

Supporting Information

Group 11 metal complexes of a dinucleating triazole appended bisphosphine, 1,4-bis(5-(diisopropylphosphaneyl)-1-phenyl-1H-1,2,3- triazol-4-yl)benzene

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NMR spectra of compounds 1a-10	S2-S30
HRMS and FT-IR spectra of compounds 2-10	S3-S32
Crystallographic information for compounds 2-5 , and 7-10	S33-S34
Computational Details	S35-S35

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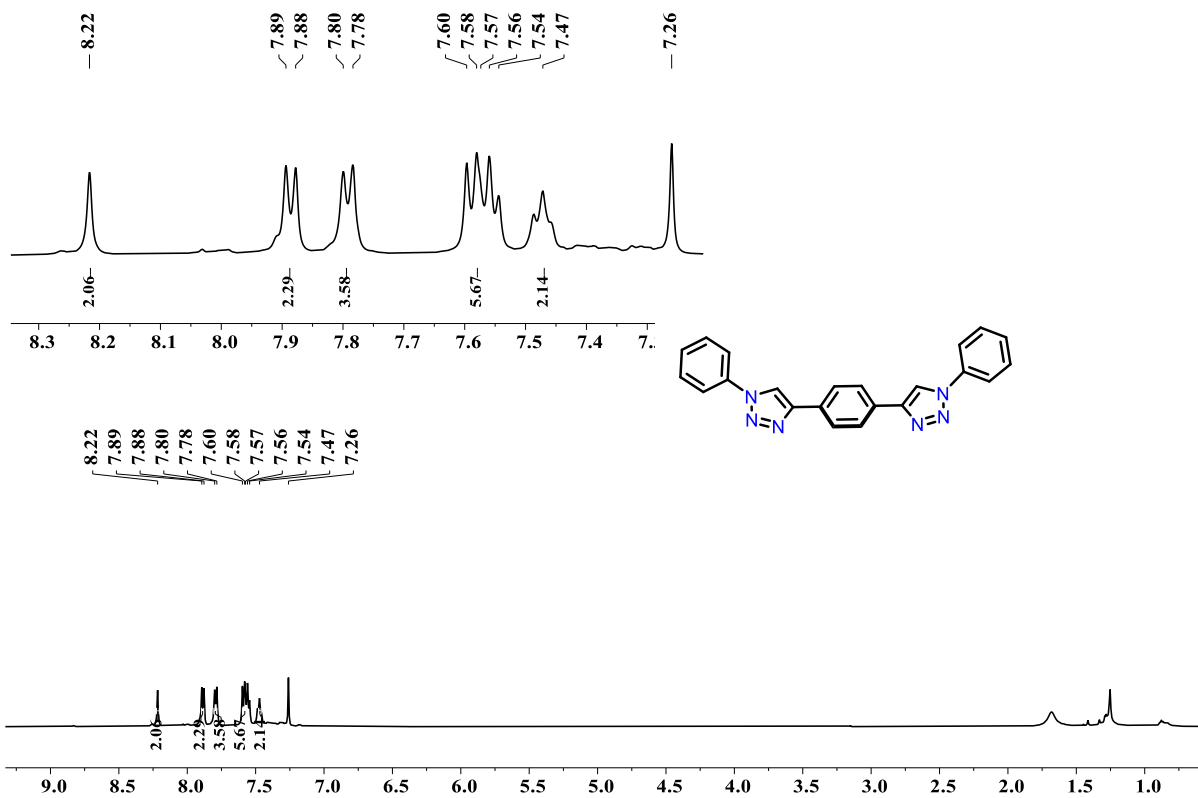


Fig. S1 ¹H NMR spectrum of **1a** in CDCl₃ (400 MHz).

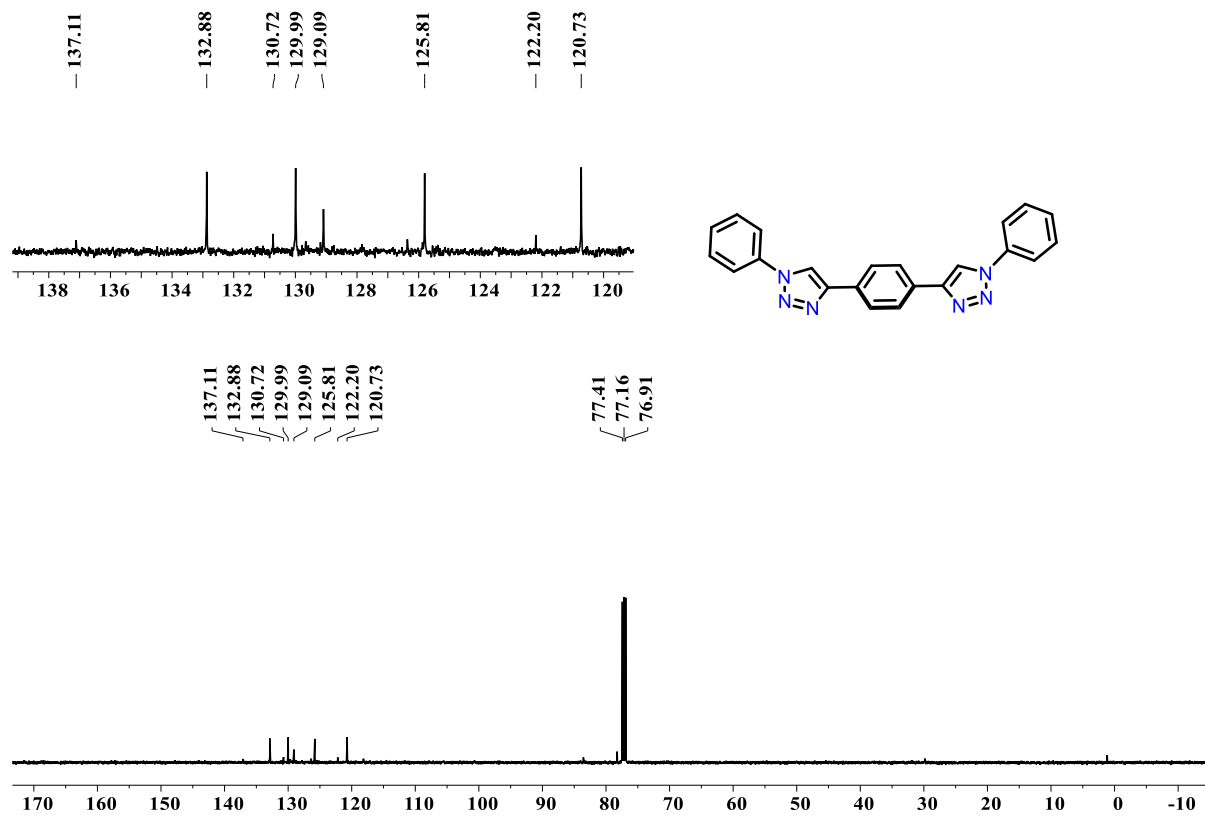


Fig. S2 ¹³C{¹H} NMR spectrum of **1a** in CDCl₃ (400 MHz).

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Analysis Info

Analysis Name D:\Data\SEP 21\MSB-BK-BISTRIAZOLE.d
 Method Low_mass- NAF.m
 Sample Name MSB-BK-BISTRIAZOLE
 Comment C22H16N6

Acquisition Date 9/17/2021 9:18:42 PM
 Operator GKL-OUT
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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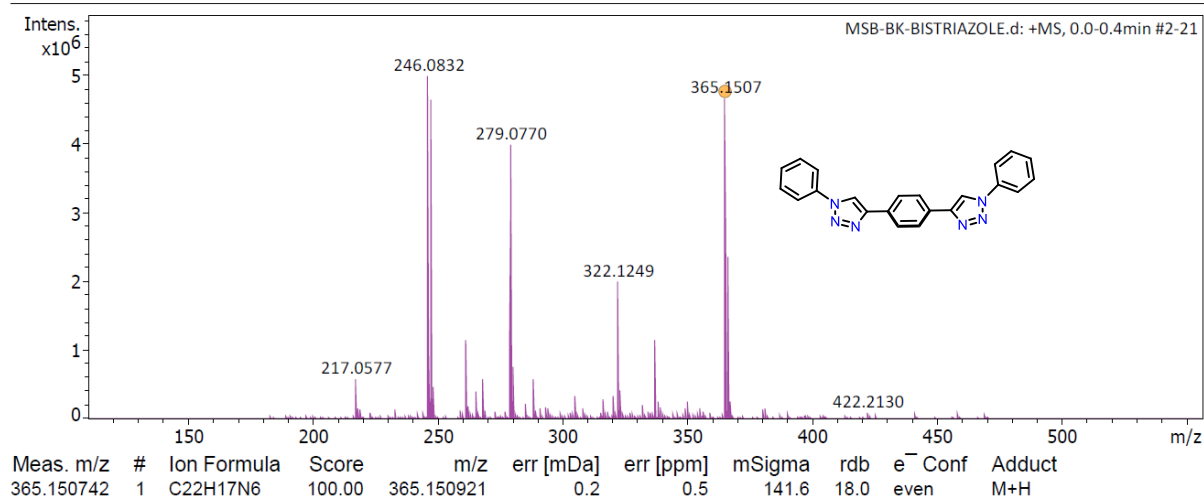


Fig. S3 HRMS spectrum of **1a**.

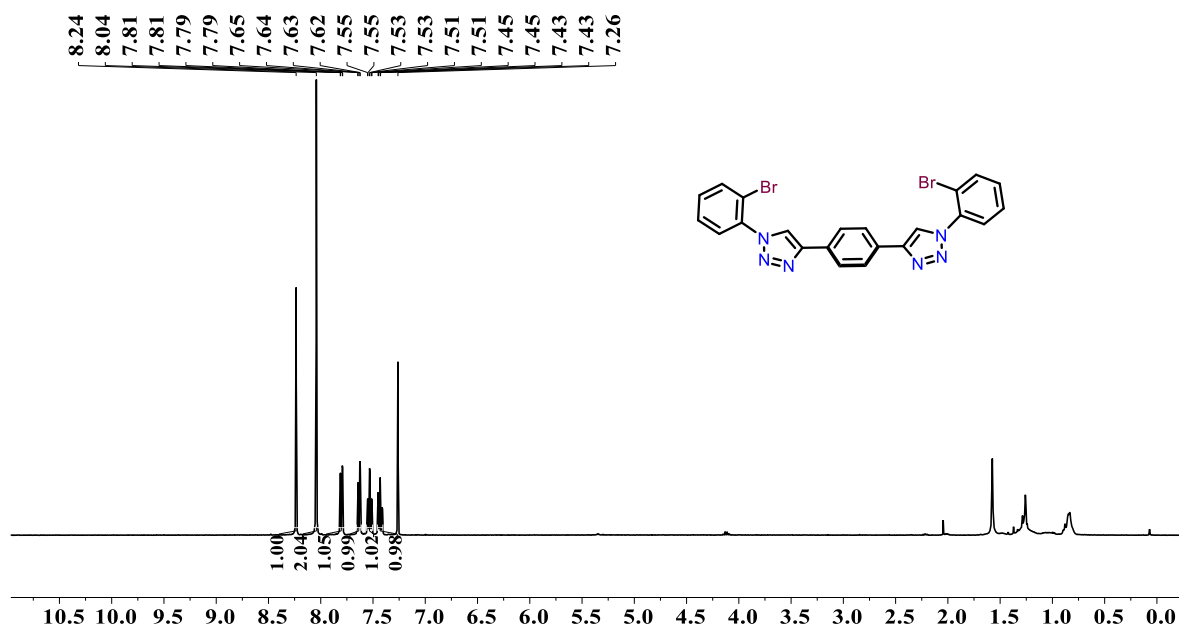


Fig. S4 ¹H NMR spectrum of **1b** in CDCl₃ (400 MHz).

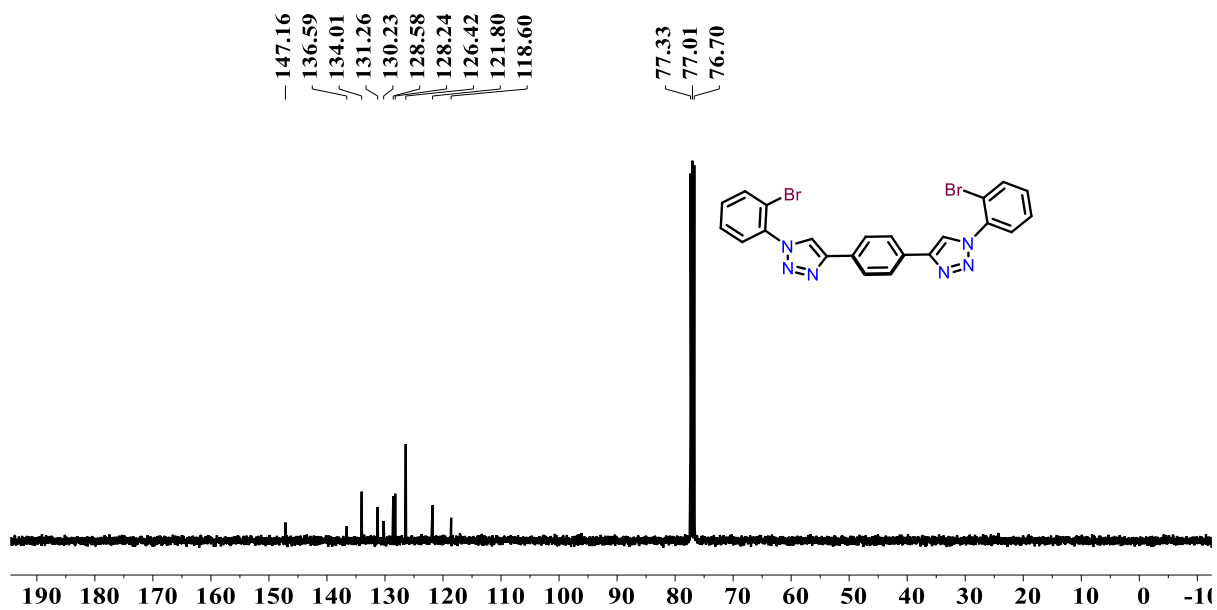


Fig. S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1b** in CDCl_3 (101 MHz).

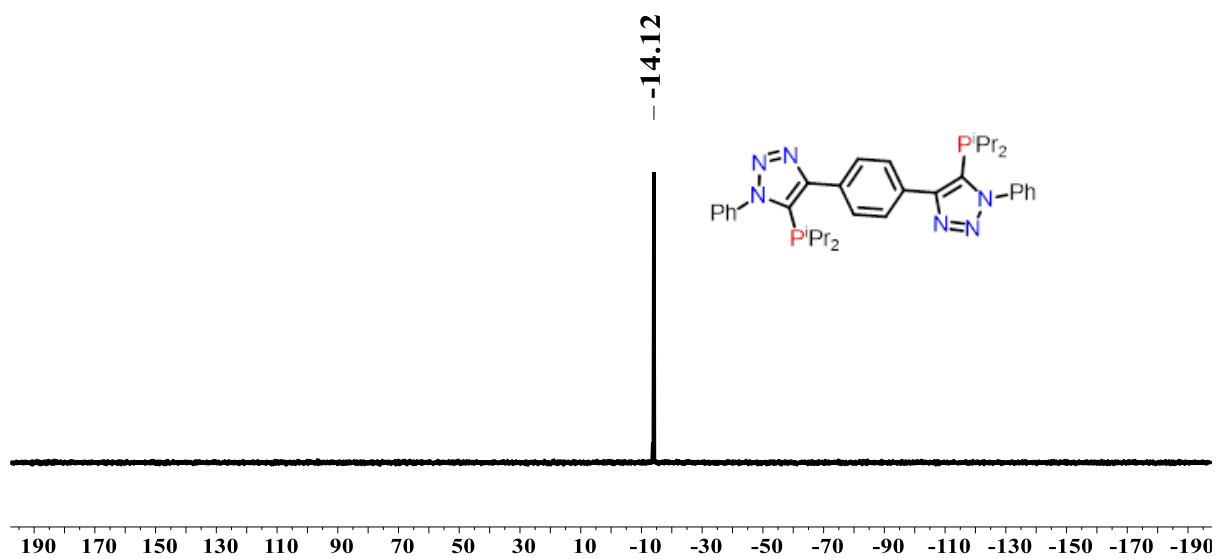


Fig. S6 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2** in CDCl_3 (162 MHz).

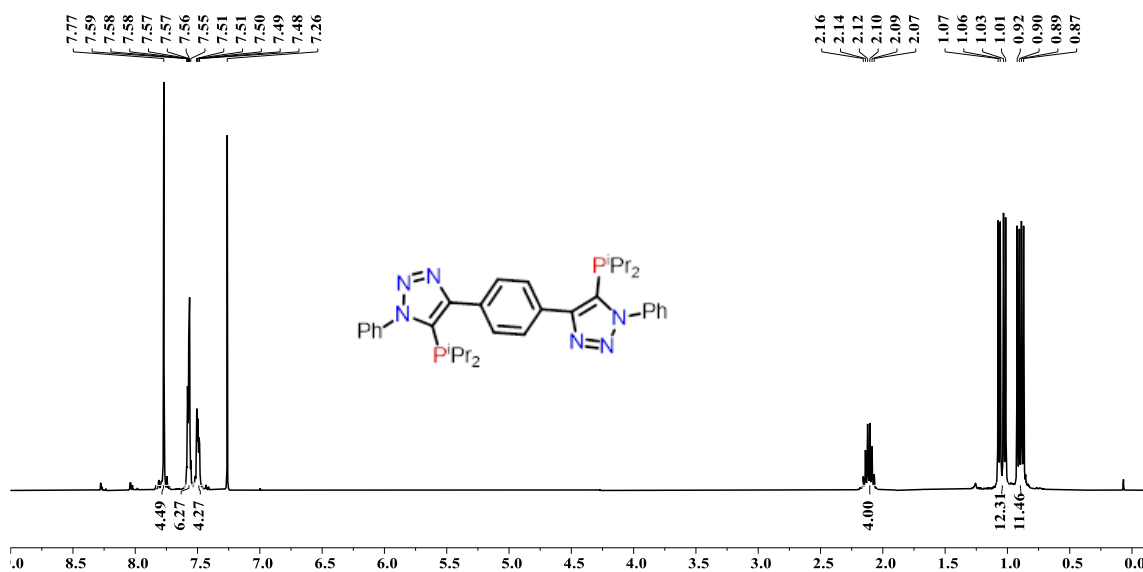


Fig. S7 ^1H NMR spectrum of **2** in CDCl_3 (400 MHz).

