Supporting information

New 1,2,3-triazole based bis- and tris-phosphine ligands: synthesis, transition metal chemistry and catalytic studies

Latchupatula Radhakrishna,[a] Harish S. Kunchur, [a§] Pavan K. Namdeo, [a§] Ray J. Butcher[b] and Maravanji S. Balakrishna[*a]

[a]*Phosphorus Laboratory, Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India.*
[b]*Department of Chemistry, Howard University, Washington, D. C. 20059, USA*
[§]Contributed equally to this work

*Author to whom correspondence should be addressed. E-mail: krishna@chem.iitb.ac.in, msb_krishna@iitb.ac.in (M. S. Balakrishna); Fax: +91-22-5172-3480/2576-7152.

NMR spectral data of compounds a-i

(E)-1,2-diphenylethene (**a**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.50 (m, 4H), 7.46 – 7.34 (m, 4H), 7.28 (ddd, *J* = 7.6, 4.0, 1.3 Hz, 2H), 7.14 (d, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.52, 128.86, 127.79, 126.70.

(E)-1-methyl-4-styrylbenzene (**b**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.4 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.26 (dd, *J* = 8.1, 6.5 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 2.5 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.71, 134.74, 129.58, 128.83, 127.89, 127.59, 126.61, 126.58, 21.44.

(E)-1-methyl-3-styrylbenzene (**c**)[1b, 2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.49 (m, 2H), 7.41 – 7.31 (m, 4H), 7.30 – 7.23 (m, 2H), 7.13 – 7.06 (m, 3H), 2.38 (d, *J* = 15.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.40, 137.61, 137.45, 128.99, 128.85, 128.76, 128.67, 128.64, 127.72, 127.39, 126.66, 123.89, 21.62.

(E)-1-chloro-4-styrylbenzene (**d**)[1b]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dt, *J* = 2.7, 1.7 Hz, 2H), 7.48 – 7.42 (m, 2H), 7.35 (ddt, *J* = 13.4, 8.9, 2.0 Hz, 4H), 7.31 – 7.25 (m, 1H), 7.13 – 7.01 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.17, 136.03, 133.35, 129.50, 129.02, 128.91, 128.05, 127.84, 127.55, 126.73.

(E)-4-styrylbenzonitrile (**e**)[3]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 7.5 Hz, 2H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.35 – 7.30 (m, 1H), 7.21 (d, *J* = 16.3 Hz, 1H), 7.09 (d, *J* = 16.3

Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.97, 136.43, 132.62, 132.54, 129.00, 128.79, 127.07, 127.01, 126.86, 119.18, 110.71.

(E)-1-methoxy-3-styrylbenzene (**f**)[4]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.48 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.16 – 7.03 (m, 4H), 6.83 (dd, *J* = 8.1, 1.8 Hz, 1H), 3.86 (s, 3H).

(E)-1-bromo-2-styrylbenzene (**g**)[5]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 – 7.65 (m, 1H), 7.62 – 7.53 (m, 3H), 7.47 (d, *J* = 16.2 Hz, 1H), 7.39 (dd, *J* = 10.4, 4.8 Hz, 2H), 7.33 – 7.27 (m, 2H), 7.15 – 7.09 (m, 1H), 7.08 – 7.02 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.36, 137.22, 133.27, 131.65, 128.98, 128.94, 128.27, 127.74, 127.68, 127.04, 126.91, 124.34.

(E)-2-styrylthiophene (**h**)[1b]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.4 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.26 (d, *J* = 3.0 Hz, 1H), 7.21 (dd, *J* = 10.9, 5.3 Hz, 2H), 7.07 (d, *J* = 3.4 Hz, 1H), 7.01 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.93 (d, *J* = 16.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.07, 137.14, 128.88, 128.52, 127.78, 126.48, 126.28, 124.52, 121.96.

(E)-3-styrylthiophene (**i**)[6]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.5 Hz, 2H), 7.38 – 7.31 (m, 4H), 7.26 (dd, *J* = 6.2, 4.3 Hz, 2H), 7.16 – 7.10 (m, 1H), 6.96 (d, *J* = 16.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.31, 137.56, 128.86, 127.64, 126.46, 126.37, 125.11, 123.08, 122.53.

