Supporting Information for:

Iridium Complexes of Perimidine-based *N*-Heterocyclic Carbene Pincer Ligands via Aminal C–H Activation

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trans-[IrH₂Cl{C(NCH₂PCy₂)₂C₁₀H₆}] (trans-5b)

¹H NMR Spectrum of Compound *trans*-5b



³¹P{¹H} Spectrum of Compound *trans*-5b

Parameter	Value
Data File	F:/ KMAb158/
lame	KMAc158c_C6D6/ 11/ fid
Drigin	Bruker BioSpin GmbH
Owner	av400bb
olvent	C6D6
emperature	300.0
ulse	zgpg30
equence	10
xperiment	10
iumper or icans	т
leceiver Gain	193
elaxation	2.0000
Delay	
ulse Width	8.0000
cquisition Time	0.5112
acquisition	2017-04-15T15:16:20
pectrometer	161.98
requency	
pectral Width	64102.6
owest	-40414.3
lucleus	31P
cauired Size	32768
pectral Size	65536

130	80	50	20	-10	-50	-90	-130	-190	
					f1 (ppm)				

¹H¹³C HMBC (carbene resonance) of Compound *trans*-5b



$[IrHCl_2{C(NCH_2PCy_2)_2C_{10}H_6}]$ (6b)

¹H NMR Spectrum of Compound 6b



³¹P{¹H} Spectrum of Compound 6b

	44	40	36	32	28	24	20	16	12	8	6	4	2	0	-4		-12
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NUCIEUS	Size	31P 32768															
Lowest F	requency	-40150.1															
Spectral	Width	64102.6															
Frequenc	сy																
Spectrom	neter	161.98	10.25.00														
Acquisitic	on Date	2017-03-31	T10.23.00														
Pulse Wie	dth an Time	8.0000															
Relaxatio	on Delay	2.0000															
Receiver	Gain	193															
Number o	of Scans	64															
Experime	ent	1D															
Pulse Sec	quence	zgpg30															
Temperat	ture	300.1															
Solvent		CDCI3															
Owner		av400bb															
Oninin		fid	Et2Owash	_CDCl3/	11/												
Data File	e Name	F:/ APhD20	15/ Abrag	am/				7									

¹³C{¹H} Spectrum of Compound 6b

-187.16	134.38 134.09 134.06 134.06 134.06 1134.02 1121.47	-106.74	53.15 53.00 52.84	22.58 22.58 22.90 27.67 27.90 27.16 27.16 27.16 26.90 26.90 26.90
Parameter Vali Data File Name F:/ APhD2015/ AI KMAc153a_Et2Ov 13/ fid Origin Bruker BioSpin Gr Owner av400bb Solvent CDC13 Temperature 300.0 Pulse Sequence zgp30 Experiment 1D Number of Scans 6000 Relaxation 2.0000 Delay Pulse Width Pulse Width 10.0000 Acquisition Time 1.3631 Acquisition Tate 2017-04-01T02:5 Spectrometer 100.61 Frequency Spectral Width Spectrol 13C Acquired Size 32768 Spectral Size 65536	Je yragam/ vash_CDCl3/ nbH 4:34			
210 190	170 150 130 f1	(ppm)	70 60 50	40 30 20 10 0
 53.15 53.00 52.84 	ParameterValueData File NameF:/ APhD2015/ Abragam/ KMAc153a_Et2Owash_CDCl3/ 13/ fidOriginBruker BioSpin GmbHOwnerav400bbSolventCDCl3Temperature300.0Pulse Sequencezgp30Experiment1DNumber of6000Scans2.0000DelayPulse WidthPulse Width10.0000Acquisition1.3631Time42038.5Lowest-1944.8Frequency32768Spectral Size65536	35.25	7_35.11 32.72 32.73 22.43	- 29.63 - 28.04 - 27.90 - 27.67 - 27.67 - 26.90
54 52 50	48 46 44 42 f1	40 38 36 (ppm)	34 32	30 28 26

