

Supporting Information

Synthesis of Silyl Iron Dinitrogen Complexes for Activation of Dihydrogen and Catalytic Silylation of Dinitrogen

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1. Table S1. Crystallographic Data for Complexes **1 - 4**

	1	2	3	4
formula	C ₂₈ H ₄₉ FeN ₂ P ₃ Si	C ₃₃ H ₅₁ FeN ₂ P ₃ Si	C ₃₀ H ₄₇ FeN ₂ P ₃ Si	C ₃₀ H ₄₇ FeP ₃ Si
<i>M_z</i>	590.54	652.61	612.54	584.52
crystal system	monoclinic	triclinic	tetragonal	monoclinic
space group	P2 ₁ /n	P-1	Pbca	P2 ₁ /n
<i>a</i> /Å	13.4753(4)	9.9876(3)	16.2215(6)	9.1689(2)
<i>b</i> /Å	17.1665(4)	10.4113(3)	16.2215(6)	16.6564(3)
<i>c</i> /Å	13.9116(4)	36.5579(6)	24.4132(11)	21.0278(5)
α /°	90	96.856(2)	90	90
β /°	105.988(2)	91.687(2)	90	101.511(2)
γ /°	90	116.430(2)	90	90
<i>V</i> [Å ³]	3093.60(15)	3365.15(16)	6424.0(4)	3146.79(12)
<i>T</i> [K]	153.15	172.99(10)	173.0(5)	180
<i>Z</i>	4	2	8	4
μ [mm ⁻¹]	5.884	5.463	5.689	3.831
total reflns	15684	32434	35686	36536
unique reflns	4868	13063	5715	7553
<i>R</i> _{int}	0.0267	0.0426	0.0851	0.0150
<i>R</i> ₁ [<i>I</i> >2 σ (<i>I</i>)]	0.0453	0.0410	0.0670	0.0270
<i>wR</i> (<i>F</i> ₂)[<i>I</i> >2 σ (<i>I</i>)]	0.1161	0.0897	0.1705	0.0741
<i>R</i> ₁ (all data)	0.0504	0.0552	0.0775	0.0290
<i>wR</i> (<i>F</i> ₂)(all data)	0.1195	0.1003	0.1829	0.0754
GOF on <i>F</i> ₂	1.040	1.073	1.087	1.026

2. Table S2. Crystallographic Data for Complexes **5 - 7**

	5	6	7
formula	C ₂₈ H ₅₁ FeP ₃ Si	C ₃₃ H ₅₃ FeP ₃ Si	C ₃₀ H ₄₉ FeP ₃ Si
<i>M</i> _z	564.53	626.64	586.54
crystal system	monoclinic	triclinic	monoclinic
space group	P2 ₁ /n	P-1	P2 ₁ /n
<i>a</i> /Å	13.3431(2)	11.0515(4)	9.1606(2)
<i>b</i> /Å	16.8555(3)	17.3189(6)	16.6565(3)
<i>c</i> /Å	14.1692(3)	19.6938(6)	21.0567(3)
α /°	90	69.372(3)	90
β /°	106.2564(19)	87.284(3)	101.548(2)
γ /°	90	74.966(3)	90
<i>V</i> [Å ³]	3059.31(10)	3402.9(2)	3147.87(10)
<i>T</i> [K]	173.00(10)	293(2)	172.99(10)
<i>Z</i>	4	2	4
μ [mm ⁻¹]	5.905	5.361	5.761
total reflns	16325	37796	19552
unique reflns	6026	13221	6230
<i>R</i> _{int}	0.0454	0.0688	0.0547
<i>R</i> ₁ [<i>I</i> >2 σ (<i>I</i>)]	0.0375	0.0500	0.0381
<i>wR</i> (<i>F</i> ₂)[<i>I</i> >2 σ (<i>I</i>)]	0.0811	0.1106	0.0770
<i>R</i> ₁ (all data)	0.0537	0.0675	0.0514
<i>wR</i> (<i>F</i> ₂)(all data)	0.0910	0.1273	0.0886
GOF on <i>F</i> ₂	1.080	1.052	1.067

