0(16)	6.0(18)	1.2(17)
C62	27(2)	22(2)	16(2)	-2.4(16)	-0.9(17)	4.3(17)
C63	22(2)	16.6(19)	20(2)	0.4(16)	2.4(17)	-2.8(16)
C64	17.0(18)	10.0(17)	19(2)	0.6(14)	2.1(15)	1.6(14)
Cl5	19.5(5)	17.6(5)	51.8(8)	1.7(5)	11.9(5)	0.1(4)
Cl6	15.7(4)	19.6(5)	23.4(5)	1.4(4)	2.0(4)	-0.2(4)
Cl7	19.7(5)	18.0(5)	32.6(6)	-0.2(4)	9.5(4)	-0.2(4)
Cl8	15.5(4)	19.9(5)	35.2(6)	2.7(4)	3.0(4)	2.6(4)
Cl9	35.5(7)	38.1(7)	66.2(10)	-6.8(7)	6.2(7)	-1.4(6)
Cl10	37.1(7)	41.2(7)	32.4(7)	-0.5(5)	6.2(5)	-5.9(6)
C65	33(3)	29(3)	42(3)	2(2)	11(2)	-4(2)

Table 4 Bond Lengths for DMMXI044A_ABS.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	Cl1	2.4116(9)	Ir3	N5	2.137(3)
Ir1	N1	2.135(3)	Ir3	N6	2.128(3)
Ir1	N2	2.120(3)	Ir3	C33	2.152(4)
Ir1	C1	2.161(4)	Ir3	C34	2.146(4)
Ir1	C2	2.152(4)	Ir3	C35	2.141(4)
Ir1	C3	2.147(4)	Ir3	C36	2.170(4)
Ir1	C4	2.157(4)	Ir3	C37	2.135(4)
Ir1	C5	2.140(4)	N5	C48	1.502(5)
N1	C16	1.514(5)	N6	C43	1.501(5)
N2	C11	1.489(5)	C33	C34	1.435(6)
C1	C2	1.418(6)	C33	C37	1.464(6)
C1	C5	1.450(6)	C33	C38	1.490(6)
C1	C6	1.502(6)	C34	C35	1.462(6)
C2	C3	1.456(6)	C34	C39	1.489(6)
C2	C7	1.497(6)	C35	C36	1.429(6)
C3	C4	1.427(6)	C35	C40	1.496(6)
C3	C8	1.504(6)	C36	C37	1.450(5)
C4	C5	1.441(6)	C36	C41	1.486(5)
C4	C9	1.498(6)	C37	C42	1.498(6)
C5	C10	1.492(6)	C43	C44	1.523(6)
C11	C12	1.510(6)	C43	C48	1.537(6)
C11	C16	1.526(6)	C44	C45	1.517(7)
C12	C13	1.524(6)	C45	C46	1.522(6)
C13	C14	1.530(7)	C46	C47	1.529(6)
C14	C15	1.535(7)	C47	C48	1.515(6)
C15	C16	1.512(6)	Ir4	Cl4	2.4027(10)
Ir2	Cl2	2.3902(10)	Ir4	N7	2.126(3)
Ir2	N3	2.148(3)	Ir4	N8	2.125(3)
Ir2	N4	2.127(3)	Ir4	C49	2.175(4)
Ir2	C17	2.178(4)	Ir4	C50	2.180(4)
Ir2	C18	2.180(4)	Ir4	C51	2.171(4)
Ir2	C19	2.168(4)	Ir4	C52	2.145(4)
Ir2	C20	2.160(4)	Ir4	C53	2.160(4)
Ir2	C21	2.144(4)	N7	C59	1.487(5)
N3	C27	1.499(5)	N8	C64	1.506(5)
N4	C32	1.485(5)	C49	C50	1.446(6)
C17	C18	1.429(6)	C49	C53	1.432(5)
C17	C21	1.448(6)	C49	C55	1.494(6)
C17	C22	1.498(6)	C50	C51	1.426(6)
C18	C19	1.454(6)	C50	C56	1.508(5)
C18	C23	1.488(6)	C51	C52	1.443(5)
C19	C20	1.444(6)	C51	C57	1.496(6)
C19	C24	1.499(6)	C52	C53	1.447(6)
C20	C21	1.448(6)	C52	C58	1.483(6)
C20	C25	1.488(6)	C53	C54	1.490(5)
C21	C26	1.501(6)	C59	C60	1.526(6)
C27	C28	1.529(6)	C59	C64	1.527(5)

C27	C32	1.527(5)	C60	C61	1.525(6)
C28	C29	1.531(6)	C61	C62	1.530(6)
C29	C30	1.524(6)	C62	C63	1.527(6)
C30	C31	1.537(6)	C63	C64	1.521(6)
C31	C32	1.516(5)	Cl9	C65	1.745(5)
Ir3	Cl3	2.4350(9)	Cl10	C65	1.773(5)

Table 5 Bond Angles for DMMXI044A_ABS.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ir1	Cl1	88.15(10)	N5	Ir3	C33	97.89(14)
N1	Ir1	C1	99.13(15)	N5	Ir3	C34	120.99(14)
N1	Ir1	C2	124.48(15)	N5	Ir3	C35	160.84(14)
N1	Ir1	C3	163.57(15)	N5	Ir3	C36	145.31(14)
N1	Ir1	C4	141.50(15)	N6	Ir3	Cl3	86.58(10)
N1	Ir1	C5	106.29(15)	N6	Ir3	N5	78.93(13)
N2	Ir1	Cl1	88.41(10)	N6	Ir3	C33	149.51(15)
N2	Ir1	N1	79.00(13)	N6	Ir3	C34	159.89(14)
N2	Ir1	C1	149.11(15)	N6	Ir3	C35	120.23(14)
N2	Ir1	C2	156.52(15)	N6	Ir3	C36	99.90(14)
N2	Ir1	C3	117.02(15)	N6	Ir3	C37	111.88(14)
N2	Ir1	C4	96.93(15)	C33	Ir3	Cl3	123.74(11)
N2	Ir1	C5	111.01(15)	C33	Ir3	C36	65.60(15)
C1	Ir1	Cl1	122.46(12)	C34	Ir3	Cl3	91.54(11)
C2	Ir1	Cl1	91.95(12)	C34	Ir3	C33	39.01(15)
C2	Ir1	C1	38.39(17)	C34	Ir3	C36	65.77(15)
C2	Ir1	C4	65.32(17)	C35	Ir3	Cl3	93.79(12)
C3	Ir1	Cl1	95.57(13)	C35	Ir3	C33	65.91(16)
C3	Ir1	C1	65.41(17)	C35	Ir3	C34	39.87(15)
C3	Ir1	C2	39.59(16)	C35	Ir3	C36	38.71(15)
C3	Ir1	C4	38.74(17)	C36	Ir3	Cl3	127.79(11)
C4	Ir1	Cl1	130.24(12)	C37	Ir3	Cl3	157.61(12)
C4	Ir1	C1	65.24(16)	C37	Ir3	N5	108.42(14)
C5	Ir1	Cl1	157.42(12)	C37	Ir3	C33	39.94(15)
C5	Ir1	C1	39.39(16)	C37	Ir3	C34	66.71(16)
C5	Ir1	C2	65.63(17)	C37	Ir3	C35	66.34(16)
C5	Ir1	C3	65.83(17)	C37	Ir3	C36	39.37(15)
C5	Ir1	C4	39.19(16)	C48	N5	Ir3	113.9(2)
C16	N1	Ir1	110.5(2)	C43	N6	Ir3	109.5(2)
C11	N2	Ir1	114.7(2)	C34	C33	Ir3	70.3(2)
C2	C1	Ir1	70.4(2)	C34	C33	C37	108.6(3)
C2	C1	C5	108.4(4)	C34	C33	C38	124.3(4)
C2	C1	C6	126.2(4)	C37	C33	Ir3	69.4(2)