Table S1. Crystallographic Information for **5**, **6**, **8**, **9**, **12** and **13**

	5	**6**	**8**	**9**	**12**	**13**
Formula	$C_{38}H_{29}N_3P_2$	$C_{38}H_{29}N_3P_2$	$C_{42}H_{29}MoN_3O_4P_2$	$C_{44}H_{33}Cl_4N_3O_4P_2W$	$C_{44}H_{32}MoN_4O_4P_2$	$C_{42}H_{29}N_3O_4P_2W$
Formula weight	589.58	589.58	797.56	1055.32	838.61	885.47
Temperature/K	150	150	150	150	150	150
Crystal system	triclinic	monoclinic	monoclinic	triclinic	triclinic	triclinic
Space group	P-1	$P2_1/c$	$P2_1/c$	P-1	P-1	P-1
a/Å	11.9846(4)	11.9547(5)	13.9968(8)	10.93180(10)	8.8012(3)	8.9297(3)
b/Å	17.0460(6)	10.9927(4)	19.0202(9)	12.0240(2)	16.0063(7)	13.0206(4)
c/Å	17.7261(5)	23.6721(10)	17.4142(8)	17.6156(3)	16.2933(7)	16.7334(5)
α/°	111.601(4)	90	90	94.8810(10)	110.228(4)	102.136(2)
β/°	93.453(3)	93.244(4)	110.220(6)	106.2740(10)	102.707(4)	99.903(2)
γ/°	110.334(3)	90	90	101.0640(10)	105.324(4)	103.182(2)
Volume/$Å^3$	3082.69(19)	3105.9(2)	4350.3(4)	2157.55(6)	1950.37(15)	1801.89(10)
Z	4	4	4	2	2	2
$\rho_{calc}g/cm^3$	1.270	1.261	1.218	1.624	1.428	1.632
μ/mm^{-1}	0.173	0.172	0.415	3.045	0.467	3.342
F(000)	1232	1232	1624	1044	856	876
Crystal size/mm^3	0.205 × 0.184 × 0.163	0.156 × 0.124 × 0.098	0.186 × 0.125 × 0.086	0.158 × 0.124 × 0.086	0.118 × 0.095 × 0.063	0.215 × 0.178 × 0.124
2Θ range	3.712 to 62.53	4.086 to 62.252	4.282 to 62.24	3.49 to 62.186	4.854 to 62.404	4.696 to 62.36
Reflections collected	32956	20849	35131	24915	22899	22495
Independent reflections	17742	9083	12655	12412	11269	10397
S	1.040	1.045	1.077	1.034	1.026	1.031
R_1	0.0769	0.0652	0.0935	0.0294	0.0823	0.0234
wR_2	0.2272	0.1615	0.1943	0.0657	0.1626	0.0537

Table S2 Crystallographic Information for **14-17** and **21**

	14	**15**	**16**	**17**	**21**
Formula	$C_{39}H_{31}Cl_4N_3P_2Pd$	$C_{39}H_{29}Cl_4N_3P_2Pt$	$C_{39}H_{29}Cl_4N_3P_2Pd$	$C_{56}H_{46}ClN_3NiP_2$	$C_{39}H_{28}N_3OP_2Rh$
Formula weight	851.81	938.48	849.79	917.06	719.49
Temperature/K	150	150	150	150	150
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/c$	P-1	P-1
a/Å	11.5130(10)	11.5113(3)	19.0043(6)	10.05434(14)	10.2700(4)
b/Å	13.1004(10)	13.1944(5)	10.0057(3)	11.14458(16)	12.3139(5)
c/Å	25.2960(4)	25.2877(8)	19.8886(6)	22.0783(3)	13.2062(5)
α/°	90	90	90	87.1739(12)	85.921(3)
β/°	103.1600(10)	103.149(3)	107.908(3)	81.6515(12)	80.350(3)
γ/°	90	90	90	71.6855(13)	74.358(3)
Volume/$Å^3$	3715.07(11)	3740.1(2)	3598.6(2)	2323.69(6)	1584.91(11)
Z	4	4	4	2	2
$\rho_{calc}g/cm^3$	1.523	1.667	1.569	1.311	1.508
μ/mm^{-1}	0.906	4.156	0.936	0.585	0.677
F(000)	1720	1840	1712	956	732
Crystal size/mm^3	0.215 × 0.178 × 0.128	0.143 × 0.095 × 0.035	0.204 × 0.202 × 0.13	0.3 × 0.26 × 0.23	0.154 × 0.1 × 0.05
2Θ range	4.782 to 62.36	4.322 to 49.994	4.504 to 49.99	4.454 to 62.428	4.584 to 62.416
Reflections collected	98012	29109	6281	46256	41851
Independent reflections	11376	6575	6281	13613	9428
S	1.04	1.066	1.136	1.038	1.054
R_1	0.0242	0.0566	0.0664	0.0347	0.0435
wR_2	0.0615	0.1278	0.1607	0.0950	0.1048