3. IR, ^1H , ^{31}P , ^{13}C , ^{29}Si NMR Spectra of Complexes **1**, **2**, **3**, **4**, **5**, **6** and **7**

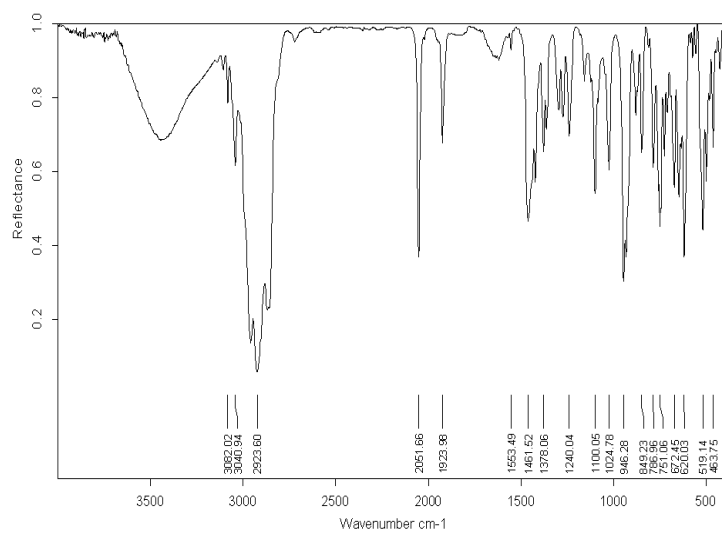


Figure S1 The IR spectrum of complex **1**

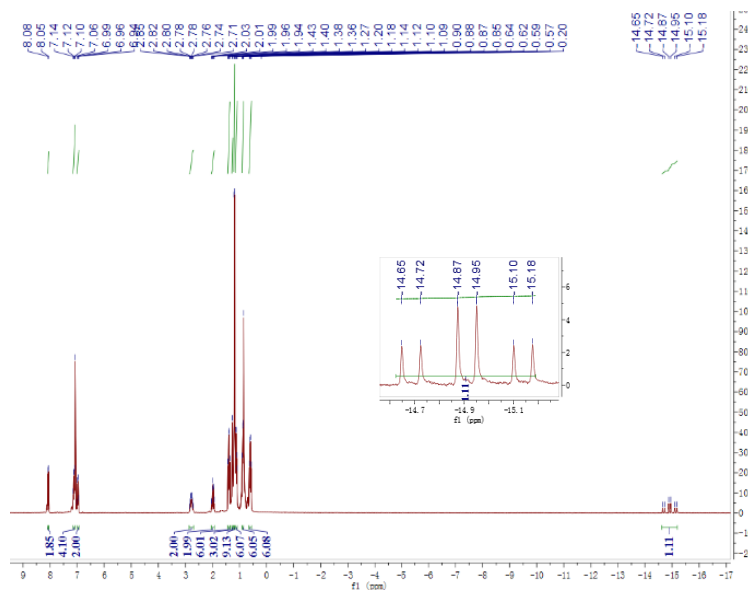


Figure S2 The ^1H NMR spectrum of complex **1**

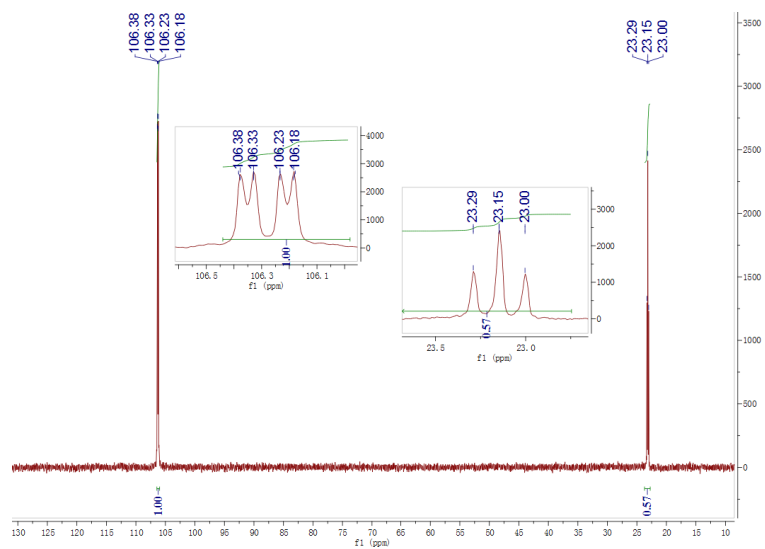


Figure S3 The ^{31}P NMR spectrum of complex 1

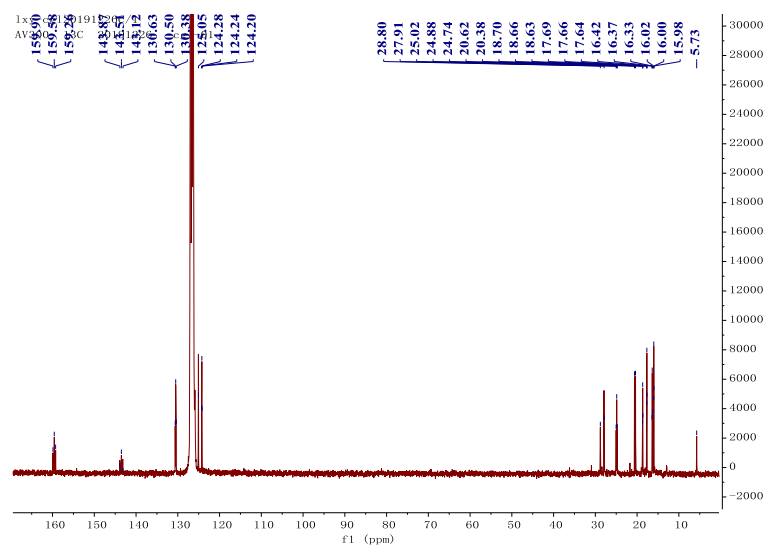


