Supporting Information for

Magnesium Complexes Supported by Dianionic Double Layer Nitrogen-Phosphorus Ligand: Synthesis and Reactivity Study

Yafei Li,[a] Pengfei Chen,[a] Qin Zhu,[b,*] and Congqing Zhu[a,*]

[a] *State Key Laboratory of Coordination Chemistry, Jiangsu Key Laboratory of Advanced Organic Materials, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China.*

[b] *Key Laboratory for Organic Electronics & Information Displays (KLOEID) and Institute of Advanced Materials (IAM), SICAM, Nanjing University of Posts & Telecommunications, Nanjing 210023, China*

*Correspondence and requests for materials should be addressed to C.Z. (E-mail: zcq@nju.edu.cn) or Q.Z. (iamqzhu@njupt.edu.cn).

Context

1. NMR spectra

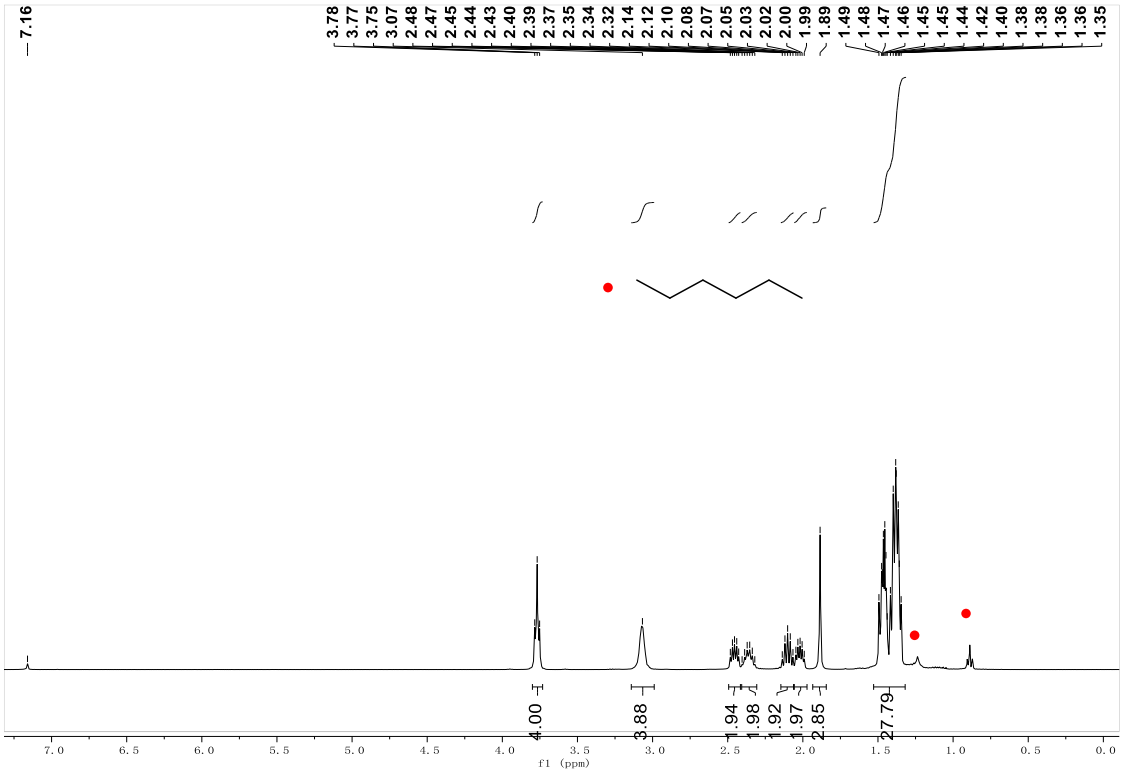


Figure S1 ^{1}H NMR spectrum of complex **1** in C_6D_6.

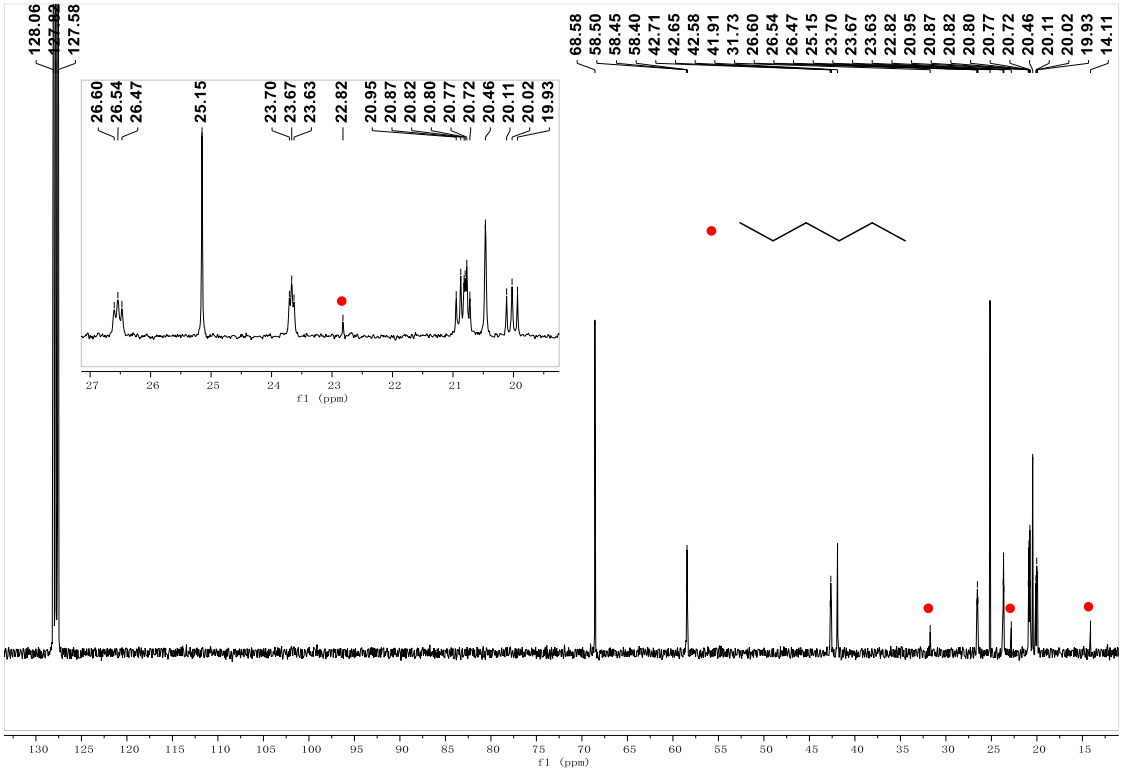


Figure S2 $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** (C_6D_6)

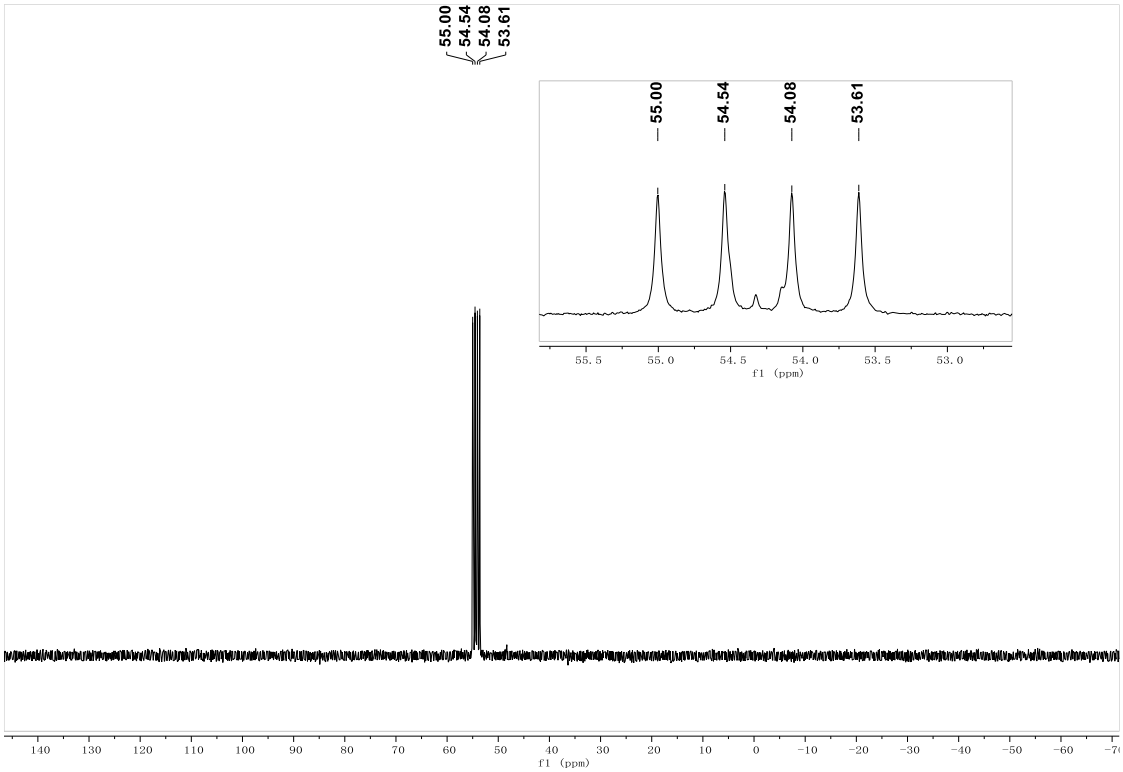


Figure S3 $^{31}P\{^{1}H\}$ NMR spectrum of complex **1** (C_6D_6)