C5	C1	Ir1	69.5(2)	C37	C33	C38	127.2(4)
C5	C1	C6	125.4(4)	C38	C33	Ir3	125.8(3)
C6	C1	Ir1	126.0(3)	C33	C34	Ir3	70.7(2)
C1	C2	Ir1	71.2(2)	C33	C34	C35	107.4(4)
C1	C2	C3	108.2(4)	C33	C34	C39	124.1(4)
C1	C2	C7	126.5(4)	C35	C34	Ir3	69.9(2)
C3	C2	Ir1	70.0(2)	C35	C34	C39	128.5(4)
C3	C2	C7	125.4(4)	C39	C34	Ir3	124.0(3)
C7	C2	Ir1	124.2(3)	C34	C35	Ir3	70.2(2)
C2	C3	Ir1	70.4(2)	C34	C35	C40	125.5(4)
C2	C3	C8	124.8(4)	C36	C35	Ir3	71.7(2)
C4	C3	Ir1	71.0(3)	C36	C35	C34	108.3(4)
C4	C3	C2	107.5(4)	C36	C35	C40	126.2(4)
C4	C3	C8	127.6(4)	C40	C35	Ir3	124.4(3)

C8	C3	Ir1	125.5(3)	C35	C36	Ir3	69.6(2)
C3	C4	Ir1	70.2(2)	C35	C36	C37	108.7(3)
C3	C4	C5	108.6(4)	C35	C36	C41	126.1(4)
C3	C4	C9	125.3(4)	C37	C36	Ir3	69.0(2)
C5	C4	Ir1	69.8(2)	C37	C36	C41	125.2(4)
C5	C4	C9	126.1(4)	C41	C36	Ir3	127.6(3)
C9	C4	Ir1	125.3(3)	C33	C37	Ir3	70.7(2)
C1	C5	Ir1	71.1(2)	C33	C37	C42	125.3(4)
C1	C5	C10	126.6(4)	C36	C37	Ir3	71.6(2)
C4	C5	Ir1	71.0(2)	C36	C37	C33	106.9(3)
C4	C5	C1	107.3(4)	C36	C37	C42	127.4(4)
C4	C5	C10	125.9(4)	C42	C37	Ir3	128.6(3)
C10	C5	Ir1	127.4(3)	N6	C43	C44	114.2(3)
N2	C11	C12	112.6(3)	N6	C43	C48	107.1(3)
N2	C11	C16	106.7(3)	C44	C43	C48	112.3(4)
C12	C11	C16	113.7(4)	C45	C44	C43	114.0(4)
C11	C12	C13	111.0(4)	C44	C45	C46	110.9(4)
C12	C13	C14	111.0(4)	C45	C46	C47	110.8(4)
C13	C14	C15	110.6(4)	C48	C47	C46	110.6(4)
C16	C15	C14	112.8(4)	N5	C48	C43	108.8(3)
N1	C16	C11	108.3(3)	N5	C48	C47	110.4(3)
C15	C16	N1	113.3(3)	C47	C48	C43	111.4(3)
C15	C16	C11	112.0(4)	N7	Ir4	Cl4	83.48(9)
N3	Ir2	Cl2	83.67(9)	N7	Ir4	C49	122.75(14)
N3	Ir2	C17	137.96(15)	N7	Ir4	C50	161.13(14)
N3	Ir2	C18	106.43(14)	N7	Ir4	C51	142.52(14)
N3	Ir2	C19	103.11(14)	N7	Ir4	C52	106.49(14)
N3	Ir2	C20	131.47(14)	N7	Ir4	C53	98.00(13)
N4	Ir2	Cl2	83.78(9)	N8	Ir4	Cl4	83.77(9)
N4	Ir2	N3	78.38(13)	N8	Ir4	N7	78.16(12)
N4	Ir2	C17	143.02(15)	N8	Ir4	C49	102.49(14)
N4	Ir2	C18	161.64(14)	N8	Ir4	C50	106.91(14)
N4	Ir2	C19	122.87(14)	N8	Ir4	C51	138.84(14)
N4	Ir2	C20	98.16(14)	N8	Ir4	C52	168.06(14)
N4	Ir2	C21	106.82(15)	N8	Ir4	C53	130.01(14)

C17	Ir2	Cl2	92.59(11)	C49	Ir4	Cl4	153.67(11)
C17	Ir2	C18	38.30(16)	C49	Ir4	C50	38.79(15)
C18	Ir2	Cl2	114.15(11)	C50	Ir4	Cl4	114.89(11)
C19	Ir2	Cl2	153.20(11)	C51	Ir4	Cl4	93.52(11)
C19	Ir2	C17	64.85(16)	C51	Ir4	C49	64.80(15)
C19	Ir2	C18	39.07(15)	C51	Ir4	C50	38.25(15)
C20	Ir2	Cl2	144.64(11)	C52	Ir4	Cl4	107.51(11)
C20	Ir2	C17	64.80(16)	C52	Ir4	C49	65.66(15)
C20	Ir2	C18	65.13(15)	C52	Ir4	C50	65.19(15)
C20	Ir2	C19	38.97(15)	C52	Ir4	C51	39.05(14)
C21	Ir2	Cl2	106.16(12)	C52	Ir4	C53	39.27(15)
C21	Ir2	N3	169.14(14)	C53	Ir4	Cl4	145.94(11)
C21	Ir2	C17	39.14(16)	C53	Ir4	C49	38.59(14)
C21	Ir2	C18	65.67(16)	C53	Ir4	C50	64.56(14)

C21	Ir2	C19	66.04(15)	C53	Ir4	C51	64.78(15)
C21	Ir2	C20	39.31(16)	C59	N7	Ir4	111.1(2)
C27	N3	Ir2	112.6(2)	C64	N8	Ir4	114.4(2)
C32	N4	Ir2	112.2(2)	C50	C49	Ir4	70.8(2)
C18	C17	Ir2	70.9(2)	C50	C49	C55	125.2(4)
C18	C17	C21	109.1(4)	C53	C49	Ir4	70.1(2)
C18	C17	C22	126.7(4)	C53	C49	C50	107.3(4)
C21	C17	Ir2	69.2(2)	C53	C49	C55	127.2(4)
C21	C17	C22	124.1(4)	C55	C49	Ir4	129.7(3)
C22	C17	Ir2	125.4(3)	C49	C50	Ir4	70.4(2)
C17	C18	Ir2	70.8(2)	C49	C50	C56	124.3(4)
C17	C18	C19	107.8(4)	C51	C50	Ir4	70.6(2)
C17	C18	C23	127.2(4)	C51	C50	C49	108.4(3)
C19	C18	Ir2	70.0(2)	C51	C50	C56	126.7(4)
C19	C18	C23	124.6(4)	C56	C50	Ir4	132.0(3)
C23	C18	Ir2	129.9(3)	C50	C51	Ir4	71.2(2)
C18	C19	Ir2	70.9(2)	C50	C51	C52	108.6(4)
C18	C19	C24	125.1(4)	C50	C51	C57	126.3(4)
C20	C19	Ir2	70.2(2)	C52	C51	Ir4	69.5(2)
C20	C19	C18	107.5(4)	C52	C51	C57	125.0(4)
C20	C19	C24	127.3(4)	C57	C51	Ir4	124.7(3)
C24	C19	Ir2	128.2(3)	C51	C52	Ir4	71.5(2)
C19	C20	Ir2	70.8(2)	C51	C52	C53	106.8(3)
C19	C20	C21	108.7(4)	C51	C52	C58	128.3(4)
C19	C20	C25	125.4(4)	C53	C52	Ir4	70.9(2)
C21	C20	Ir2	69.8(2)	C53	C52	C58	124.7(4)
C21	C20	C25	125.8(4)	C58	C52	Ir4	126.1(3)
C25	C20	Ir2	127.1(3)	C49	C53	Ir4	71.3(2)
C17	C21	Ir2	71.7(2)	C49	C53	C52	108.9(3)
C17	C21	C26	126.5(4)	C49	C53	C54	126.2(4)
C20	C21	Ir2	70.9(2)	C52	C53	Ir4	69.8(2)
C20	C21	C17	106.8(4)	C52	C53	C54	124.8(3)
C20	C21	C26	126.6(4)	C54	C53	Ir4	127.5(3)
C26	C21	Ir2	125.4(3)	N7	C59	C60	111.1(3)
N3	C27	C28	113.7(3)	N7	C59	C64	106.8(3)