Figure S4 The ^{13}C NMR spectrum of complex 1

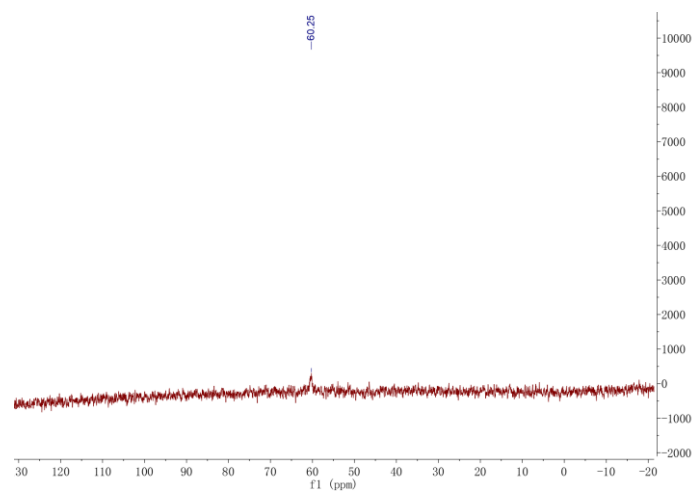


Figure S5 The ^{29}Si NMR spectrum of complex **1**

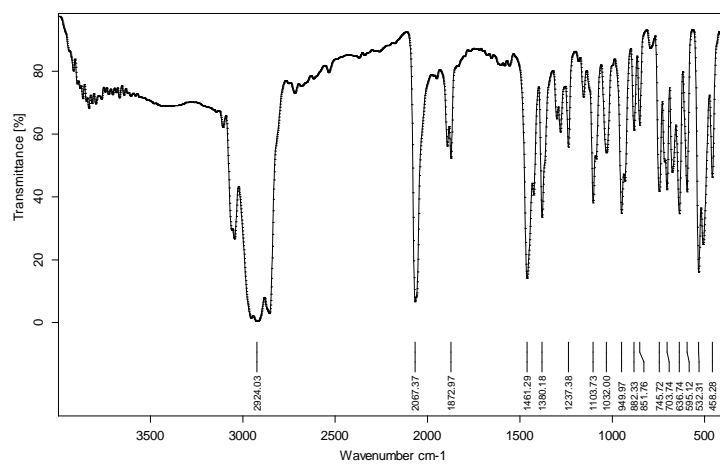


Figure S6 The IR spectrum of complex **2**

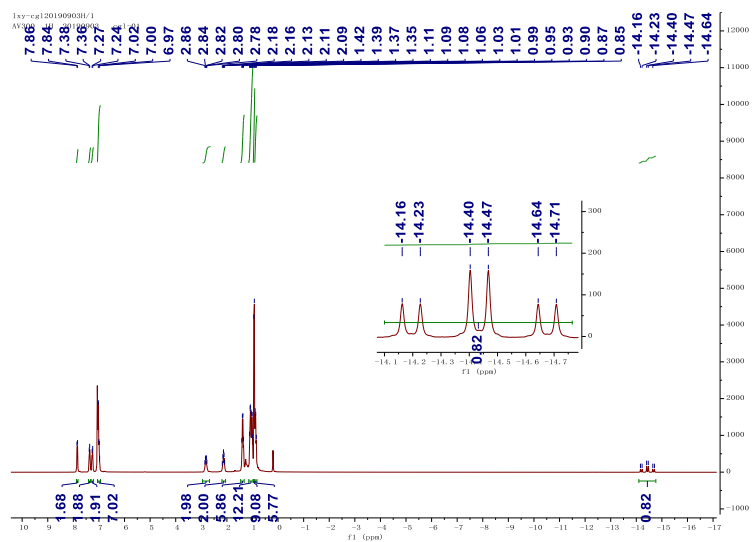


Figure S7 The ^1H NMR spectrum of complex 2

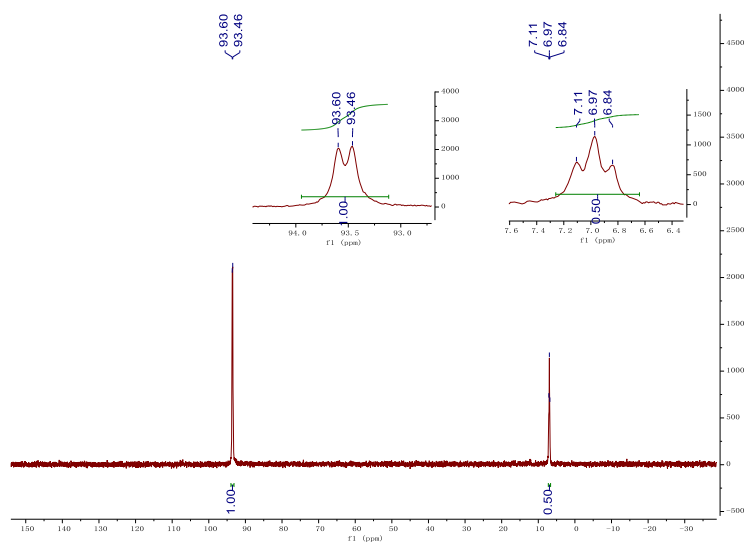


Figure S8 The ^{31}P NMR spectrum of complex 2

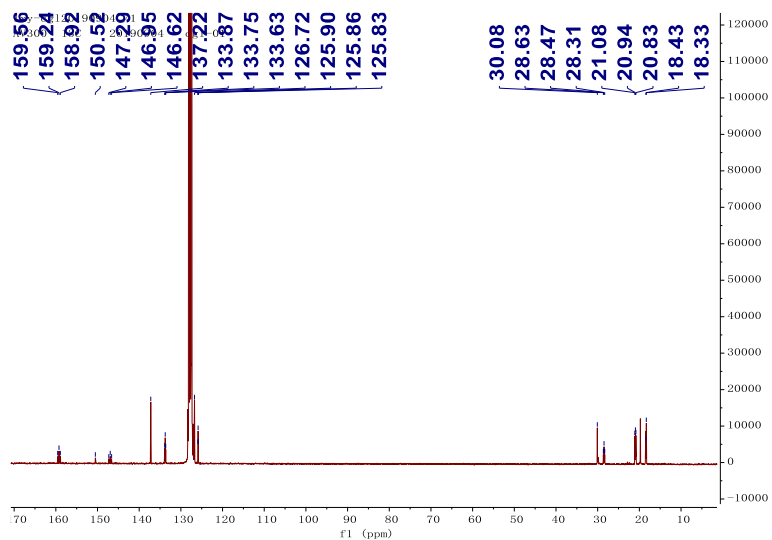