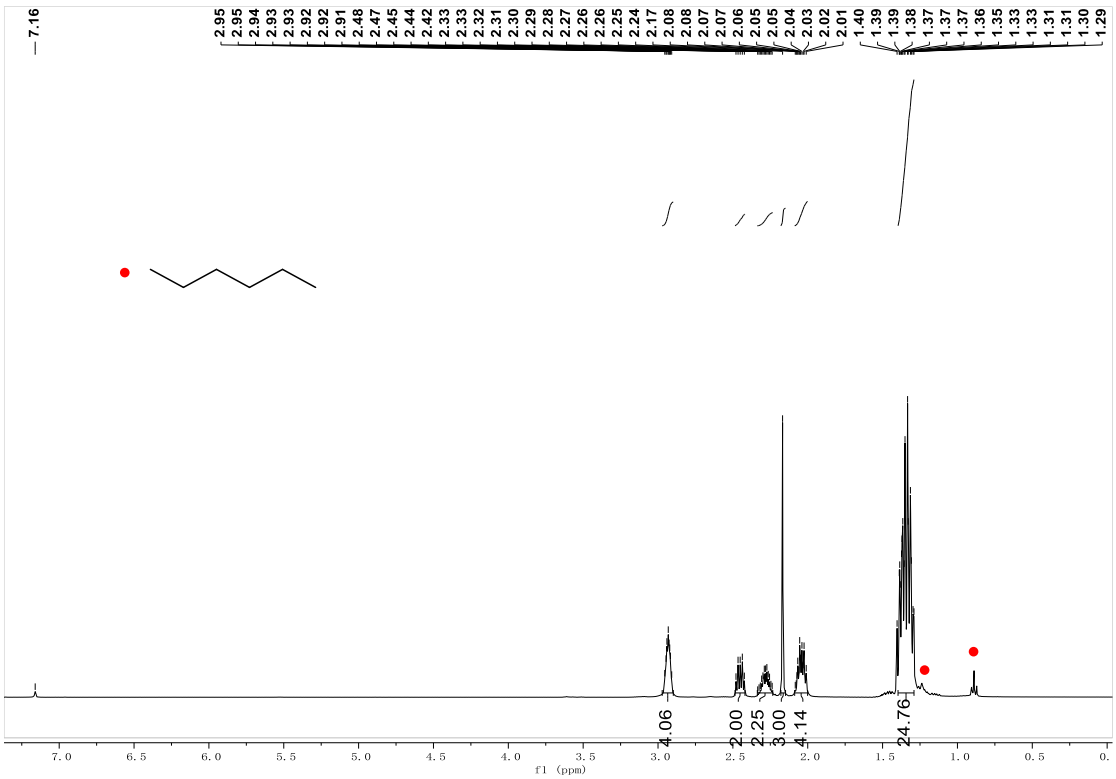


Figure S4 ^{1}H NMR spectrum of complex **2** (C_6D_6)

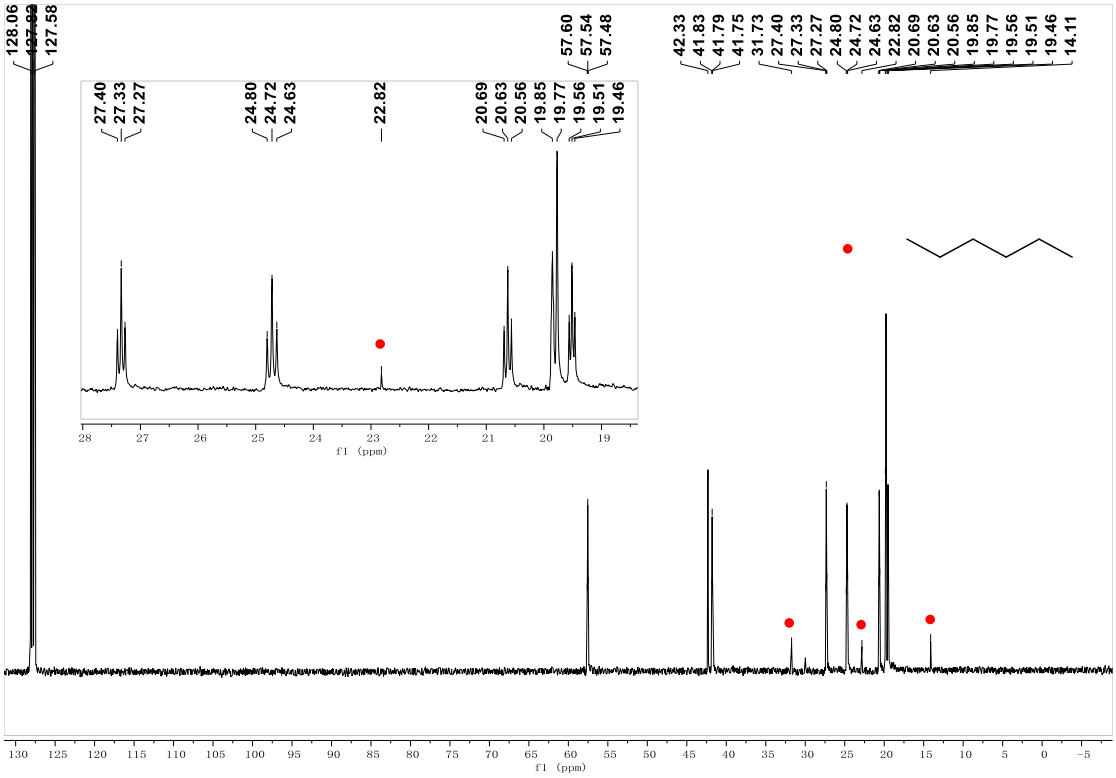


Figure S5 $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** (C_6D_6)

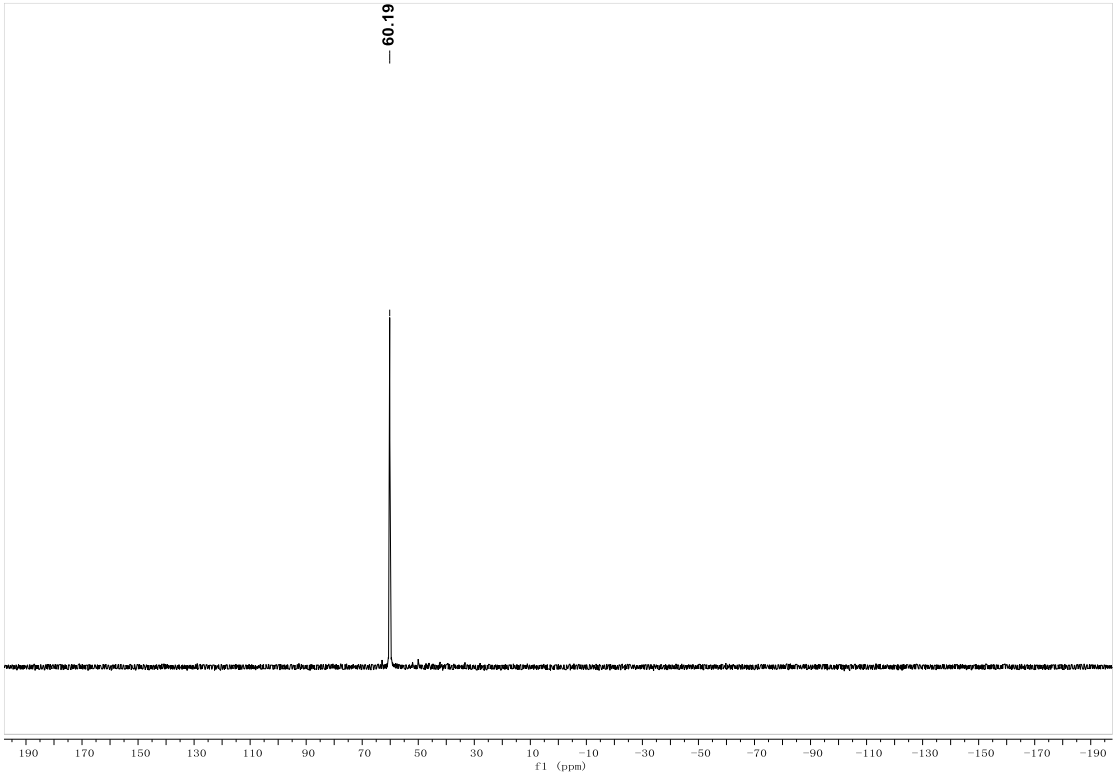


Figure S6 $^{31}P\{^{1}H\}$ NMR spectrum of complex **2** (C_6D_6)

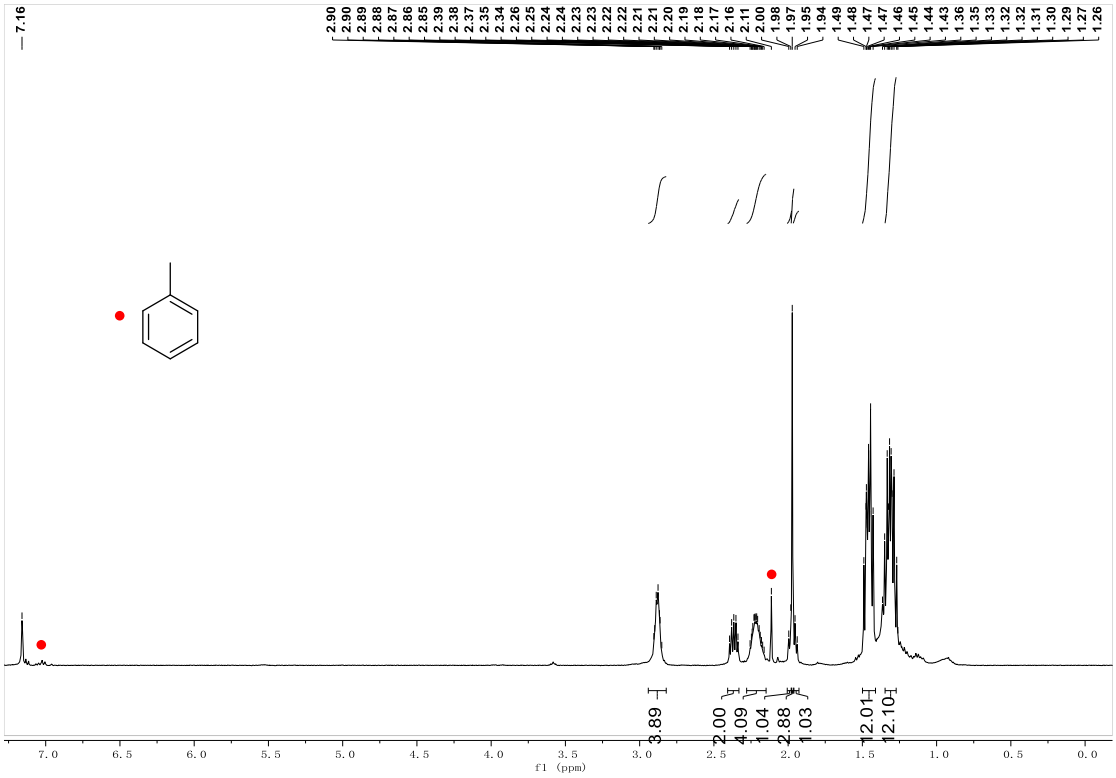


Figure S7 ^{1}H NMR spectrum of complex **3** (C_6D_6)