$[IrCl{CH_2(NCH_2PPh_2)_2C_{10}H_6}(COD)]$ (8a)

¹H NMR Spectrum of Compound 8a



³¹P{¹H} Spectrum of Compound 8a

raraffeter	Valla
Data File Name	/ Users/ kathym/ Documents/ Abragam/ CMA5f_CD2Cl2/ 2/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CD2Cl2
Temperature	300.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	16
Receiver Gain	193
Relaxation Delay	2.0000
Pulse Width	8.0000
Acquisition Time	0.5112
Acquisition Date	2014-10-09T14:04:00
Spectrometer Frequency	161.97
Spectral Width	64102.6
Lowest Frequency	-40020.0
Nucleus	31P
Acquired Size	32768
Spectral Size	65536

140 110 80 60 40 20 0 -30 -60 -90 -120 -150 f1 (ppm)

¹³C{¹H} Spectrum of Compound 8a

Parameter Data File Name	Value C:/ Users/ Kathy/ Desktop/ PhD Thesis/	144.30 135.73	133./0 129.45 127.81 126.11	7119.20 118.92	-108.43	r65.36	65.29	50.30 50.22	-32.59		
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Origin	Bruker BioSpin GmbH										
Owner	av400bb										
Solvent	CD2Cl2										
Temperature	300.0										
Pulse Sequence	zgpg30										
Experiment	1D										
Number of Scans	4000										
Receiver Gain	193										
Relaxation Delay	2.0000										
Pulse Width	10.0000										
Acquisition Time	1.3631										
Acquisition Date	2014-10-13T01:54:00										
Spectrometer Frequency	100.61										
Spectral Width	24038.5										
Lowest Frequency	-1916.1		1.1								
Nucleus	13C										
Acquired Size	32768								1		
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¹H(400 MHz)-¹³C{100 MHz) HSQC and HMBC spectra of (8a) in the COD methylene region.

$[IrH{CH(NCH_2PPh_2)_2C_{10}H_6}(\eta^4-C_8H_{12})][BAr_F] [9a][BAr_F]$

¹H NMR Spectrum of Compound [9a][BAr_F]



$^{31}\text{P}\{^{1}\text{H}\}$ Spectrum of Compound [9a][BAr_F]

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Spectral Size	05530											
Acquired Size	32768											
Nucleus	31P											
Lowest Frequency	-40150.1											
Spectral Width	64102.6											
Spectrometer	161.97											
Acquisition Date	2014-10-10T08:24:00											
Acquisition Time	0.5112											
Pulse Width	8.0000											
Relaxation Delay	2.0000											
Receiver Gain	193											
Number of Scans	16											
Experiment	1D											
Pulse Sequence	zapa30											
Temperature	300.1											
Solvent												
Ouper	pruker biospin GMDH											
Origin	Abragam/ CMA30b_char2_CD2Cl2/ 6/ fid				I							
Data File Name	(users/ (atn/m/ uocuments/											

¹³C{¹H} Spectrum of Compound [9a][BAr_F]



$[IrCl{C(NCH_2PPh_2)_2C_{10}H_6}]$ (10a)

¹H NMR Spectrum of Compound 10a



³¹P{¹H} Spectrum of Compound 10a

Parameter	Value			Х.								
Data File Name	C:/ Users/ Kathy/ Desktop/ PhD Thesis/ Articles/ Ir paper/ Abragam/ CM33b_colid_C6D6/ 2/ fid			-23								
Origin	CMASSD_Solid_COD0/ 2/ IId Bruker BioSpin GmbH											
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Solvent	CEDE											
Tomporature	300.0											
remperature	300.0											
Pulse Sequence	zgpg30											
Experiment	1D											
Number of Scans	128											
Receiver Gain	193											
Relaxation Delay	2.0000											
Pulse Width	8.0000											
Acquisition Time	0.5112											
Acquisition Date	2014-10-02T15:55:00											
Spectrometer Frequency	161.98											
Spectral Width	64102.6											
Lowest Frequency	-40046.9											
Nucleus	31P											
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Spectral Size	65536											
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85	75 65 55	45	35	25 f1 (nnm)	15	5	0	-5	-10	-20	-30	-4(