Figure S9 The ^{13}C NMR spectrum of complex 2

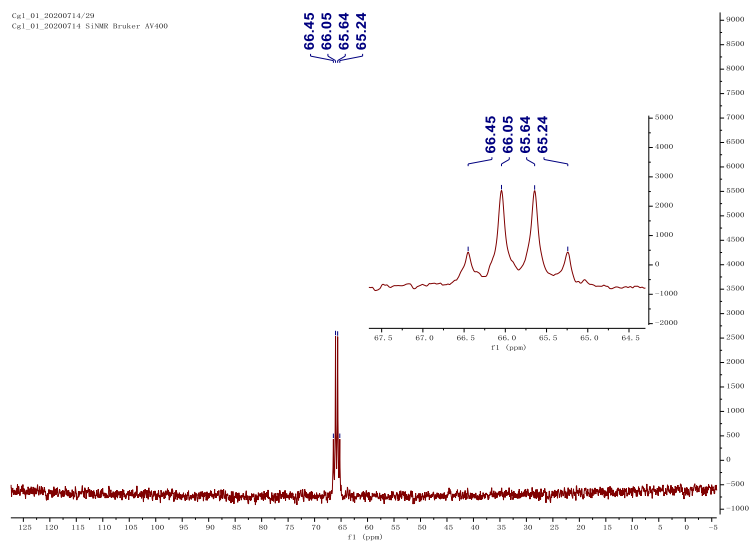


Figure S10 The ^{29}Si NMR spectrum of complex 2

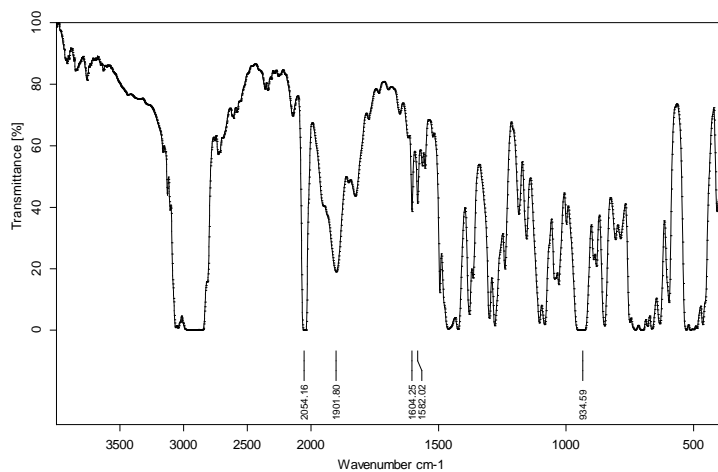


Figure S11 The IR spectrum of complex 3

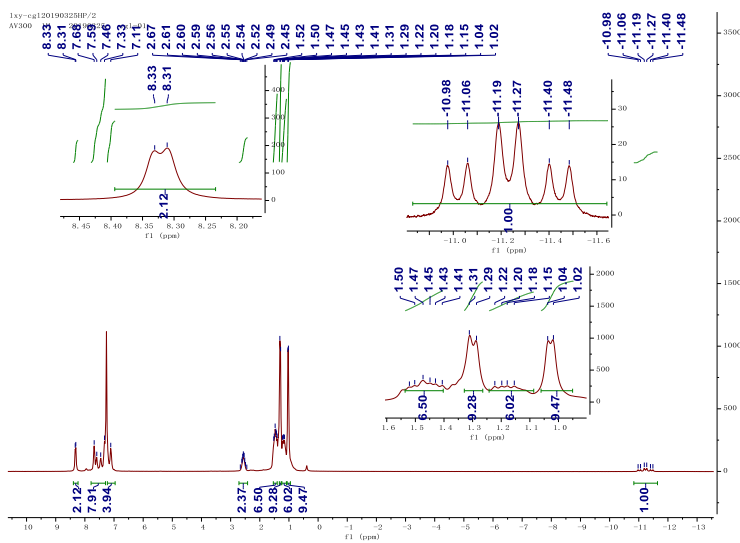


Figure S12 The ¹H NMR spectrum of complex 3

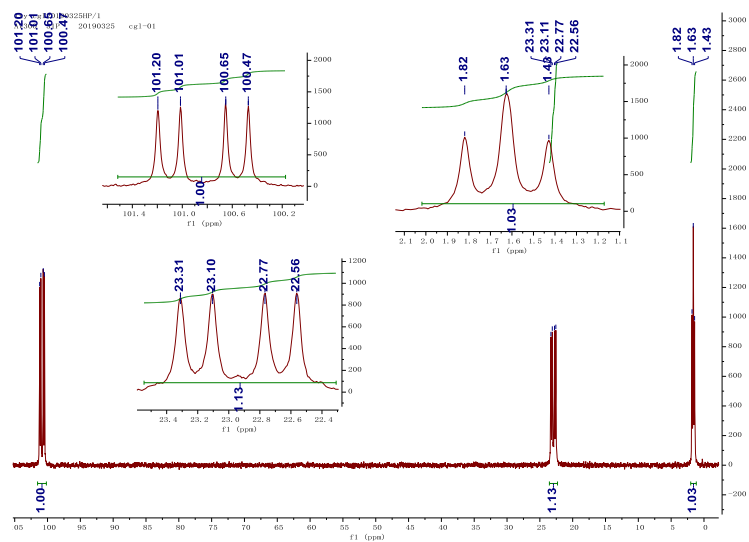


Figure S13 The ^{31}P NMR spectrum of complex 3

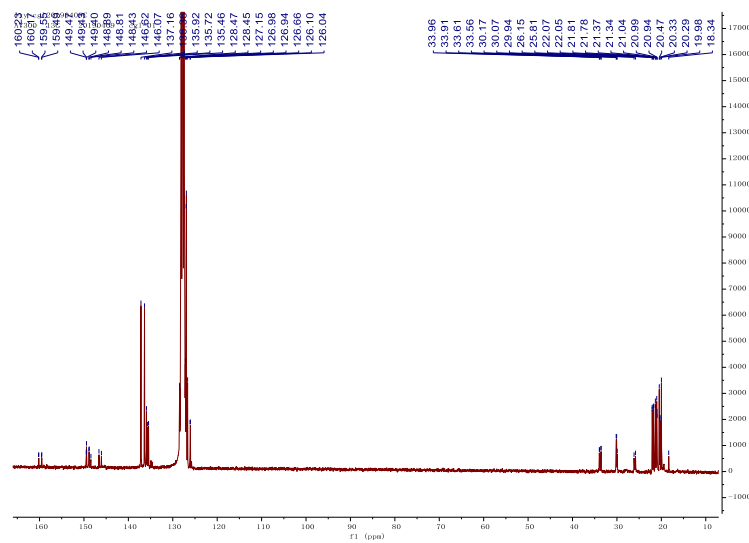