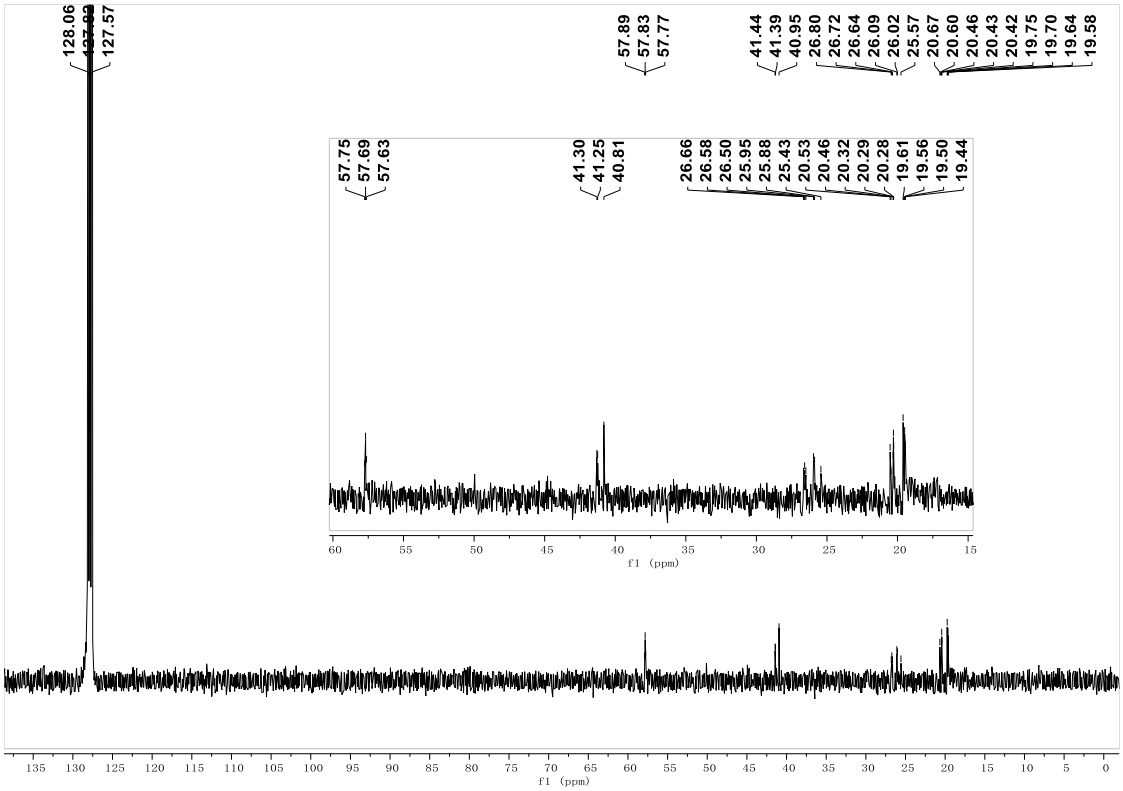


Figure S8 $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** (C_6D_6)

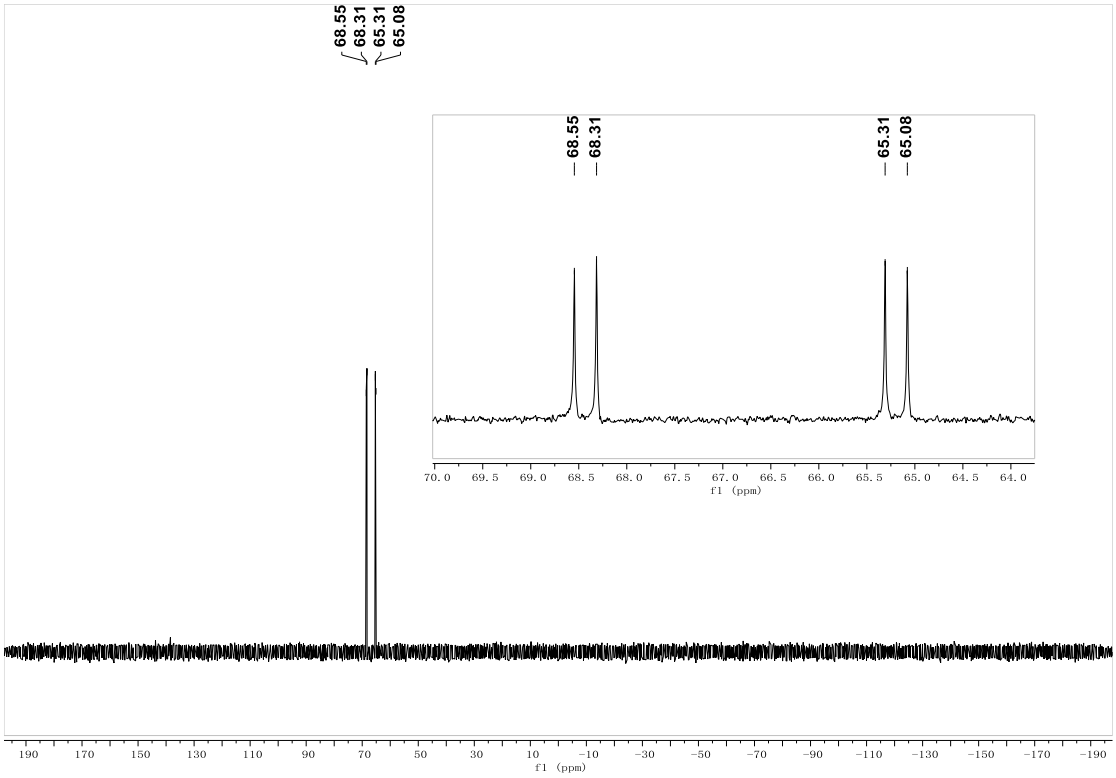


Figure S9 $^{31}P\{^{1}H\}$ NMR spectrum of complex **3** (C_6D_6)

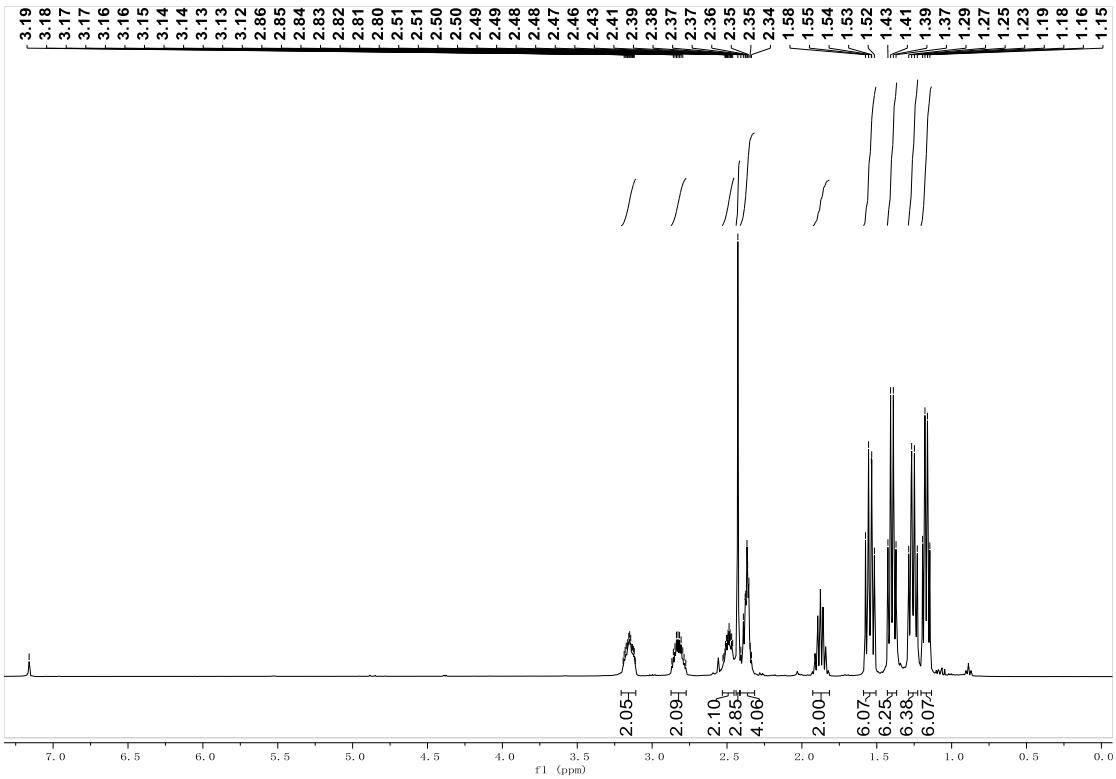


Figure S10 ^{1}H NMR spectrum of complex **4** (C_6D_6)

