2-Pyridone-Stabilized Iridium Silylene Complexes: Structure and Bonding

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1. Characterization of compound NSi^{iPr2}-H **(1)**

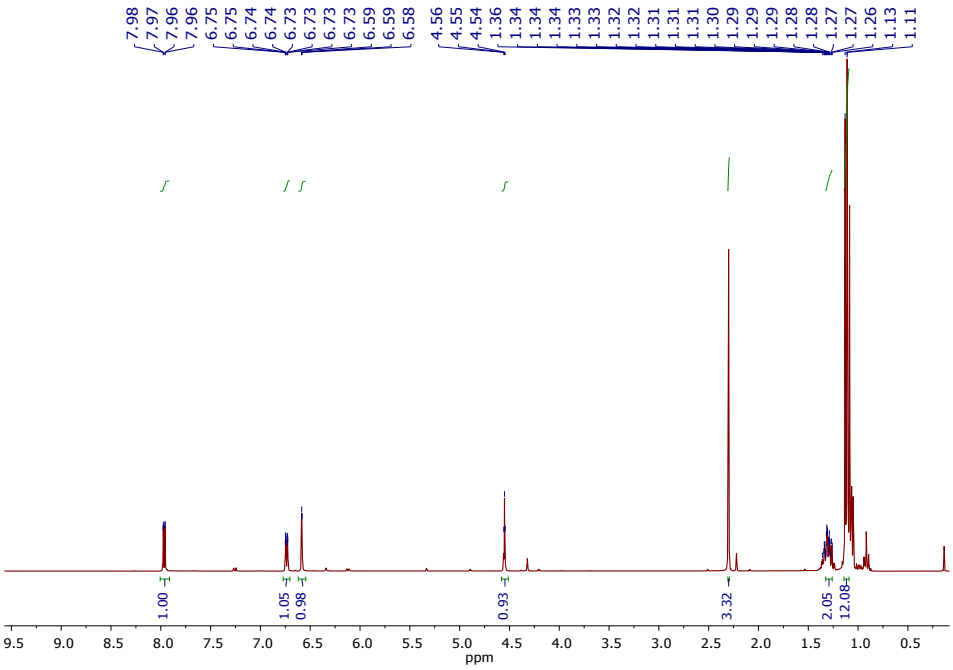

Figure S1. ^{1}H NMR spectrum of compound **1**

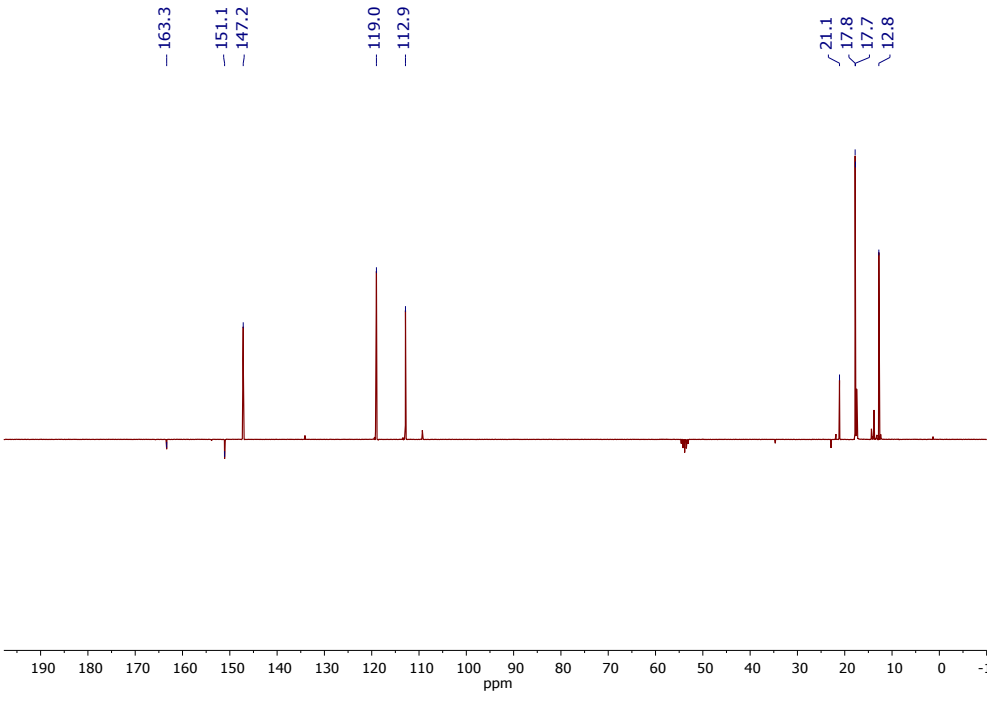

Figure S2. ^{13}C APT NMR spectrum of compound **1**

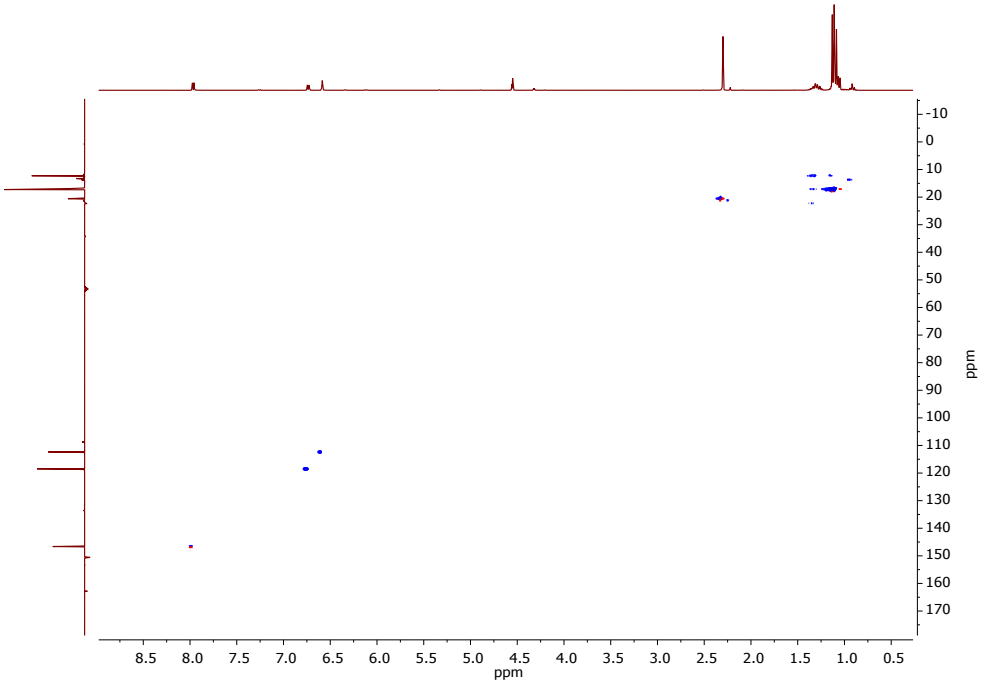

Figure S3. $^{1}H–^{13}C$ HSQC spectrum of compound **1**

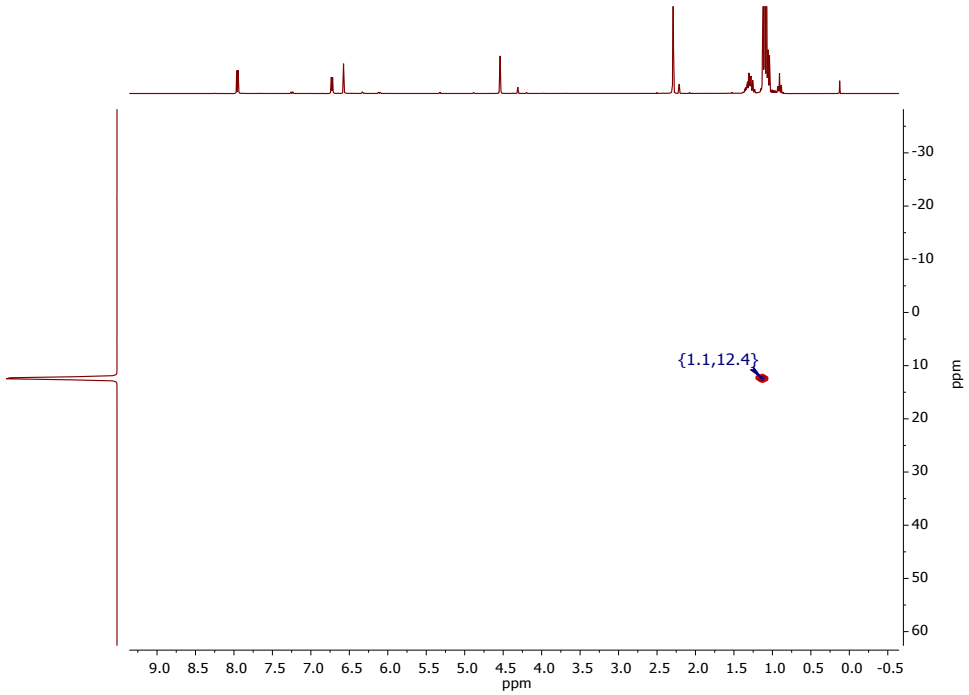

Figure S4. ^{1}H-^{29}Si HMBC NMR spectrum of compound **1**

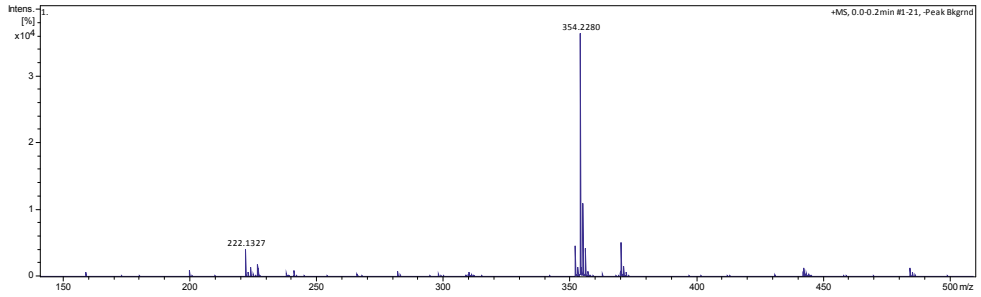

Figure S5. HR-MS of compound **1**. (11 %)