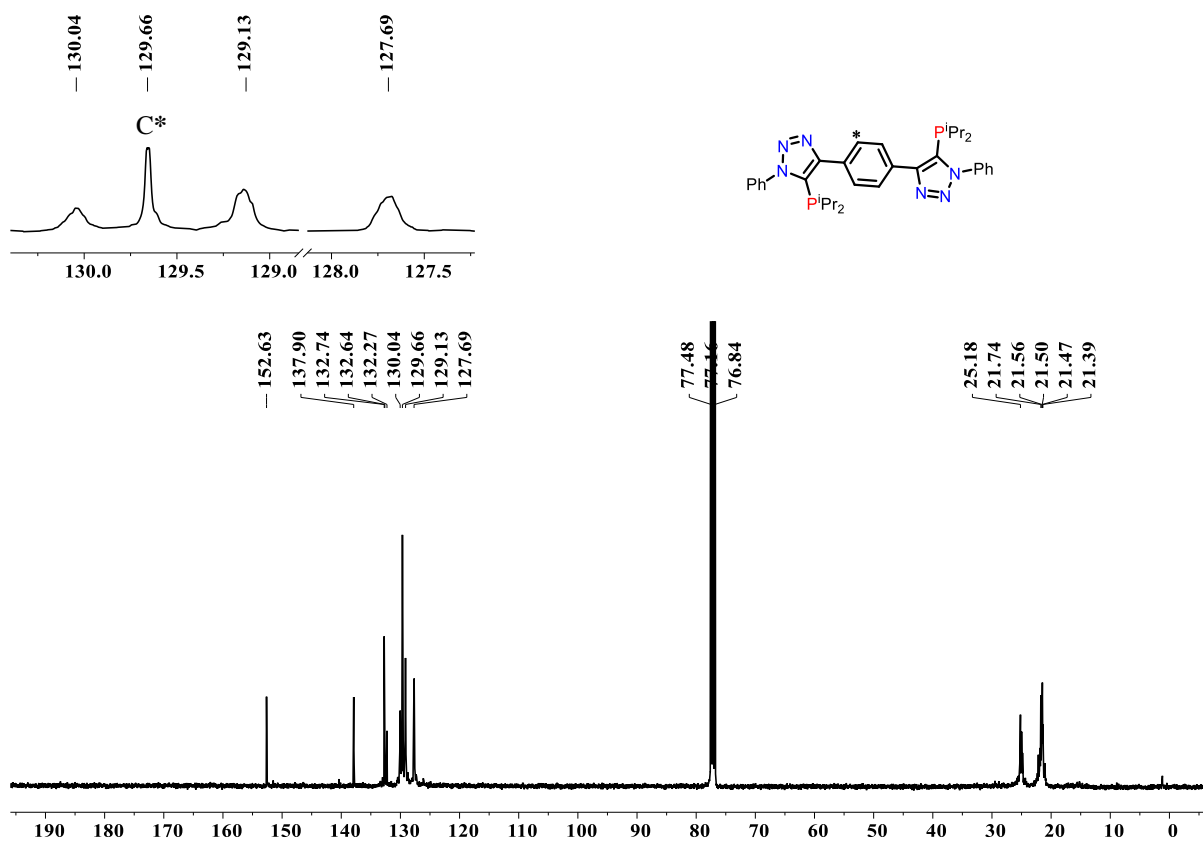


Fig. S8 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in CDCl_3 (101 MHz).

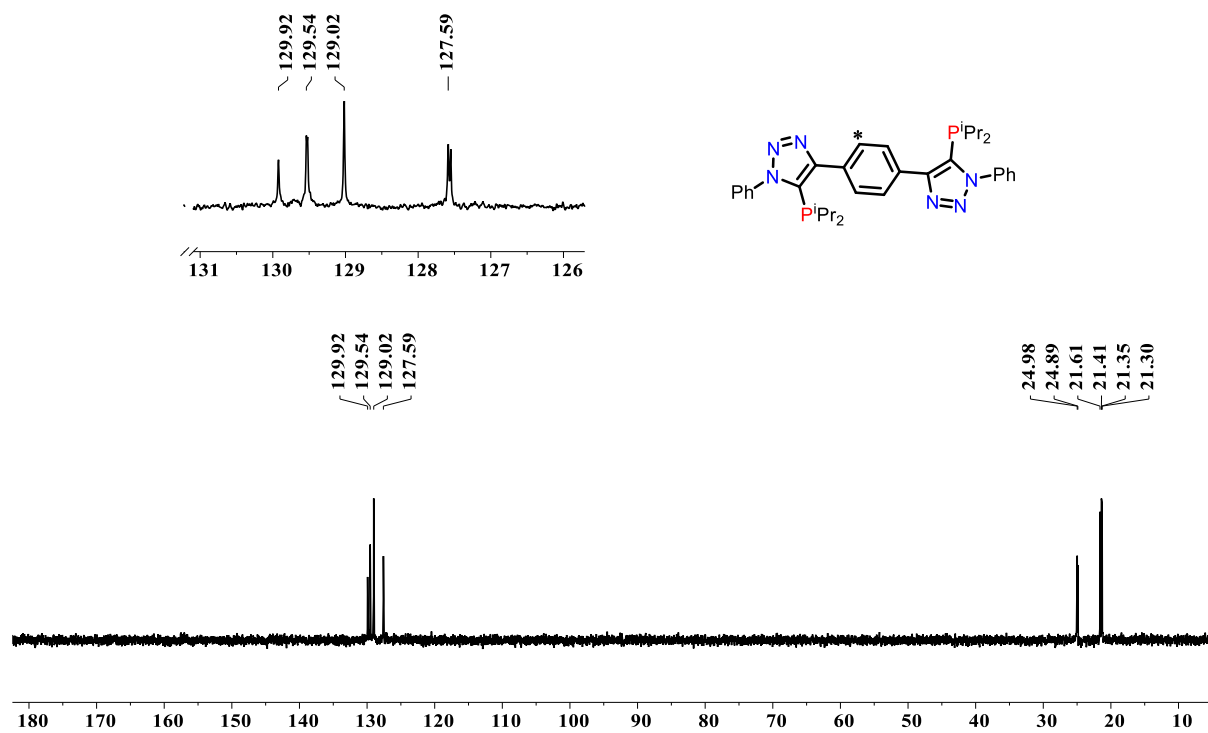


Fig. S9 $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 spectrum of **2** in CDCl_3 (101 MHz).

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Analysis Info

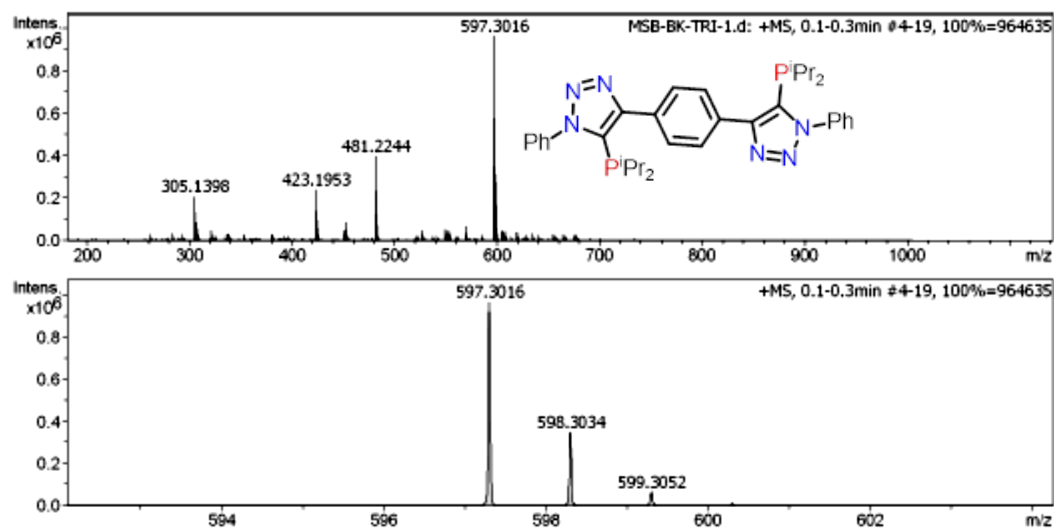
Analysis Name D:\Data\OCT-2018\MSB-BK-TRI-1.d
 Method Tune_pos_NAF-1000.m
 Sample Name MSB-BK-TRI-1
 Comment C34H42N6P2

Acquisition Date 10/3/2018 8:37:18 PM

Operator MSB IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
597.3016	1	C34H43N6P2	597.3019	-0.4	19.3	1	100.00	17.5	even	ok

Fig. S10 HRMS spectrum of 2.

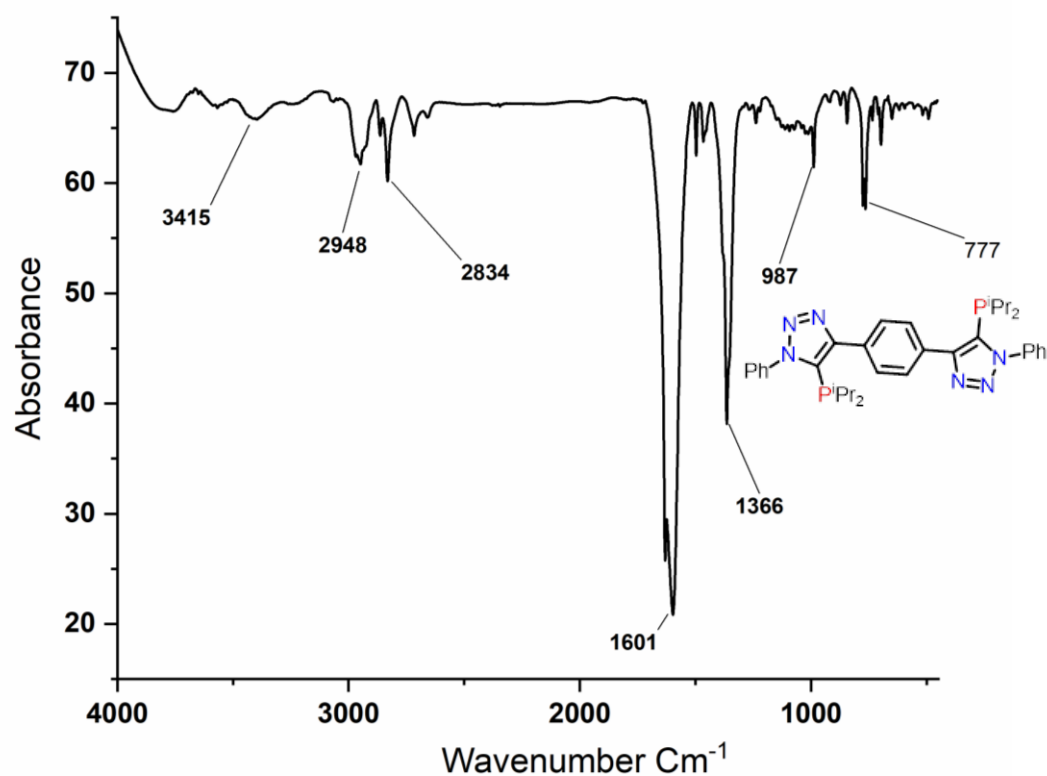


Fig. S11 FT-IR spectrum of ligand **2**.

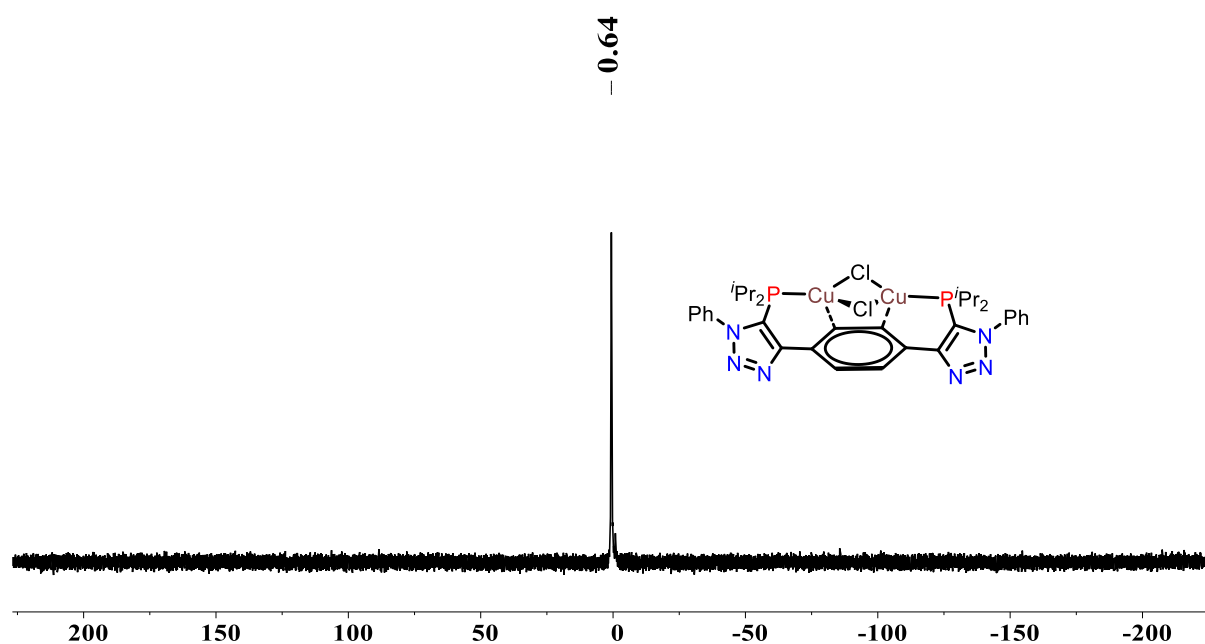


Fig. S12 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **3** in CDCl_3 (162 MHz).

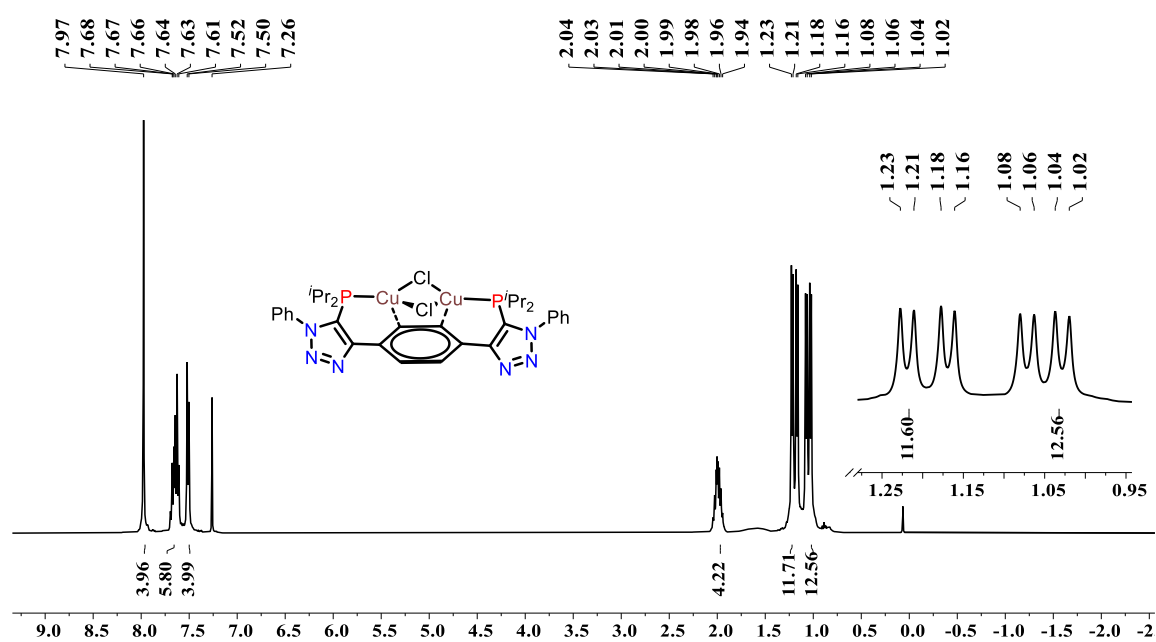


Fig. S13 ^1H NMR spectrum of **3** in CDCl_3 (400 MHz).

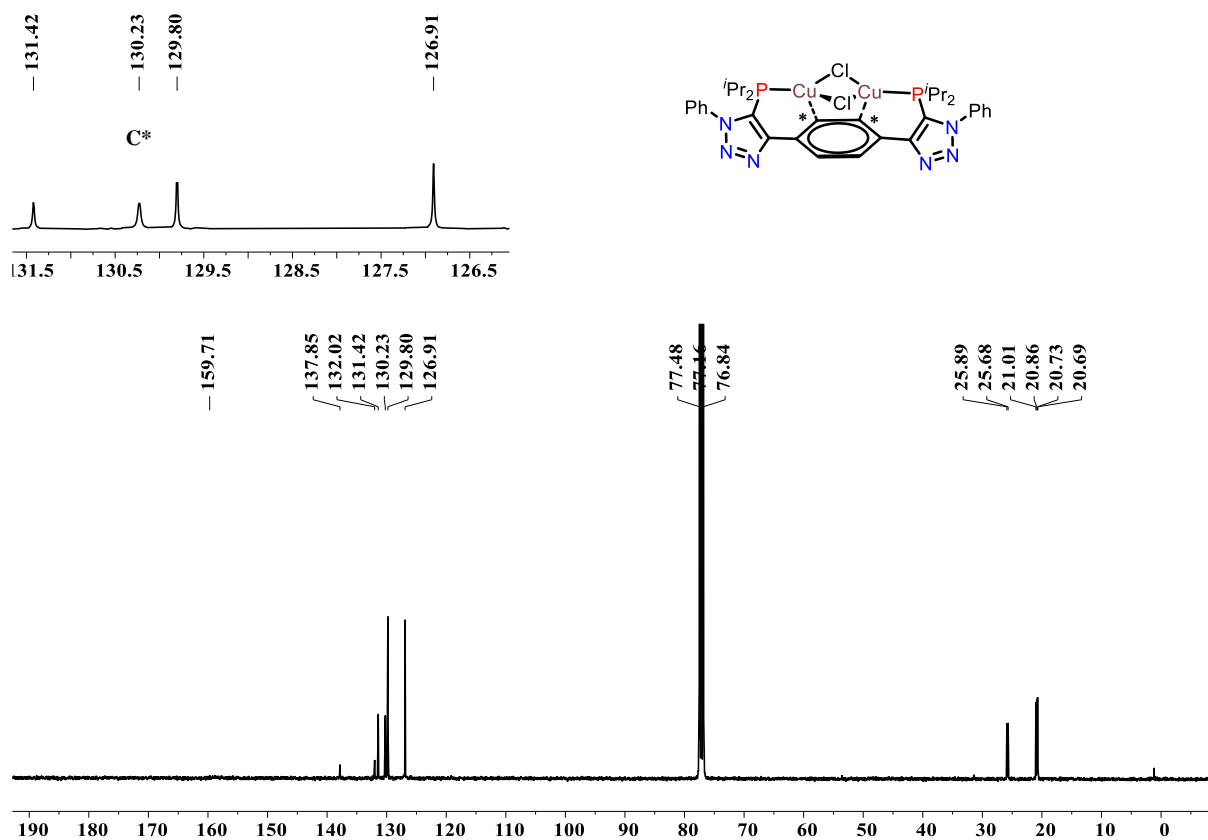


Fig. S14 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in CDCl_3 (101 MHz).