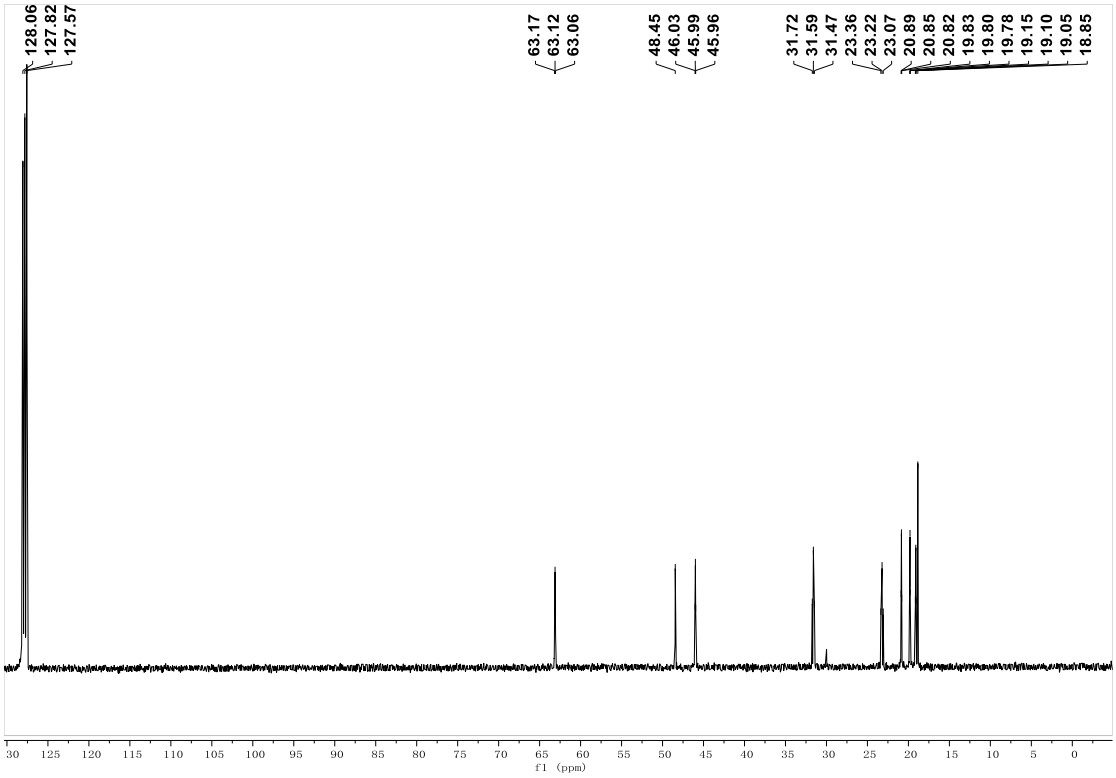


Figure S11 $^{13}C\{^{1}H\}$ NMR spectrum of complex **4** (C_6D_6)

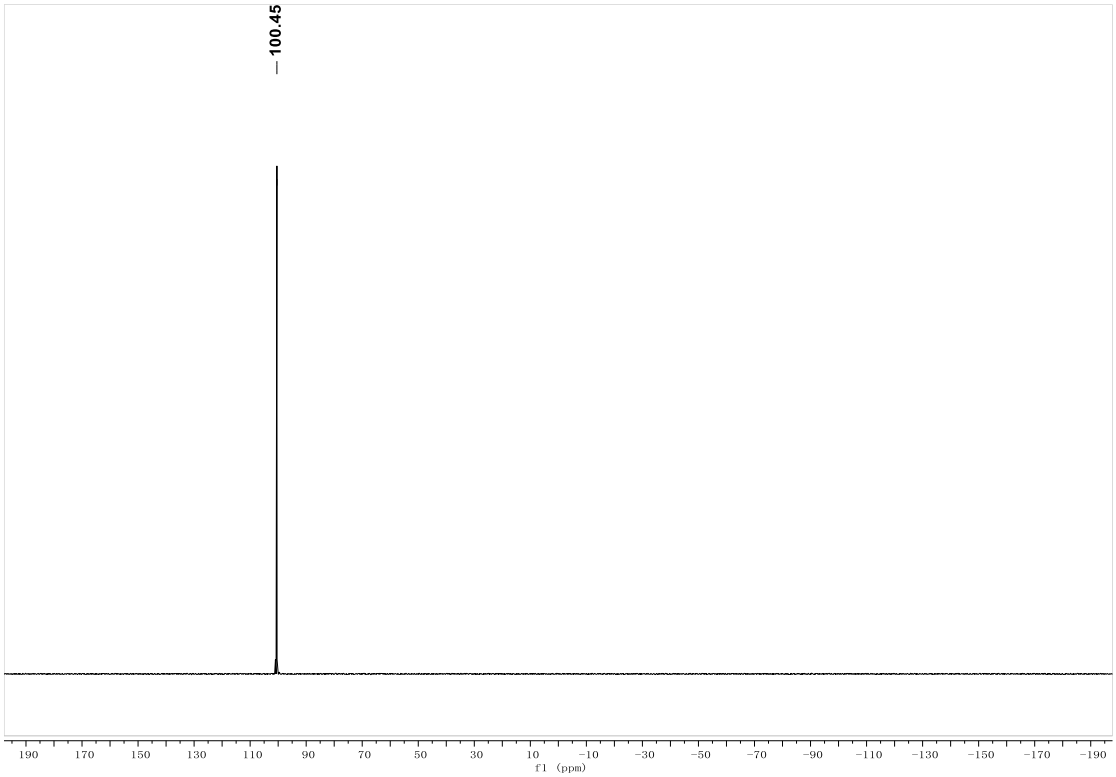


Figure S12 $^{31}P\{^{1}H\}$ NMR spectrum of complex **4** (C_6D_6)

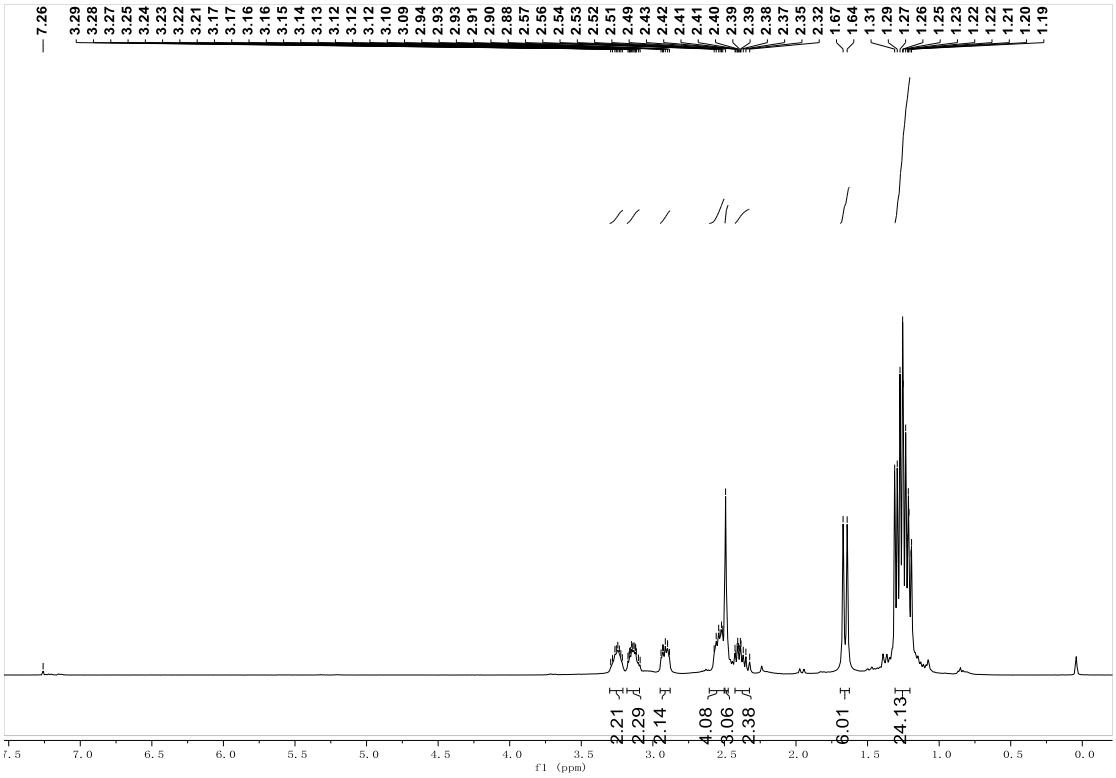


Figure S13 ^{1}H NMR spectrum of complex **5** ($CDCl_3$)

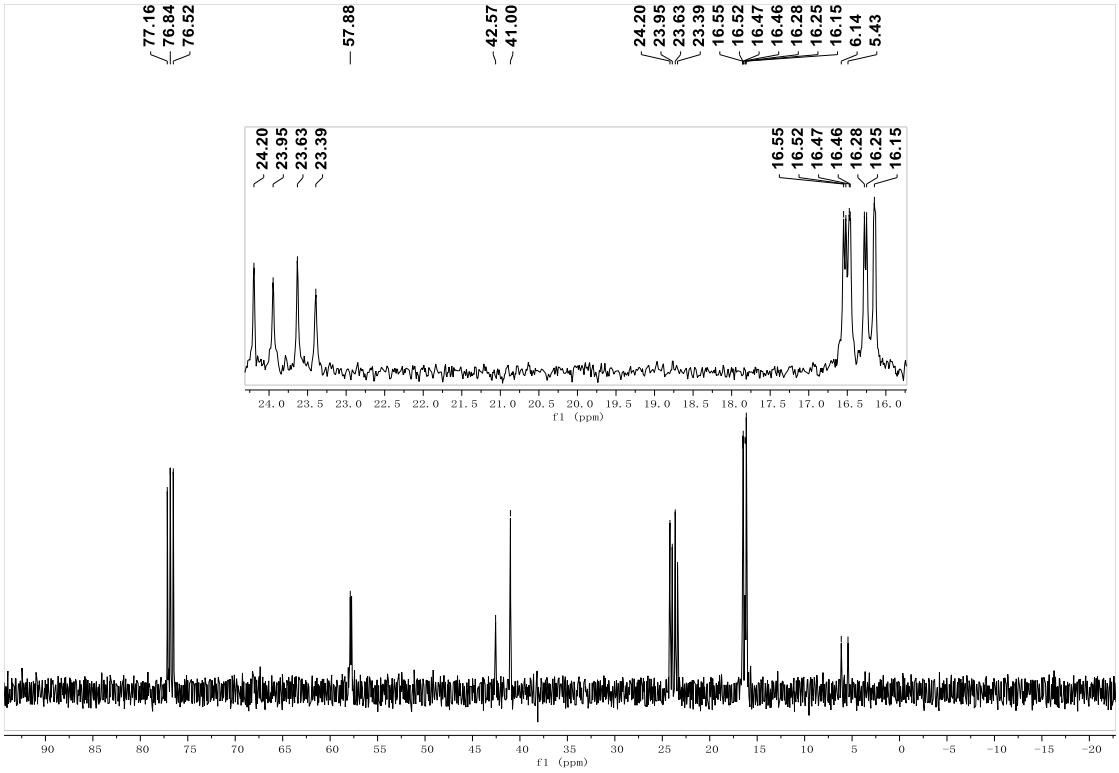


Figure S14 $^{13}C\{^{1}H\}$ NMR spectrum of complex **5** ($CDCl_3$)