2. Characterization of complex $[Ir(Cl)(\kappa^2\text{-}NSi^{iPr2})_2]$ **(3)**

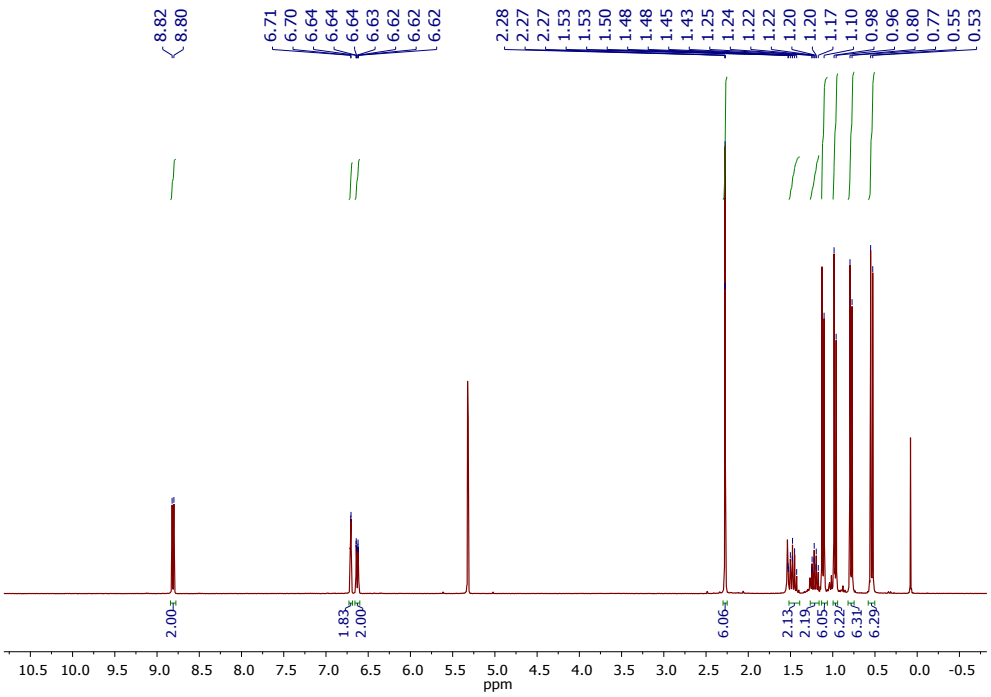

Figure S6. ^{1}H-NMR spectrum of complex **3**

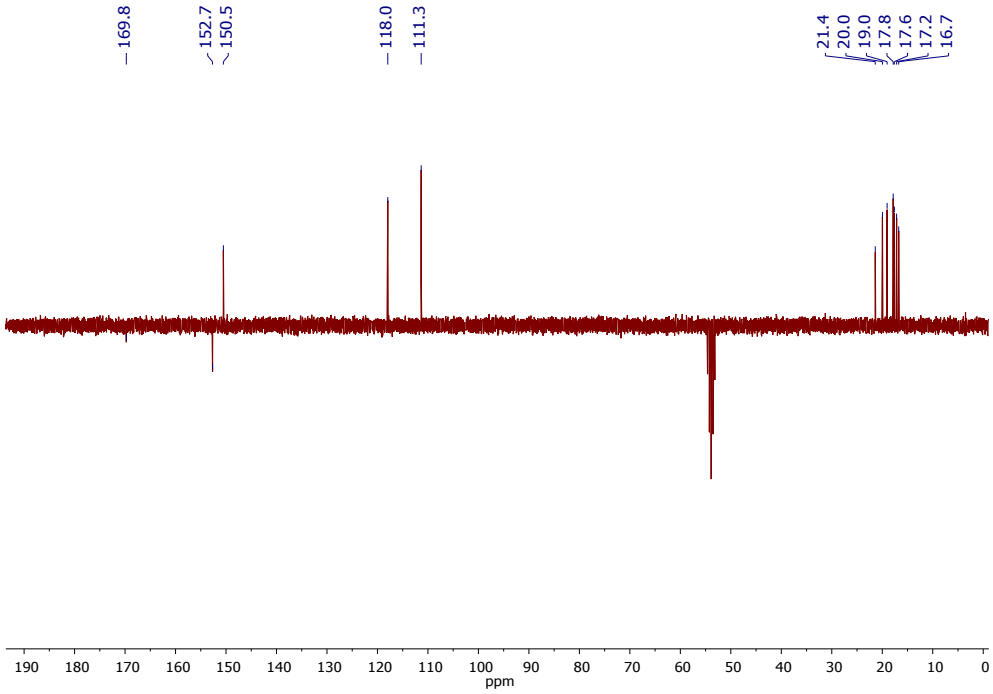

Figure S7. ^{13}C APT NMR spectrum of complex **3**

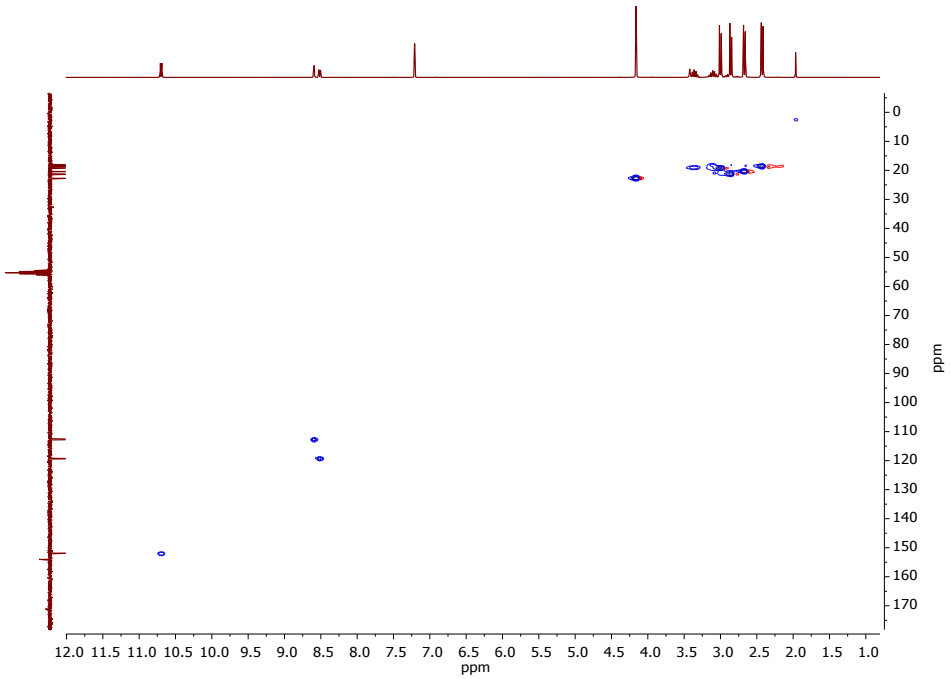

Figure S8. ^{1}H–^{13}C HSQC spectrum of complex **3**

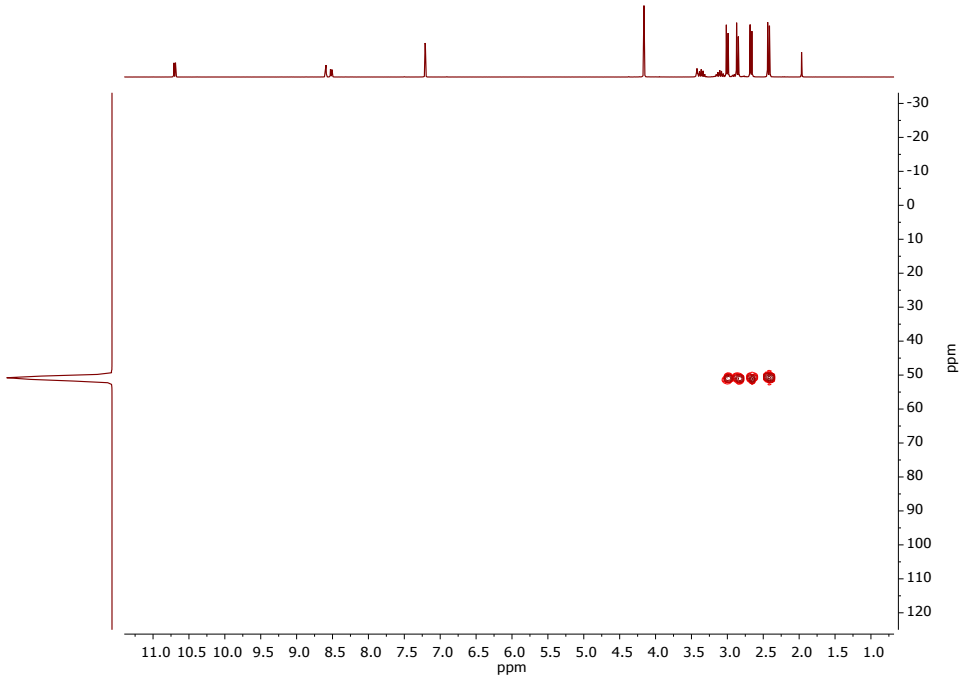

Figure S9. ^{1}H-^{29}Si HMBC NMR spectrum of complex **3**

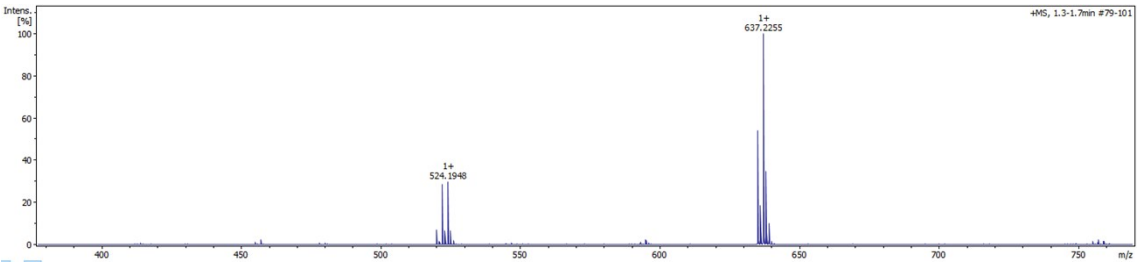

Figure S10. HR-MS of complex **3**

3. Characterization of complex $[Ir(CF_3CO_2)(\kappa^2\text{-}NSi^{iPr2})_2]$ **(5)**