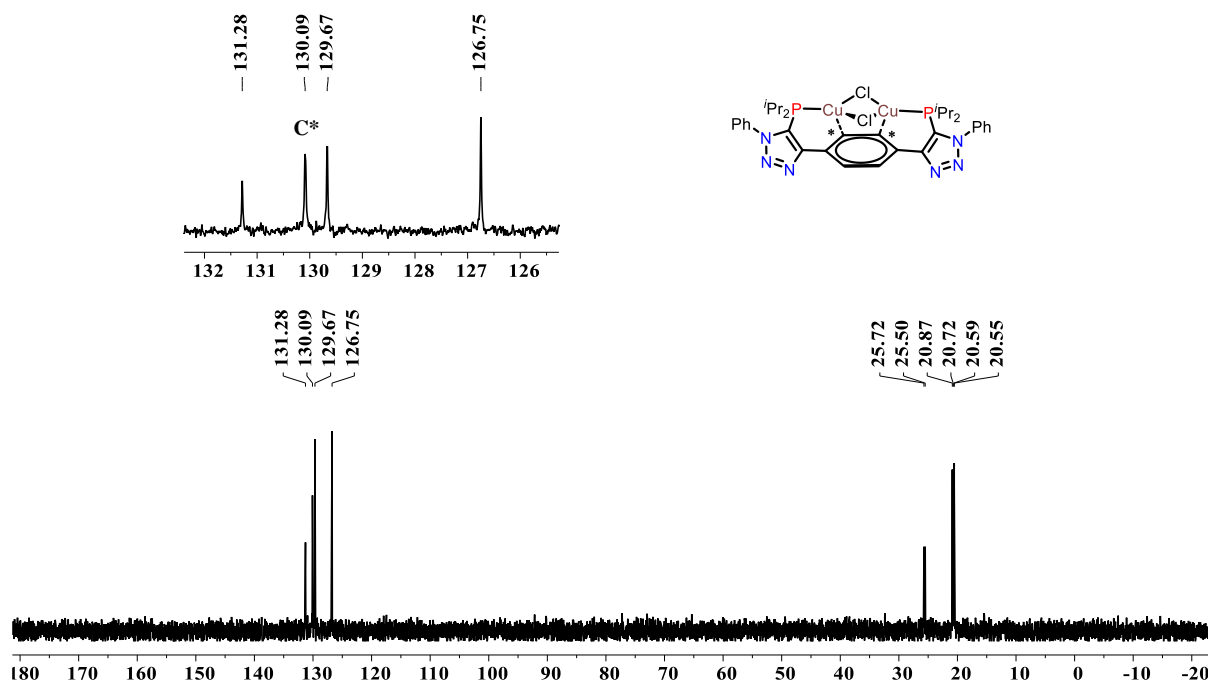


Fig. S15 $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 spectrum of **3** in CDCl_3 (101 MHz).

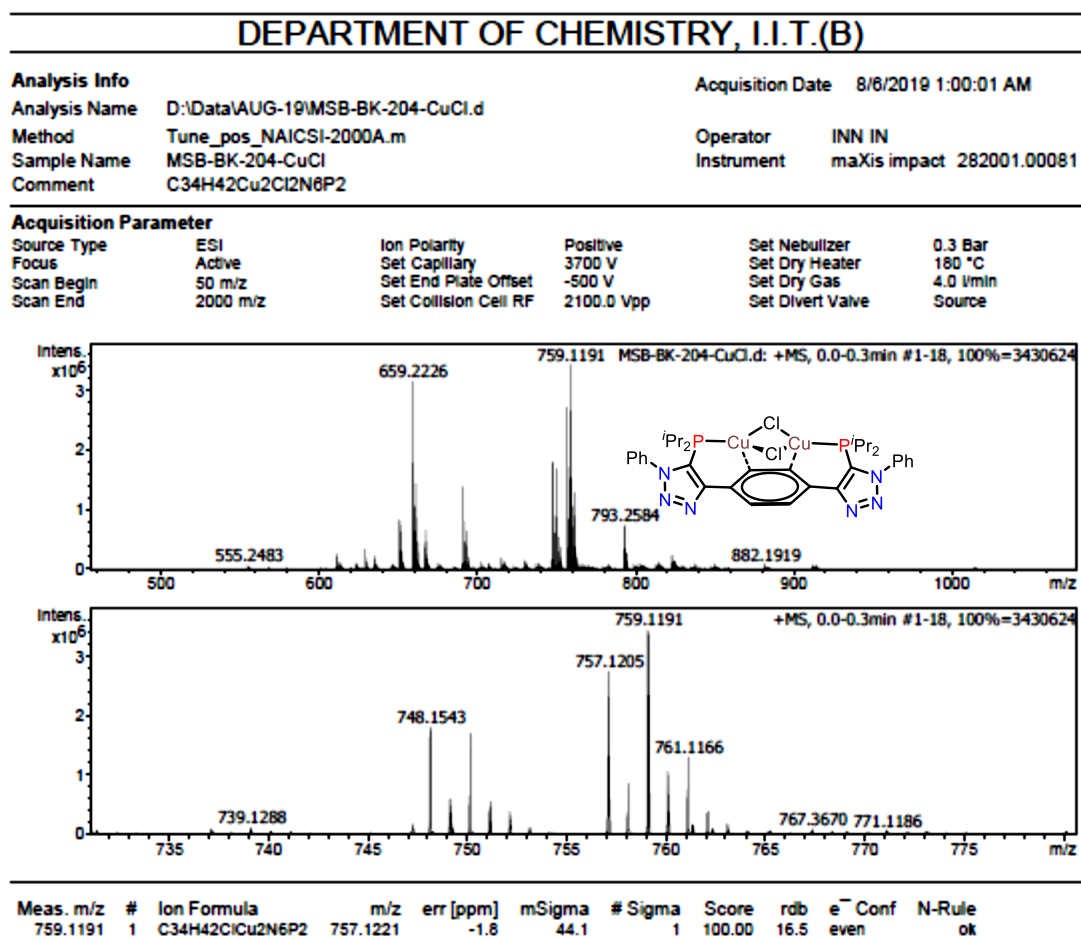


Fig. S16 HRMS spectrum of **3**.

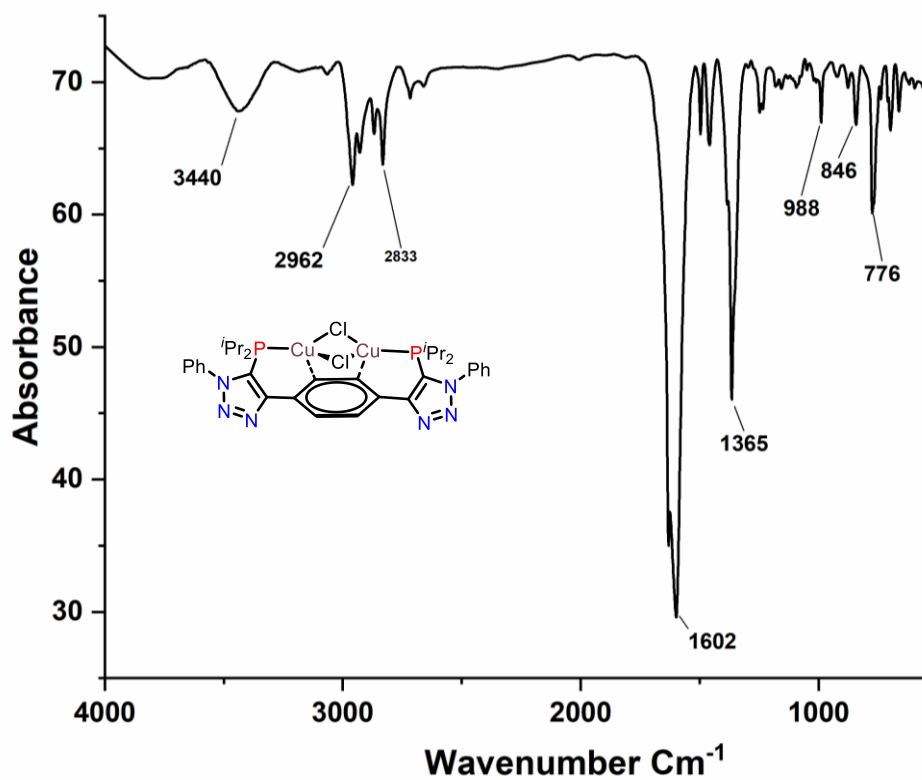


Fig. S17 FT-IR spectrum of **3**.

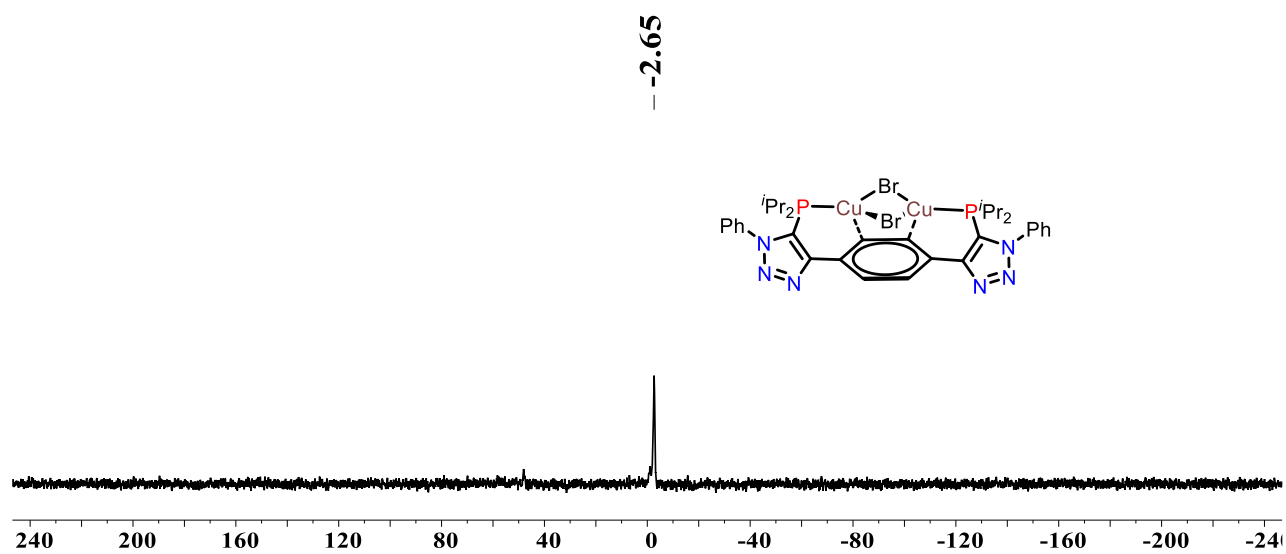


Fig. S18 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **4** in CDCl_3 (162 MHz).

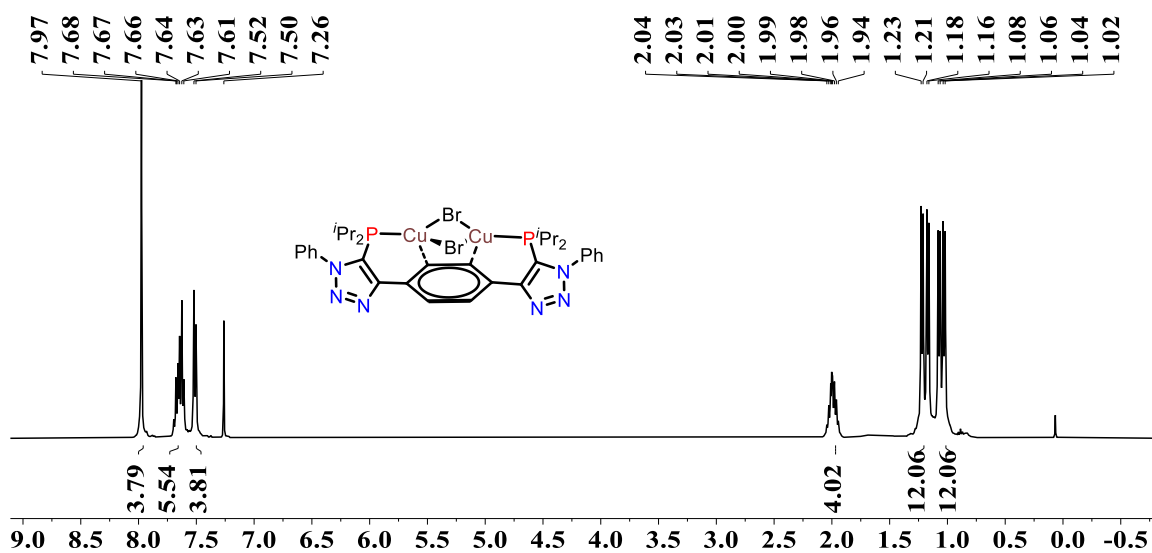


Fig. S19 ^1H NMR spectrum of **4** in CDCl_3 (400 MHz).

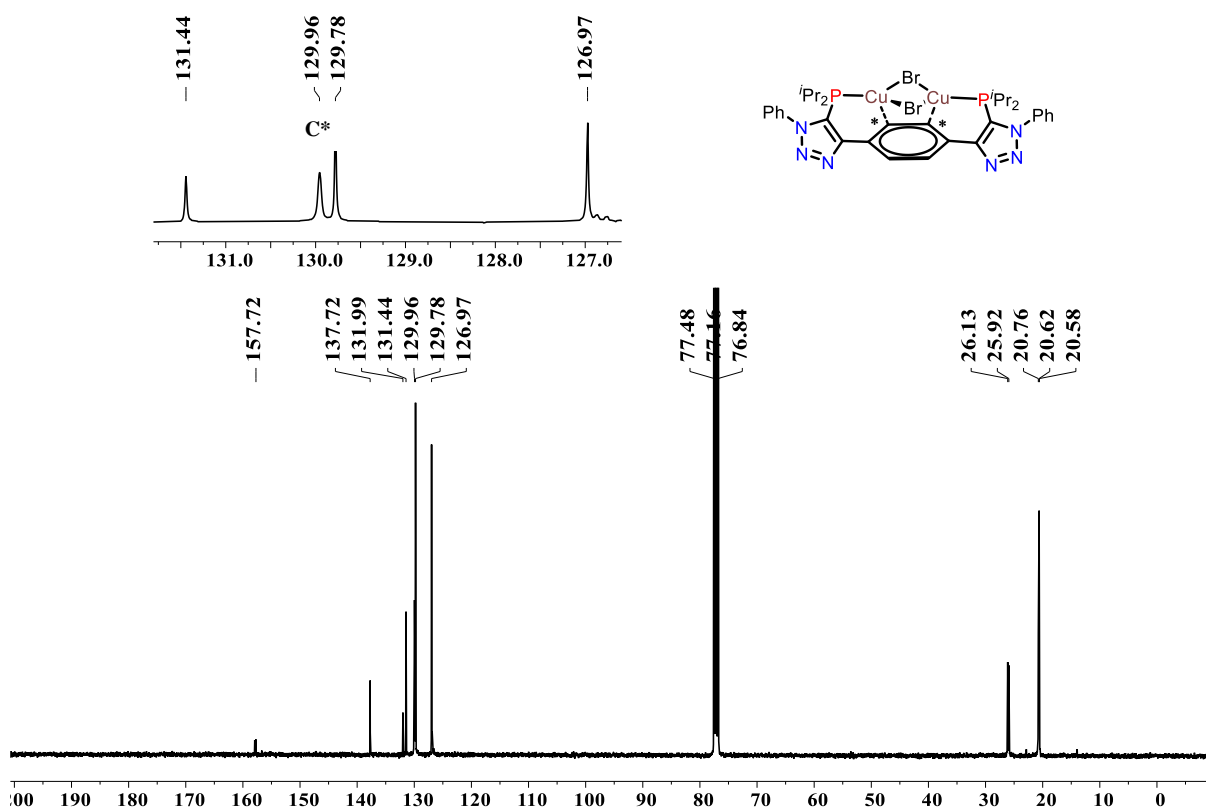


Fig. S20 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** in CDCl_3 (101 MHz).

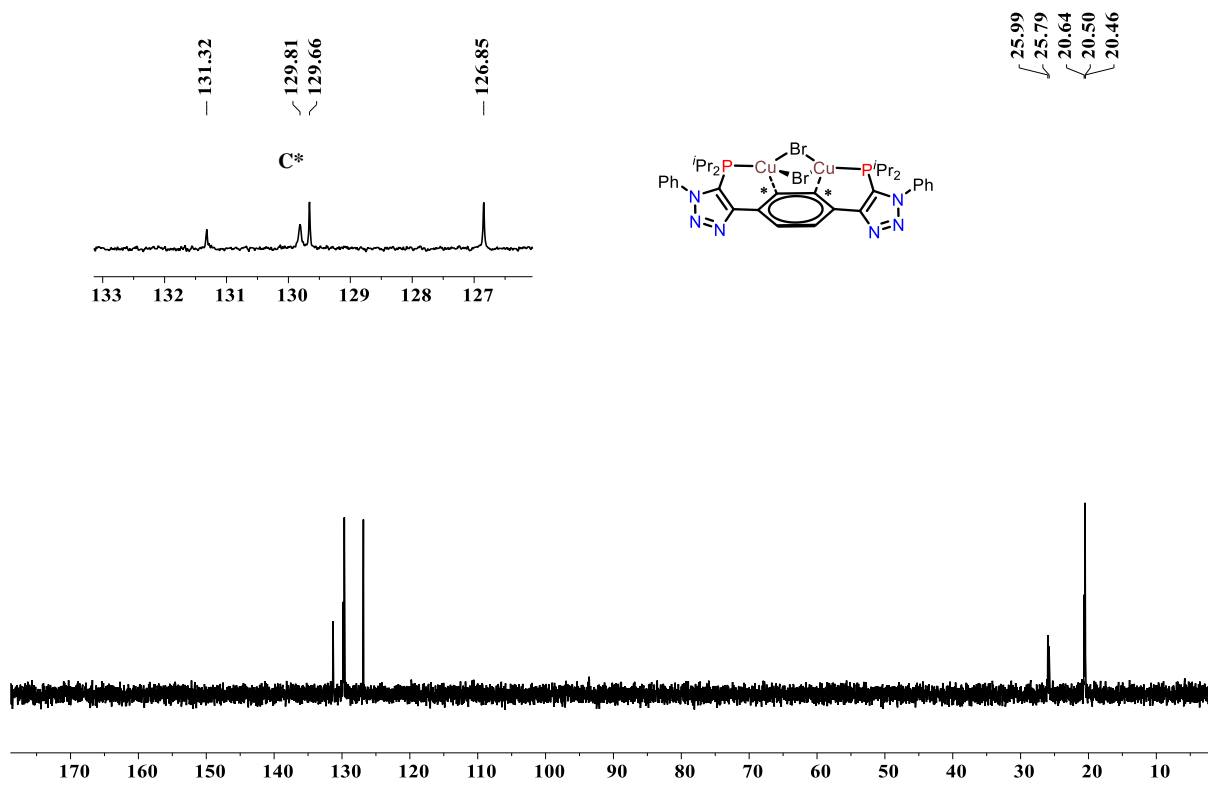


Fig. S21 $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 spectrum of **5** in CDCl_3 (101 MHz).