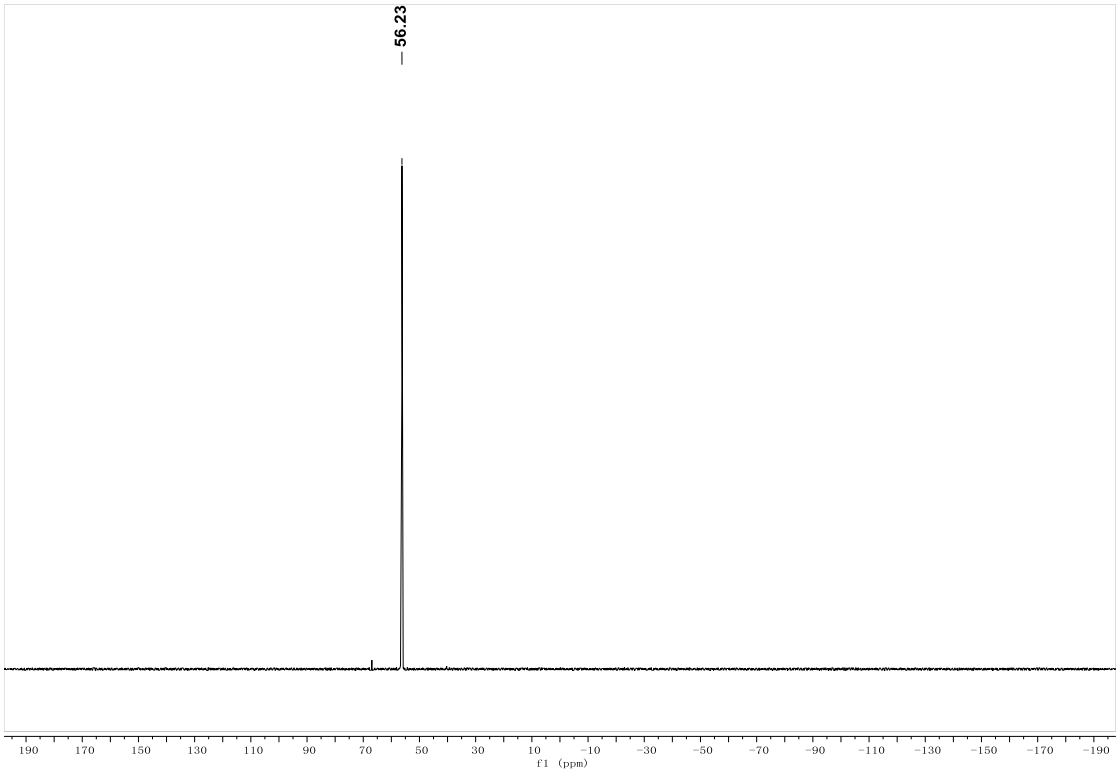


Figure S15 $^{31}P\{^{1}H\}$ NMR spectrum of complex **5** ($CDCl_3$)

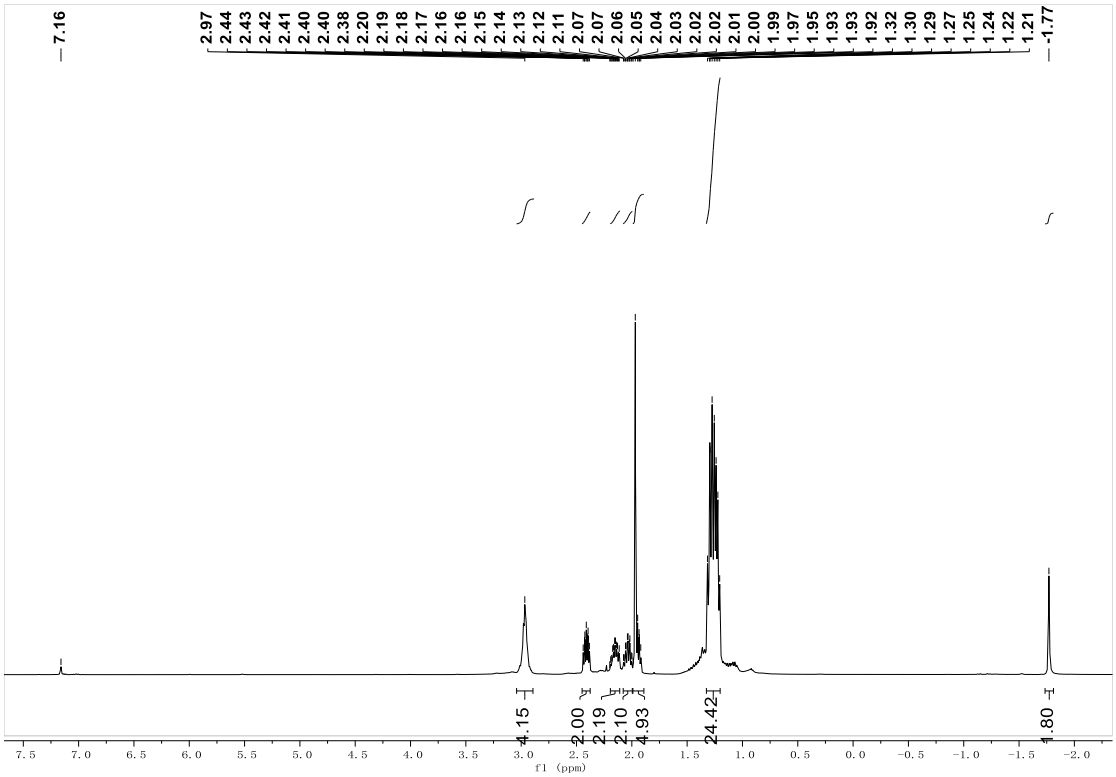


Figure S16 ^{1}H NMR spectrum of complex **6** (C_6D_6)

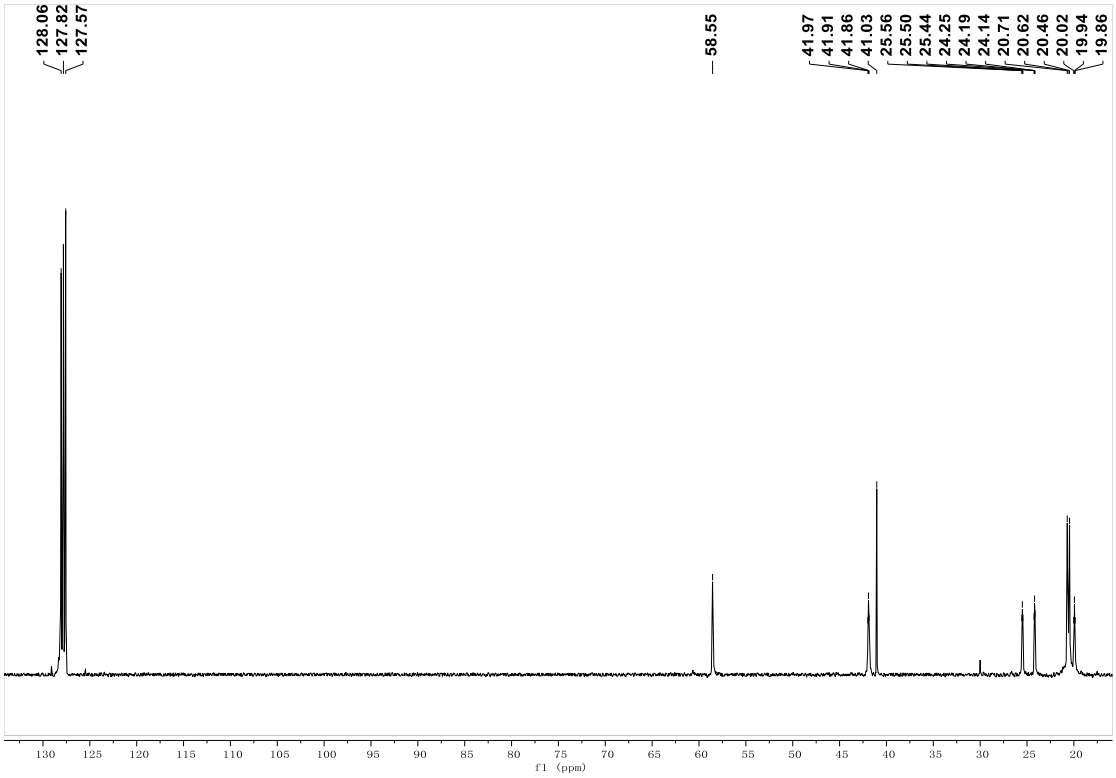


Figure S17 $^{13}C\{^{1}H\}$ NMR spectrum of complex **6** (C_6D_6)