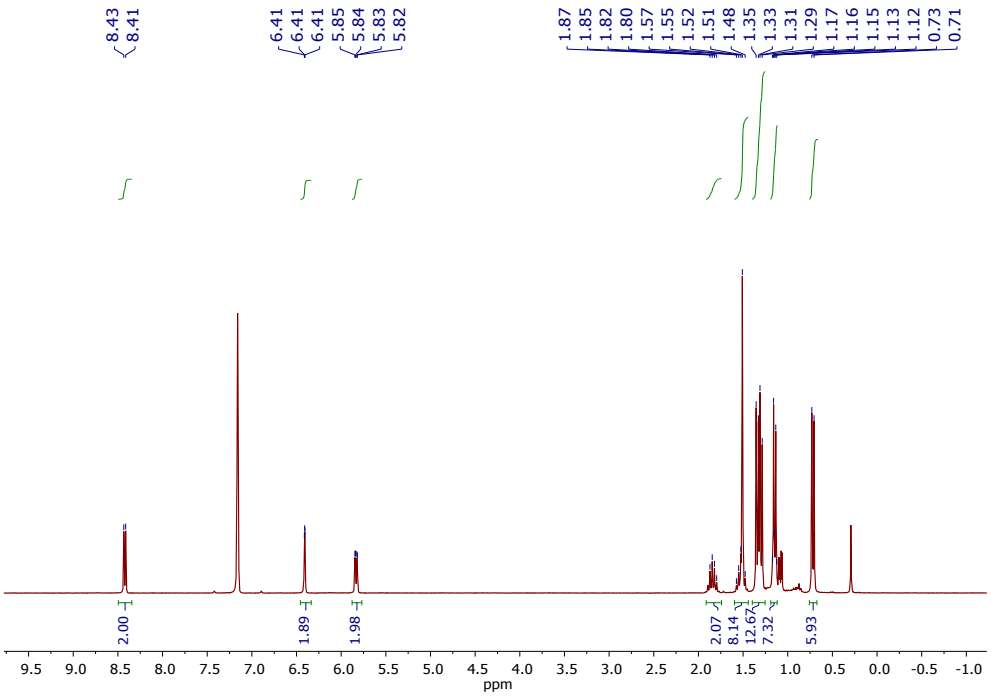

Figure S11. ^{1}H-NMR spectrum of complex **5**

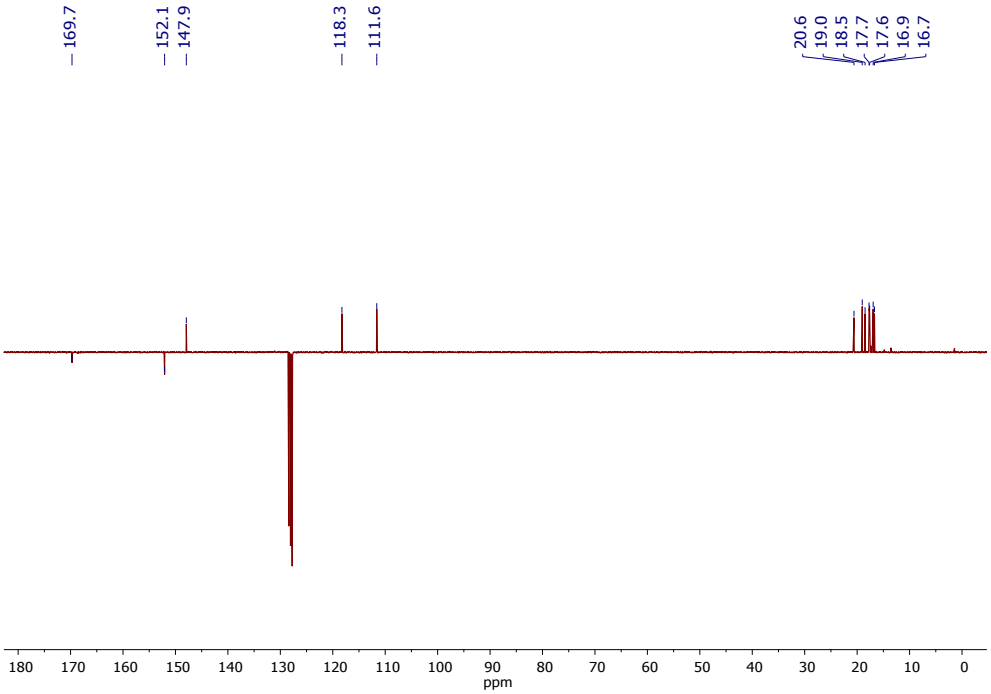

Figure S12. ^{13}C APT NMR spectrum of complex **5**

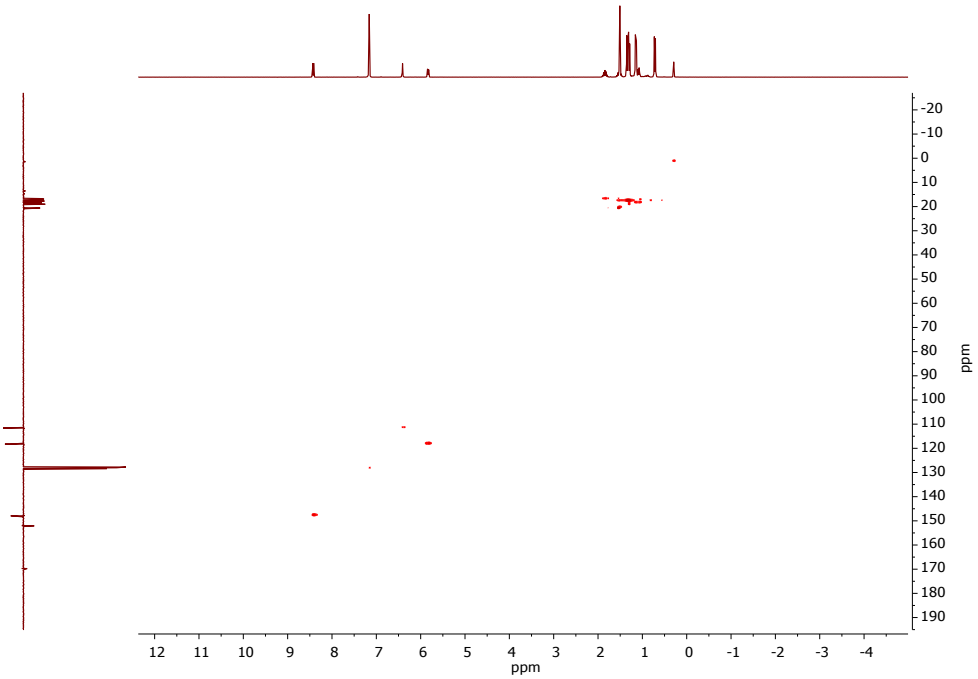

Figure S13. $^{1}H–^{13}C$ HSQC spectrum of complex **5**

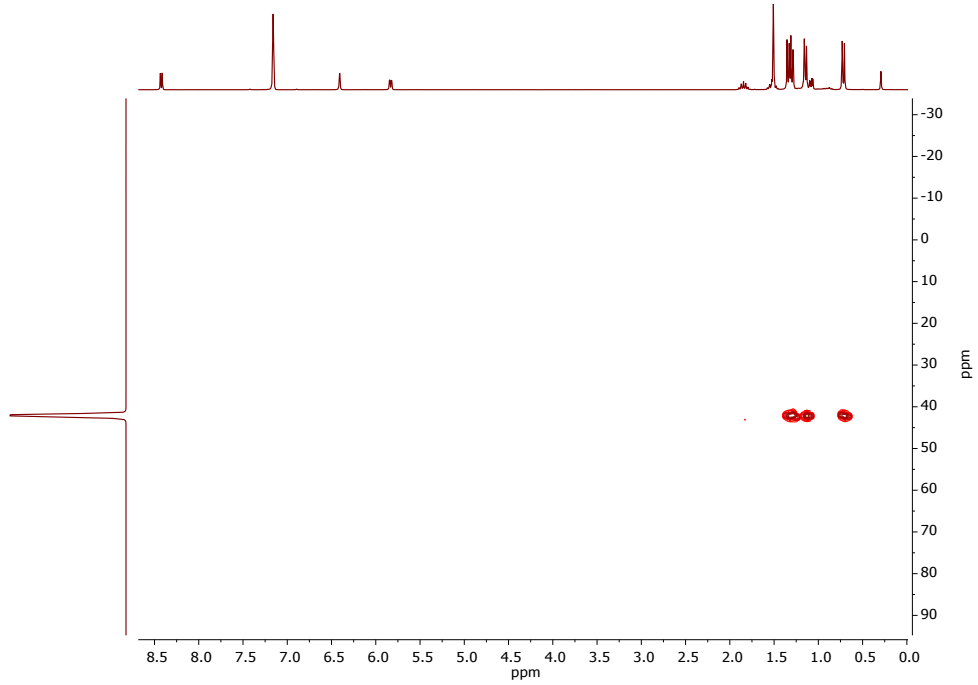

Figure S14. ^{1}H-^{29}Si HMBC NMR spectrum of complex **5**

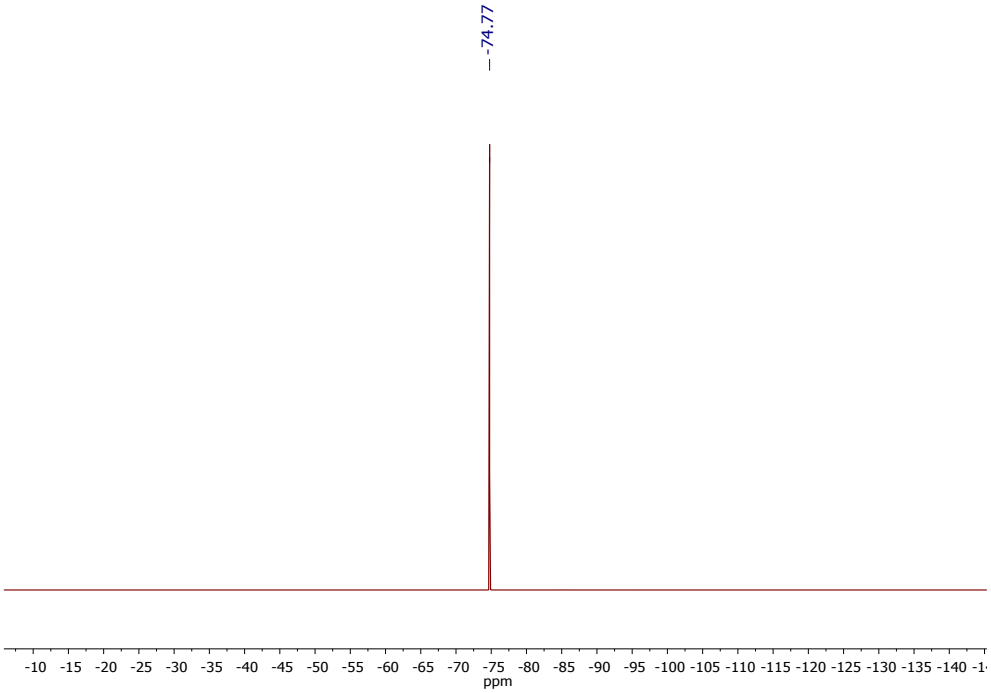

Figure S15. ^{19}F NMR spectrum of complex **5**

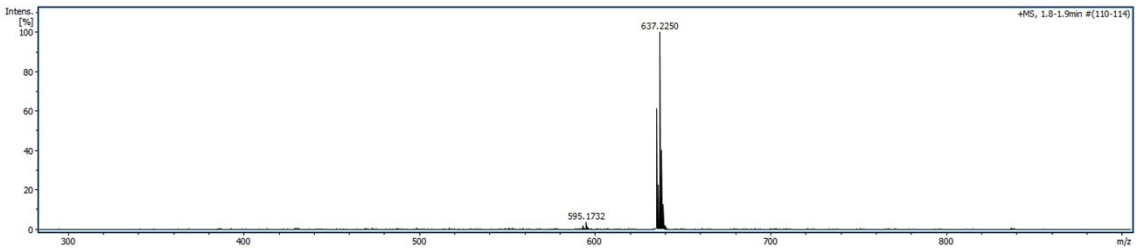

Figure S16. HR-MS of complex **5**