N3	C27	C32	108.0(3)	C60	C59	C64	112.5(3)
C32	C27	C28	111.1(3)	C61	C60	C59	111.3(3)
C27	C28	C29	112.9(3)	C60	C61	C62	109.5(3)
C30	C29	C28	111.8(3)	C63	C62	C61	111.2(4)
C29	C30	C31	110.6(3)	C64	C63	C62	112.8(3)
C32	C31	C30	109.4(3)	N8	C64	C59	107.4(3)
N4	C32	C27	106.4(3)	N8	C64	C63	112.5(3)
N4	C32	C31	111.3(3)	C63	C64	C59	111.9(3)
C31	C32	C27	112.9(3)	Cl9	C65	Cl10	112.4(3)
N5	Ir3	Cl3	86.89(9)				

Table 6 Torsion Angles for DMMXI044A_ABS.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ir1	N1	C16	C11	42.6(4)	Ir3	N5	C48	C43	23.6(4)
Ir1	N1	C16	C15	167.6(3)	Ir3	N5	C48	C47	-98.9(3)
Ir1	N2	C11	C12	-90.9(4)	Ir3	N6	C43	C44	174.1(3)
Ir1	N2	C11	C16	34.5(4)	Ir3	N6	C43	C48	49.1(4)
Ir1	C1	C2	C3	60.5(3)	Ir3	C33	C34	C35	60.5(3)
Ir1	C1	C2	C7	-119.1(4)	Ir3	C33	C34	C39	-118.6(4)
Ir1	C1	C5	C4	-62.2(3)	Ir3	C33	C37	C36	-62.9(3)
Ir1	C1	C5	C10	123.1(5)	Ir3	C33	C37	C42	124.2(4)
Ir1	C2	C3	C4	61.7(3)	Ir3	C34	C35	C36	62.0(3)
Ir1	C2	C3	C8	-120.2(4)	Ir3	C34	C35	C40	-118.7(4)
Ir1	C3	C4	C5	59.4(3)	Ir3	C35	C36	C37	58.0(3)
Ir1	C3	C4	C9	-119.8(5)	Ir3	C35	C36	C41	-122.3(4)
Ir1	C4	C5	C1	62.3(3)	Ir3	C36	C37	C33	62.3(3)
Ir1	C4	C5	C10	-123.0(5)	Ir3	C36	C37	C42	-125.0(4)
N2	C11	C12	C13	174.8(4)	N6	C43	C44	C45	-73.3(5)
N2	C11	C16	N1	-49.2(4)	N6	C43	C48	N5	-46.8(4)
N2	C11	C16	C15	-175.0(3)	N6	C43	C48	C47	75.1(4)
C1	C2	C3	Ir1	-61.3(3)	C33	C34	C35	Ir3	-61.1(3)
C1	C2	C3	C4	0.4(5)	C33	C34	C35	C36	0.9(5)
C1	C2	C3	C8	178.5(4)	C33	C34	C35	C40	-179.8(4)
C2	C1	C5	Ir1	60.0(3)	C34	C33	C37	Ir3	59.6(3)
C2	C1	C5	C4	-2.3(5)	C34	C33	C37	C36	-3.3(4)
C2	C1	C5	C10	-177.0(4)	C34	C33	C37	C42	-176.3(4)
C2	C3	C4	Ir1	-61.3(3)	C34	C35	C36	Ir3	-61.0(3)
C2	C3	C4	C5	-1.8(5)	C34	C35	C36	C37	-3.0(5)
C2	C3	C4	C9	178.9(4)	C34	C35	C36	C41	176.6(4)
C3	C4	C5	Ir1	-59.7(3)	C35	C36	C37	Ir3	-58.4(3)
C3	C4	C5	C1	2.5(5)	C35	C36	C37	C33	3.9(4)
C3	C4	C5	C10	177.3(4)	C35	C36	C37	C42	176.6(4)
C5	C1	C2	Ir1	-59.4(3)	C37	C33	C34	Ir3	-59.0(3)
C5	C1	C2	C3	1.2(5)	C37	C33	C34	C35	1.5(4)
C5	C1	C2	C7	-178.5(4)	C37	C33	C34	C39	-177.6(4)
C6	C1	C2	Ir1	120.9(4)	C38	C33	C34	Ir3	120.6(4)
C6	C1	C2	C3	-178.6(4)	C38	C33	C34	C35	-178.9(4)
C6	C1	C2	C7	1.7(7)	C38	C33	C34	C39	2.0(6)
C6	C1	C5	Ir1	-120.3(4)	C38	C33	C37	Ir3	-120.0(4)

C6	C1	C5	C4	177.5(4)	C38	C33	C37 C36	177.1(4)
C6	C1	C5	C10	2.8(7)	C38	C33	C37 C42	4.2(7)
C7	C2	C3	Ir1	118.4(4)	C39	C34	C35 Ir3	118.0(4)
C7	C2	C3	C4	-179.9(4)	C39	C34	C35 C36	180.0(4)
C7	C2	C3	C8	-1.8(7)	C39	C34	C35 C40	-0.7(7)
C8	C3	C4	Ir1	120.7(5)	C40	C35	C36 Ir3	119.7(4)
C8	C3	C4	C5	-179.9(4)	C40	C35	C36 C37	177.7(4)
C8	C3	C4	C9	0.8(8)	C40	C35	C36 C41	-2.7(7)
C9	C4	C5	Ir1	119.5(5)	C41	C36	C37 Ir3	122.0(4)
C9	C4	C5	C1	-178.2(4)	C41	C36	C37 C33	-175.8(4)
C9	C4	C5	C10	-3.4(7)	C41	C36	C37 C42	-3.0(7)

C11	C12	C13	C14	-56.4(5)	C43	C44	C45 C46	-51.4(5)
C12	C11	C16	N1	75.5(4)	C44	C43	C48 N5	-172.9(3)
C12	C11	C16	C15	-50.2(5)	C44	C43	C48 C47	-51.0(5)
C12	C13	C14	C15	56.7(5)	C44	C45	C46 C47	56.2(5)
C13	C14	C15	C16	-54.1(5)	C45	C46	C47 C48	-59.6(5)
C14	C15	C16	N1	-72.7(5)	C46	C47	C48 N5	177.4(3)
C14	C15	C16	C11	50.3(5)	C46	C47	C48 C43	56.5(5)
C16	C11	C12	C13	53.3(5)	C48	C43	C44 C45	48.9(5)
Ir2	N3	C27	C28	158.3(3)	Ir4	N7	C59 C60	75.2(3)
Ir2	N3	C27	C32	34.5(4)	Ir4	N7	C59 C64	-47.8(3)
Ir2	N4	C32	C27	45.0(3)	Ir4	N8	C64 C59	-29.0(4)
Ir2	N4	C32	C31	-78.4(3)	Ir4	N8	C64 C63	-152.5(3)
Ir2	C17	C18	C19	60.5(3)	Ir4	C49	C50 C51	60.6(3)
Ir2	C17	C18	C23	-126.0(4)	Ir4	C49	C50 C56	-128.1(4)
Ir2	C17	C21	C20	-62.7(3)	Ir4	C49	C53 C52	-59.9(3)
Ir2	C17	C21	C26	120.9(4)	Ir4	C49	C53 C54	123.3(4)
Ir2	C18	C19	C20	61.1(3)	Ir4	C50	C51 C52	59.7(3)
Ir2	C18	C19	C24	-123.8(4)	Ir4	C50	C51 C57	-119.7(4)
Ir2	C19	C20	C21	59.7(3)	Ir4	C51	C52 C53	62.5(3)
Ir2	C19	C20	C25	-122.4(4)	Ir4	C51	C52 C58	-121.8(4)
Ir2	C20	C21	C17	63.2(3)	Ir4	C52	C53 C49	60.8(3)
Ir2	C20	C21	C26	-120.4(4)	Ir4	C52	C53 C54	-122.3(4)
N3	C27	C28	C29	-72.1(4)	N7	C59	C60 C61	-174.8(3)
N3	C27	C32	N4	-50.8(4)	N7	C59	C64 N8	48.7(4)
N3	C27	C32	C31	71.7(4)	N7	C59	C64 C63	172.6(3)
C17	C18	C19	Ir2	-61.0(3)	C49	C50	C51 Ir4	-60.6(3)
C17	C18	C19	C20	0.1(4)	C49	C50	C51 C52	-0.9(4)
C17	C18	C19	C24	175.2(4)	C49	C50	C51 C57	179.7(4)
C18	C17	C21	Ir2	59.8(3)	C50	C49	C53 Ir4	61.4(3)
C18	C17	C21	C20	-2.8(5)	C50	C49	C53 C52	1.5(4)
C18	C17	C21	C26	-179.3(4)	C50	C49	C53 C54	-175.3(4)
C18	C19	C20	Ir2	-61.5(3)	C50	C51	C52 Ir4	-60.7(3)
C18	C19	C20	C21	-1.8(4)	C50	C51	C52 C53	1.8(4)
C18	C19	C20	C25	176.1(4)	C50	C51	C52 C58	177.5(4)
C19	C20	C21	Ir2	-60.3(3)	C51	C52	C53 Ir4	-62.9(3)
C19	C20	C21	C17	2.8(5)	C51	C52	C53 C49	-2.0(4)
C19	C20	C21	C26	179.3(4)	C51	C52	C53 C54	174.8(4)
C21	C17	C18	Ir2	-58.8(3)	C53	C49	C50 Ir4	-61.0(3)