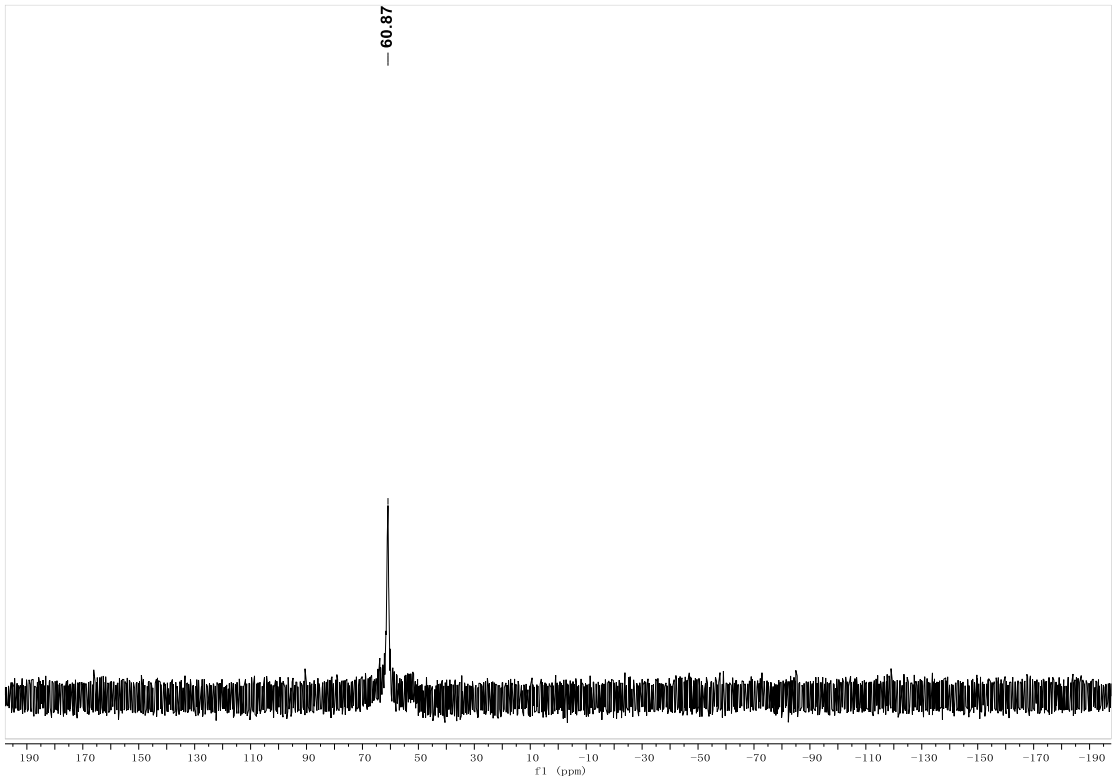


Figure S18 $^{31}P\{^{1}H\}$ NMR spectrum of complex **6** (C_6D_6)

2. **Crystal data and structure refinement**

Table S1. Crystal data and structure refinements for **1** and **2.**

	Compound **1**	Compound **2**
Empirical formula	$C_{47}H_{106}Cl_2Li_2Mg_2N_6O_2P_4$	$C_{37}H_{85}Cu_2I_2Mg_2N_6P_4$
Formula weight	1044.65	1167.48
Temperature [K]	190.0	193.00
Crystal system	triclinic	orthorhombic
Space group	*P*-1	*F*dd2
a/Å	11.7919(8)	23.6804(7)
b/Å	12.9748(9)	63.6047(17)
c/Å	22.3011(15)	13.9335(4)
α/°	93.839(2)	90
β/°	98.412(2)	90
γ/°	109.612(2)	90
Volume/Å^3	3154.7(4)	20986.4(10)
Z	2	16
ρ_{calc}/g cm^{-3}	1.100	1.478
μ/mm^{-1}	0.261	11.801
F(000)	1140.0	9552.0
Crystal size/mm^3	0.2 × 0.18 × 0.16	0.2 × 0.18 × 0.16
Radiation	MoKα (λ = 0.71073)	GaKα (λ = 1.34139)
2Θ range for data collection/°	3.856 to 49.998	4.834 to 107.984
Index ranges	-14 ≤ h ≤ 14, -15 ≤ k ≤ 12, -26 ≤ l ≤ 26	-28 ≤ h ≤ 28, 76 ≤ k ≤ 73, -16 ≤ l ≤ 16
Reflections collected	24096	65160
Independent reflections	11061 [Rint = 0.0898]	9212 [Rint = 0.0386]
Data/restraints/parameters	11061/200/654	9212/83/526
Goodness−of−fit on F^2	1.008	1.045
Final *R* indexes [*I*>=2σ (*I*)]	R1 = 0.0720, wR2 = 0.1631	R1 = 0.0191, wR2 = 0.0437
Final R indexes [all data]	R1 = 0.1368, wR2 = 0.1924	R1 = 0.0207, wR2 = 0.0441
Largest diff. peak/hole / e Å^{-3}	0.61/-0.36	0.40/-0.48

Table S2. Crystal data and structure refinements for **3** and **4**.

	Compound **3**	Compound **4**
Empirical formula	$C_{34}H_{78}Ag_2I_2Mg_2N_6P_4$	$C_{34}H_{77}Au_2Cl_2Mg_2N_6P_4$
Formula weight	606.53	1207.34
Temperature [K]	190.00	190.00
Crystal system	monoclinic	triclinic
Space group	*C*2/c	*P*-1
a/Å	23.870(3)	12.441(18)
b/Å	14.5992(17)	13.95(3)
c/Å	14.7309(16)	16.13(3)
α/°	90	78.19(5)
β/°	94.704(4)	87.56(4)
γ/°	90	65.18(7)
Volume/Å^3	5116.2(10)	2483(8)
Z	8	2
ρ_{calc}/g cm^{-3}	1.575	1.615
μ/mm^{-1}	2.151	6.193
F(000)	2432.0	1198.0
Crystal size/mm^3	0.22 × 0.2 × 0.18	0.2 × 0.18 × 0.18
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.58 to 55.016	3.724 to 54.982
Index ranges	-30 ≤ h ≤ 30, -18 ≤ k ≤ 16, -19 ≤ l ≤ 18	-16 ≤ h ≤ 13, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	24208	23756
Independent reflections	5869 [Rint = 0.0570]	11309 [Rint = 0.0720]
Data/restraints/parameters	5869/283/316	11309/81/502
Goodness−of−fit on F^2	1.011	1.017
Final *R* indexes [*I*>=2σ (*I*)]	R1 = 0.0398, wR2 = 0.0741	R1 = 0.0557, wR2 = 0.1116
Final R indexes [all data]	R1 = 0.0782, wR2 = 0.0868	R1 = 0.1067, wR2 = 0.1324
Largest diff. peak/hole / e Å^{-3}	0.75/-0.70	1.41/-1.55

Table S3. Crystal data and structures refinements for **5** and **6**.

	Compound **5**	Compound **6**
Empirical formula	$C_{19}H_{45}I_2MgN_3P_2$	$C_{34}H_{82}Mg_2N_8Na_2P_4$
Formula weight	655.63	821.55
Temperature [K]	296.15	193.00
Crystal system	monoclinic	monoclinic
Space group	*I*a	*P*21/n
a/Å	13.868(3)	12.9772(6)
b/Å	15.384(5)	15.3074(7)
c/Å	14.660(9)	13.8680(6)
α/°	90	90
β/°	110.85(3)	114.657(3)
γ/°	90	90
Volume/Å^3	2923(2)	2503.7(2)
Z	4	2
ρ_{calc}/g cm^{-3}	1.490	1.090
μ/mm^{-1}	2.292	1.321
F(000)	1312.0	896.0
Crystal size/mm^3	0.2 × 0.18 × 0.16	0.2 × 0.18 × 0.16
Radiation	MoKα (λ = 0.71073)	GaKα (λ = 1.34139)
2Θ range for data collection/°	3.98 to 49.992	6.822 to 107.922
Index ranges	-16 ≤ h ≤ 14, -18 ≤ k ≤ 18, -17 ≤ l ≤ 17	-15 ≤ h ≤ 15, -18 ≤ k ≤ 13, -16 ≤ l ≤ 16
Reflections collected	11066	18150
Independent reflections	4085 [Rint = 0.0930]	4588 [Rint = 0.0775]
Data/restraints/parameters	4085/484/364	4588/0/243
Goodness−of−fit on F^2	0.943	1.032
Final *R* indexes [*I*>=2σ (*I*)]	R1 = 0.0545, wR2 = 0.0682	R1 = 0.0551, wR2 = 0.1273
Final R indexes [all data]	R1 = 0.1411, wR2 = 0.0809	R1 = 0.1243, wR2 = 0.1548
Largest diff. peak/hole / e Å^{-3}	0.40/-0.33	0.25/-0.47

3. **Molecular Structure, Bond Lengths and Angles**

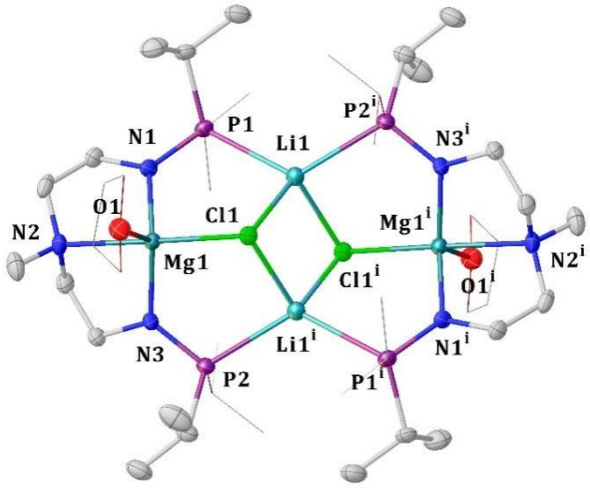


Figure S19 Molecular structure of **1** from X-ray diffraction. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 30% probability level.

Table S4 Selected Bond Lengths [Å] and Angles [°] for **1**

Bond lengths			
Mg1-N1	2.028(3)	Mg1-Cl1	2.4919(15)
Mg1-N2	2.271(3)	Li1-Cl1	2.380(6)
Mg1-N3	2.026(4)	Li1-P1	2.609(7)
Mg1-O1	2.123(3)		
Angles			
O1-Mg1-N2	85.59(13)	N1-Mg1-N2	80.83(12)
O1-Mg1-Cl1	85.40(9)	N2-Mg1-Cl^{i}	170.98(11)
N3-Mg1-Cl1	103.14(10)	Cl1-Li1-$Cl1^{i}$	96.5(3)
N3-Mg1-O1	117.54(13)	Cl1-Li1-$P2^{i}$	119.0(2)
N3-Mg1-N1	125.58(14)	$Cl1^{i}$-Li1-$P2^{i}$	96.8(2)
N3-Mg1-N2	80.89(14)	Cl1-Li1-P1	97.7(2)
N1-Mg1-Cl1	102.75(10)	$Cl1^{i}$-Li1-P1	120.4(3)
N1-Mg1-O1	111.53(15)	$P2^{i}$-Li1-P1	124.3(3)

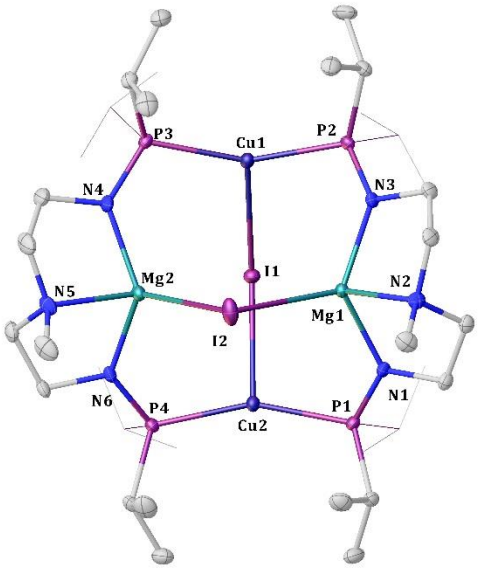


Figure S20 Molecular structure of **2** from X-ray diffraction. Hydrogen atoms and solvent are omitted for clarity. Thermal ellipsoids are drawn at the 30% probability level.