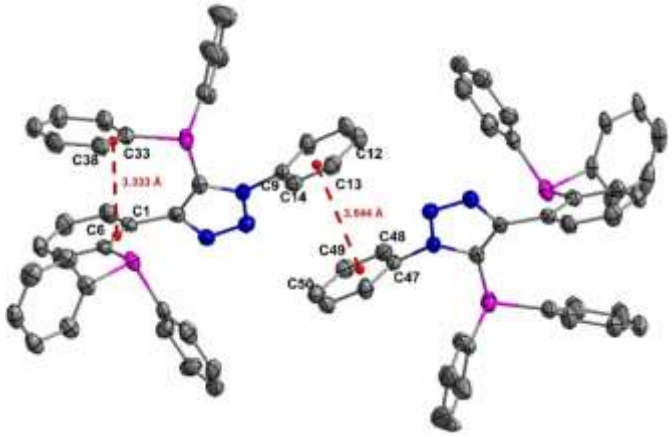


Fig. S1 Molecular structure of **5** showing inter- and intramolecular aromatic π–π interaction.

NMR and mass spectra of 2-21

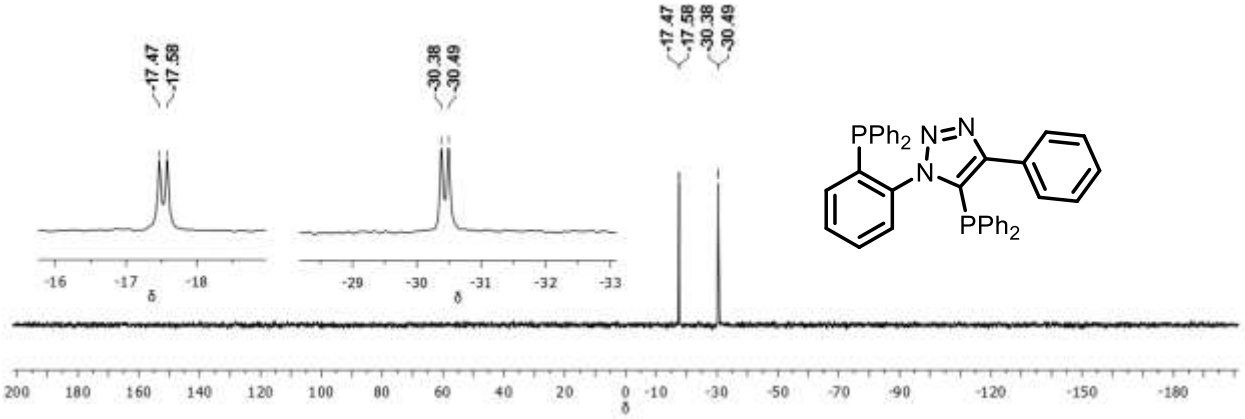


Fig. S2 $^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$ (202 MHz)