Figure S14 The ^{13}C NMR spectrum of complex 3

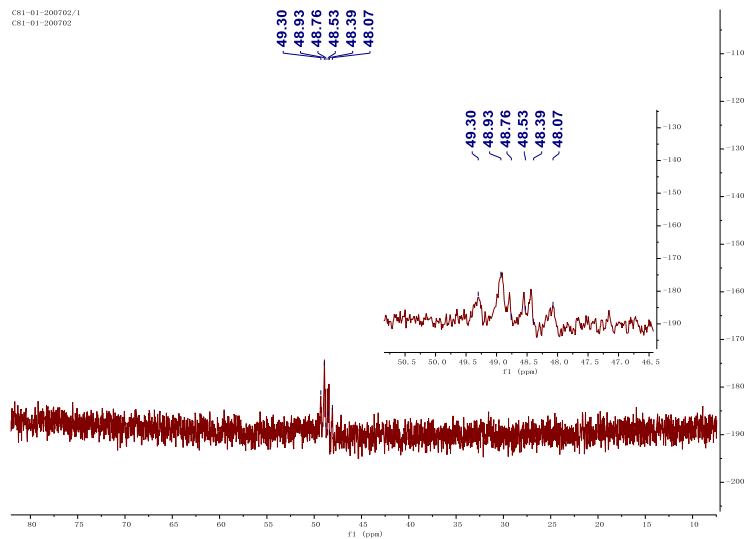


Figure S15 The ^{29}Si NMR spectrum of complex **3**

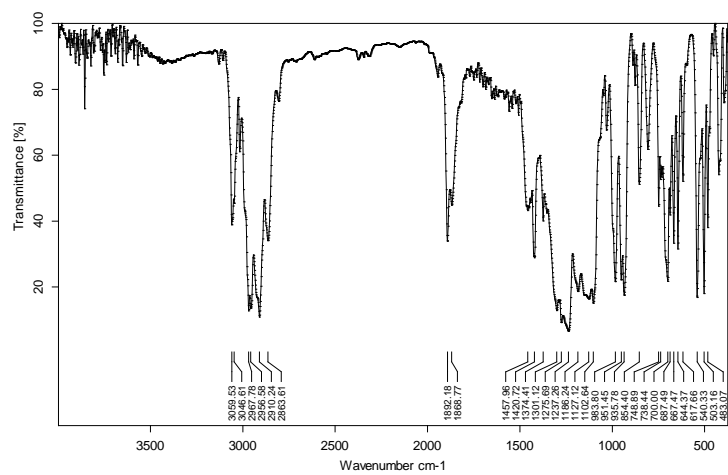


Figure S16 The IR spectrum of complex **4**

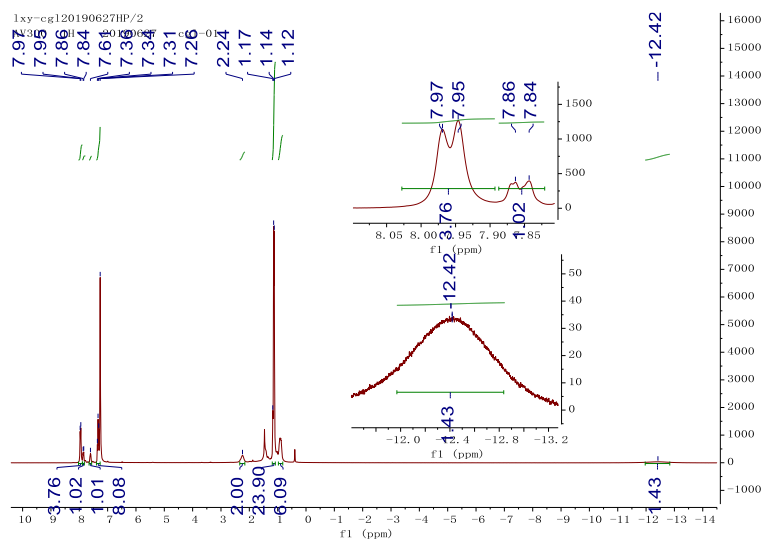


Figure S17 The ¹H NMR spectrum of complex 4

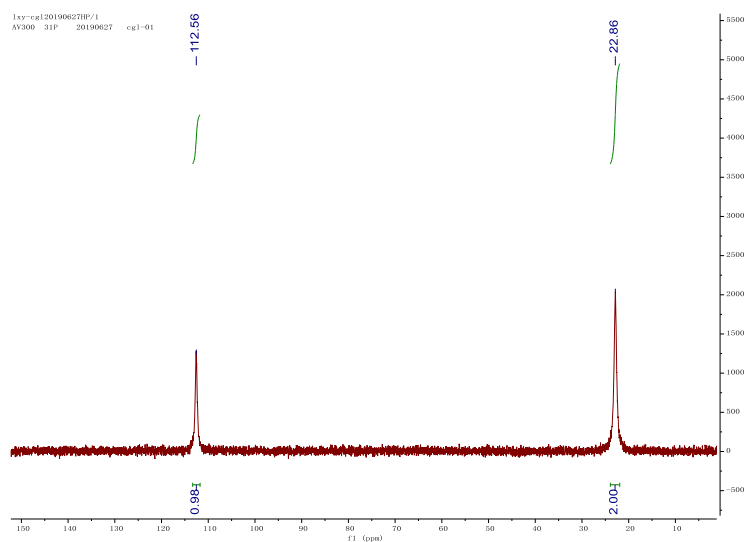


Figure S18 The ³¹P NMR spectrum of complex 4

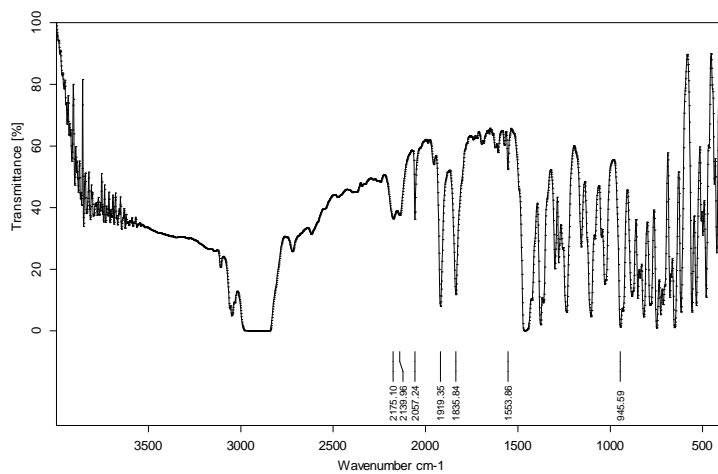