4. Characterization of complex $[Ir(CF_3SO_3)(\kappa^2\text{-}NSi^{iPr2})_2]$ (**6**)

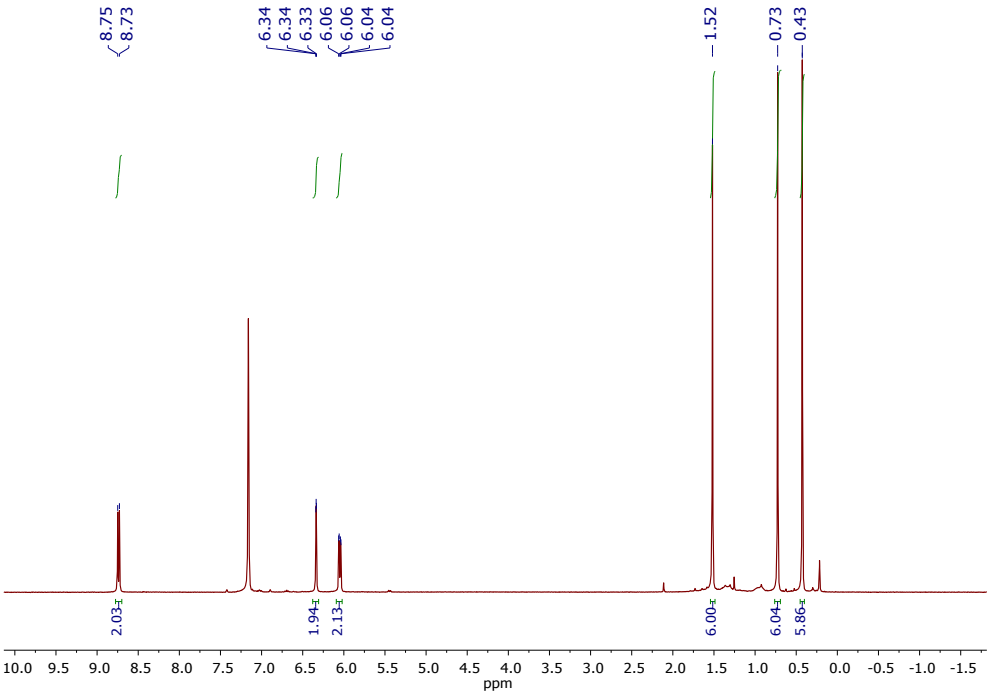

Figure S17. ^{1}H NMR spectrum of complex **6**

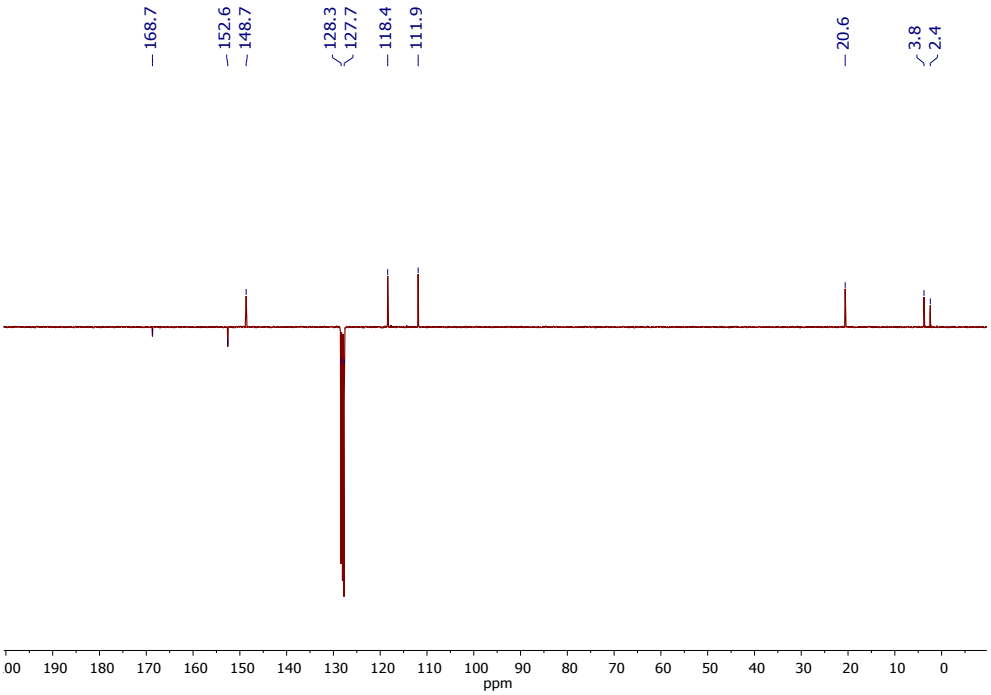

Figure S18. ^{13}C APT NMR spectrum of complex **6**

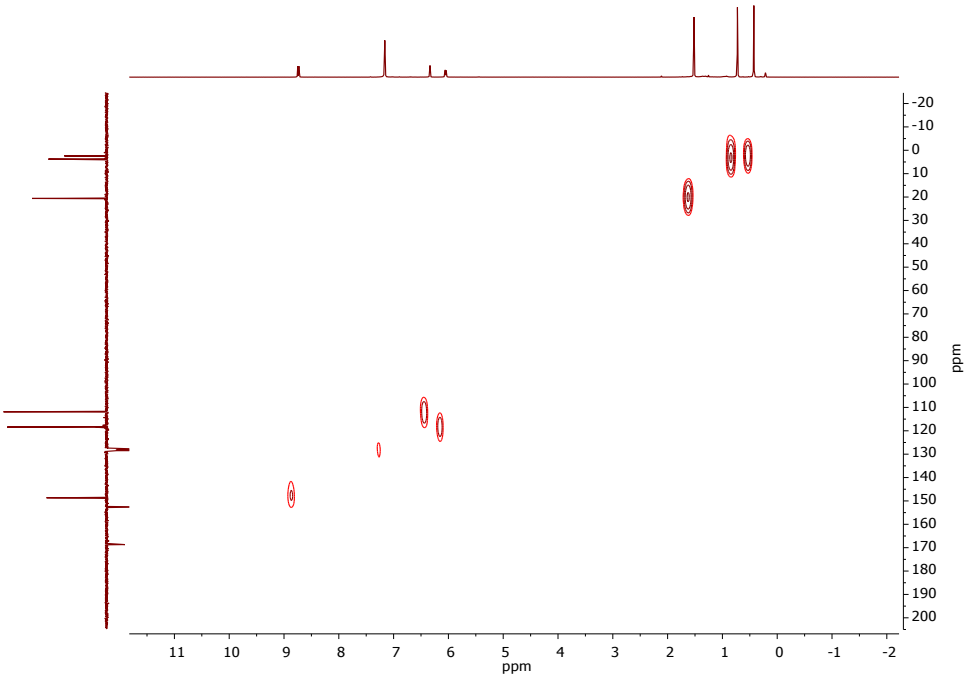

Figure S19. $^{1}H–^{13}C$ HSQC spectrum of complex **6**

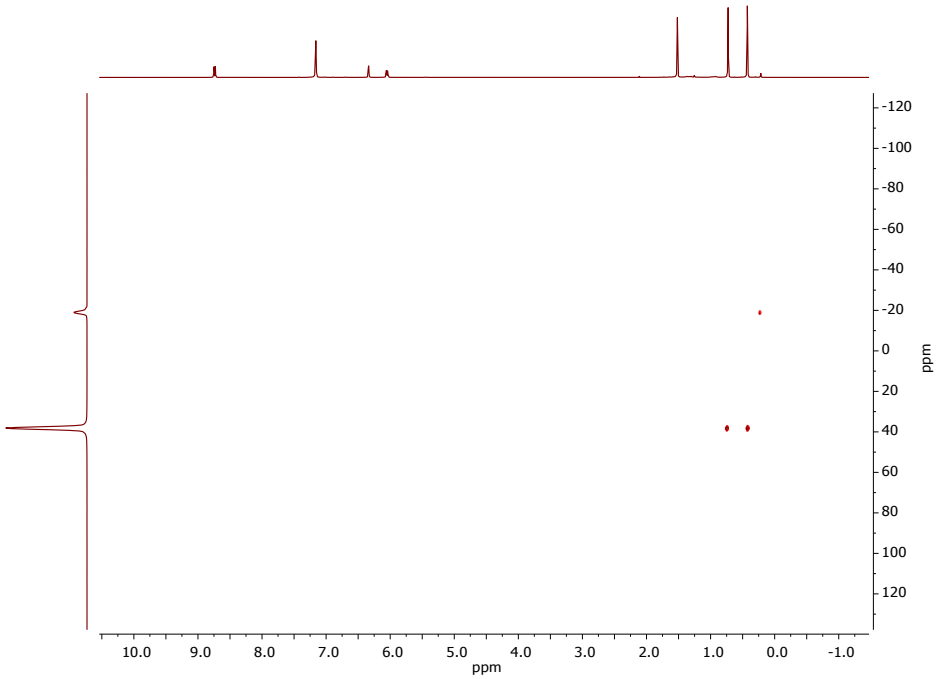

Figure S20. ^{1}H-^{29}Si HMBC NMR spectrum of complex **6**

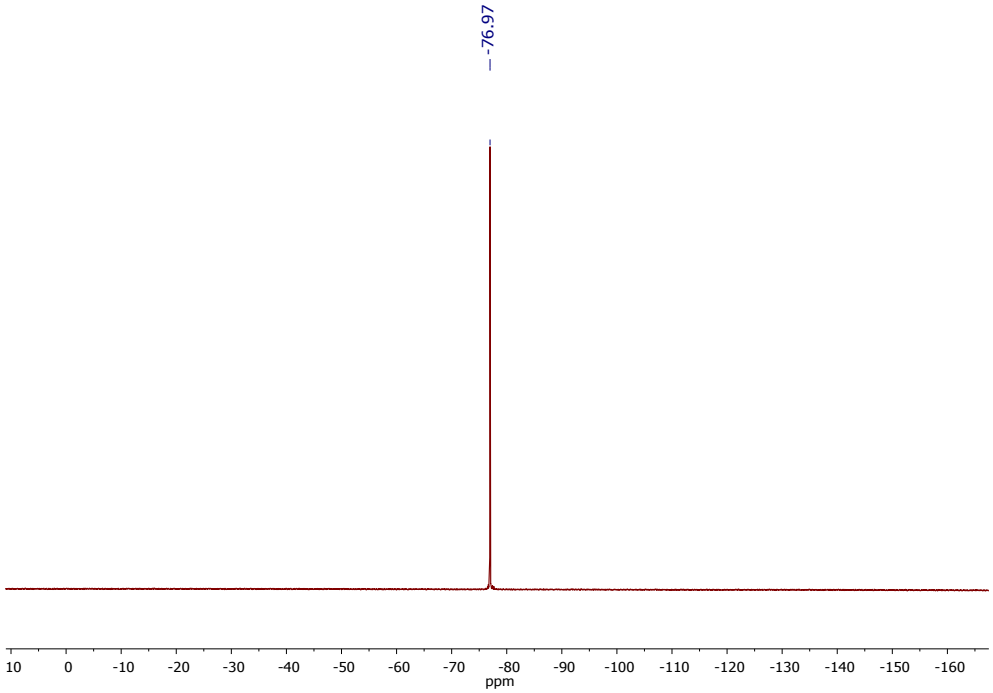

Figure S21. ^{19}F NMR spectrum of complex **6**

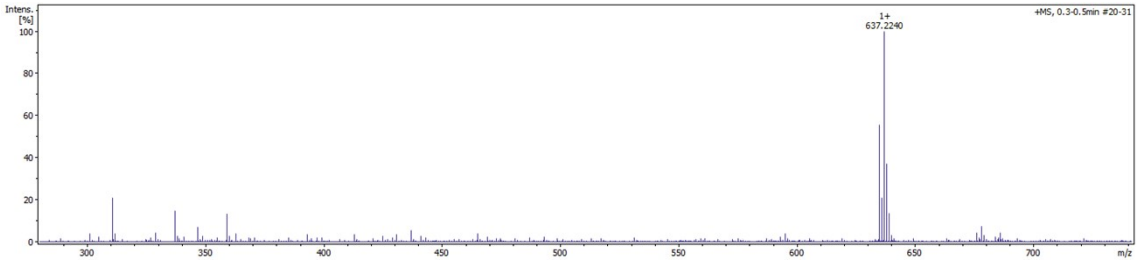