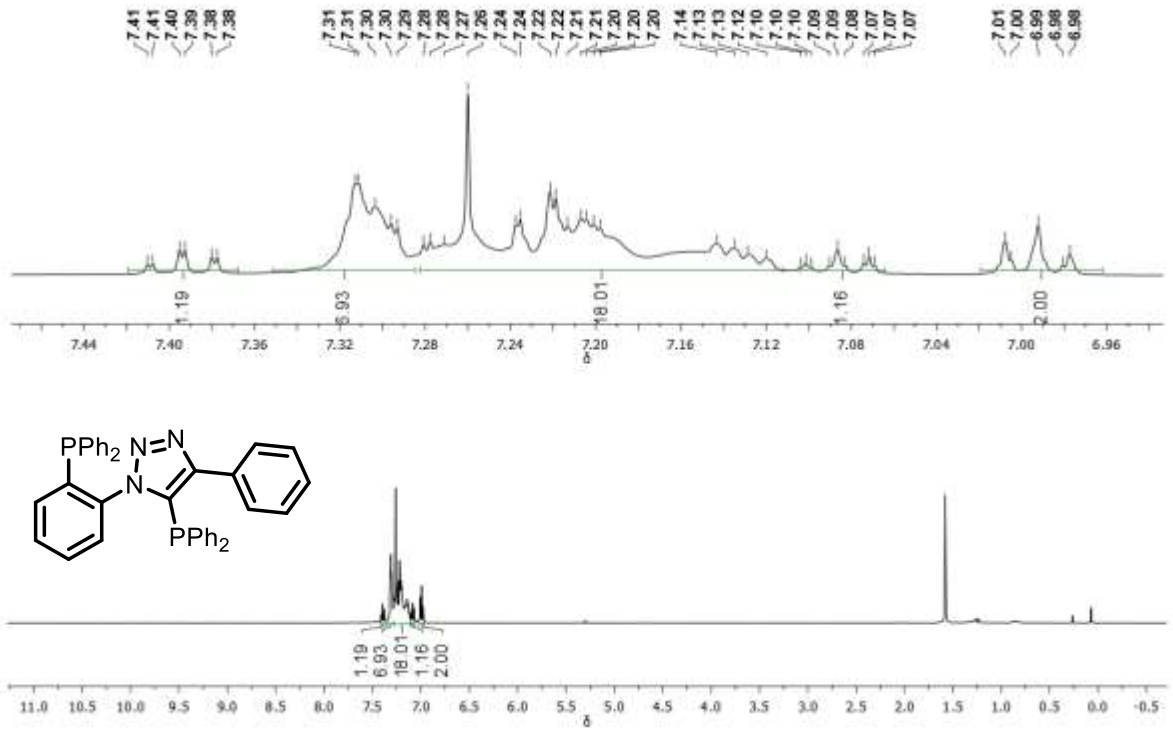


Fig. S3 ^{1}H NMR spectrum of **5** in $CDCl_3$ (500 MHz)

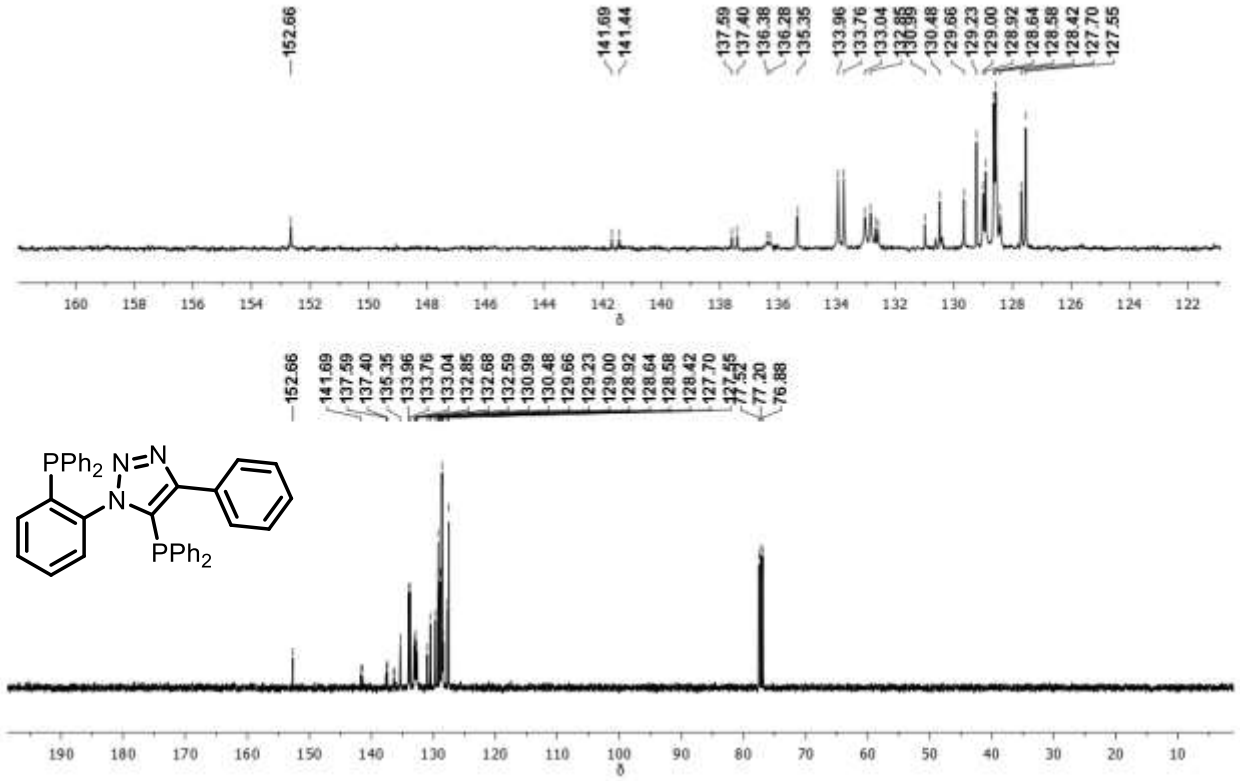
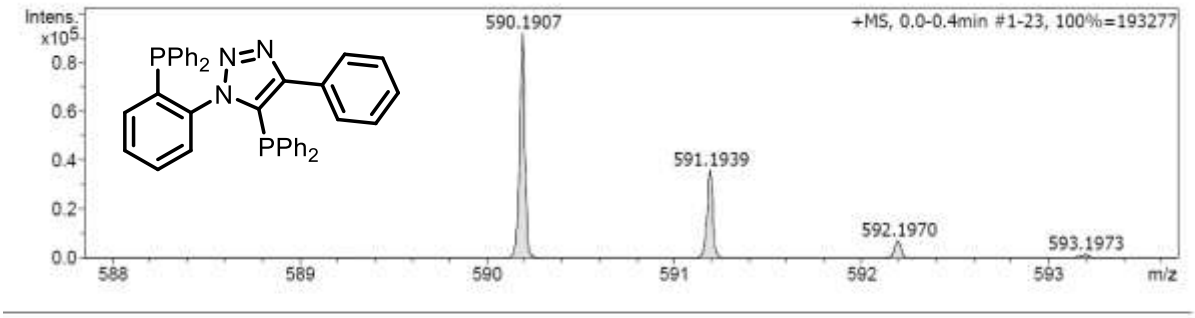