Figure S19 The IR spectrum of complex 5

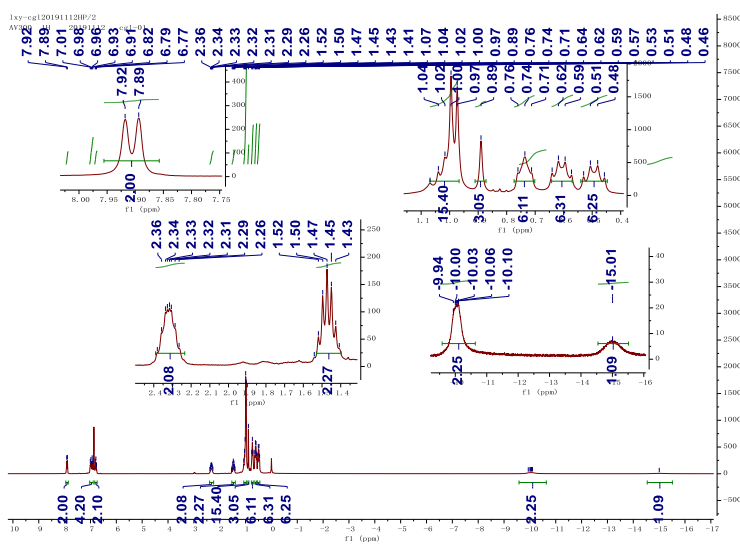


Figure S20 The ¹H NMR spectrum of complex 5

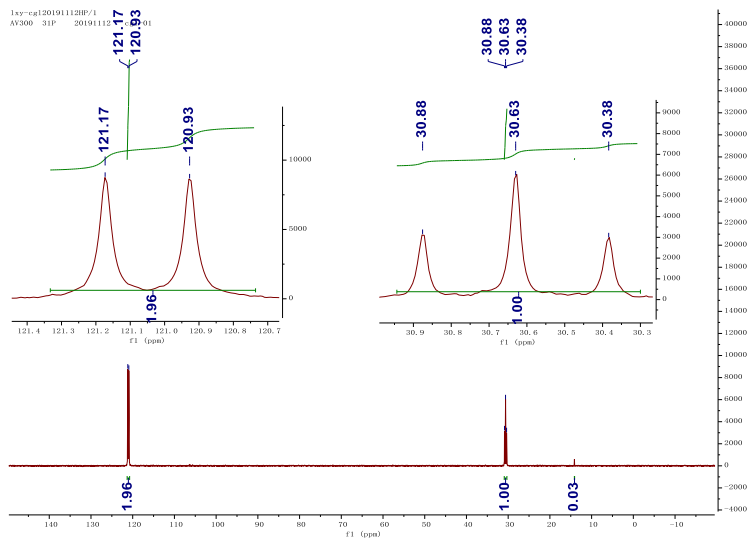


Figure S21 The ^{31}P NMR spectrum of complex 5

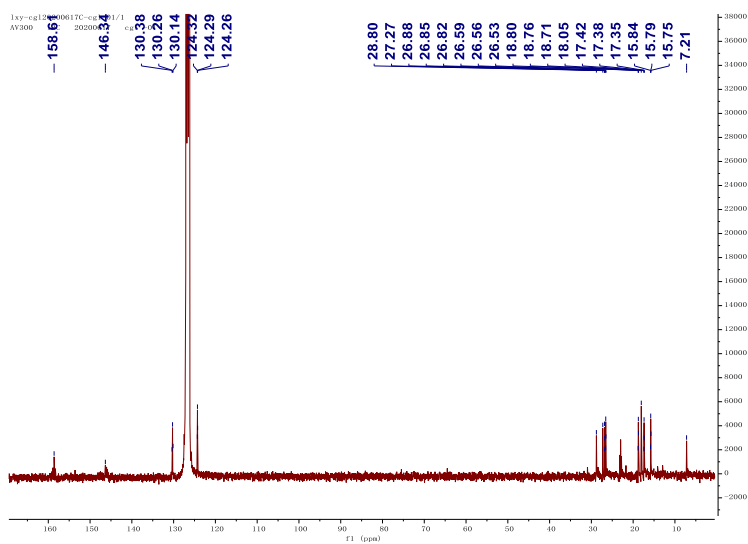


Figure S22 The ^{13}C NMR spectrum of complex 5

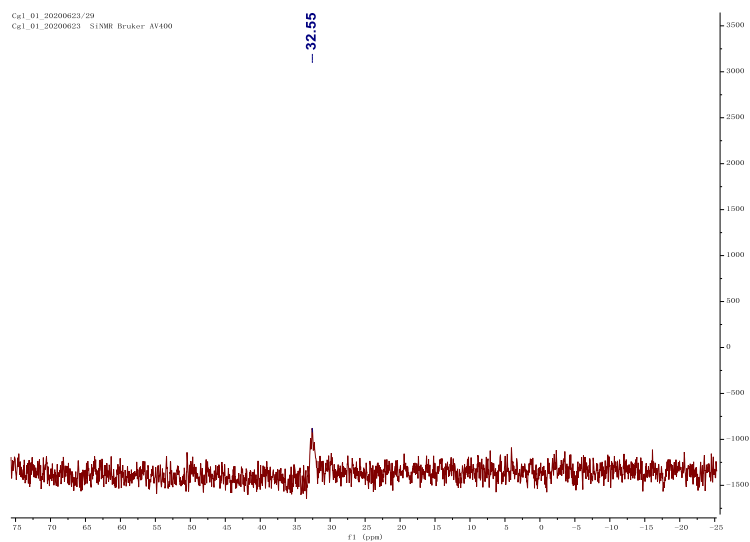


Figure S23 The ^{29}Si NMR spectrum of complex **5**

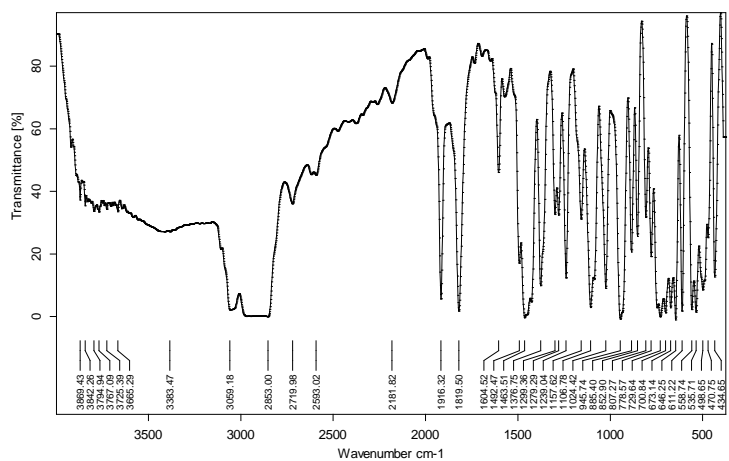