Figure S22. HR-MS of complex **6**

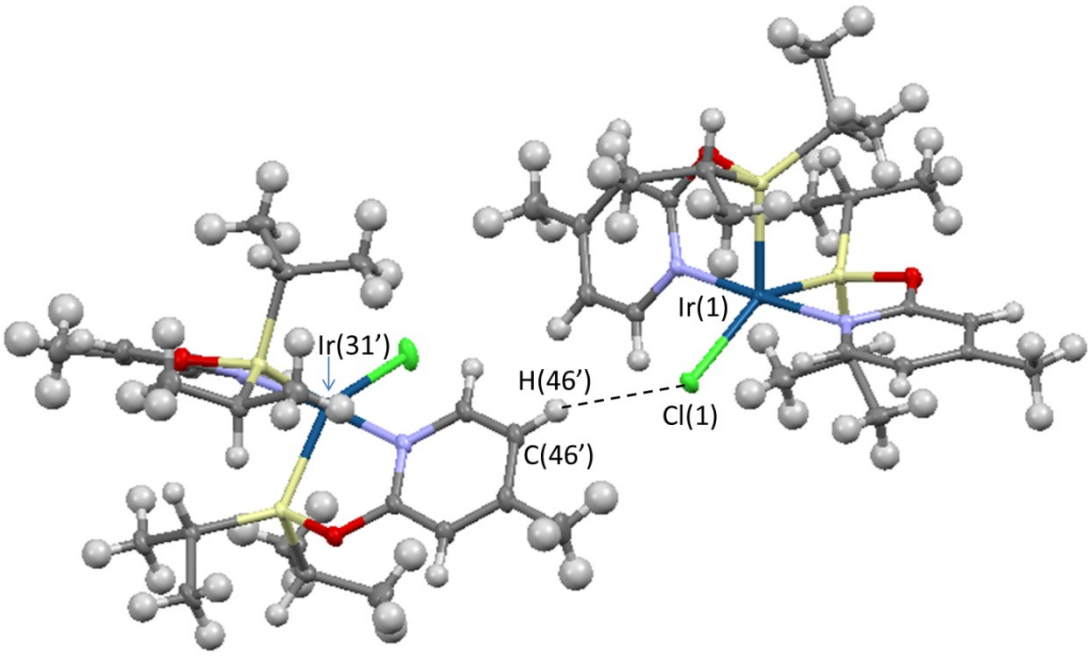

Figure S23. Intermolecular C-H··Cl interactions in complex **3**. Geometrical parameters: C(46')-H(46'): 0.95 Å; C(46')···Cl(1): 3.645(1) Å;C(46')-H(46')···Cl(1): 159.0°. Symmetry operation: ')-*x*,2-*y*, 1-*z*.

Table S1. Ring puckering parameters for Ir-NSi^{R2} (R = tBu, Me, iPr) complexes.

	[Ir(μ-Cl)(κ^2-NSi^{Me2})$_2$]$_2$	[Ir(CF$_3$CO$_2$)(κ^2-NSi^{Me2})$_2$]		[Ir(μ-CF$_3$SO$_3$)(κ^2-NSi^{Me2})$_2$]$_2$	Cmpnd **3**		Cmpnd **5**	Cmpnd **6**	[Ir(H)(Cl)(κ^2-NSi^{tBu2})(coe)]
	Ref. 13a	Ref. 13a		Ref. 13b	This work		This work	This work	Ref. 14