C21 C17 C18 C19	1.7(4)	C53 C49 C50 C51	-0.4(4)
C21 C17 C18 C23	175.2(4)	C53 C49 C50 C56	170.9(4)
C22 C17 C18 Ir2	120.4(4)	C55 C49 C50 Ir4	125.6(4)
C22 C17 C18 C19	-179.0(4)	C55 C49 C50 C51	-173.8(4)
C22 C17 C18 C23	-5.6(7)	C55 C49 C50 C56	-2.5(6)
C22 C17 C21 Ir2	-119.4(4)	C55 C49 C53 Ir4	-125.4(4)
C22 C17 C21 C20	177.9(4)	C55 C49 C53 C52	174.7(4)
C22 C17 C21 C26	1.5(7)	C55 C49 C53 C54	-2.1(7)
C23 C18 C19 Ir2	125.3(4)	C56 C50 C51 Ir4	128.5(4)
C23 C18 C19 C20	-173.6(4)	C56 C50 C51 C52	-171.9(4)
C23 C18 C19 C24	1.5(6)	C56 C50 C51 C57	8.7(7)

C24 C19 C20 Ir2	123.5(4)	C57 C51 C52 Ir4	118.7(4)
C24 C19 C20 C21	-176.8(4)	C57 C51 C52 C53	-178.8(4)
C24 C19 C20 C25	1.1(7)	C57 C51 C52 C58	-3.1(7)
C25 C20 C21 Ir2	121.8(4)	C58 C52 C53 Ir4	121.3(4)
C25 C20 C21 C17	-175.1(4)	C58 C52 C53 C49	-177.9(4)
C25 C20 C21 C26	1.4(7)	C58 C52 C53 C54	-1.1(6)
C27 C28 C29 C30	-52.0(5)	C59 C60 C61 C62	58.0(4)
C28 C27 C32 N4	-176.1(3)	C60 C59 C64 N8	-73.4(4)
C28 C27 C32 C31	-53.7(4)	C60 C59 C64 C63	50.5(4)
C28 C29 C30 C31	56.0(5)	C60 C61 C62 C63	-57.6(4)
C29 C30 C31 C32	-58.4(4)	C61 C62 C63 C64	54.5(5)
C30 C31 C32 N4	177.5(3)	C62 C63 C64 N8	70.7(4)
C30 C31 C32 C27	57.9(4)	C62 C63 C64 C59	-50.3(4)
C32 C27 C28 C29	50.0(4)	C64 C59 C60 C61	-55.1(4)

Table 7 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for DMMXI044A_ABS.

Atom	*x*	*y*	*z*	U(eq)
H1A	9540.81	3608.74	7807.72	22
H1B	10021.64	3469.66	7449.83	22
H2A	9896.36	6069.59	7396.31	22
H2B	9339.63	6057.61	7558.5	22
H6A	10255.39	2929.77	6333.08	46
H6B	10018.09	2742.63	5595.95	46
H6C	9665.83	2546.01	6205.15	46
H7A	8784.31	2986	6029.07	48
H7B	8679.91	3358.46	5292.41	48
H7C	8402.53	3838.28	5885.45	48
H8A	8361.75	5352.25	5871.7	47
H8B	8605.01	5783.02	5235.8	47
H8C	8698.14	6270.31	5937.35	47
H9A	9557.19	6815.78	6158.36	46
H9B	9909.79	6658.82	5543.73	46
H9C	10166.52	6532.41	6279.14	46

H10A	10726.05	5311.31	6447.88	50
H10B	10790.63	4784.11	5769.99	50
H10C	10757.48	4227.87	6441.81	50
H11	10037.96	5809.43	8426.37	23
H12A	9062.78	4830.83	8379.95	29
H12B	9165.21	5811.91	8701.91	29
H13A	9193.78	4667.25	9531.87	36
H13B	9749.09	5189.53	9533.51	36
H14A	9537.65	3442.37	8944.77	40
H14B	9913.03	3614.33	9599.7	40
H15A	10536.11	4379.56	9000.55	34
H15B	10420.88	3420.01	8653.23	34
H16	10450.03	4671.91	7903.65	25
H3A	6763.94	8672.52	2897.54	19
H3B	6862.58	9573.99	3189.6	19
H4A	8253.21	9151.21	2962.6	21
H4B	8266.97	8159.39	2889.36	21
H22A	8019.28	9236.06	5233.23	45
H22B	7807.54	8515.87	5742.2	45
H22C	7404.49	9214.03	5372.95	45
H23A	6605.36	8764.16	4905.51	38
H23B	6472.05	7717.88	5020.29	38
H23C	6329.11	8175.58	4317.02	38
H24A	6482.69	7136.58	3470.55	30
H24B	6656.75	6224.44	3852.41	30
H24C	6920.99	6490.35	3185.51	30
H25A	7825.23	6363.1	3136.11	36
H25B	8072.18	5863.93	3784.86	36
H25C	8389.43	6671.79	3463.85	36

H26A	8808.32	7599.83	4230.23	44
H26B	8723.79	7413	4991.45	44
H26C	8708.32	8428.71	4714.3	44
H27	7435.9	9994.06	2486.74	19
H28A	7058.33	9797.02	1442.8	23
H28B	6573.98	9821.48	1909.26	23
H29A	6466.77	8254.73	1837.72	24
H29B	6482.71	8632.38	1100.89	24
H30A	7369.08	8168.69	1056.68	24
H30B	7022.86	7314.61	1256.91	24
H31A	7313.62	7514.39	2388.09	21
H31B	7819.23	7399.17	1959.76	21
H32	7941.08	8980.47	1934.99	18
H5A	4475.03	4947.48	2647.71	21
H5B	5047.57	5090.88	2618.13	21
H6D	4953.89	7407.73	2822.67	22
H6E	4400.44	7683.69	2659.34	22
H38A	5456.15	4621.26	1540.37	33
H38B	5317.83	4509.83	764.81	33
H38C	4881.24	4277.54	1273.5	33

H39A	4031.07	4750.81	956.37	36
H39B	4129.65	5025.77	213.04	36
H39C	3704.95	5569.55	608.53	36
H40A	3645.88	7137.67	813.48	38
H40B	3968.77	7572.64	241.15	38
H40C	3988.78	8037.06	953.81	38
H41A	4784.47	8542.14	1387.59	31
H41B	5240.32	8412.84	886.87	31
H41C	5365.78	8236.02	1658.28	31
H42A	5903.52	6969.6	1938.68	36
H42B	6077.66	6543.33	1262.46	36
H42C	5935.69	5892.67	1855.28	36
H43	4063.77	6528.86	3238.45	26
H44A	4352.64	7813.9	3901.54	31
H44B	4303.76	6887.82	4300.98	31
H45A	5082.97	7572.59	4692.99	32
H45B	5268.06	7718.26	3962.03	32
H46A	5186.76	5993.83	4601.03	34
H46B	5731.33	6475.24	4441.74	34
H47A	5510.89	6316.25	3291.78	28
H47B	5515.19	5341.25	3639.99	28
H48	4588.15	5359.9	3657.56	25
H7D	3148.12	8457.48	2412.06	19
H7E	3103.23	7480.93	2547.97	19
H8D	1766.24	7110.67	2835.84	19
H8E	1623.34	7967.8	2502.08	19
H54A	3211.41	10023.83	2753.54	27
H54B	2952.76	10902.98	3062.84	27
H54C	2642.44	10372.72	2468.37	27