Table S5 Selected Bond Lengths [Å] and Angles [°] for **2**

Bond lengths			
Mg1-N1	2.044(3)	Mg1-I2	2.8348(12)
Mg1-N2	2.205(3)	Mg2-I2	2.8475(12)
Mg1-N3	2.048(3)	Cu1-P2	2.2256(10)
Mg2-N4	2.037(4)	Cu1-P3	2.2271(10)
Mg2-N5	2.215(3)	Cu2-P1	2.2199(10)
Mg2-N6	2.036(3)	Cu2-P4	2.2224(10)
Mg1-I1	3.2074(11)	Cu1-I1	2.7543(6)
Mg2-I1	3.1443(12)	Cu2-I1	2.7822(6)
Angles			
Cu1-I1-Mg1	76.41(2)	N1-Mg1-N3	131.08(13)
Cu1-I1-Mg2	78.89(3)	N1-Mg1-I2	114.00(10)
Cu2-I1-Cu1	144.471(18)	N1-Mg1-N2	80.29(12)
Cu2-I1-Mg2	77.60(3)	N2-Mg1-I2	104.61(9)
Cu2-I1-Mg1	76.38(2)	N3-Mg1-I2	114.41(10)

Mg2-I1-Mg1	87.68(3)	N6-Mg2-I2	112.71(10)
Mg2-I2-Mg1	101.48(3)	N3-Mg1-N2	81.41(12)
P2-Cu1-I1	101.51(3)	N4-Mg2-I2	112.81(10)
P3-Cu1-I1	104.28(3)	N4-Mg2-N5	80.81(13)
P2-Cu1-P3	153.43(4)	N5-Mg2-I2	104.85(10)
P1-Cu2-I1	102.84(3)	N6-Mg2-I1	93.97(9)
P1-Cu2-P4	156.69(5)	N6-Mg2-N4	133.75(13)
P4-Cu2-I1	100.44(3)	N6-Mg2-N5	80.26(12)

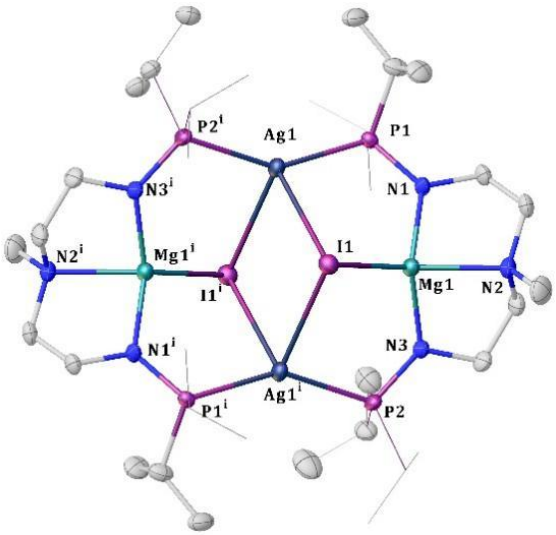


Figure S21 Molecular structure of **3** from X-ray diffraction. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 30% probability level.

Table S6 Selected Bond Lengths [Å] and Angles [°] for **3**

Bond lengths			
Mg1-N1	2.000(4)	$Ag1^{i}$-I1	3.1413(5)
Mg1-N2	2.203(4)	Ag1-$I1^{i}$	3.1412(5)
Mg1-N3	2.002(4)	Ag1-P1	2.4271(12)
Mg1-I1-	2.7152(15)	Ag1-$P2^{i}$	2.4320(13)

Ag1-I1	3.2203(5)		
Angles			
$Ag1^{i}$-I1-Ag1	93.920(14)	$P2^{i}$-Ag1-$I1^{i}$	97.07(4)
Mg1-I1-Ag1	79.20(3)	N1-Mg1-I1	109.18(11)
Mg1-I1-$Ag1^{i}$	81.13(3)	N1-Mg1-N2	82.53(15)
$I1^{i}$-Ag1-I1	86.081(14)	N1-Mg1-N3	135.25(16)
P1-Ag1-$I1^{i}$	106.93(3)	N2-Mg1-I1	134.22(12)
P1-Ag1-I1	97.05(3)	N3-Mg1-I1	111.18(12)
P1-Ag1-$P2^{i}$	148.29(4)	N3-Mg1-N2	83.06(16)
$P2^{i}$-Ag1-I1	105.12(3)		

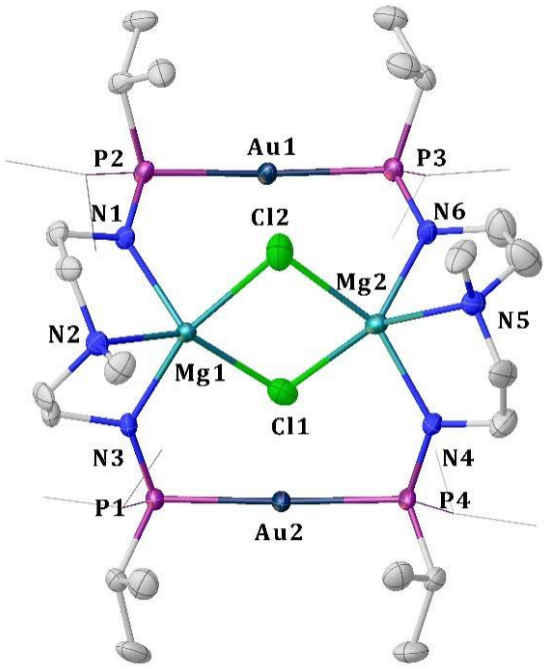


Figure S22 Molecular structure of **4** from X-ray diffraction. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 30% probability level.

Table S7 Selected Bond Lengths [Å] and Angles [°] for **4**

Bond lengths			
Mg1-N1	2.082(8)	Mg2-N6	2.107(8)
Mg1-N2	2.385(8)	Mg2-Cl1	2.43(2)

Mg1-N3	2.072(8)	Mg2-Cl2	2.44(2)
Mg1-Cl1	2.49(2)	Mg2-Cl1A	2.440(6)
Mg1-Cl2	2.42(2)	Mg2-Cl2A	2.424(5)
Mg1-Cl1A	2.487(5)	Au1-P2	2.300(4)
Mg1-Cl2A	2.412(6)	Au1-P3	2.310(4)
Mg2-N4	2.097(8)	Au2-P1	2.307(4)
Mg2-N5	2.339(9)	Au2-P4	2.313(4)
Angles			
P1-Au2-P4	174.33(9)	N4-Mg2-N6	117.4(3)
P2-Au1-P3	171.06(10)	N4-Mg2-N5	78.9(3)
N3-Mg1-Cl1A	96.6(2)	N4-Mg2-Cl2	148(2)
N3-Mg1-Cl2A	129.0(3)	N4-Mg2-Cl1A	103.7(3)
Cl2-Mg1-Cl1	87.8(8)	N4-Mg2-Cl2A	113.0(3)
Cl2A-Mg1-Cl1A	88.3(2)	N5-Mg2-Cl1	158.4(19)
Cl1-Mg2-Cl2	88.6(9)	N5-Mg2-Cl2	101.0(12)
N6-Mg2-Cl1	120.8(19)	N5-Mg2-Cl1A	175.0(3)
N6-Mg2-N5	78.2(4)	N5-Mg2-Cl2A	93.6(3)
N6-Mg2-Cl2	93.6(18)	Cl2A-Mg2-Cl1A	89.1(2)
N6-Mg2-Cl1A	96.8(3)	Mg2-Cl1A-Mg1	90.2(2)
N6-Mg2-Cl2A	125.9(3)	Mg2-Cl1-Mg1	90.3(7)
N4-Mg2-Cl1	82.7(13)	Mg1-Cl2A-Mg2	92.3(2)

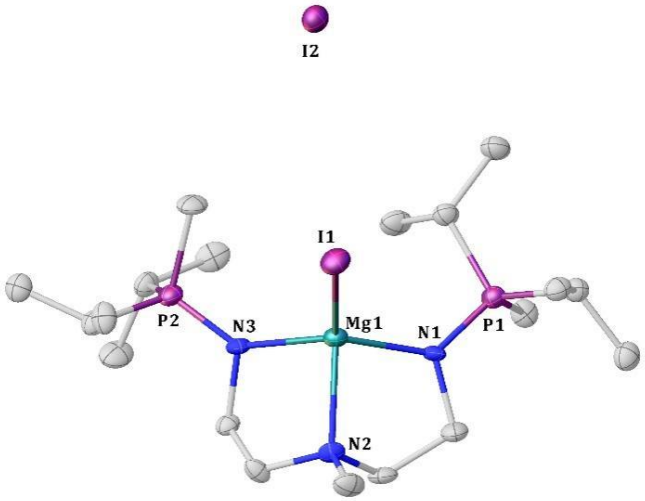


Figure S23 Molecular structure of **5** from X-ray diffraction. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 30% probability level.