¹³C{¹H} Spectrum of Compound 10a



¹H¹³C HMBC (carbene resonance)



[IrCl{C(NCH₂PPh₂)₂C₁₀H₆}] (10a)

¹H NMR Spectrum of Compound 10b



$^{31}\text{P}\{^{1}\text{H}\}$ NMR Spectrum of Compound 10b

Peaks at δ_P = 4.58, 1.82 and -1.90 correspond to minor but inseparable impurities.



¹³C-¹H HMBC NMR Spectrum of Compound 10b



PCH₂N (δ_{H} = 3.31) Correlation to NHC Carbene (δ_{C} = 199.3)

$[Ir_{2}{\mu-H_{2}C(NCH_{2}PPh_{2})_{2}C_{10}H_{6}}CI_{2}(\eta-C_{8}H_{12})_{2}]$ (11a)

¹H NMR Spectrum of Compound 11a



³¹P{¹H} Spectrum of Compound 11a

Data File NameC:/ Users/ Kathy/ Desktop/ PhD Thesis/ Articles/ Ir paper/ Abragam/ CMA32a_proton_C6D6/ 2/ fidOriginBruker BioSpin GmbHOwnerav400bbSolventC6D6Temperature300.0Pulse Sequencezpg30Experiment1DNumber of Scans128Receiver Gain193Relaxion Delay2.0000Pulse Width8.0000Acquisition Time0.5112Acquisition Time0.5112Spectral Width64102.6Lowest Frequency40045.9Nucleus31PAcquired Size32768Spectral Width32768Spectral Width32768Spectral Width32768Spectral Width32768Spectral Width312Acquired Size32768Spectral Width312Acquired Size32768Ac	Parameter	Value					9.					
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Relaxation Delay 2.0000 Pulse Width 8.0000 Acquisition Time 0.5112 Acquisition Data 2014-10-09T12:37:00 Spectrometer 161.98 Frequency	Receiver Gain	193										
Pulse Width 8.0000 Acquisition Time 0.5112 Acquisition Date 2014-10-09T12:37:00 Spectrometer 161.98 Frequency 161.93 Spectral Width 64102.6 Lowest Frequency -40045.9 Nucleus 31P Acquired Size 25766	Relaxation Delay	2.0000										
Acquisition Time 0.5112 Acquisition Date 2014-10-09T12:37:00 Spectrometer 161.98 Frequency - Spectral Width 64102.6 Lowest Frequency -40045.9 Nucleus 31P Acquired Size 32768 Spectral Size 6556	Pulse Width	8.0000										
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Frequency Spectral Width 64102.6 Lowest Frequency -40045.9 Nucleus 31P Acquired Size 32768 Snetral Size 6556	Spectrometer	161.98										
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¹³C{¹H} Spectrum of Compound 11a



$[IrH_{3}{C(NCH_{2}PPh_{2})_{2}C_{10}H_{6}}]$ (14a)

¹H NMR Spectrum of Compound 14a



³¹P{¹H} NMR Spectrum of Compound 14a

130	80	50	20	-10	-50	-90	-130	-190
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ectral Width	64102.6							
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pectrometer	161.98							
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$[Ir_{2}{\mu-H_{2}C(NCH_{2}PPh_{2})_{2}C_{10}H_{6}}Cl_{2}(\eta-C_{5}Me_{5})_{2}]$ (12a)

¹H NMR Spectrum of Compound 12a



³¹P{¹H} NMR Spectrum of Compound 12a

Parameter	Value
Data File Name	C:/ Users/ Kathy/ Desktop/ PhD Thesis/
	Fids Ir Paper/ Newer/ CMA011_CDCl3/ 10/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	109
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	4.0894
Acquisition Date	2017-10-02T17:07:26
Spectrometer Frequency	400.13
Spectral Width	8012.8
Lowest Frequency	-1535.6
Nucleus	1H
Acquired Size	32768
Snectral Size	65536