Fig. S4 ^{13}C NMR spectrum of **5** in $CDCl_3$ (101 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
590.1907	1	C38H30N3P2	590.1909	0.5	17.0	1	100.00	26.5	even	ok

Fig. S5 EI mass spectrum of **5**

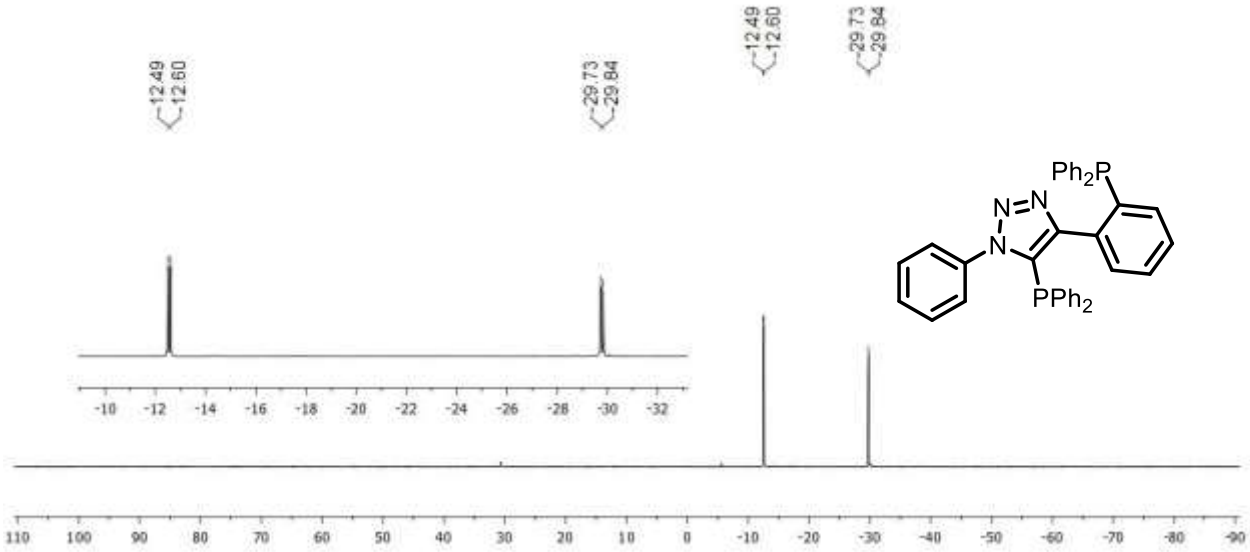


Fig. S6 $^{31}P\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$ (202 MHz)