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Analysis Info

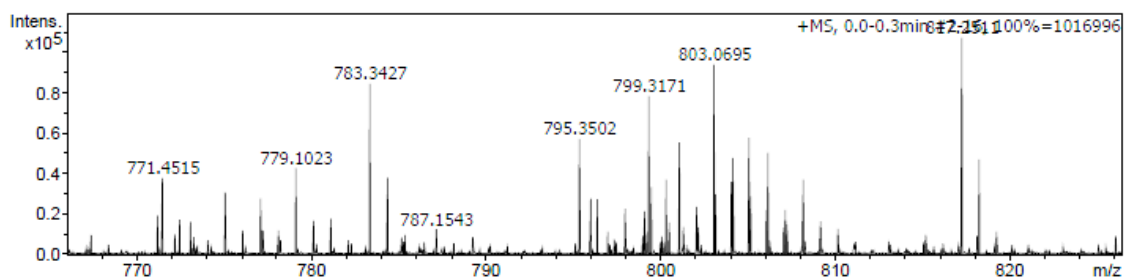
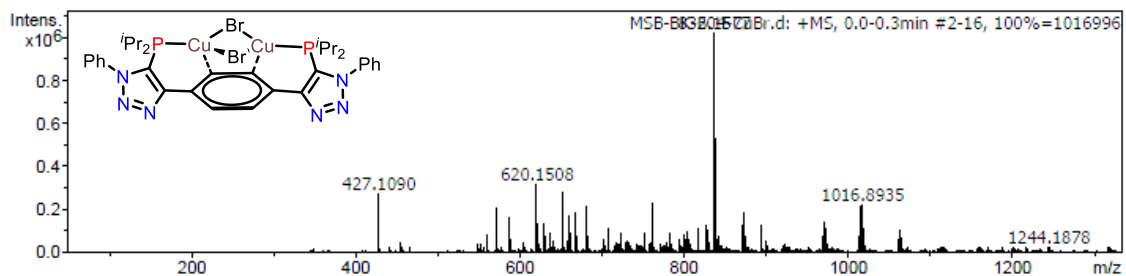
Analysis Name D:\Data\JULY-19\MSB-BK-204-CuBr.d
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 Sample Name MSB-BK-204-CuBr
 Comment C34H42Cu2Br2N6P2

Acquisition Date 7/18/2019 12:19:44 AM

Operator kpk
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
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Scan End	3000 m/z	Set Collision Cell RF	2100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
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Fig. S22 HRMS spectrum of **4**.

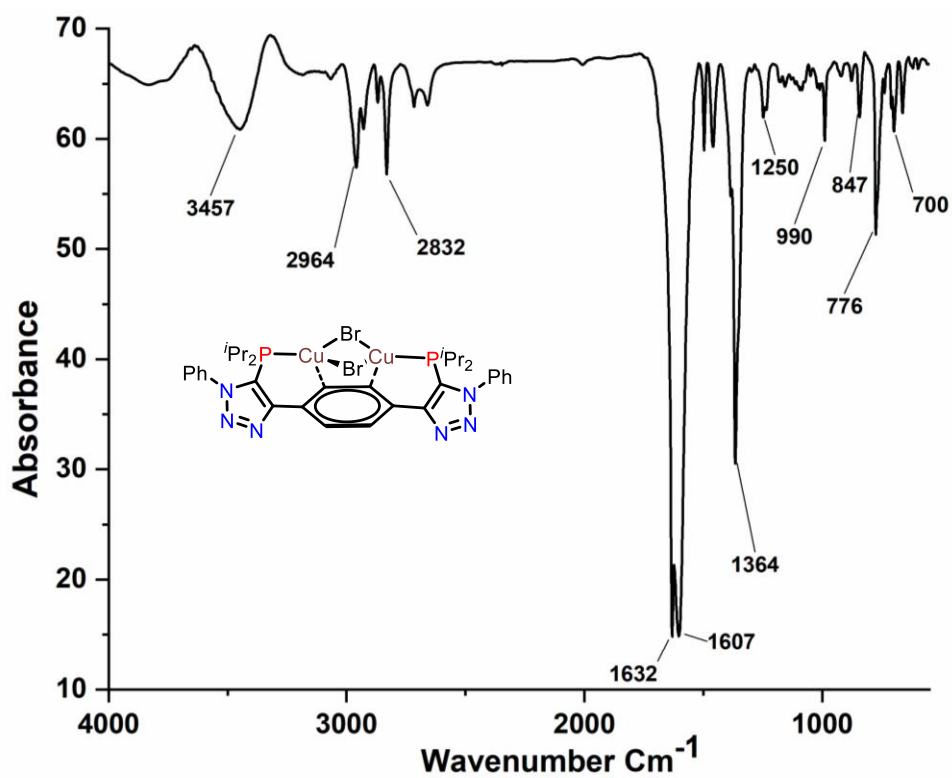


Fig. S23 FT-IR spectrum of **4**.

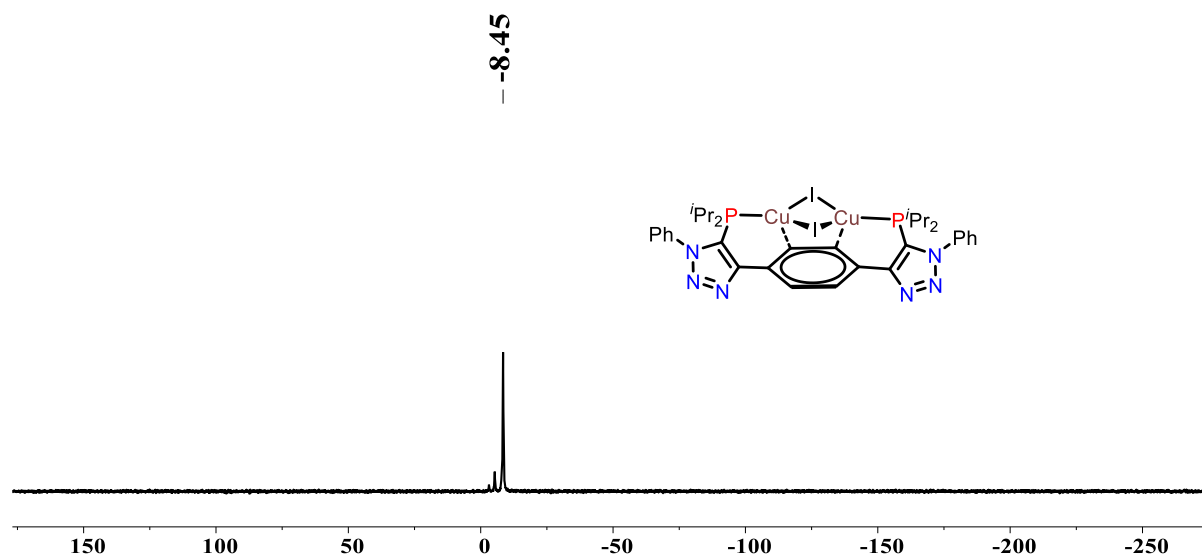
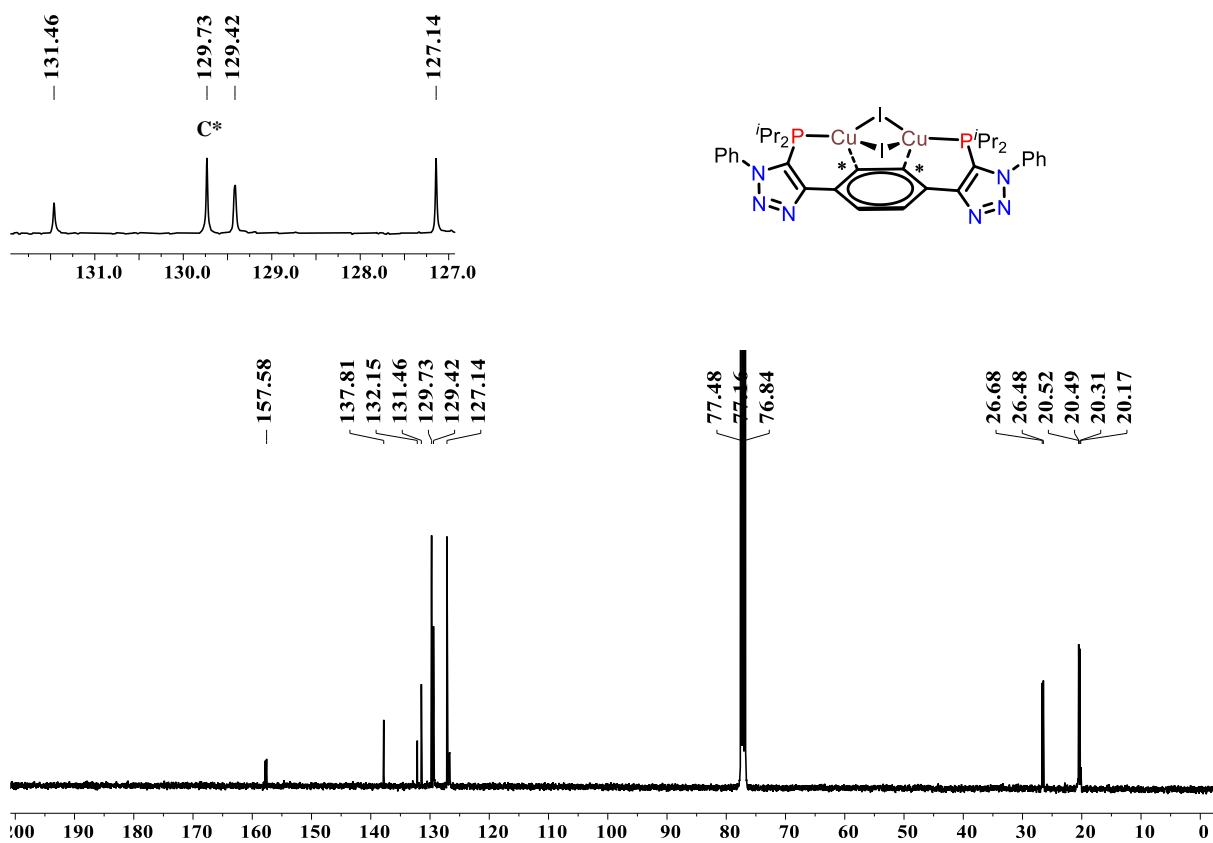
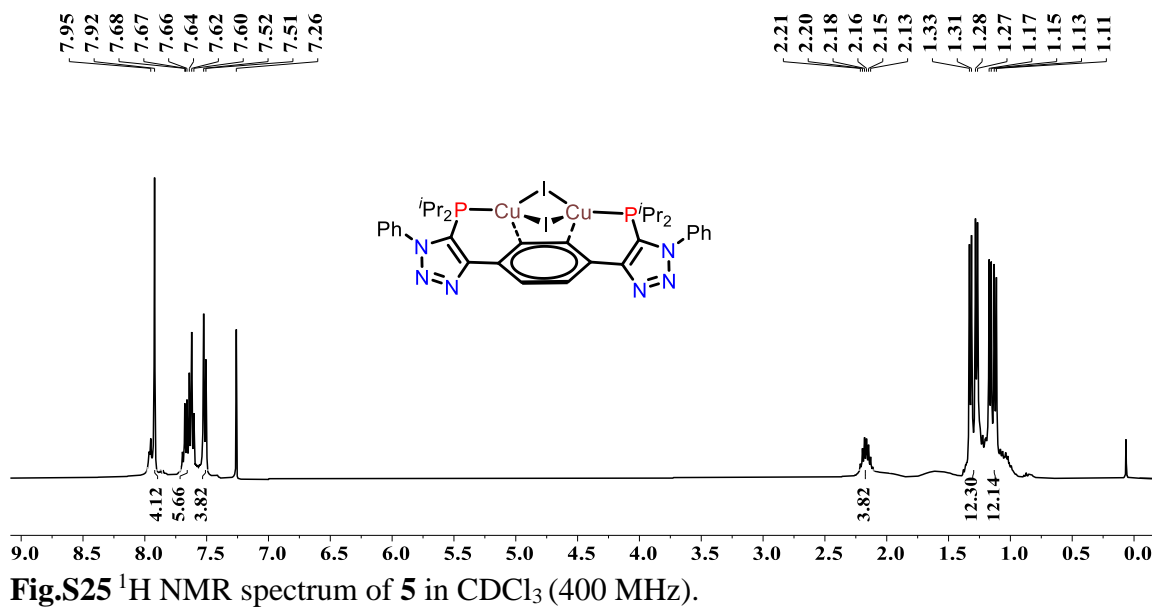


Fig. S24 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **5** in CDCl_3 (162 MHz).



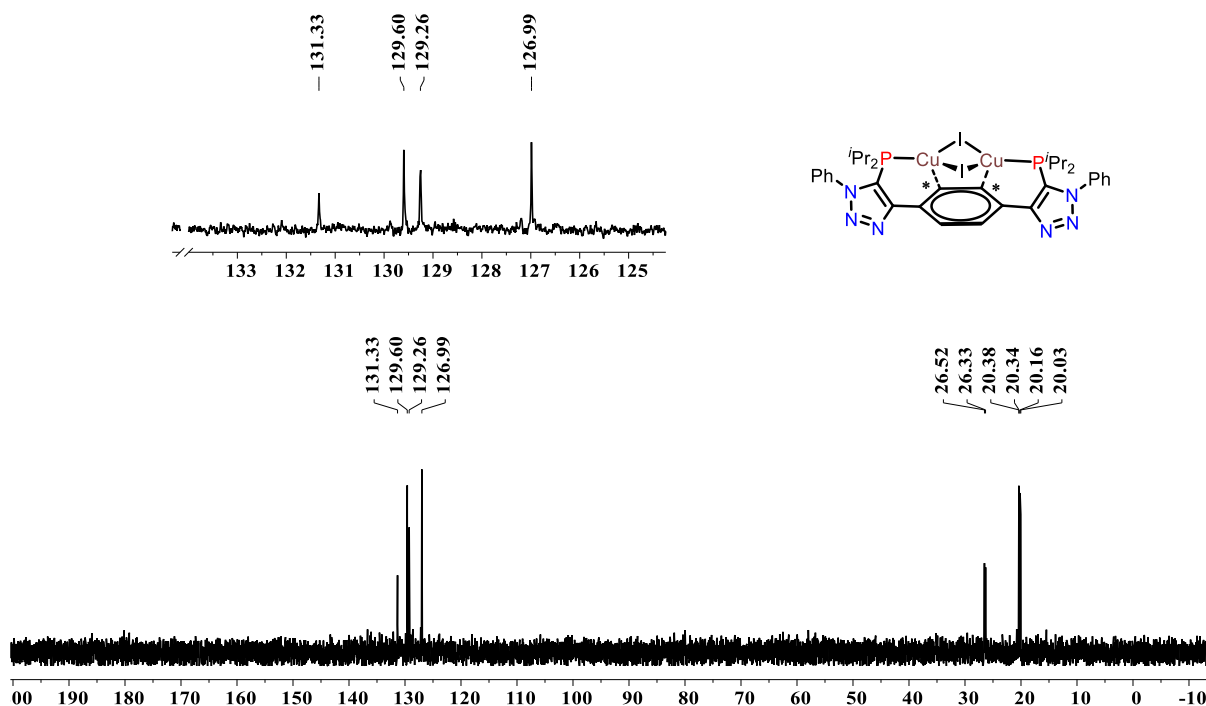


Fig. S27 $^{13}\text{C}\{^1\text{H}\}$ DEPT-135 spectrum of **5** in CDCl_3 (101 MHz).

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Analysis Info

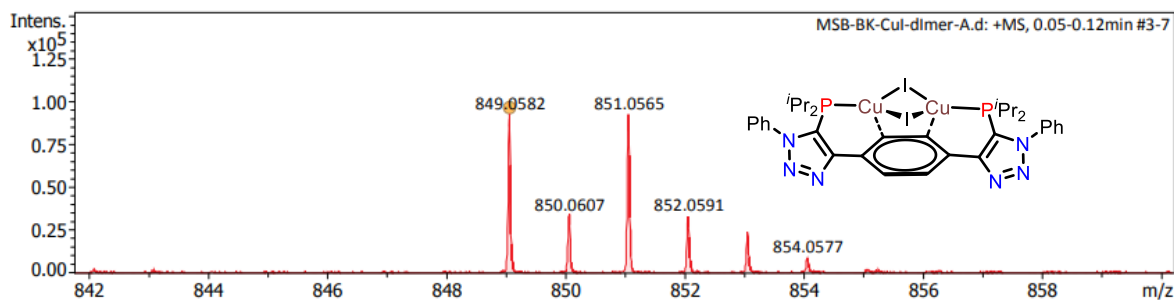
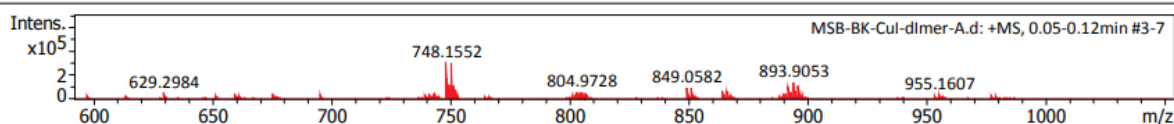
Analysis Name D:\Data\JUNE 2021\MSB-BK-Cul-dlmer-A.d
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 Sample Name MSB-BK-Cul-dlmer-A
 Comment C34H42Cu2I2N6P2

Acquisition Date 6/29/2021 1:25:16 PM

Operator GKL-IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
849.0582	1	C34H42Cu2I2N6P2	849.0577	-0.6	17.6	1	100.00	23.0	even	ok

Fig. S28 HRMS spectrum of **5**.