H55A	1758.87	10205.84	2543.98	31
H55B	1501.1	10567.04	3192.09	31
H55C	1332.85	9599.13	2890.35	31
H56A	1204.68	8669.91	3871.98	40
H56B	1335.49	9395.4	4445.22	40
H56C	1498.69	8355.65	4555.71	40
H57A	2332.18	7807.84	4902.03	39
H57B	2611.65	8662.86	5263.55	39
H57C	2954.01	7972.58	4858.6	39
H58A	3581.12	8726.16	4320.3	32
H58B	3591.48	9804.01	4232.85	32
H58C	3653.07	9158.58	3609.93	32
H59	2789.46	7588.56	1504.76	20
H60A	2197.64	9122.47	1924.19	23
H60B	2679.19	9166.32	1452.5	23
H61A	2167.88	8384.3	613.4	26
H61B	1855.82	9276.75	817.78	26
H62A	1326.08	8405.63	1498.13	26
H62B	1273.78	7999.95	765.72	26

H63A	1402.09	6825.55	1569.93	23
H63B	1859.97	6821.16	1064.3	23
H64	2277.93	6629.52	2090.28	18
H65A	6787.69	4125.83	4504.29	41
H65B	6921.11	3943.01	5273.56	41

Experimental

Single crystals of $C_{32.5}H_{59}N_4Cl_5Ir_2$ [DMMXI044A_ABS] were []. A suitable crystal was selected and [] on a Gemini_Mo_Eos diffractometer. The crystal was kept at 99.9 K during data collection. Using Olex2 [1], the structure was solved with the Unknown [2] structure solution program using Unknown and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [DMMXI044A_ABS]

Crystal Data for $C_{32.5}H_{59}N_4Cl_5Ir_2$ (M =1067.48 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 25.3023(2) Å, b = 14.75173(12) Å, c = 20.32938(18) Å, β = 93.8630(8)°, V = 7570.75(11) Å^3, Z = 8, T = 99.9 K, μ(MoKα) = 7.405 mm^{-1}, *Dcalc* = 1.873 g/cm^3, 161024 reflections measured (6.956° ≤ 2Θ ≤ 64.946°), 25813 unique (R_{int} = 0.0659, R_{sigma} = 0.0486) which were used in all calculations. The final R_1 was 0.0338 (I > 2σ(I)) and wR_2 was 0.0669 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Ternary CH refined with riding coordinates:
 C11(H11), C16(H16), C27(H27), C32(H32), C43(H43), C48(H48), C59(H59), C64(H64)
2.b Secondary CH2 refined with riding coordinates:
 N1(H1A,H1B), N2(H2A,H2B), C12(H12A,H12B), C13(H13A,H13B), C14(H14A,H14B),
 C15(H15A,H15B), N3(H3A,H3B), N4(H4A,H4B), C28(H28A,H28B), C29(H29A,H29B),
 C30(H30A,H30B), C31(H31A,H31B), N5(H5A,H5B), N6(H6D,H6E), C44(H44A,H44B),
 C45(H45A,H45B), C46(H46A,H46B), C47(H47A,H47B), N7(H7D,H7E), N8(H8D,H8E),
 C60(H60A,H60B), C61(H61A,H61B), C62(H62A,H62B), C63(H63A,H63B), C65(H65A,H65B)
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2.c Idealised Me refined as rotating group:
 C6(H6A,H6B,H6C), C7(H7A,H7B,H7C), C8(H8A,H8B,H8C), C9(H9A,H9B,H9C), C10(H10A,
 H10B,H10C), C22(H22A,H22B,H22C), C23(H23A,H23B,H23C), C24(H24A,H24B,H24C),
 C25(H25A,H25B,H25C), C26(H26A,H26B,H26C), C38(H38A,H38B,H38C), C39(H39A,H39B, H39C),
 C40(H40A,H40B,H40C), C41(H41A,H41B,H41C), C42(H42A,H42B,H42C), C54(H54A, H54B,H54C),
 C55(H55A,H55B,H55C), C56(H56A,H56B,H56C), C57(H57A,H57B,H57C), C58(H58A,H58B,H58C)
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This report has been created with Olex2, compiled on May 18 2018 14:05:52 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

Entry 8S. Tables of Data and Bond Lengths and Angles for Compound 2. CCDC1901125

Table 1 Crystal data and structure refinement for DMMXI059a_abs.

Identification code	DMMXI059a_abs
Empirical formula	$C_{16}H_{31}Cl_2IrN_2O$
Formula weight	530.53
Temperature/K	100.0(6)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.16689(15)
b/Å	20.2059(4)
c/Å	21.1011(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3908.44(12)
Z	8
ρ_{calc}g/cm^3	1.803
μ/mm ^{1}	7.109
F(000)	2080.0
Crystal size/mm^3	0.3217 × 0.2996 × 0.0683
Radiation	MoKα (λ = 0.71073) 2Θ
range for data collection/°	7.058 to 64.952
Index ranges	-13 ≤ h ≤ 13, -28 ≤ k ≤ 30, -31 ≤ l ≤ 31
Reflections collected	86880
Independent reflections	13359 [R_{int} = 0.0662, R_{sigma} = 0.0432] Data/restraints/parameters
13359/0/421	
Goodness-of-fit on F^2	1.087
Final R indexes [I>=2σ (I)]	R_1 = 0.0311, wR_2 = 0.0626
Final R indexes [all data]	R_1 = 0.0356, wR_2 = 0.0646
Largest diff. peak/hole / e Å^{-3}	1.37/-1.13
Flack parameter	-0.006(4)

DMMXI059a_abs

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for DMMXI059a_abs. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ir1	7489.2(2)	6306.8(2)	6206.9(2)	9.53(4)
Cl1	6873.0(14)	5131.4(6)	6225.0(7)	16.6(2)
N1	9260(5)	6050(2)	5599(2)	10.9(9)
N2	6457(4)	6329(2)	5307.4(19)	10.6(8)
C1	7827(6)	7300(2)	6541(2)	14.6(10)

C2	6309(6)	7115(3)	6635(3)	13.8(10)
C3	6246(6)	6553(3)	7037(3)	16.4(11)
C4	7741(6)	6388(3)	7227(2)	15.4(10)
C5	8699(6)	6848(3)	6920(3)	14.9(11)
C6	8404(6)	7898(3)	6202(3)	19.6(11)
C7	5040(6)	7446(3)	6320(3)	20.7(13)
C8	4881(6)	6204(3)	7261(3)	26.2(13)
C9	8175(7)	5832(3)	7653(3)	24.9(13)
C10	10317(6)	6865(3)	6981(3)	21.1(13)
C11	7286(6)	5921(2)	4845(2)	10.6(9)
C12	8875(6)	6093(3)	4914(2)	12.1(10)
C13	9823(6)	5647(3)	4504(3)	15.0(11)
C14	9324(6)	5653(3)	3813(3)	19.3(11)
C15	7691(6)	5521(2)	3749(2)	17.7(10)
C16	6788(6)	5996(3)	4163(2)	13.6(10)
Ir2	2320.5(2)	3740.7(2)	6161.9(2)	9.41(4)
Cl3	1443.1(14)	4877.1(6)	6137.5(7)	16.9(2)
N3	4066(5)	4101(2)	5585(2)	11.0(9)
N4	1448(5)	3596(2)	5236(2)	10.7(8)
C17	3579(6)	3276(3)	6906(3)	14.0(11)
C18	2527(6)	3717(3)	7183(2)	16.0(10)
C19	1072(6)	3487(3)	6996(3)	14.5(11)
C20	1251(6)	2912(3)	6610(3)	13.8(10)
C21	2808(6)	2781(2)	6542(2)	12.9(10)
C22	5203(6)	3322(3)	6971(3)	21.5(13)
C23	2827(7)	4311(3)	7586(3)	21.6(12)
C24	-342(6)	3792(3)	7196(3)	22.8(12)
C25	66(6)	2513(3)	6313(3)	21.1(13)
C26	3476(6)	2195(2)	6220(3)	17.0(11)
C27	3485(6)	4311(2)	4965(2)	10.0(9)
C28	2521(5)	3756(2)	4727(2)	11.5(9)
C29	1772(6)	3945(3)	4102(3)	15.8(11)
C30	2903(6)	4173(3)	3605(2)	15.9(11)
C31	3910(5)	4715(2)	3869(3)	13.7(10)
C32	4661(6)	4481(3)	4477(3)	13.7(11)
Cl2	1653.9(14)	7212.0(6)	5363.4(7)	15.7(3)
Cl4	6441.8(15)	2931.4(6)	5312.4(7)	16.6(3)
O1	3475(5)	5928(2)	5351(3)	30.2(11)
O2	8515(5)	4156(2)	5180(2)	23.6(9)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for DMMXI059a_abs. The Anisotropic displacement factor exponent takes the form:

$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir1	11.50(8)	7.61(8)	9.48(8)	0.74(7)	0.44(7)	0.16(7)

Cl1	20.4(6)	9.6(5)	19.7(6)	1.6(5)	1.1(5)	-2.1(4)
N1	13(2)	9(2)	11(2)	-1.0(17)	-1.4(16)	-0.6(17)
N2	13.6(18)	9(2)	8.8(19)	-0.4(17)	2.6(15)	0.0(18)
C1	20(3)	13(2)	12(2)	-3.0(19)	-3(2)	0(2)
C2	19(3)	11(2)	11(3)	-2(2)	0(2)	2(2)
C3	18(3)	15(3)	17(3)	-5(2)	4(2)	-1(2)
C4	20(2)	16(2)	11(2)	-2.2(18)	-2.9(19)	3(2)
C5	22(3)	12(3)	10(3)	-1(2)	-1(2)	0(2)
C6	29(3)	15(2)	15(3)	1(2)	-3(3)	-5(2)
C7	23(3)	24(3)	16(3)	-1(2)	2(2)	9(2)
C8	24(3)	29(3)	25(3)	0(3)	9(2)	-4(3)
C9	32(3)	28(3)	15(3)	8(2)	-1(3)	5(3)
C10	16(3)	32(3)	15(3)	-1(2)	-4(2)	-2(2)
C11	15(2)	6.6(19)	10(2)	-1.5(16)	3.8(19)	-0.6(19)
C12	14(2)	12(2)	11(2)	-2.4(19)	0.9(18)	-1.7(18)
C13	15(3)	15(3)	15(3)	-4(2)	2(2)	0(2)
C14	26(3)	14(2)	18(3)	-3(2)	10(3)	0(2)
C15	28(3)	16(2)	9(2)	-4.5(19)	0(2)	0(2)
C16	19(3)	13(2)	9(2)	0.1(19)	-2.7(19)	1(2)
Ir2	10.82(7)	7.87(8)	9.54(8)	-0.24(7)	0.16(7)	0.16(7)
Cl3	20.1(6)	10.1(5)	20.4(7)	-0.7(5)	0.7(6)	4.5(4)
N3	16(2)	7.1(19)	9(2)	0.5(16)	-1.4(16)	-2.4(16)
N4	13.6(19)	8.6(19)	10(2)	1.1(16)	-0.7(16)	-1.4(16)
C17	16(3)	14(3)	12(3)	2(2)	1(2)	1(2)
C18	22(2)	19(2)	8(2)	1.5(18)	-1.3(18)	1(3)
C19	15(2)	15(3)	13(3)	5(2)	4(2)	-1(2)
C20	18(3)	14(3)	10(3)	3(2)	1(2)	-1(2)
C21	18(2)	11(2)	9(2)	2.9(18)	2(2)	1(2)
C22	17(3)	29(3)	18(3)	1(3)	-3(2)	2(2)
C23	29(3)	24(3)	12(2)	-8(2)	2(2)	-4(2)
C24	22(3)	25(3)	21(3)	-2(3)	8(2)	2(3)
C25	24(3)	21(3)	18(3)	-4(2)	2(3)	-9(2)
C26	21(2)	11(2)	19(3)	1(2)	1(2)	3.9(19)
C27	9(2)	10(2)	10(2)	-0.2(18)	-0.5(17)	-2.9(18)
C28	12(2)	10(2)	13(2)	-2.2(17)	-0.2(17)	0(2)
C29	17(2)	14(2)	16(3)	0(2)	-2(2)	-4(2)
C30	26(3)	12(2)	9(2)	0.2(18)	-3(2)	0(2)
C31	16(2)	14(2)	11(2)	-1(2)	2(2)	-3.5(18)
C32	13(2)	13(2)	15(3)	1(2)	-1.5(19)	-3(2)
Cl2	16.9(6)	12.2(6)	18.1(7)	1.3(5)	0.6(5)	-1.3(5)
Cl4	19.2(6)	12.0(6)	18.7(7)	-2.4(5)	3.4(5)	0.6(5)
O1	17(2)	17(2)	57(3)	3(2)	2(2)	2.3(18)
O2	18(2)	17(2)	36(3)	-4.2(19)	3.0(19)	-1.5(17)

Table 4 Bond Lengths for DMMXI059a_abs.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

Ir1	Cl1	2.4415(12)	Ir2	Cl3	2.4335(12)
Ir1	N1	2.132(5)	Ir2	N3	2.138(4)
Ir1	N2	2.121(4)	Ir2	N4	2.131(4)
Ir1	C1	2.149(5)	Ir2	C17	2.163(5)
Ir1	C2	2.157(5)	Ir2	C18	2.163(5)
Ir1	C3	2.149(6)	Ir2	C19	2.161(5)
Ir1	C4	2.171(5)	Ir2	C20	2.158(5)
Ir1	C5	2.166(6)	Ir2	C21	2.146(5)
N1	C12	1.492(7)	N3	C27	1.476(6)
N2	C11	1.486(6)	N4	C28	1.492(6)
C1	C2	1.455(8)	C17	C18	1.437(7)
C1	C5	1.454(7)	C17	C21	1.448(7)
C1	C6	1.501(7)	C17	C22	1.498(8)
C2	C3	1.420(8)	C18	C19	1.467(7)
C2	C7	1.496(8)	C18	C23	1.496(7)
C3	C4	1.466(8)	C19	C20	1.427(8)
C3	C8	1.511(8)	C19	C24	1.497(8)
C4	C5	1.433(8)	C20	C21	1.459(7)
C4	C9	1.493(7)	C20	C25	1.492(8)
C5	C10	1.489(8)	C21	C26	1.496(7)
C11	C12	1.505(7)	C27	C28	1.513(6)
C11	C16	1.518(7)	C27	C32	1.529(7)
C12	C13	1.521(7)	C28	C29	1.535(7)
C13	C14	1.527(8)	C29	C30	1.545(7)
C14	C15	1.526(8)	C30	C31	1.537(7)
C15	C16	1.538(7)	C31	C32	1.531(7)

Table 5 Bond Angles for DMMXI059a_abs.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ir1	Cl1	87.08(13)	N3	Ir2	Cl3	85.04(12)
N1	Ir1	C1	108.3(2)	N3	Ir2	C17	99.32(19)
N1	Ir1	C2	144.8(2)	N3	Ir2	C18	120.59(18)
N1	Ir1	C3	161.9(2)	N3	Ir2	C19	160.17(19)
N1	Ir1	C4	122.24(19)	N3	Ir2	C20	148.62(19)
N1	Ir1	C5	98.7(2)	N3	Ir2	C21	111.40(18)
N2	Ir1	Cl1	86.05(12)	N4	Ir2	Cl3	89.22(12)
N2	Ir1	N1	78.85(16)	N4	Ir2	N3	78.81(16)
N2	Ir1	C1	109.76(18)	N4	Ir2	C17	143.72(18)
N2	Ir1	C2	97.76(18)	N4	Ir2	C18	160.52(18)
N2	Ir1	C3	119.2(2)	N4	Ir2	C19	121.0(2)
N2	Ir1	C4	158.91(18)	N4	Ir2	C20	97.17(19)
N2	Ir1	C5	147.11(19)	N4	Ir2	C21	107.22(18)
C1	Ir1	Cl1	159.47(15)	C17	Ir2	Cl3	126.94(15)
C1	Ir1	C2	39.5(2)	C17	Ir2	C18	38.81(19)
C1	Ir1	C4	65.8(2)	C18	Ir2	Cl3	94.04(14)
C1	Ir1	C5	39.4(2)	C19	Ir2	Cl3	93.79(15)
C2	Ir1	Cl1	127.88(15)	C19	Ir2	C17	65.7(2)
C2	Ir1	C4	65.2(2)	C19	Ir2	C18	39.7(2)
C2	Ir1	C5	65.4(2)	C20	Ir2	Cl3	126.23(15)