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130	80	50	20	-10	-50	-90	-130	-190	
					f1 (ppm)				

¹³C{¹H} NMR Spectrum of Compound 12a

Parameter	Value).62 1.75	69.1	.12	.33	.00	.68	10 08		80	84	64			8		
Data File Name	C:/ Users/ Kathy/ Desktop/ PhD Thesis/ Articles/ Ir paper/ Raw Fids Ir Paper/ Newer/ CMA011_CDCl3/ 2/ fid	140 134 134	131	128	127	×113	-102	92. 92.		-67.	49.	49.			-8.2		
Origin	Bruker BioSpin GmbH																
Owner	hill																
Solvent	CDCI3																
Temperature	298.1																
Pulse Sequence	1D_C.go														1		
Experiment	1D																
Number of Scans	8000																
Receiver Gain	64																
Relaxation Delay	2.0000																
Pulse Width	12.0000																
Acquisition Time	1.7083																
Acquisition Date	2017-10-03T11:47:00																
Spectrometer Frequency	150.88																
Spectral Width	36057.7																
Lowest Frequency	-2919.2																
Nucleus	13C																
Acquired Size	32768																
Spectral Size	65536				1												
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$[Rh_{2}{\mu-H_{2}C(NCH_{2}PPh_{2})_{2}C_{10}H_{6}}Cl_{2}(\eta-C_{5}Me_{5})_{2}]$ (13a)

¹H NMR Spectrum of Compound 13a



³¹P{¹H} NMR Spectrum of Compound 13a

Parameter	Value
Data File	C:/ Users/ Kathy/
Name	Desktop/ PhD Thesis/
	Fids Ir Paper/ Newer/
	CMA001 CDCl3/ 12/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse	zgpg30
Sequence	
Experiment	1D
Number of	6000
Receiver Gain	193
Relaxation	2.0000
Delay	
Pulse Width	10.0000
Acquisition	1.3631
Time	2017 10 02702-51-40
Acquisition Date	2017-10-03103:51:48
Spectrometer	100.61
Frequency	
Spectral Width	24038.5
Lowest	-1946.1
Frequency	100
Nucleus	130
Acquired Size	32/68
spectral size	05550

130	80	50	20	-10	-50	-90	-130	-190	
					f1 (ppm)				

¹³C{¹H} NMR Spectrum of Compound 13a

Parameter	Value	4.85	1.79 1.79	3.32	.32	7.4	2.73	66		05		14 92				2		
Data File Name	C:/ Users/ Kathy/ Desktop/ PhD Thesis/ Articles/ Ir paper/ Raw Fids Ir Paper/ Newer/ CMA001_CDCl3/ 12/ fid	1.13	113 113 1131	128	127		√102 298.	98		-67.	1	50.						
Origin	Bruker BioSpin GmbH																	
Owner	av400bb																	
Solvent	CDCl3																	
Temperature	300.0																	
Pulse Sequence	zgpg30																	
Experiment	1D																	
Number of Scans	6000																	
Receiver Gain	193								_ I									
Relaxation Delav	2.0000																	
Pulse Width	10.0000								_ I									
Acquisition Time	1.3631								_ I									
Acquisition Date	2017-10-03T03: 51:48																	
Spectrometer Frequency	100.61																	
Spectral Width	24038.5								_ I									
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NMR scale reaction: Compound 1b with 0.5 $Ir_2Cl_2(COD)_2$

SP = 10b



NMR scale reaction: Hydrogenation of 10b to provide cis-5b



NB: Traces of *trans*-**5b** observed at $\delta_{H} = -7.17$.

Time Course ¹H and ³¹P NMR Spectra for Hydrogenation of 10b to afford *cis*-5b



1 Atmosphere, $t_{0.5} \approx 8$ minutes.