		Molecule 1	Molecule 2		Molecule 1	Molecule 2			
Ir-Si(1)-O(1)-C(1)-N(1)									
Q_T (Å)	0.050(4) / 0.175(3)	0.0212(1)	0.202(1)	0.2213(6)	0.220(1)	0.251(1)	0.308(1)	0.223(1)	0.118(1)
ø (º)	154(5) / -157(3)	12.51(13)	-146.08(1)	26.72(6)	29.26(8)	16.65(8)	32.8(7)	19.11(8)	-158.4(1)
conformation	$^5T_1$ - ^5E / $^2T_1$	$^1T_2$	^2E	$^1T_2$ - E_2	E_2	$^1T_2$	E_2	$^1T_2$	$^2T_1$
Ir-Si(2)-O(2)-C(13)-N(2)									
Q_T (Å)	0.154(3) 0.120(3)	0.0700(1)	0.133(1)	0.1249(6)	0.262(1)	0.214(1)	0.235(1)	0.308(1)	
ø (º)	-148(2)/ -164(2)	-141.93(5)	-162.01(1)	19.34(6)	14.73(8)	33.48(8)	11.8(5)	25.32	
conformation	^2E / $^2T_1$	^2E	$^2T_1$	$^1T_2$	$^1T_2$	E_2	$^1T_2$/^1E	$^1T_2$ - E_2	

D. Cremer and J.A Pople, J.Am. Chem. Soc., 1975, 97, 6, 1354-1358.

Table contains the value of both crystallographically independent molecules for complexes **3** and [Ir(CF$_3$CO$_2$)(κ^2-NSi^{Me2})$_2$]. Compound [Ir(μ-Cl)(κ^2-NSi^{Me2})$_2$]$_2$ corresponds to a binuclear complex, with crystallographically independent moieties. Both values are indicated in the table, separated by a forward slash symbol.

Table S2. Bond lengths (Å) along the Ir-Si-O-C-N iridacycle for Ir-NSi^{R2} (R = tBu, Me, iPr) complexes.