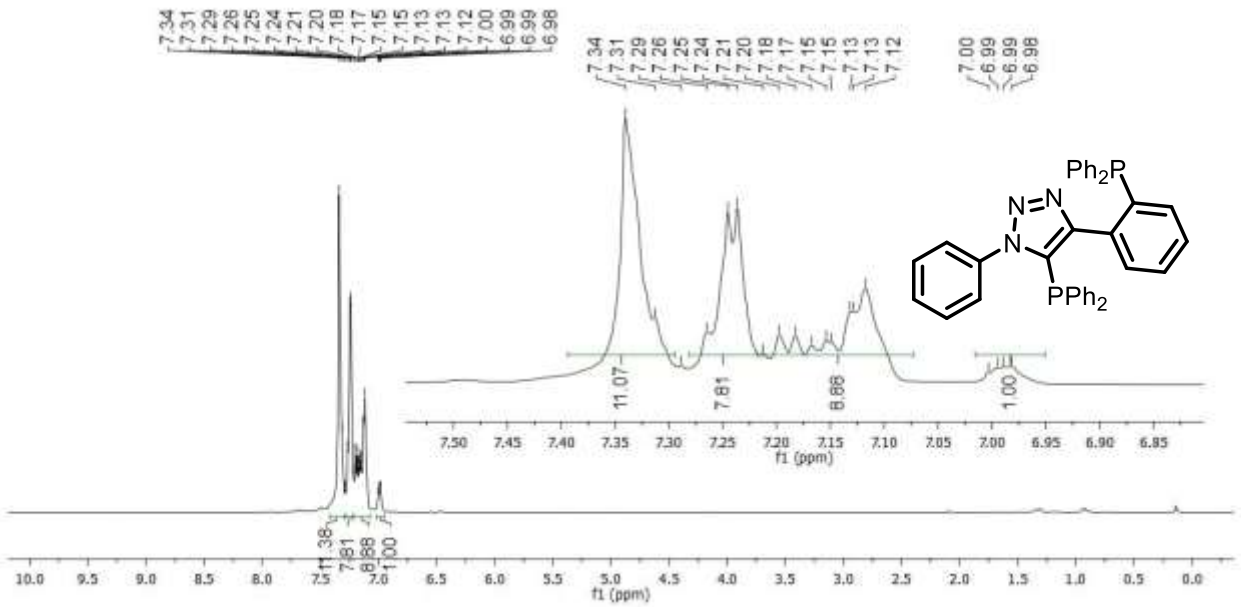


Fig. S7 ^{1}H NMR spectrum of **5** in $CDCl_3$ (500 MHz)