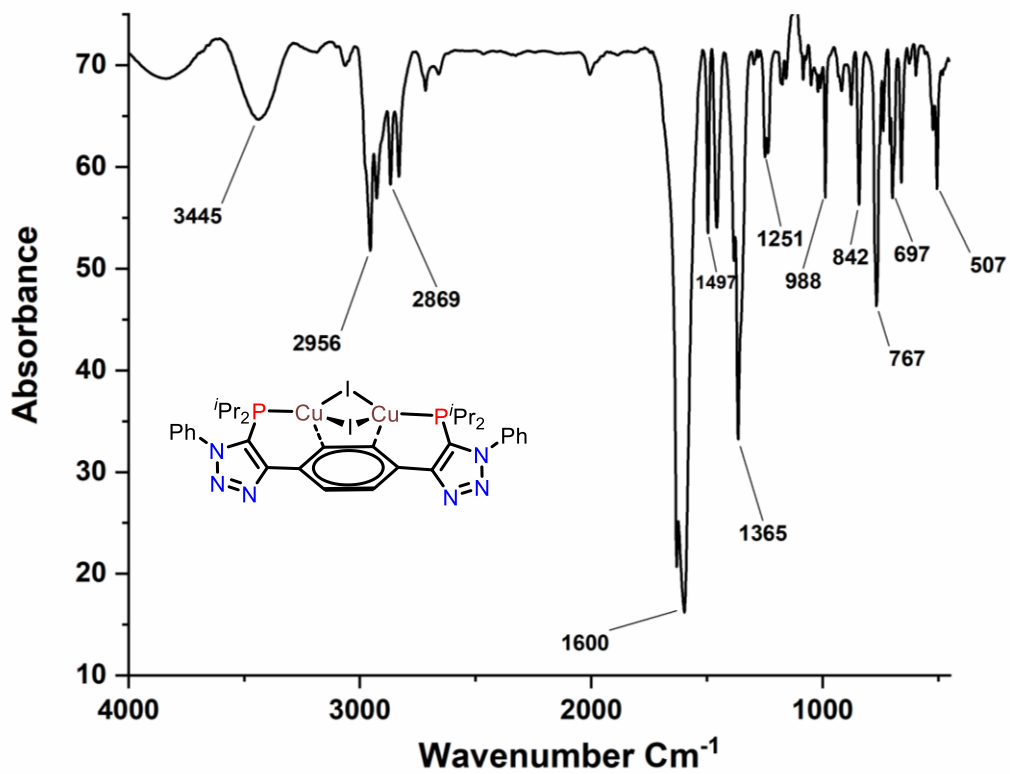


Fig. S29 FT-IR spectrum of **5**.

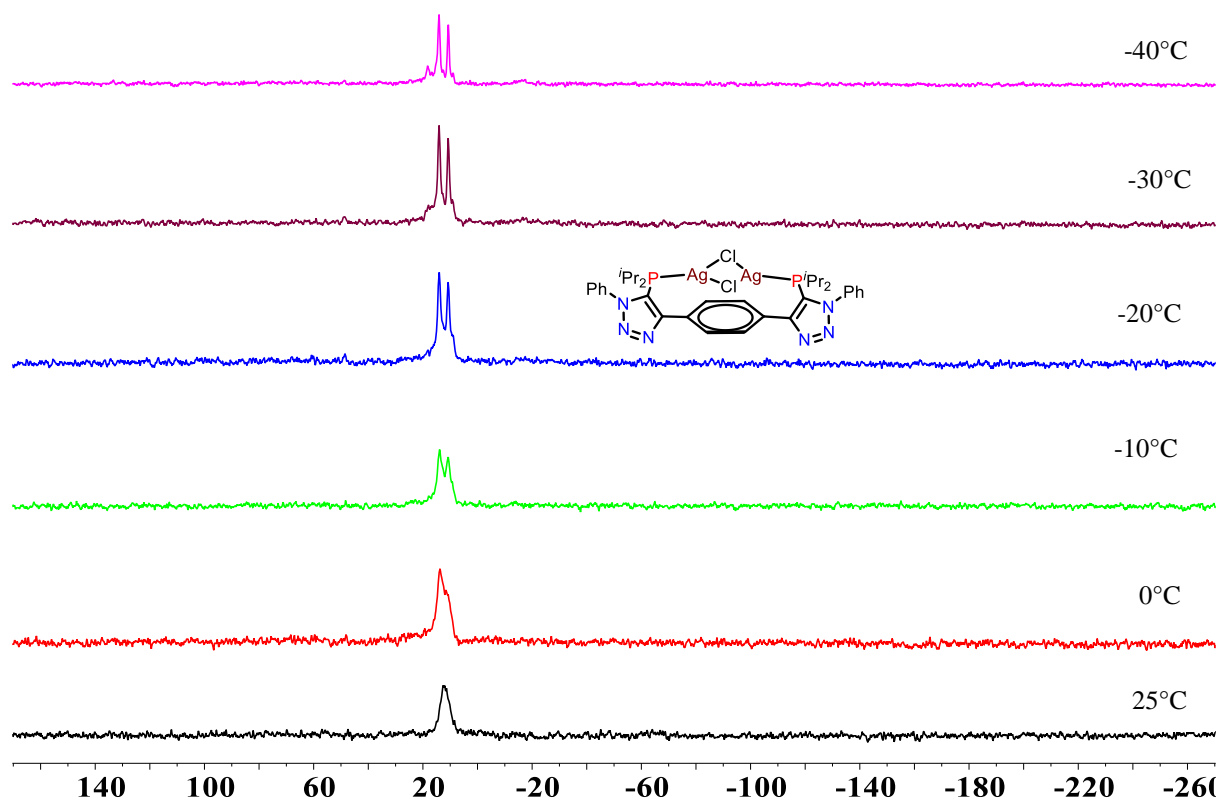


Fig. S30 $^{31}\text{P}\{^1\text{H}\}$ VT NMR data for **6**.

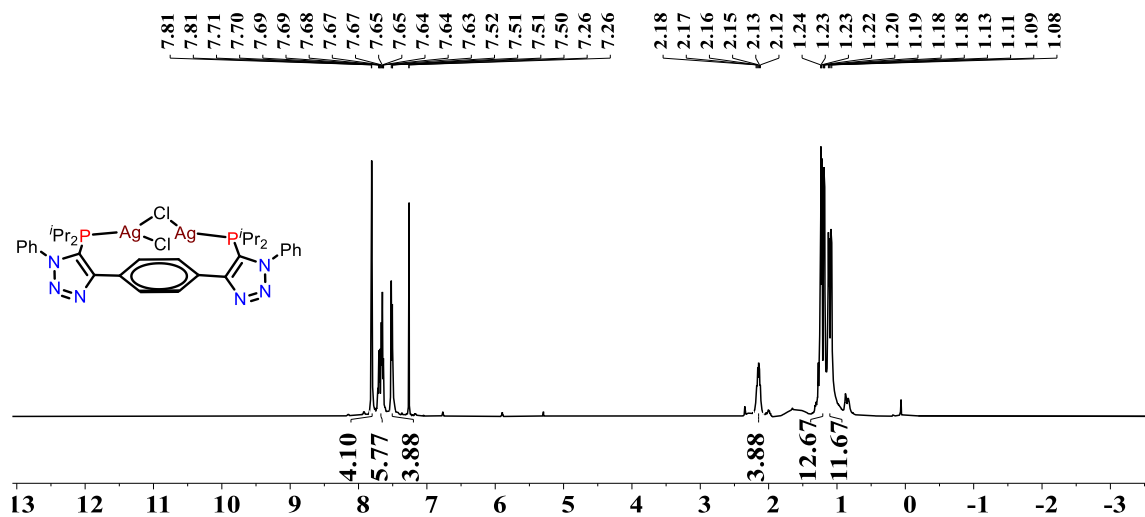


Fig. S31 ^1H NMR spectrum of **6** in CDCl_3 (400 MHz).

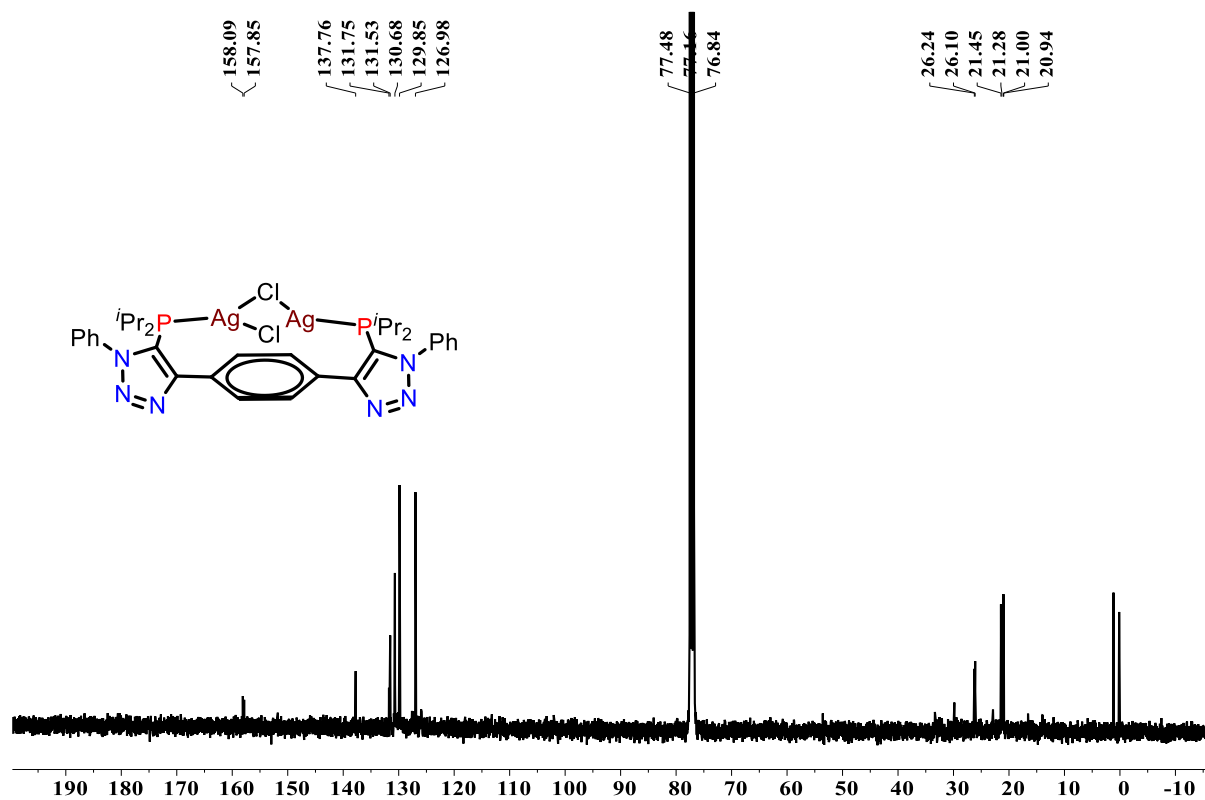


Fig. S32 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** in CDCl_3 (101 MHz).

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info
 Analysis Name D:\Data\MAY 2021\MSB-BK-BISPHOS-AgCl-CUBANE-B.d
 Method NaICsl_pos_1500hplc.m
 Sample Name MSB-BK-BISPHOS-AgCl-CUBANE-B
 Comment C34H42Ag2Cl2N6P2
 Acquisition Date 5/6/2021 5:50:58 PM
 Operator SJG-IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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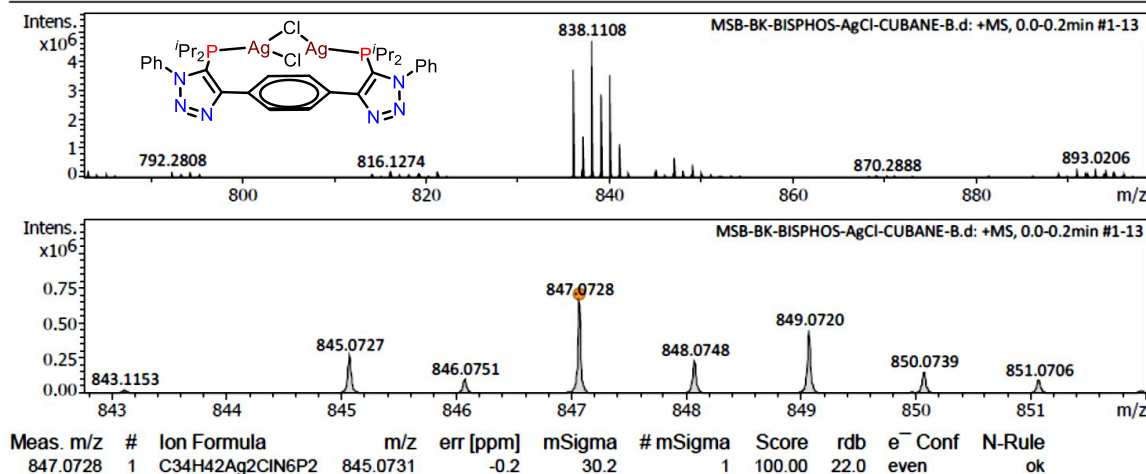


Fig. S33 HRMS spectrum of 6.

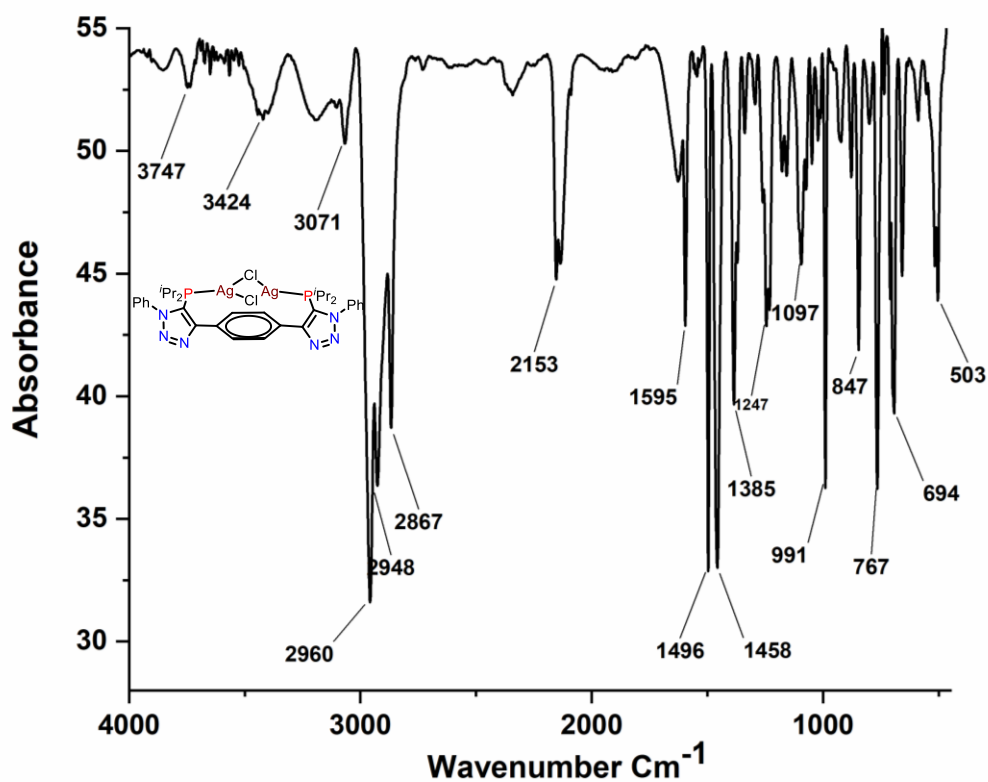


Fig. S34 FT-IR spectrum 6.

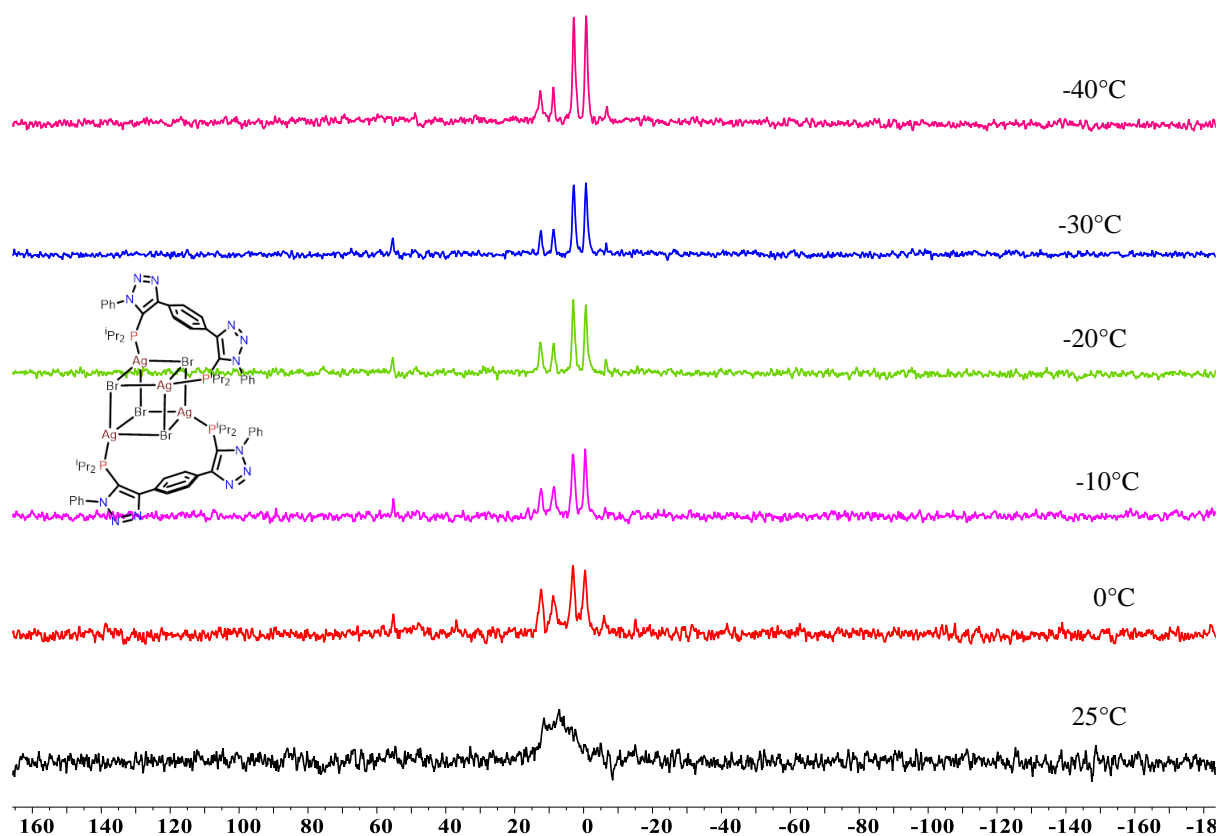


Fig. S35 $^{31}\text{P}\{^1\text{H}\}$ VT NMR data for 7.