Table S8 Selected Bond Lengths [Å] and Angles [°] for **5**

Bond lengths			
Mg1-I1	2.706(5)	N1-P1	1.596(15)
Mg1-N1	2.009(13)	N1-P1A	1.60(2)
Mg1-N2	2.112(12)	N3-P2	1.586(12)
Mg1-N3	2.025(12)		
Angles			
N1-Mg1-I1	115.5(4)	N2-Mg1-I1	117.0(4)
N1-Mg1-N2	85.0(5)	N3-Mg1-I1	116.1(4)
N1-Mg1-N3	126.0(5)	N3-Mg1-N2	85.4(5)

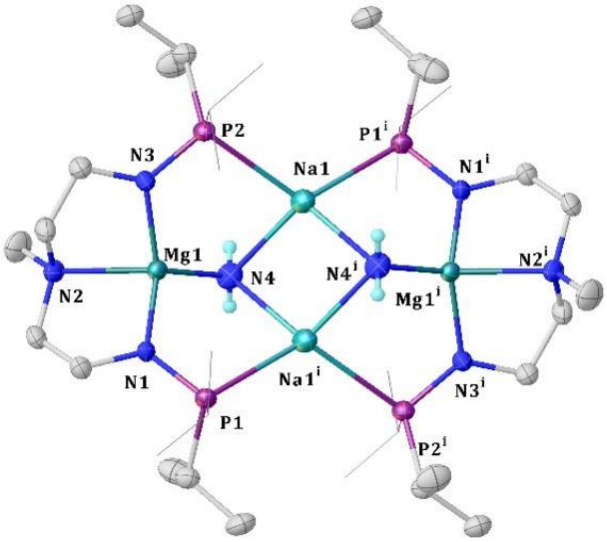
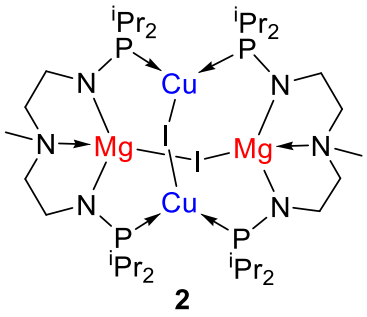


Figure S24 Molecular structure of **6** from X-ray diffraction. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 30% probability level.

Table S9 Selected Bond Lengths [Å] and Angles [°] for **6**

Bond lengths			
Mg1-N1	2.015(3)	Na1-N4	2.391(4)
Mg1-N2	2.189(3)	P1-Na1^{i}	2.8360(17)
Mg1-N3	2.006(3)	P2-Na1	2.8482(18)
Mg1-N4	2.018(4)	Na1-P1^{i}	2.8359(17)
Na1-N4^{i}	2.418(4)		
Angles			
N1-Mg1-N2	82.05(11)	P2-Na1-Mg1^{i}	154.12(7)
N1-Mg1-N4	111.08(15)	N4-Na1-P1^{i}	124.88(11)
N3-Mg1-N1	129.26(13)	N4^{i}-Na1-P1^{i}	90.77(10)
N3-Mg1-N2	82.84(12)	N4-Na1-P2	91.89(10)
N3-Mg1-N4	111.00(16)	N4^{i}-Na1-P2	124.25(11)
N4-Mg1-N2	140.94(14)	Mg1-N4-Na1^{i}	102.50(15)
P1^{i}-Na1-P2	122.86(6)	Mg1-N4-Na1	102.13(16)
P1^{i}-Na1-Mg1^{i}	60.22(4)	Na1-N4-Na1^{i}	76.27(12)

4. Cartesian Coordinates



2

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P	3.12798500	2.30465900	-0.41018500
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C	-3.47514300	-3.19283500	-2.09686200
H	-4.17403300	-4.01283600	-1.87727300
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C	3.79050100	-2.15549900	-3.29004300	H	3.08863500	1.48824800	-3.36604300
H	3.93034700	-2.68164900	-4.24405600	H	4.76886500	1.78288400	-2.90119300
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C	3.34327000	-3.13711100	-2.19391000	H	2.12431700	4.37583200	-3.48570600
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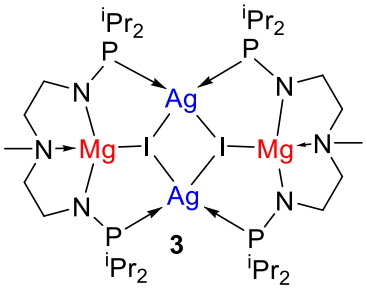

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N	-3.83504500	-0.87848600	0.16402300
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H	-2.30177600	4.83558000	2.58629900
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H	-0.26718500	-3.21934900	-3.09638100	C	2.36710000	3.55961500	-3.09746800
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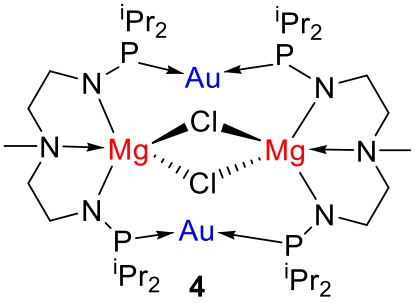

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Mg	0.00328700	1.88241100	0.88069300
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Cl	0.00006600	0.00026800	-0.84405900
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H	4.73567200	3.96535200	0.76888000
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H	-0.82529100	4.83486700	0.07039500
C	4.75109900	2.25028000	2.06871200
H	4.80349900	1.15658700	2.00975200
H	3.84630700	2.50338800	2.62845600
H	5.62025400	2.60036700	2.64061000
C	4.65404100	-3.07356000	0.31406000
H	4.54672900	-4.16553000	0.36068000
C	-3.37794600	-3.21533200	-1.95953100
H	-4.25427000	-2.72478100	-2.40612800
C	1.20316900	4.23979400	2.50740400
H	1.89141600	3.67266300	3.14143200
H	1.14179500	5.26548200	2.91382300
C	2.15714600	2.89963600	-2.83368100
H	1.25052300	3.34152000	-2.40649600
H	1.98474400	1.82192200	-2.92147700
H	2.29315200	3.31116800	-3.84224700
C	-3.18292100	3.07541400	-2.27940100
H	-4.09568500	2.62232200	-2.69103500
C	3.18302900	-3.07472300	-2.27972700
H	4.09672500	-2.62253800	-2.69026900
C	-0.33824700	3.08286200	3.96344600
H	-1.27764200	2.52711900	4.00567900
H	-0.37908800	3.91248600	4.68995500

H	0.46430800	2.39910000	4.24675700	H	6.11195900	3.01642200	-1.06170500
C	5.91801200	-2.74446800	-0.49576800	H	6.03695500	1.40710400	-0.32259900
H	5.93386100	-3.24076500	-1.47117100	C	-3.30302900	4.60477000	-2.36978700
H	6.81168700	-3.06898200	0.05296900	H	-4.16729600	4.99585500	-1.82146200
H	6.00646900	-1.66372600	-0.66418600	H	-3.41395700	4.91170300	-3.41822700
C	-4.75236300	-2.87210600	0.66359900	H	-2.40450100	5.09605600	-1.98074300
H	-4.73733700	-3.96485500	0.76741600	C	-1.98525500	2.56763600	-3.09428000
C	-6.02056500	-2.48167400	-0.11201900	H	-1.04393200	2.94810200	-2.68456900
H	-6.91230500	-2.71742300	0.48317800	H	-2.06455600	2.90448900	-4.13620700
H	-6.11124400	-3.01434400	-1.06414700	H	-1.92278000	1.47485600	-3.08873800
H	-6.03622500	-1.40545400	-0.32412400	C	1.98672400	-2.56484200	-3.09529800
C	-5.91866600	2.74077500	-0.49688400	H	2.06618600	-2.90160500	-4.13724200
H	-5.93462500	3.23680100	-1.47243000	H	1.92608700	-1.47196200	-3.08958700
H	-6.81296200	3.06442000	0.05135100	H	1.04447900	-2.94379200	-2.68631700
H	-6.00579300	1.65989500	-0.66507700	C	-3.63511900	-4.72881700	-1.89241700
C	-4.77068600	2.53342200	1.74739700	H	-2.78380700	-5.25697200	-1.44889600
H	-4.93854800	1.44978400	1.74282700	H	-3.77717500	-5.13150100	-2.90408100
H	-5.61627700	3.00443300	2.26527500	H	-4.52945300	-4.98105900	-1.31219400
H	-3.86334300	2.72124800	2.32832300	C	3.63625600	4.72761800	-1.89401400
C	-4.65546400	3.07155700	0.31345300	H	3.78034100	5.12920400	-2.90582400
H	-4.54965100	4.16366100	0.35997000	H	4.52928500	4.98075300	-1.31217400
C	4.76934700	-2.53536300	1.74796900	H	2.78387100	5.25605800	-1.45289500
H	4.93899900	-1.45199700	1.74329000	C	-4.75263400	-2.25017100	2.06776300
H	5.61386100	-3.00766100	2.26643200	H	-4.80321900	-1.15637900	2.00909700
H	3.86134800	-2.72160100	2.32839300	H	-3.84896400	-2.50489900	2.62858100
C	6.02063500	2.48321000	-0.10994500	H	-5.62305300	-2.59905700	2.63847000
H	6.91174800	2.71900500	0.48617600	C	-2.15444900	-2.90207000	-2.83206900

H	-1.98120500	-1.82449900	-2.92002400
H	-2.28974800	-3.31381300	-3.84064600
H	-1.24855800	-3.34449500	-2.40387000
C	3.30131000	-4.60417100	-2.37110000
H	2.40183300	-5.09464900	-1.98325200
H	4.16460200	-4.99670600	-1.82226100
H	3.41282100	-4.91046200	-3.41966500
Cl	-0.00053800	0.00043100	2.52664400
C	1.23132600	-4.44904000	2.16886900
H	1.01625700	-5.49818100	2.43528100
H	2.11385400	-4.14388700	2.73810600
C	1.58721800	-4.32987600	0.67762400
H	2.50488100	-4.91934000	0.53208800
H	0.81977300	-4.83158900	0.06763100
C	0.34411700	-3.08181600	3.96301200
H	1.28432500	-2.52719900	4.00222000
H	0.38622000	-3.91135400	4.68955800
H	-0.45672700	-2.39705100	4.24871500
C	-1.20359400	-4.23601300	2.51154300
H	-1.88968200	-3.66566300	3.14506200
H	-1.14392000	-5.26081400	2.92053400
C	-1.79231000	-4.25487700	1.09610400
H	-1.21423500	-4.94796300	0.46377400
H	-2.78991000	-4.70983300	1.18605100
H	-2.11413500	4.13893400	2.74126900