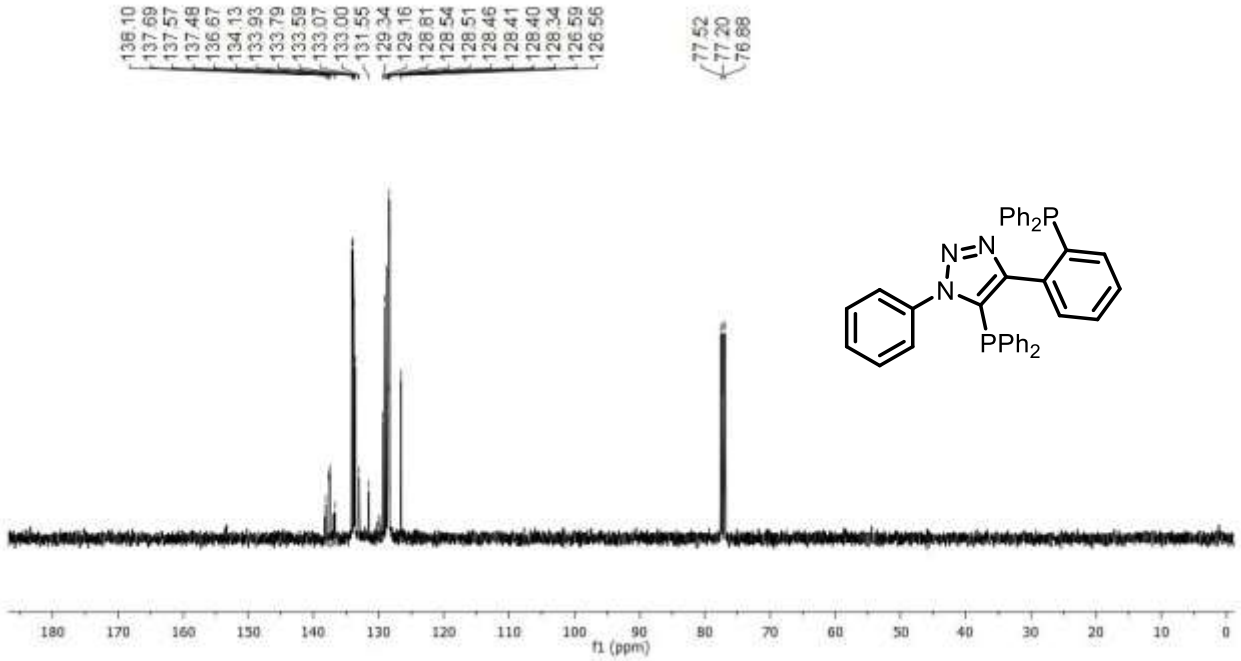
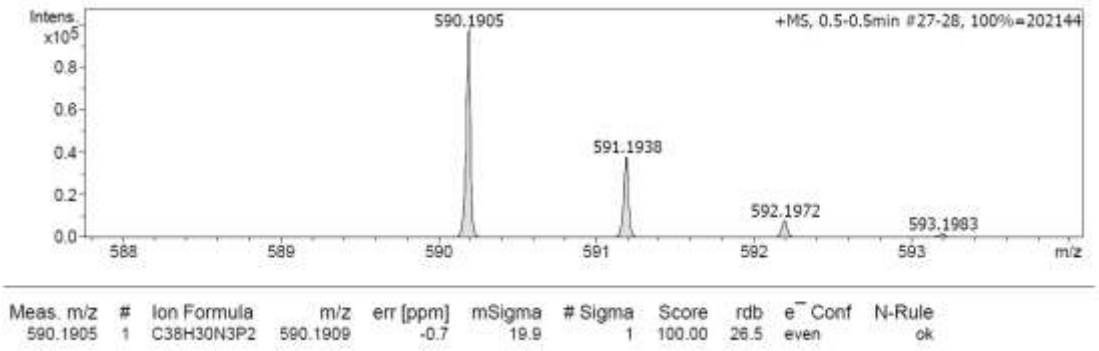


Fig. S8 ^{13}C NMR spectrum of **5** in $CDCl_3$ (101 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
590.1905	1	C38H30N3P2	590.1909	-0.7	19.9	1	100.00	26.5	even	ok

Fig. S9 EI mass spectrum of **5**

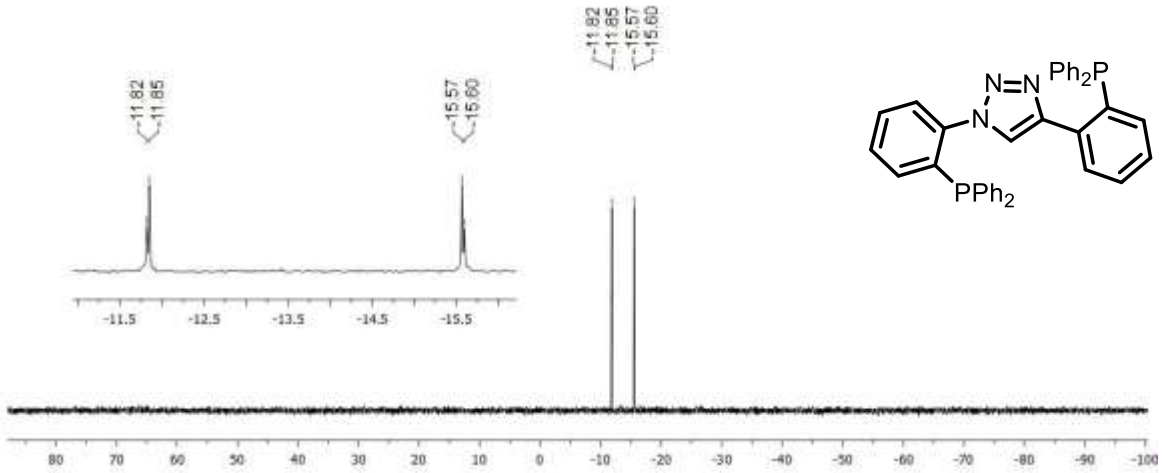


Fig. S10 $^{31}P\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$ (162 MHz)