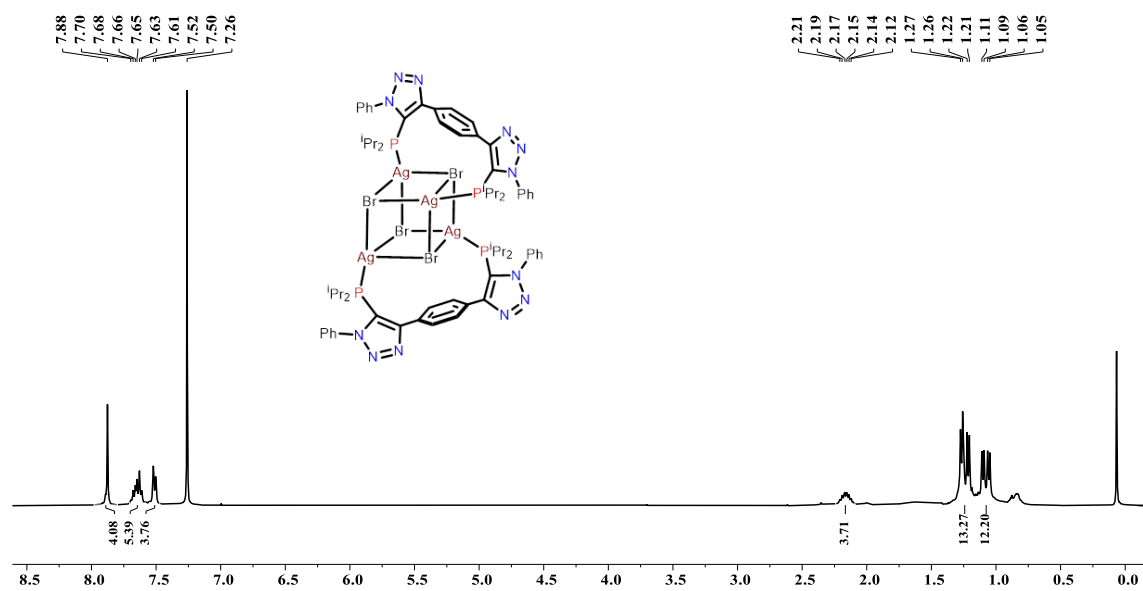


Fig. S36 ^1H NMR spectrum of 7 in CDCl_3 (400 MHz).

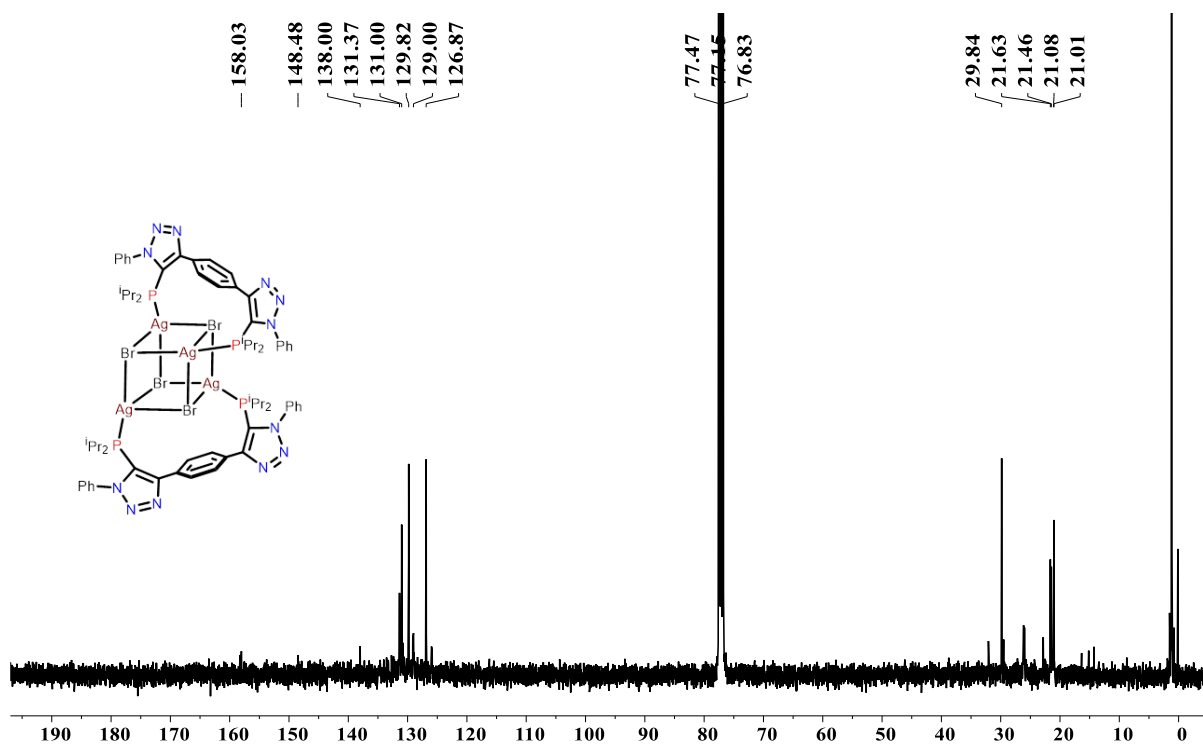


Fig. S37 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7** in CDCl_3 (101 MHz).

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

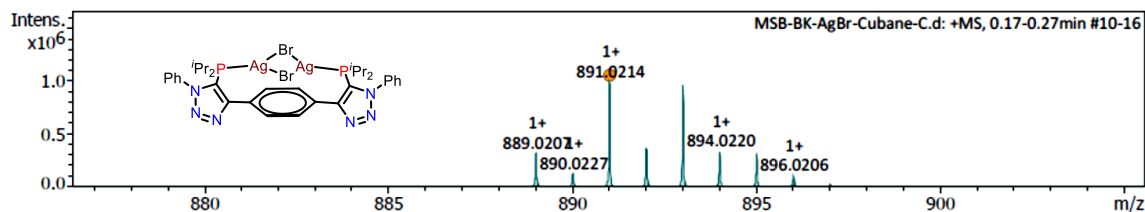
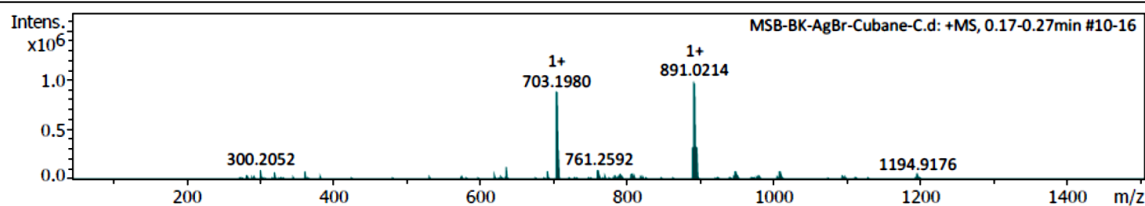
Analysis Name D:\Data\MAR-21\MSB-BK-AgBr-Cubane-C.d
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Acquisition Date 3/16/2021 9:19:18 AM

Operator AK IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	Adduct
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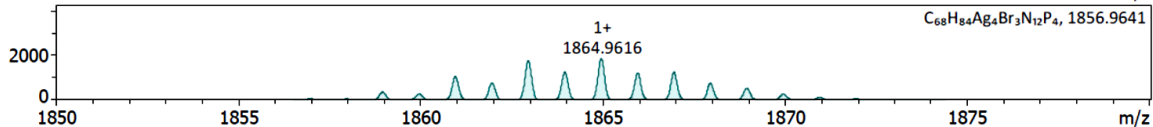
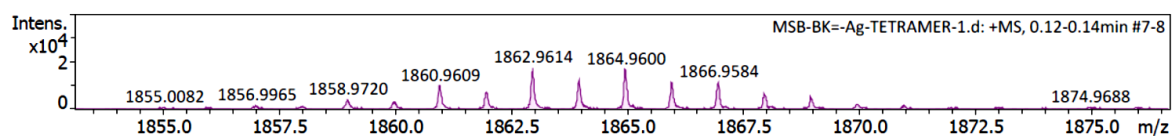
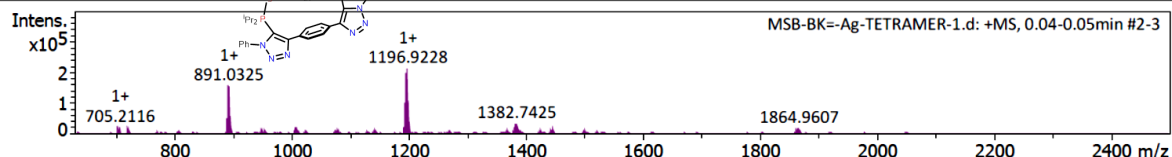
Fig. S38 HRMS spectrum of **7**.

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info
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 Method NaICsl_pos_3000.m
 Sample Name MSB-BK=-Ag-TETRAMER-1
 Comment C68H84N16P4Ag4Br4
 Acquisition Date 7/19/2021 7:41:19 PM
 Operator SJG-IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	Adduct
1862.961363	1	C68H84Ag4Br3N12P4	100.00	1856.964069	0.7	0.4	46.4	42.0	even	M

Fig. S39 HRMS spectrum of 7.

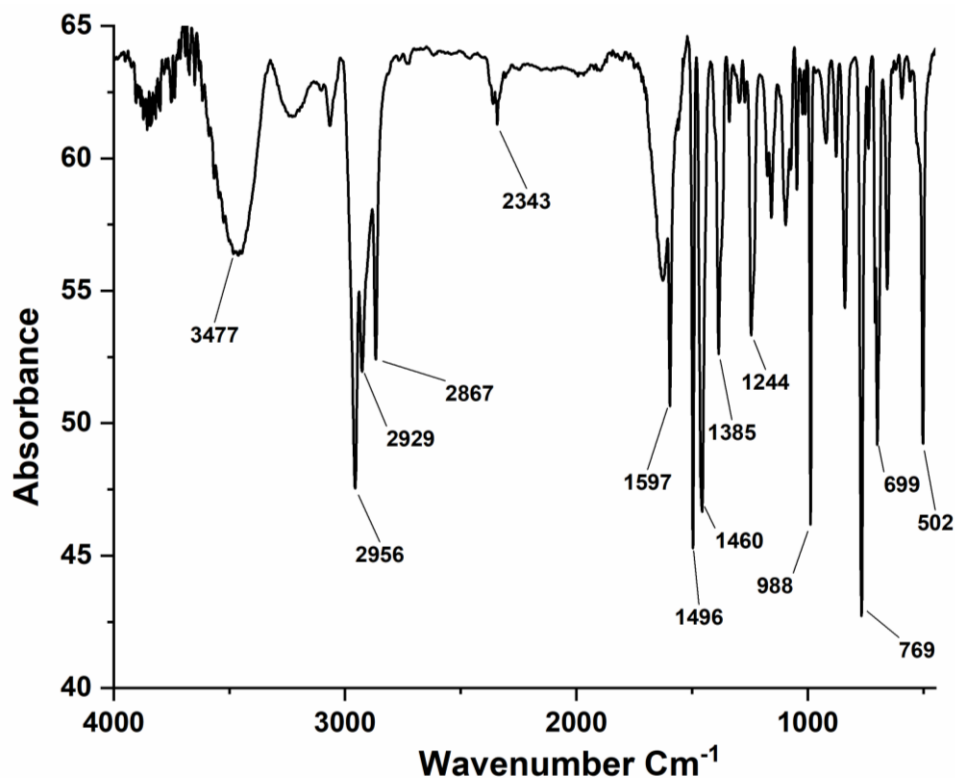


Fig. S40 FT-IR spectrum of **7**.

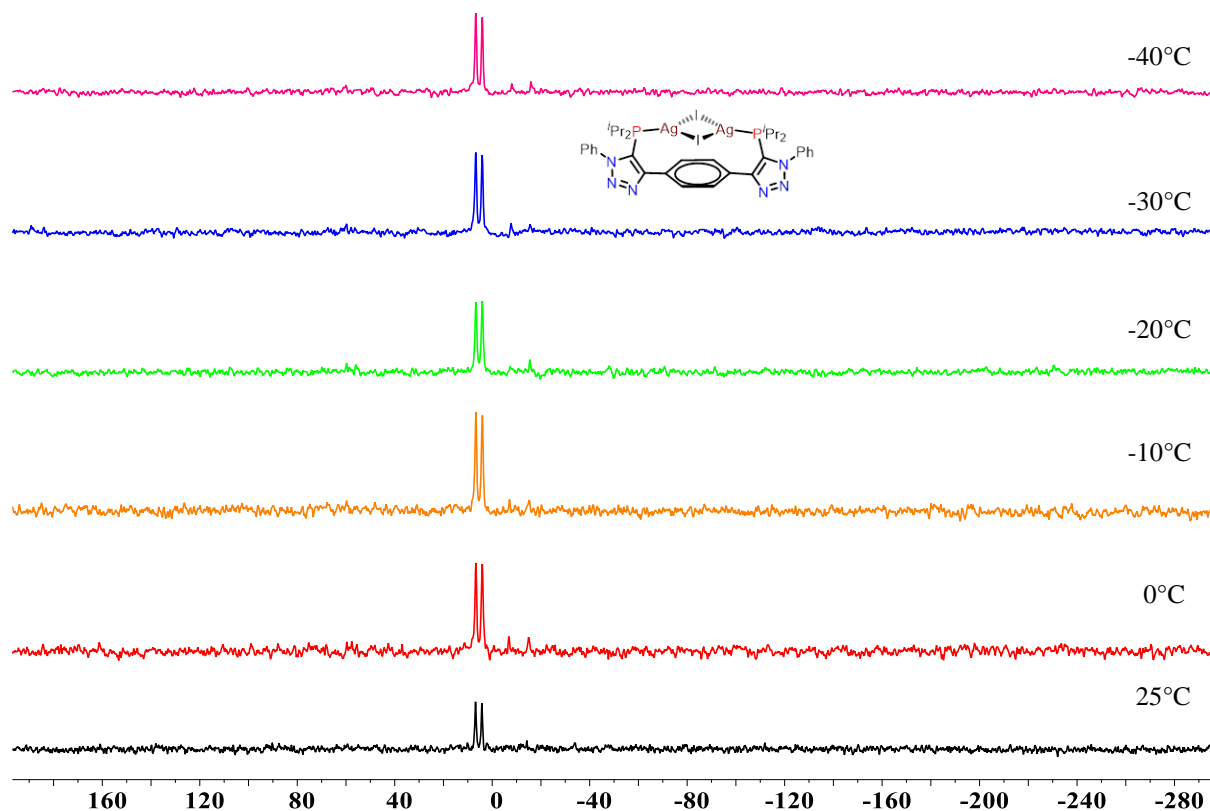


Fig. S41 $^{31}\text{P}\{^1\text{H}\}$ VT NMR data for **8**.

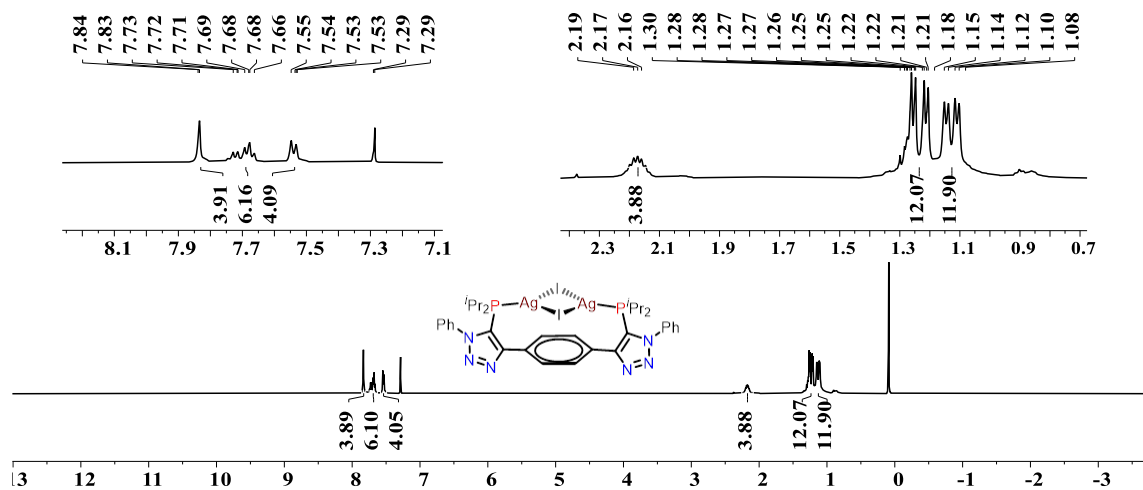


Fig. S42 ^1H NMR spectrum of **8** in CDCl_3 (400 MHz).