C3	Ir1	Cl1	95.14(16)	C20	Ir2	C17	65.6(2)
C3	Ir1	C1	66.0(2)	C20	Ir2	C18	65.6(2)
C3	Ir1	C2	38.5(2)	C20	Ir2	C19	38.6(2)
C3	Ir1	C4	39.7(2)	C21	Ir2	Cl3	158.40(14)
C3	Ir1	C5	65.7(2)	C21	Ir2	C17	39.3(2)
C4	Ir1	Cl1	94.73(15)	C21	Ir2	C18	65.82(19)
C5	Ir1	Cl1	126.77(15)	C21	Ir2	C19	65.9(2)
C5	Ir1	C4	38.6(2)	C21	Ir2	C20	39.6(2)
C12	N1	Ir1	112.9(3)	C27	N3	Ir2	109.5(3)
C11	N2	Ir1	110.4(3)	C28	N4	Ir2	112.5(3)
C2	C1	Ir1	70.6(3)	C18	C17	Ir2	70.6(3)
C2	C1	C6	127.5(5)	C18	C17	C21	108.5(5)
C5	C1	Ir1	70.9(3)	C18	C17	C22	126.3(5)
C5	C1	C2	106.8(5)	C21	C17	Ir2	69.8(3)
C5	C1	C6	125.1(5)	C21	C17	C22	125.2(5)
C6	C1	Ir1	130.3(4)	C22	C17	Ir2	124.7(4)
C1	C2	Ir1	69.9(3)	C17	C18	Ir2	70.6(3)
C1	C2	C7	124.7(5)	C17	C18	C19	107.7(5)
C3	C2	Ir1	70.4(3)	C17	C18	C23	127.2(5)
C3	C2	C1	109.0(5)	C19	C18	Ir2	70.1(3)
C3	C2	C7	126.2(5)	C19	C18	C23	125.1(5)
C7	C2	Ir1	122.8(4)	C23	C18	Ir2	124.4(4)
C2	C3	Ir1	71.1(3)	C18	C19	Ir2	70.3(3)
C2	C3	C4	107.9(5)	C18	C19	C24	125.5(5)
C2	C3	C8	126.4(5)	C20	C19	Ir2	70.6(3)
C4	C3	Ir1	71.0(3)	C20	C19	C18	107.9(5)
C4	C3	C8	125.7(5)	C20	C19	C24	126.6(5)

C8	C3	Ir1	125.8(4)	C24	C19	Ir2	126.2(4)
C3	C4	Ir1	69.3(3)	C19	C20	Ir2	70.8(3)
C3	C4	C9	125.8(5)	C19	C20	C21	108.5(5)
C5	C4	Ir1	70.5(3)	C19	C20	C25	126.6(5)
C5	C4	C3	107.6(5)	C21	C20	Ir2	69.7(3)
C5	C4	C9	126.6(5)	C21	C20	C25	124.9(5)
C9	C4	Ir1	124.6(4)	C25	C20	Ir2	124.4(4)
C1	C5	Ir1	69.7(3)	C17	C21	Ir2	71.0(3)
C1	C5	C10	125.5(5)	C17	C21	C20	107.4(5)
C4	C5	Ir1	70.9(3)	C17	C21	C26	126.1(5)
C4	C5	C1	108.6(5)	C20	C21	Ir2	70.6(3)
C4	C5	C10	125.9(5)	C20	C21	C26	126.2(5)
C10	C5	Ir1	125.5(4)	C26	C21	Ir2	129.1(4)
N2	C11	C12	107.7(4)	N3	C27	C28	106.9(4)
N2	C11	C16	114.5(4)	N3	C27	C32	114.0(4)
C12	C11	C16	111.1(4)	C28	C27	C32	110.8(4)
N1	C12	C11	108.0(4)	N4	C28	C27	107.9(4)
N1	C12	C13	112.5(4)	N4	C28	C29	112.2(4)
C11	C12	C13	111.2(4)	C27	C28	C29	111.2(4)
C12	C13	C14	111.6(5)	C28	C29	C30	110.9(4)
C15	C14	C13	112.1(5)	C31	C30	C29	111.7(4)
C14	C15	C16	111.7(4)	C32	C31	C30	110.7(4)

C11	C16	C15	108.3(4)	C27	C32	C31	108.4(4)

Table 6 Hydrogen Bonds for DMMXI059a_abs.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2	H2A	O1	0.91	1.95	2.854(6)	172.6
N4	H4B	O2[1]	0.91	2.05	2.920(6)	160.9
O1	H1D	Cl2	0.85	2.26	3.086(4)	163.7
O2	H2D	Cl4	0.85	2.32	3.133(4)	160.2

[1]-1+X,+Y,+Z

Table 7 Torsion Angles for DMMXI059a_abs.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ir1	N1	C12	C11	-32.0(5)	Ir2	N3	C27	C28	-48.5(4)
Ir1	N1	C12	C13	-155.0(3)	Ir2	N3	C27	C32	-171.3(3)
Ir1	N2	C11	C12	-46.1(4)	Ir2	N4	C28	C27	-32.4(4)
Ir1	N2	C11	C16	-170.2(3)	Ir2	N4	C28	C29	-155.2(3)
Ir1	C1	C2	C3	59.8(4)	Ir2	C17	C18	C19	60.5(3)
Ir1	C1	C2	C7	-116.7(5)	Ir2	C17	C18	C23	-119.0(5)
Ir1	C1	C5	C4	-60.5(4)	Ir2	C17	C21	C20	-61.6(4)
Ir1	C1	C5	C10	119.8(6)	Ir2	C17	C21	C26	125.1(5)
Ir1	C2	C3	C4	61.8(4)	Ir2	C18	C19	C20	60.9(4)
Ir1	C2	C3	C8	-121.1(6)	Ir2	C18	C19	C24	-121.0(6)
Ir1	C3	C4	C5	60.4(4)	Ir2	C19	C20	C21	59.8(4)
Ir1	C3	C4	C9	-118.5(5)	Ir2	C19	C20	C25	-119.2(6)
Ir1	C4	C5	C1	59.7(4)	Ir2	C20	C21	C17	61.9(4)
Ir1	C4	C5	C10	-120.6(6)	Ir2	C20	C21	C26	-124.9(5)
N1	C12	C13	C14	175.0(4)	N3	C27	C28	N4	52.6(5)
N2	C11	C12	N1	50.4(5)	N3	C27	C28	C29	176.0(4)
N2	C11	C12	C13	174.2(4)	N3	C27	C32	C31	-177.8(4)
N2	C11	C16	C15	-177.2(4)	N4	C28	C29	C30	174.5(4)
C1	C2	C3	Ir1	-59.5(4)	C17	C18	C19	Ir2	-60.9(4)
C1	C2	C3	C4	2.3(6)	C17	C18	C19	C20	0.0(6)
C1	C2	C3	C8	179.4(5)	C17	C18	C19	C24	178.2(5)
C2	C1	C5	Ir1	61.8(4)	C18	C17	C21	Ir2	60.2(4)
C2	C1	C5	C4	1.4(6)	C18	C17	C21	C20	-1.4(6)
C2	C1	C5	C10	-178.4(5)	C18	C17	C21	C26	-174.7(5)
C2	C3	C4	Ir1	-61.9(4)	C18	C19	C20	Ir2	-60.7(4)
C2	C3	C4	C5	-1.4(6)	C18	C19	C20	C21	-0.9(6)
C2	C3	C4	C9	179.7(5)	C18	C19	C20	C25	-179.9(5)
C3	C4	C5	Ir1	-59.7(4)	C19	C20	C21	Ir2	-60.4(4)
C3	C4	C5	C1	0.0(6)	C19	C20	C21	C17	1.4(6)
C3	C4	C5	C10	179.8(5)	C19	C20	C21	C26	174.7(5)
C5	C1	C2	Ir1	-62.1(4)	C21	C17	C18	Ir2	-59.7(4)
C5	C1	C2	C3	-2.3(6)	C21	C17	C18	C19	0.8(6)
C5	C1	C2	C7	-178.8(5)	C21	C17	C18	C23	-178.6(5)
C6	C1	C2	Ir1	126.5(5)	C22	C17	C18	Ir2	119.4(6)