Figure S24 The IR spectrum of complex **6**

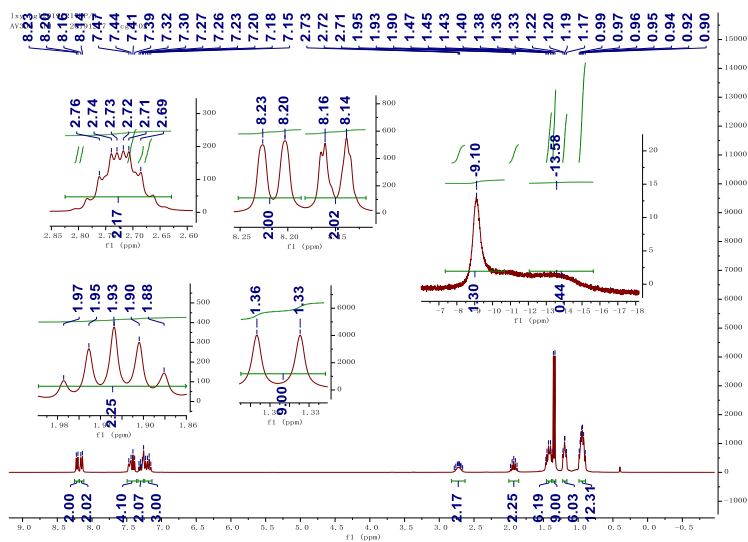


Figure S25 The ^1H NMR spectrum of complex 6

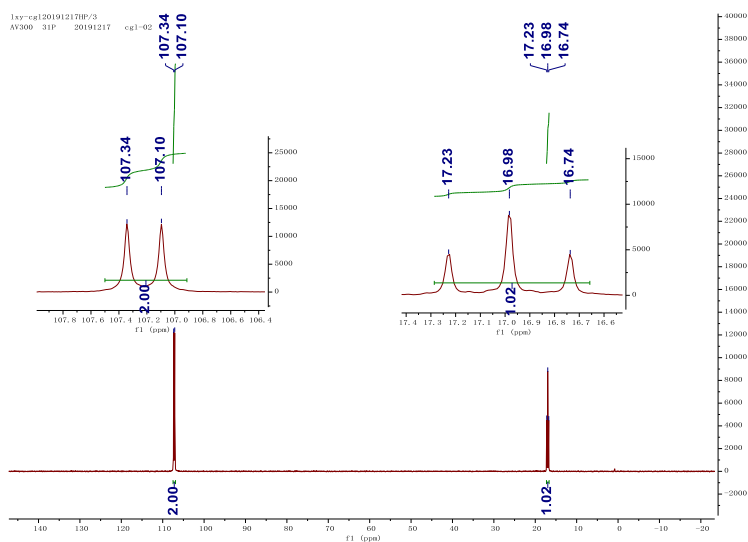


Figure S26 The ^{31}P NMR spectrum of complex 6

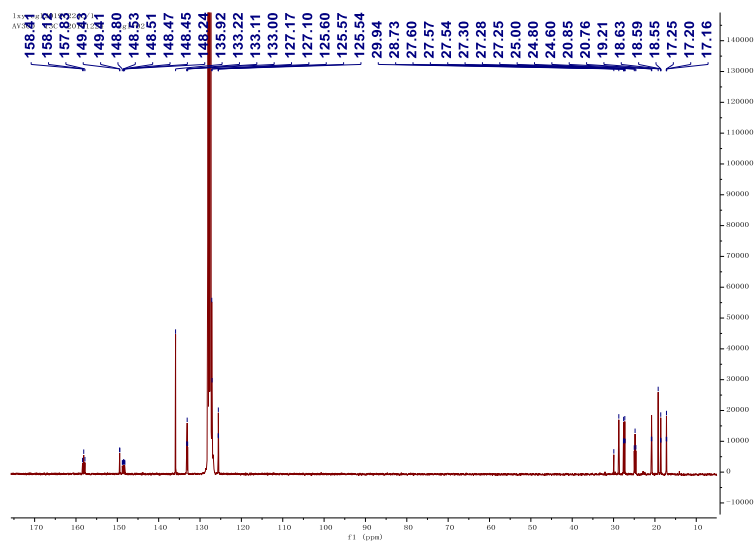


Figure S27 The ^{13}C NMR spectrum of complex 6

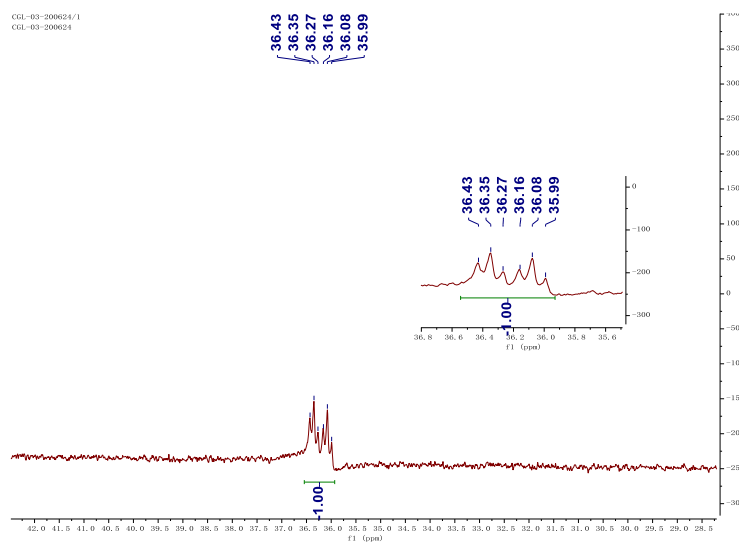


Figure S28 The ^{29}Si NMR spectrum of complex 6