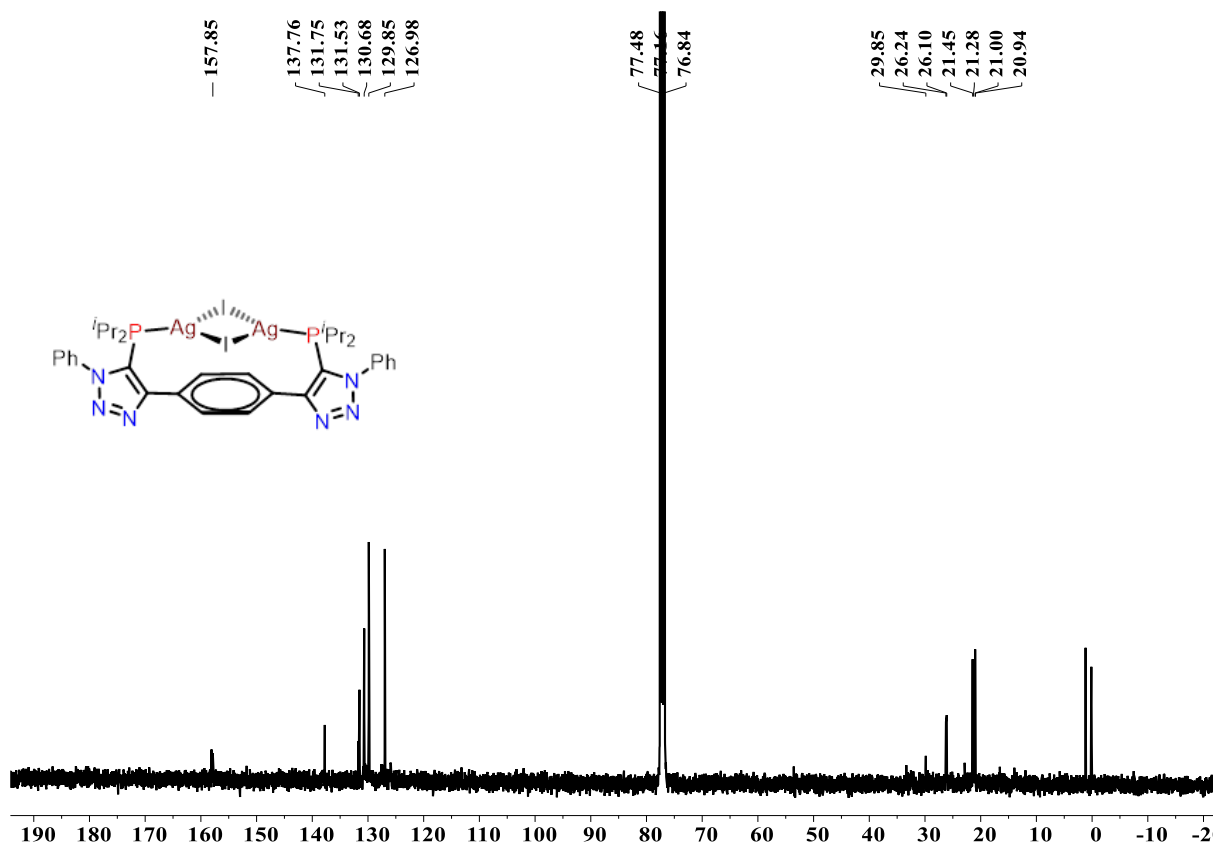


Fig. S43 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8** in CDCl_3 (101 MHz).

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

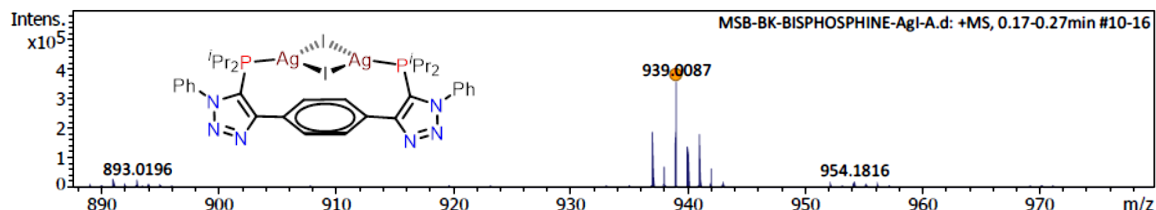
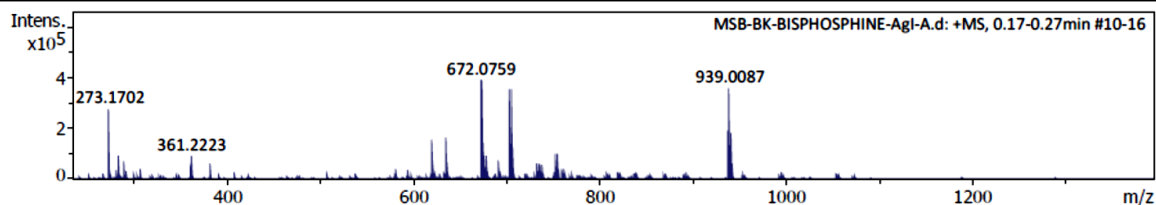
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 Comment C34H42Ag2I2P2N6

Acquisition Date 3/16/2021 9:39:53 AM

Operator AK IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
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Fig. S44 HRMS spectrum of **8**.

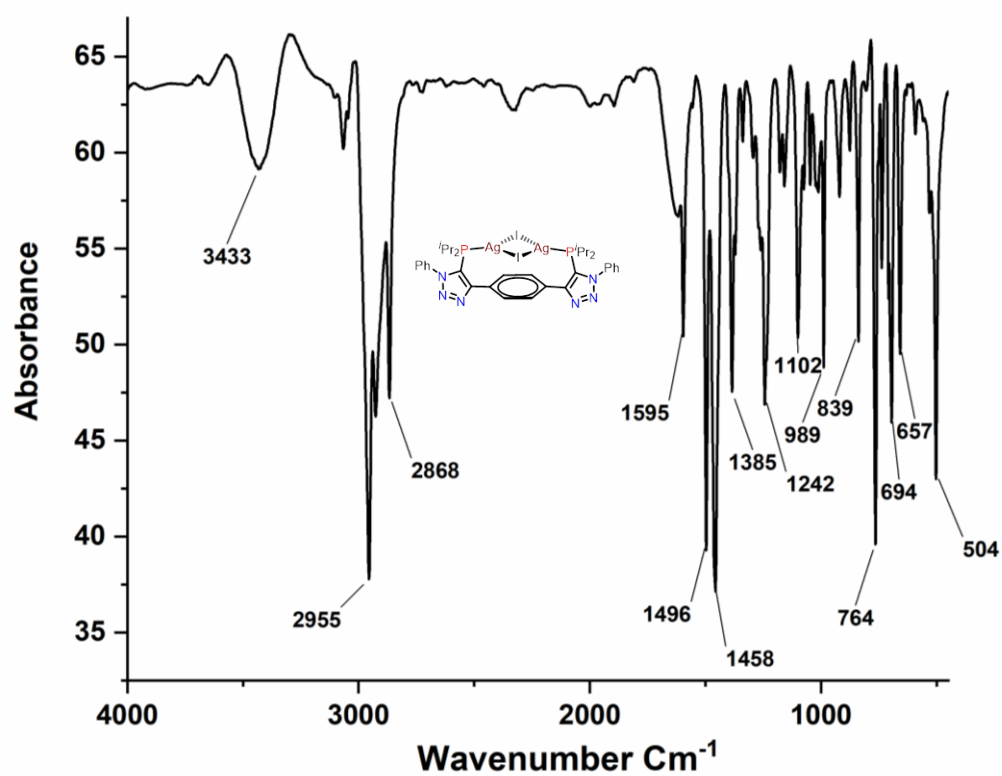


Fig. S45 FT-IR spectrum **8**.

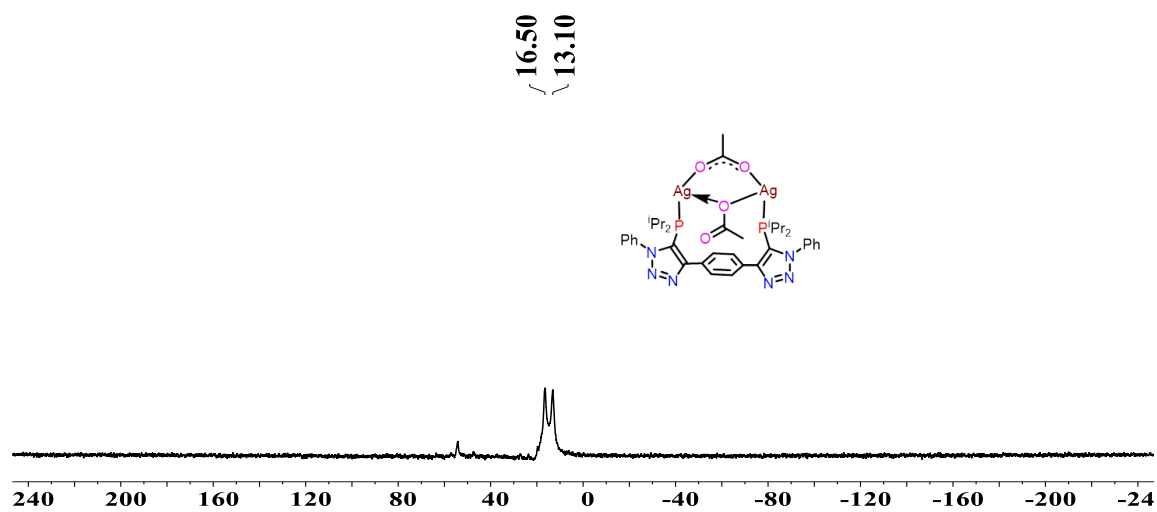


Fig. S46 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **9** in CDCl_3 (162 MHz).

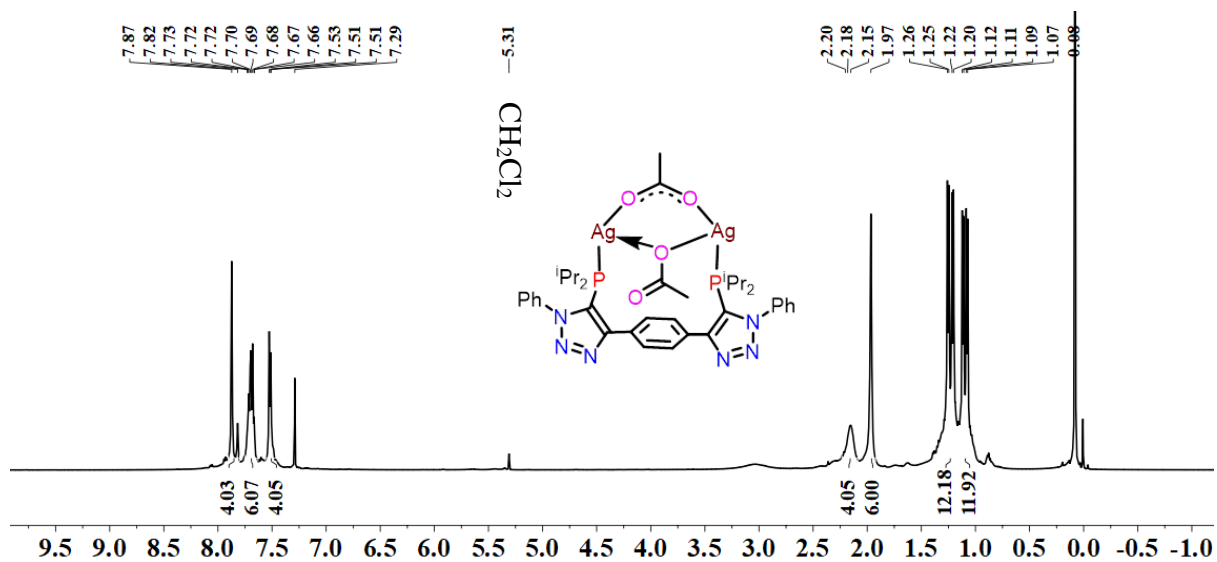


Fig. S47 ^1H NMR spectrum of **9** in CDCl_3 (400 MHz).

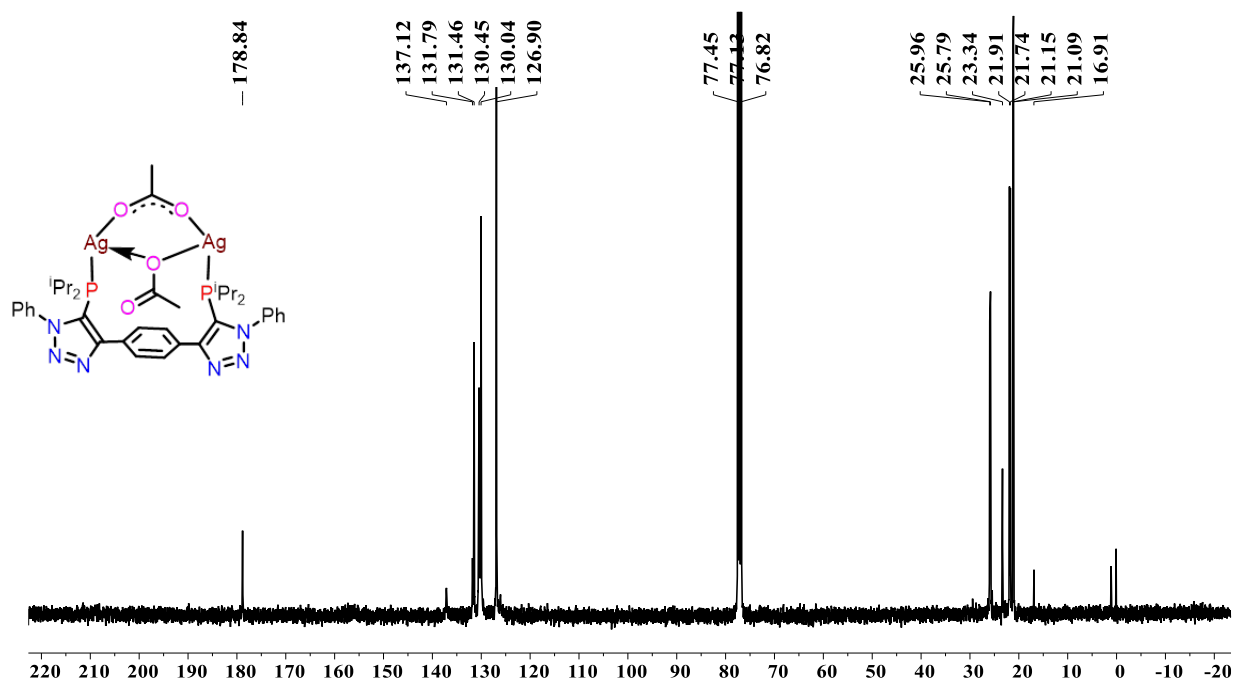


Fig. S48 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** in CDCl_3 (101 MHz).

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Analysis Info		Acquisition Date	3/16/2021 10:07:18 AM	
Analysis Name	D:\Data\MAR-21\MSB-BK-AgOAc-BRIDGING-B.d	Operator	AK IN	
Method	NaICSI_pos_1500hplc.m	Instrument	maXis impact 282001.00081	
Sample Name	MSB-BK-AgOAc-BRIDGING-B			
Comment	C38H48Ag2P2N6O4			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

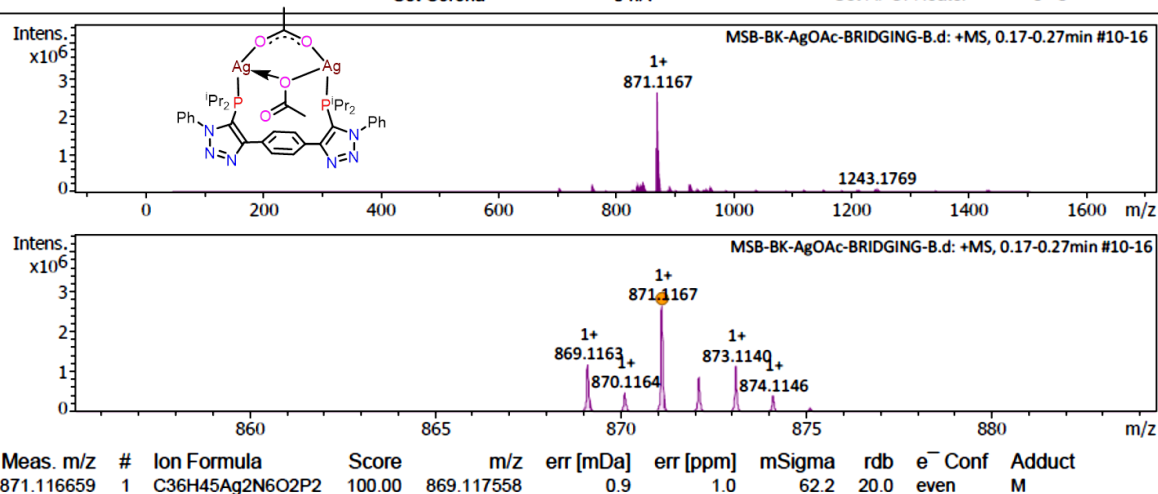


Fig. S49 HRMS spectrum of **9**.

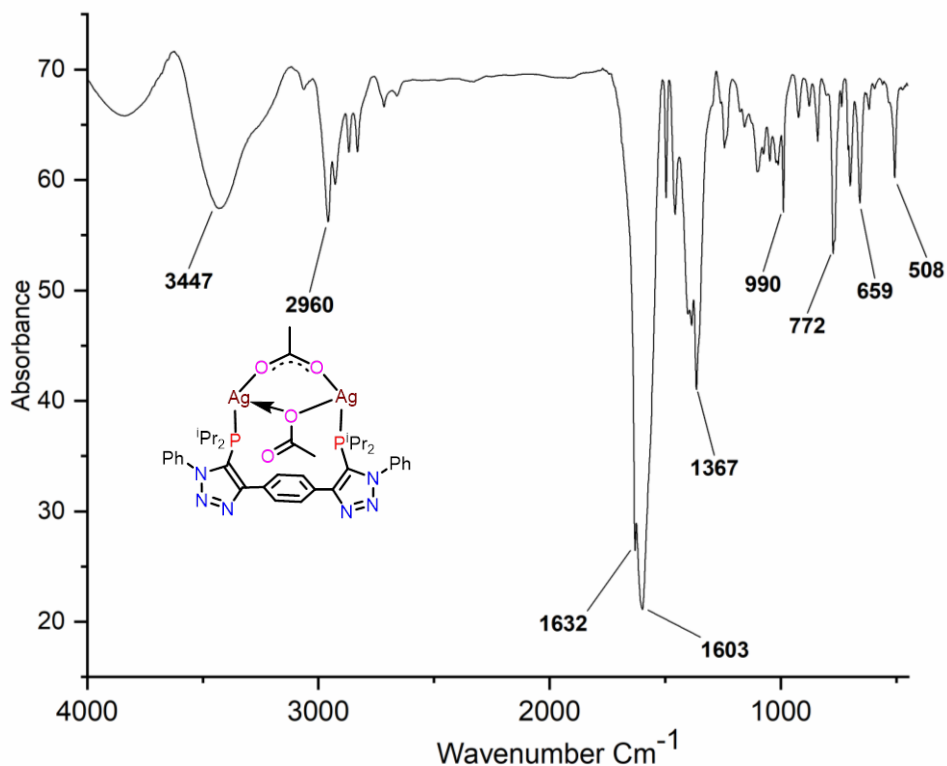


Fig. S50 FT-IR spectrum of **9**.