C6	C1	C2	C3	-173.7(5)	C22	C17	C18 C19 179.9(5)
C6	C1	C2	C7	9.8(9)	C22	C17	C18 C23 0.5(9)
C6	C1	C5	Ir1	-126.5(5)	C22	C17	C21 Ir2 -118.9(6)
C6	C1	C5	C4	173.1(5)	C22	C17	C21 C20 179.5(5)
C6	C1	C5	C10	-6.7(9)	C22	C17	C21 C26 6.2(9)
C7	C2	C3	Ir1	116.9(6)	C23	C18	C19 Ir2 118.6(5)
C7	C2	C3	C4	178.7(5)	C23	C18	C19 C20 179.6(5)
C7	C2	C3	C8	-4.2(9)	C23	C18	C19 C24 -2.3(9)
C8	C3	C4	Ir1	121.0(6)	C24	C19	C20 Ir2 121.2(6)
C8	C3	C4	C5	-178.6(5)	C24	C19	C20 C21 -179.0(5)
C8	C3	C4	C9	2.5(9)	C24	C19	C20 C25 2.1(9)
C9	C4	C5	Ir1	119.2(5)	C25	C20	C21 Ir2 118.5(5)
C9	C4	C5	C1	178.9(5)	C25	C20	C21 C17 -179.6(5)

C9	C4	C5	C10	-1.4(9)	C25	C20	C21 C26 -6.3(9)
C11	C12	C13	C14	53.8(6)	C27	C28	C29 C30 53.6(5)
C12	C11	C16	C15	60.5(5)	C28	C27	C32 C31 61.5(5)
C12	C13	C14	C15	-50.8(6)	C28	C29	C30 C31 -51.9(6)
C13	C14	C15	C16	53.3(6)	C29	C30	C31 C32 55.6(6)
C14	C15	C16	C11	-57.2(6)	C30	C31	C32 C27 -59.4(6)
C16	C11	C12	N1	176.5(4)	C32	C27	C28 N4 177.4(4)
C16	C11	C12	C13	-59.7(5)	C32	C27	C28 C29 -59.2(5)

Table 8 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for DMMXI059a_abs.

Atom	*x*	*y*	*z*	U(eq)
H1A	9640(60)	5650(30)	5680(30)	7(15)
H1B	9900(70)	6290(30)	5680(30)	17(17)
H2A	5532.11	6169.84	5342.69	13
H2B	6405.73	6753.71	5166.6	13
H6A	7757.92	8008.46	5847.24	29
H6B	9385.39	7805	6040.5	29
H6C	8446.09	8272.69	6496.69	29
H7A	4626.34	7778.21	6606.69	31
H7B	4295.69	7114.42	6218.69	31
H7C	5368.26	7661.41	5929.34	31
H8A	5107.34	5740.17	7353.38	39
H8B	4135.92	6226.14	6928.48	39
H8C	4516.04	6420.31	7644.96	39
H9A	7485.4	5464.48	7602.94	37
H9B	8164.88	5983.43	8093.98	37
H9C	9158.33	5681.57	7541.36	37
H10A	10750.17	6974.93	6569.28	32
H10B	10669.42	6430.29	7118.79	32
H10C	10595.8	7200.35	7293.23	32
H11	7164.12	5446.3	4967	13

H12	9017.2	6560.96	4771.43	14
H13A	9778.96	5189.11	4668.98	18
H13B	10848.48	5798.17	4527.66	18
H14A	9555.29	6088.08	3623	23
H14B	9869.25	5310.39	3574.8	23
H15A	7481.97	5059.09	3876.02	21
H15B	7399.9	5573.98	3300.25	21
H16A	6932.07	6457.68	4019.44	16
H16B	5737.67	5887.32	4127.15	16
H3A	4505.41	4450.2	5780.21	13
H3B	4742.89	3777.4	5529.85	13
H4A	1162.53	3166.49	5194.54	13
H4B	645.13	3855.54	5187.53	13
H22A	5479.84	3781.12	7061.49	32
H22B	5665.35	3178.98	6575.45	32
H22C	5527.31	3036.5	7319.08	32
H23A	3816.79	4472.1	7501.54	32
H23B	2740.49	4190.07	8034.11	32
H23C	2121.31	4660.16	7486.19	32
H24A	-240.02	4275.08	7205.06	34
H24B	-604.22	3632.41	7619.1	34
H24C	-1108.43	3669.71	6893.88	34
H25A	422.41	2318.08	5916.71	32
H25B	-772.11	2799.11	6222.86	32
H25C	-231.26	2159.42	6603.34	32

H26A	4403.14	2324.6	6024.73	25
H26B	2811.23	2030.63	5891.76	25
H26C	3652.13	1844.47	6532.04	25
H27	2863.02	4711.97	5030.75	12
H28	3144.02	3357.34	4651.03	14
H29A	1064.62	4305.48	4180.42	19
H29B	1228.58	3558.22	3936.48	19
H30A	3498.72	3788.59	3471.32	19
H30B	2385.94	4343.76	3227.25	19
H31A	4657.74	4828.53	3548.36	16
H31B	3332.12	5117.76	3958.81	16
H32A	5266.73	4086.17	4388.67	16
H32B	5302.39	4834.54	4644.02	16
H1C	3207.9	5777.5	5708.95	45
H1D	3025.05	6286.81	5274.77	45
H2C	8240.27	4367.83	5507.85	35
H2D	7941.37	3833.82	5114.63	35

Experimental

Single crystals of $C_{16}H_{31}Cl_2IrN_2O$ [DMMXI059a_abs] were []. A suitable crystal was selected and [] on a Xcalibur, Eos, Gemini ultra diffractometer. The crystal was kept at 100.0(6) K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341. 2.
3.

Crystal structure determination of [DMMXI059a_abs]

Crystal Data for $C_{16}H_{31}Cl_2IrN_2O$ (M =530.53 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 9.16689(15) Å, b = 20.2059(4) Å, c = 21.1011(4) Å, V = 3908.44(12) Å^3, Z = 8, T = 100.0(6) K, μ(MoKα) = 7.109 mm^{-1}, *Dcalc* = 1.803 g/cm^3, 86880
reflections measured (7.058° ≤ 2Θ ≤ 64.952°), 13359 unique (R_{int} = 0.0662, R_{sigma} = 0.0432) which were used in all calculations. The
final R_1 was 0.0311 (I > 2σ(I)) and wR_2 was 0.0646 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups,
 All N(H,H) groups At 1.5 times of:
  All C(H,H,H) groups, All O(H,H) groups
2.a
 Free
```

```
rotat
ing
group
:
O1(H1
C,H1D
),
O2(H2
C,H2D
)
2.b Ternary CH refined with
 riding coordinates:
 C11(H11), C12(H12),
 C27(H27), C28(H28)
2.c Secondary CH2 refined with riding coordinates:
 N2(H2A,H2B), C13(H13A,H13B), C14(H14A,H14B), C15(H15A,H15B),
 C16(H16A,H16B), N3(H3A,H3B), N4(H4A,H4B), C29(H29A,H29B),
 C30(H30A,H30B), C31(H31A,H31B), C32(H32A,H32B)
2.d Idealised Me refined as rotating group:
 C6(H6A,H6B,H6C), C7(H7A,H7B,H7C), C8(H8A,H8B,H8C), C9(H9A,H9B,H9C),
 C10(H10A, H10B,H10C), C22(H22A,H22B,H22C), C23(H23A,H23B,H23C),
 C24(H24A,H24B,H24C), C25(H25A,H25B,H25C), C26(H26A,H26B,H26C)
```

This report has been created with Olex2, compiled on May 18 2018 14:05:52 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.