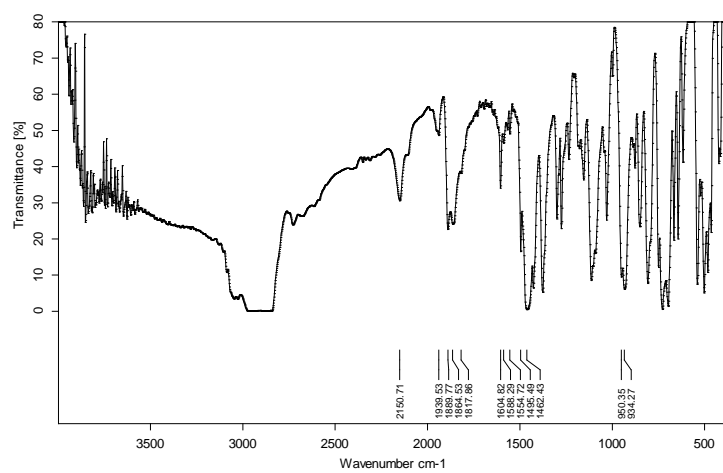


Figure S29 The IR spectrum of complex **7**

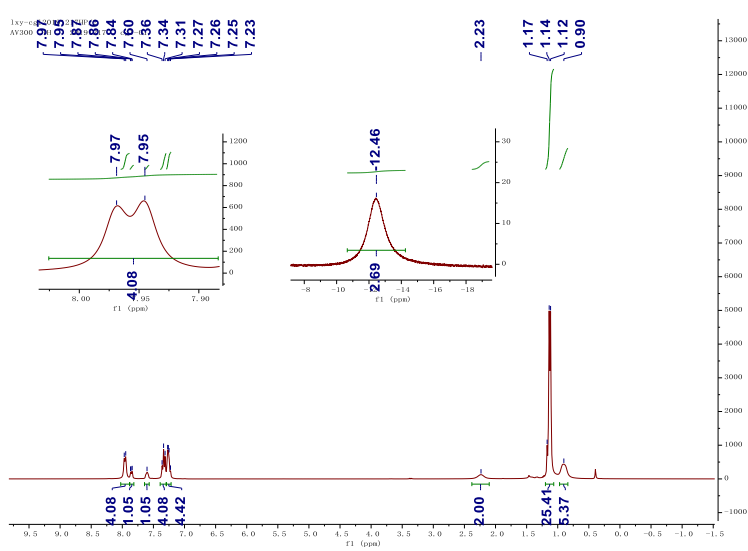


Figure S30 The ¹H NMR spectrum of complex **7**

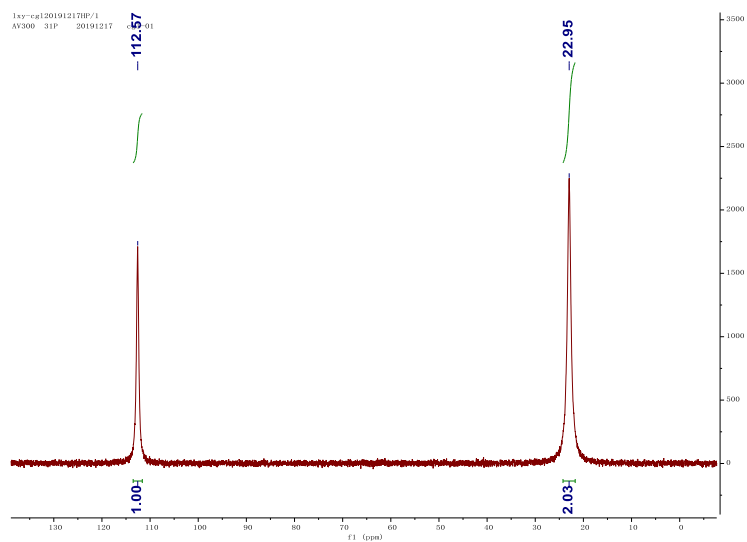


Figure S31 The ^{31}P NMR spectrum of complex 7

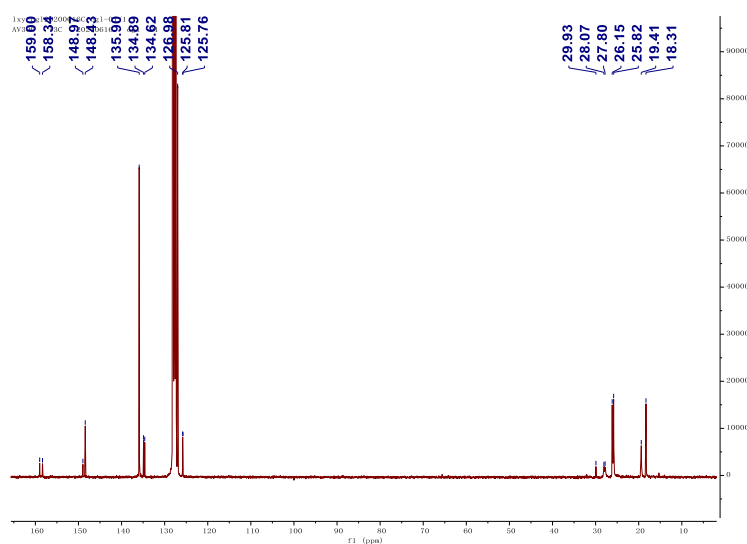


Figure S32 The ^{13}C NMR spectrum of complex 7

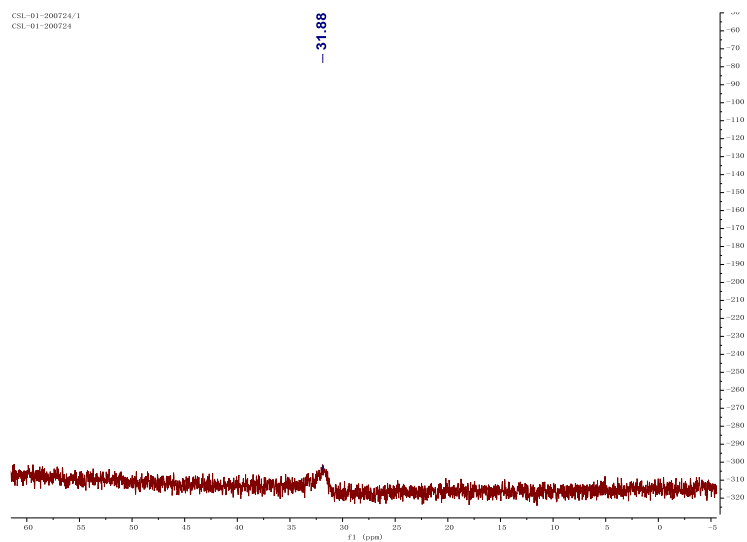


Figure S33 The ^{29}Si NMR spectrum of complex **7**