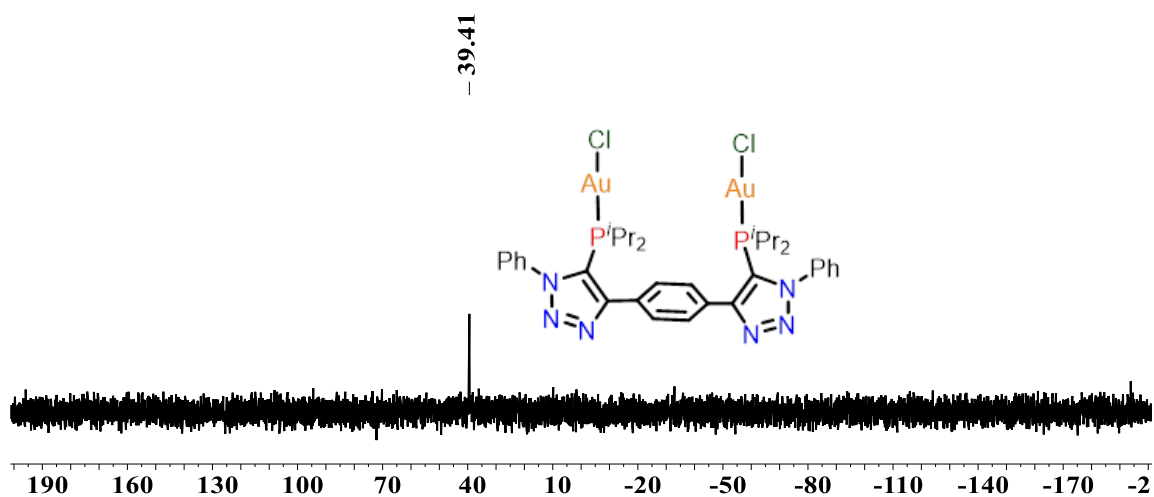


Fig. S51 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **10** in CDCl_3 (162 MHz).

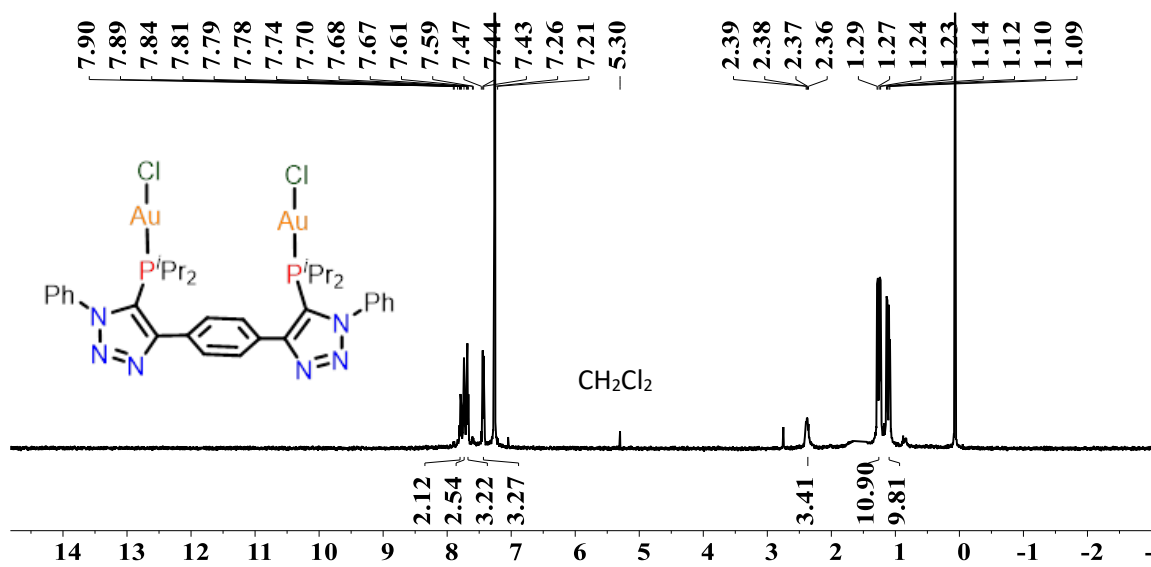


Fig. S52 ^1H NMR spectrum of **10** in CDCl_3 (400 MHz).

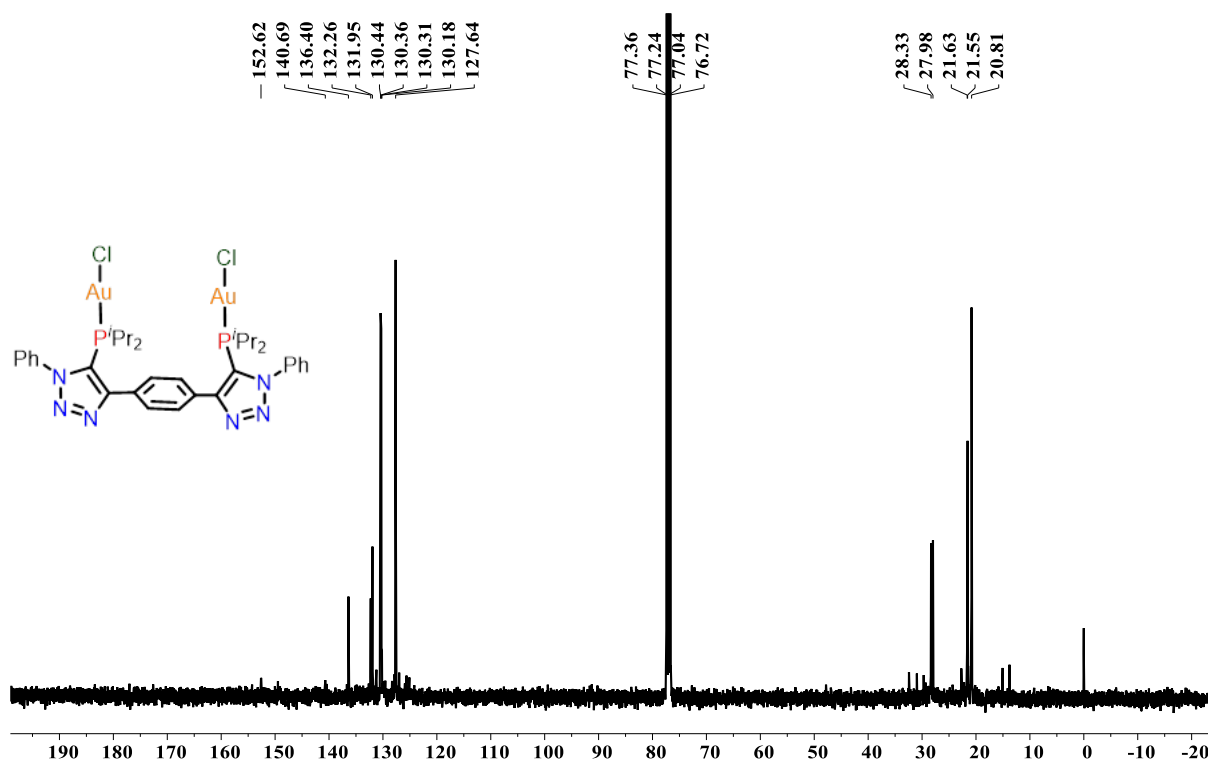


Fig. S53 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** in CDCl_3 (101 MHz).

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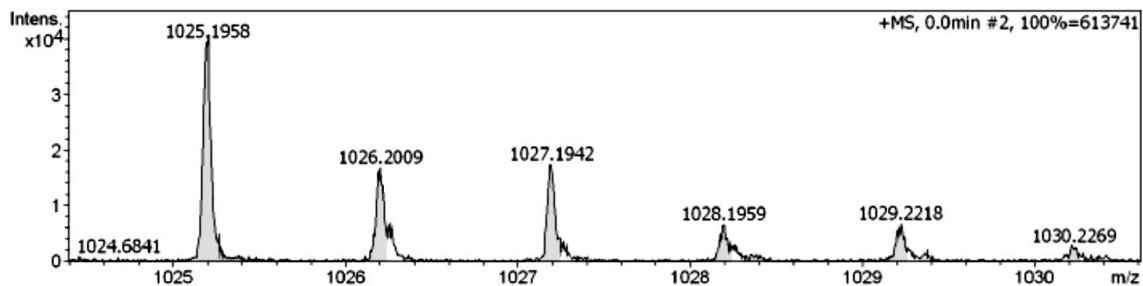
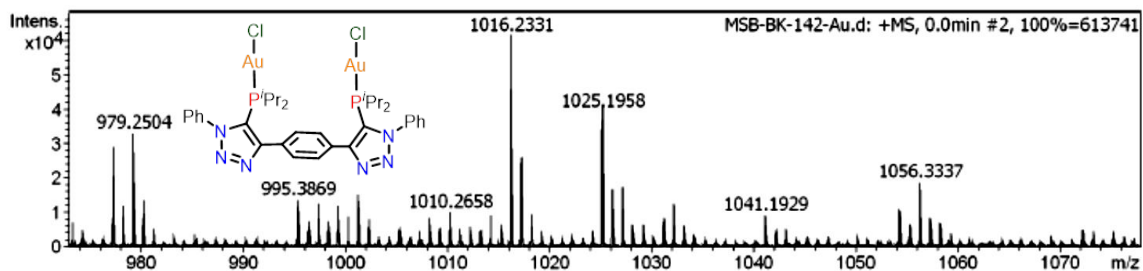
Analysis Info

Analysis Name D:\Data\JULY-19\MSB-BK-142-Au.d
 Method Tune_pos_NAICSI-2000A.m
 Sample Name MSB-BK-142-Au
 Comment C34H42Au2Cl2IN6P2

Acquisition Date 7/30/2019 1:41:50 AM
 Operator MSB-SS OUT
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
1025.1958	1	C34H42Au2Cl2IN6P2	1025.1961	-0.2	70.2	1	100.00	16.5	even	ok

Fig. S54 HRMS spectrum of 10.

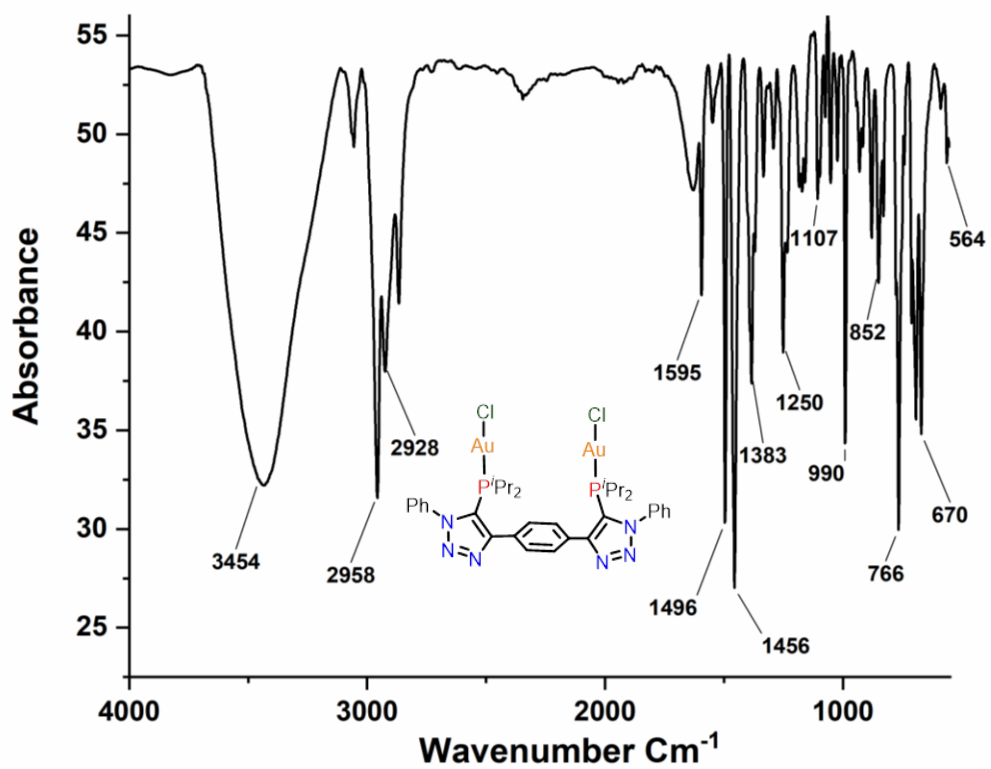


Fig. S55 FT-IR spectrum of 10.

Table S1 Crystallographic information for compounds 2–5.

	2	3·(CH₂Cl₂)	4	5·1.334(CH₂Cl₂)
Formula	C ₃₄ H ₄₂ N ₆ P ₂	C ₃₅ H ₄₄ Cl ₄ Cu ₂ N ₆ P ₂	C ₃₄ H ₄₂ Br ₂ Cu ₂ N ₆ P ₂	C _{35.33} H _{44.67} Cl _{2.86} Cu ₂ I _{1.81} N ₆ P ₂
Formula Weight	596.67	879.58	883.57	1073.66
Crystal System	triclinic	monoclinic	monoclinic	orthorhombic
Space group	P-1	P2 ₁ /n	P2 ₁ /c	Pbca
<i>a</i> , Å	9.4624(9)	12.1164(3)	10.3774(7)	19.0847(3)
<i>b</i> , Å	9.4943(9)	12.6359(3)	13.1298(5)	16.9234(2)
<i>c</i> , Å	10.6255(9)	26.3943(7)	27.1445(13)	26.5829(4)
<i>α</i> , deg	79.746(7)	90	90	90
<i>β</i> , deg	73.045(8)	102.446(3)	100.700(6)	90
<i>γ</i> , deg	61.024(9)	90	90	90
<i>V</i> , Å ³	798.03(15)	3946.06(17)	3634.2(3)	8585.7(2)
<i>Z</i>	1	4	4	8
<i>ρ</i> _{calc.} (g cm ⁻³)	1.242	1.481	1.615	1.513
<i>μ</i> (Mo Kα), mm ⁻¹	0.170	1.464	3.491	2.532
<i>F</i> (000)	318.0	1808.0	1784.0	3856.0
crystal size, mm	0.123 × 0.08 × 0.068	0.250 × 0.105 × 0.085	0.19 × 0.11 × 0.09	0.125 × 0.118 × 0.075
<i>T</i> (K)	150	150	150	150
2 <i>θ</i> range, deg	5.068 to 49.992	2.358 to 31.0145°	4.556 to 49.994	3.065 to 31.208
Total no. reflns	7245	29108	29523	223620
No. of indep reflns	2789 [R _{int} = 0.0738]	6918 [R _{int} = 0.0963]	6393 [R _{int} = 0.1138]	13598 [R _{int} = 0.0888]
<i>S</i>	1.052	1.054	1.101	1.063
<i>R</i> ₁	0.0701	0.0390	0.0863	0.0474
<i>wR</i> ₂	0.1835	0.0966	0.1842	0.1167

Table S2. Crystallographic information for compounds 7–10.

	7 ·3(CH ₂ Cl ₂)	8 ·(C ₂ H ₄ Cl ₂)	9 ·0.66(CHCl ₃), 2.34(CH ₂ Cl ₂)	10 ·(CH ₂ Cl ₂)
Empirical formula	C ₇₁ H ₉₀ Ag ₄ Br ₄ Cl ₆ N ₁₂ P ₄	C ₃₆ H ₄₆ Ag ₂ Cl ₂ I ₂ N ₆ P ₂	C ₄₁ H _{53.34} Ag ₂ Cl _{6.66} N ₆ O ₄ P ₂	C ₃₅ H ₄₄ Au ₂ Cl ₄ N ₆ P ₂
Formula weight	2199.24	1065.17	1208.056	1146.43
Crystal system	triclinic	orthorhombic	triclinic	monoclinic
Space group	P-1	Pbca	P-1	P2 ₁ /c
a/Å	13.3674(4)	18.9149(5)	12.6903(3)	9.2017(2)
b/Å	17.7306(8)	17.4523(5)	13.7105(3)	32.7903(6)
c/Å	20.2898(6)	26.6732(7)	16.3337(4)	13.2599(3)
α/°	83.651(3)	90	67.733(2)	90
β/°	74.880(3)	90	85.412(2)	98.888(2)
γ/°	70.200(3)	90	75.516(2)	90
Volume/Å ³	4366.7(3)	8805.0(4)	2546.05(11)	3952.82(15)
Z	2	8	2	4
ρ _{calc.} (g cm ⁻³)	1.673	1.758	1.576	1.926
μ (Mo Kα), mm ⁻¹	3.016	2.518	1.226	7.800
F(000)	2182.0	4544	1220.05	2208.0
Size	0.123 × 0.023 × 0.012	0.103 × 0.078 × 0.075	0.123 × 0.053 × 0.024	0.089 × 0.067 × 0.065
T (K)	150	150	150	150
2θ range, deg	3.438 to 49.998	3.524 to 145.528	4.086 to 50	3.348 to 53.996
Reflections collected	168363	97689	142218	119124
Independent reflections	15366 [R _{int} = 0.1353]	7751 [R _{int} = 0.0833]	8975 [R _{int} = 0.1213]	8615 [R _{int} = 0.0832]
S	1.021	1.035	1.046	1.018
R _I ^a	0.0778	0.0363	0.0458	0.0358
wR ₂	0.2249	0.0931	0.1223	0.0889

Table S3. Important bond distances in the Cu(I) complexes (3–5) as obtained from the X-ray crystal structure and DFT optimization (wb97xd/Def2SVP). All distances in Å.

System	Cu1–P1	Cu2–P2	C1–C2	Cu1–C2	Cu2–C1	Cu1–Cu2
Complex 3 (found)	2.1757	2.1835	1.391	2.950	2.746	2.7617
Complex 3 (calc.)	2.1761	2.1835	1.3896	2.9298	2.7661	2.7615
Complex 4 (found)	2.191	2.207	1.407	2.794	2.640	2.7036
Complex 4 (calc.)	2.1913	2.2065	1.4076	2.7987	2.6398	2.7035
Complex 5 (found)	2.2244	2.2245	1.402	2.856	2.852	2.8316
Complex 5 (calc.)	2.2246	2.2243	1.4029	2.8518	2.856	2.8315

Table S4. Selected topological properties of complexes 3, 4, and 5.

Complex	$\rho(r)$	λ_2	$\nabla^2 \rho(r)$	G(r)
3-BCP-1	0.0133	-0.0065	0.0322	0.0083
3-BCP-2	0.0175	-0.0100	0.0479	0.0121
4-BCP-1	0.0166	-0.0084	0.0444	0.0112
4-BCP-2	0.0220	-0.0139	0.06f	0.0167
5-BCP-1	0.0159	-0.0073	0.0382	0.0100
5-BCP-2	0.0159	-0.0078	0.0387	0.0101