	[Ir(μ-Cl)(κ^2-NSi^{Me2})$_2$]$_2$	[Ir(CF$_3$CO$_2$)(κ^2-NSi^{Me2})$_2$]		[Ir(μ-CF$_3$SO$_3$)(κ^2-NSi^{Me2})$_2$]$_2$	Cmpnd **3**		Cmpnd **5**	Cmpnd **6**	[Ir(H)(Cl)(κ^2-NSi^{tBu2})(coe)]
	Ref. 13a	Ref. 13a		Ref. 13b	This work		This work	This work	Ref. 14
		Molecule 1	Molecule 2		Molecule 1	Molecule 2			
Ir(1)-Si(1)	2.2634(14) 2.2552(14)	2.2645(10)	2.2505(10)	2.2570(5)	2.2700(7)	2.2515(7)	2.2702(10)	2.2573(8)	2.2853(6)
Si(1)-O(1)	1.723(4) 1.728(4)	1.734(3)	1.719(3)	1.7281(14)	1.7282(18)	1.7333(19)	1.733(3)	1.727(2)	1.7285(16)
O(1)-C(1)	1.320(6) 1.316(6)	1.329(4)	1.331(4)	1.336(2)	1.330(3)	1.332(3)	1.332(5)	1.329(3)	1.334(3)
C(1)-N(1)	1.343(6) 1.351(6)	1.359(4)	1.351(5)	1.359(2)	1.359(3)	1.355(3)	1.367(5)	1.367(4)	1.347(3)
N(1)-Ir(1)	2.078(4) 2.069(4)	2.052(3)	2.053(3)	2.0591(15)	2.065(2)	2.058(2)	2.068(3)	2.048(2)	2.0947(18)
Ir(1)-Si(2)	2.2695(14) 2.2747(14)	2.2505(11)	2.2570(10)	2.2615(5)	2.2499(7)	2.2579(7)	2.2668(11)	2.2498(8)	
Si(2)-O(2)	1.721(4) 1.731(4)	1.729(3)	1.732(3)	1.7330(15)	1.7338(18)	1.7320(19)	1.742(3)	1.733(2)	
O(2)-C(13)	1.326(6) 1.338(6)	1.331(5)	1.328(5)	1.335(2)	1.333(3)	1.328(3)	1.333(5)	1.340(4)	
C(13)-N(2)	1.355(6) 1.354(6)	1.347(5)	1.364(5)	1.352(2)	1.363(3)	1.361(3)	1.352(5)	1.359(4)	
N(2)-Ir(1)	2.074(4) 2.073(4)	2.056(3)	2.049(3)	2.0581(15)	2.057(2)	2.061(2)	2.065(3)	2.052(2)	

Table contains the value of both crystallographically independent molecules for complexes **3** and [Ir(CF$_3$CO$_2$)(κ^2-NSi^{Me2})$_2$]. Compound [Ir(μ-Cl)(κ^2-NSi^{Me2})$_2$]$_2$ corresponds to a binuclear complex, with crystallographically independent moieties. Both values are indicated in the table in two correlative lines.

Table S3 Sum of the angles (°) around the Si atom, excluding Ir-Si-O angle, for Ir-NSi^{R2} (R = tBu, Me, iPr) complexes.

	$[Ir(\mu\text{-}Cl)(\kappa^2\text{-}NSi^{Me2})_2]_2$	$[Ir(CF_3CO_2)(\kappa^2\text{-}NSi^{Me2})_2]$		$[Ir(\mu\text{-}CF_3SO_3)(\kappa^2\text{-}NSi^{Me2})_2]_2$	Cmpnd **3**		Cmpnd **5**	Cmpnd **6**	$[Ir(H)(Cl)(\kappa^2\text{-}NSi^{tBu2})(coe)]$
	Ref. 13a	Ref. 13a		Ref. 13b	This work		This work	This work	Ref. 14
		Molecule 1	Molecule 2		Molecule 1	Molecule 2			
Ir-Si(1)-C	115.68(19) 114.8(2)	109.71(13)	109.57(14)	113.84(7)	109.74(8)	107.86(9)	112.21(13)	108.05(10)	111.07(8)
Ir-Si(1)-C	125.0(2) 123.8(2)	129.56(15)	127.00(15)	124.35(7)	128.46(8)	127.45(9)	122.05(13)	127.84(11)	121.84(8)
C-Si(1)-C	104.2(3) 104.7(3)	107.19(19)	108.1(2)	105.84(10)	108.15(11)	108.47(12)	109.67(19)	108.98(13)	116.49(11)
sum	**344.9(4)** **343.3(4)**	**346.5(3)**	**344.7(3)**	**344.03(14)**	**346.35(16)**	**343.78(17)**	**343.9(3)**	**344.9(2)**	**349.4(16)**
Ir-Si(2)-C	115.15(19) 116.47(19)	108.51(16)	108.77(13)	113.80(7)	107.79(9)	109.53(8)	111.91(14)	110.95(11)	
Ir-Si(2)-C	125.1(2) 124.9(2)	130.44(16)	128.20(14)	126.21(7)	127.17(8)	128.33(9)	125.91(13)	124.00(11)	
C-Si(2)-C	103.9(3) 104.3(3)	105.5(2)	107.58(19)	104.31(9)	108.90(12)	107.44(11)	108.94(19)	109.19(16)	
sum	**344.1(4)** **345.7(4)**	**344.4(3)**	**344.5(3)**	**344.32(13)**	**343.86(17)**	**345.30(16)**	**346.8(3)**	**344.1(2)**	

Table contains the value of both crystallographically independent molecules for complexes **3** and $[Ir(CF_3CO_2)(\kappa^2\text{-}NSi^{Me2})_2]$. Compound $[Ir(\mu\text{-}Cl)(\kappa^2\text{-}NSi^{Me2})_2]_2$ corresponds to a binuclear complex, with crystallographically independent moieties. Both values are indicated in the table in two correlative lines.

5. Cartesian coordinates (in Å) of DFT optimized species

A

77	0.000000	0.000000	0.757592
17	0.000000	0.000000	3.210744
14	0.393777	1.520472	-0.891183
14	-0.393777	-1.520472	-0.891183
8	-1.286295	1.937800	-1.284621
8	1.286295	-1.937800	-1.284621
7	-1.891603	0.885307	0.681454
7	1.891603	-0.885307	0.681454
6	-2.212783	1.666319	-0.387847
6	-3.513621	2.174758	-0.545527
1	-3.712809	2.784877	-1.426882
6	-4.496294	1.902829	0.399607
6	-4.130380	1.119816	1.514008
1	-4.852183	0.886778	2.298510
6	-2.838793	0.642394	1.619784
1	-2.498218	0.058158	2.474681
6	-5.897108	2.428857	0.255109
1	-6.018093	3.020108	-0.663129
1	-6.164568	3.065319	1.114382
1	-6.623384	1.600043	0.231396
6	1.263921	1.268733	-2.564530
1	1.015194	0.253943	-2.910316
6	0.763931	2.272143	-3.613899
1	0.972720	3.311720	-3.309874
1	-0.321860	2.189870	-3.772578
1	1.265171	2.109498	-4.583935
6	2.791578	1.331515	-2.406338
1	3.290952	1.101305	-3.363033
1	3.165374	0.612599	-1.660768
1	3.127269	2.334875	-2.098702
6	1.082255	3.119082	-0.083012
1	1.434435	3.746330	-0.924015
6	2.277121	2.823240	0.837788
1	2.749304	3.758900	1.184214
1	3.056766	2.219862	0.347943
1	1.944509	2.271129	1.730775
6	0.000000	3.898454	0.676554
1	-0.420245	3.293361	1.496640
1	-0.829790	4.199808	0.020053
1	0.419739	4.813474	1.129187
6	2.212783	-1.666319	-0.387847
6	3.513621	-2.174758	-0.545527
1	3.712809	-2.784877	-1.426882
6	4.496294	-1.902829	0.399607
6	4.130380	-1.119816	1.514008
1	4.852183	-0.886778	2.298510
6	2.838793	-0.642394	1.619784
1	2.498218	-0.058158	2.474681
6	5.897108	-2.428857	0.255109
1	6.623384	-1.600043	0.231396
1	6.164568	-3.065319	1.114382
1	6.018093	-3.020108	-0.663129
6	-1.263921	-1.268733	-2.564530
1	-1.015194	-0.253943	-2.910316
6	-2.791578	-1.331515	-2.406338
1	-3.290952	-1.101305	-3.363033
1	-3.165374	-0.612599	-1.660768
1	-3.127269	-2.334875	-2.098702
6	-0.763931	-2.272143	-3.613899
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