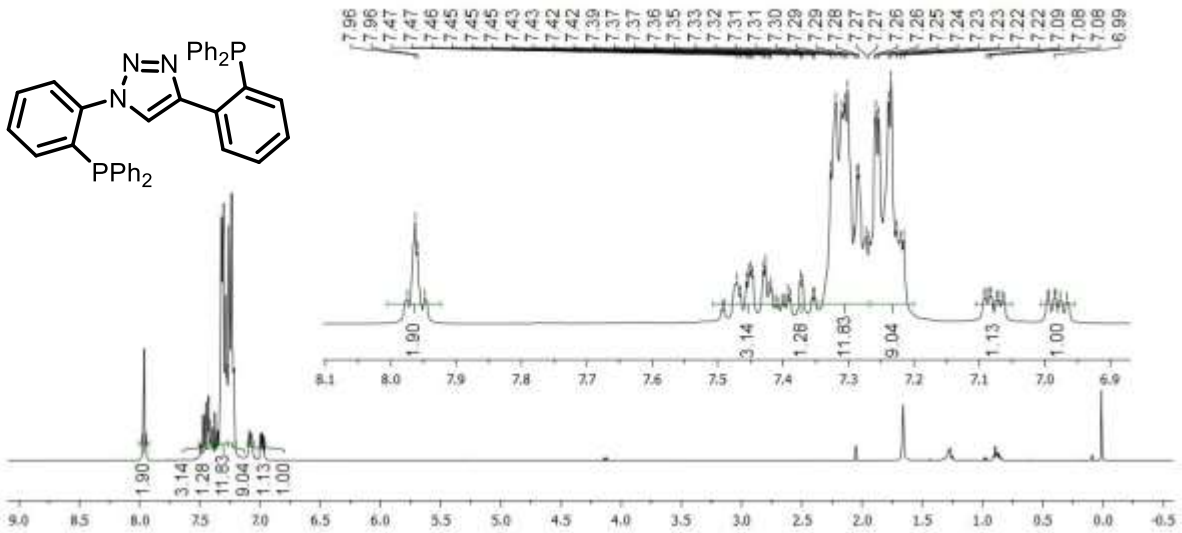


Fig. S11 ^{1}H NMR spectrum of **6** in $CDCl_3$ (400 MHz)

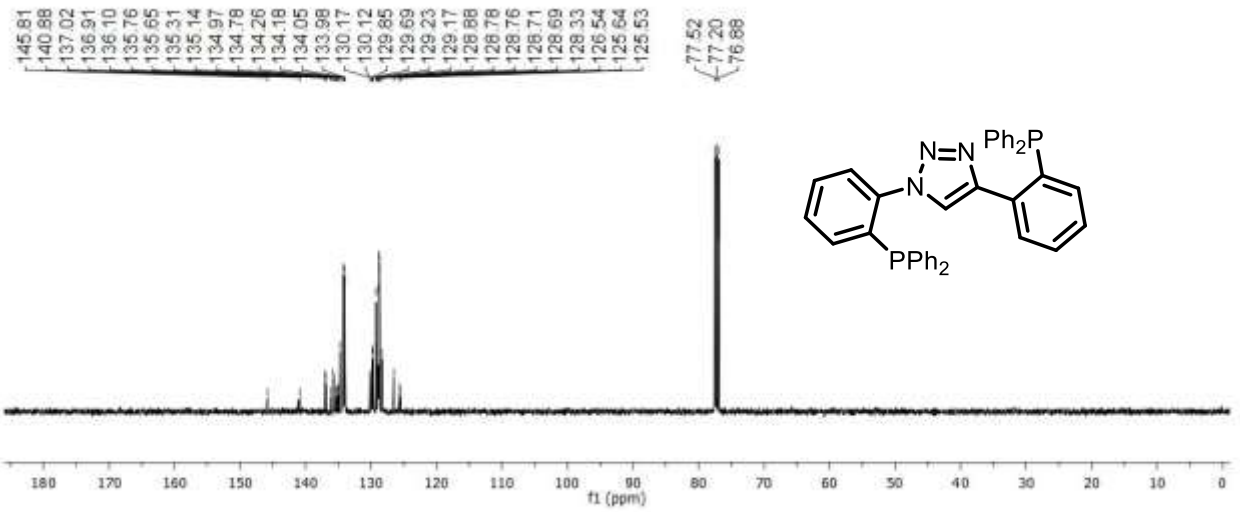
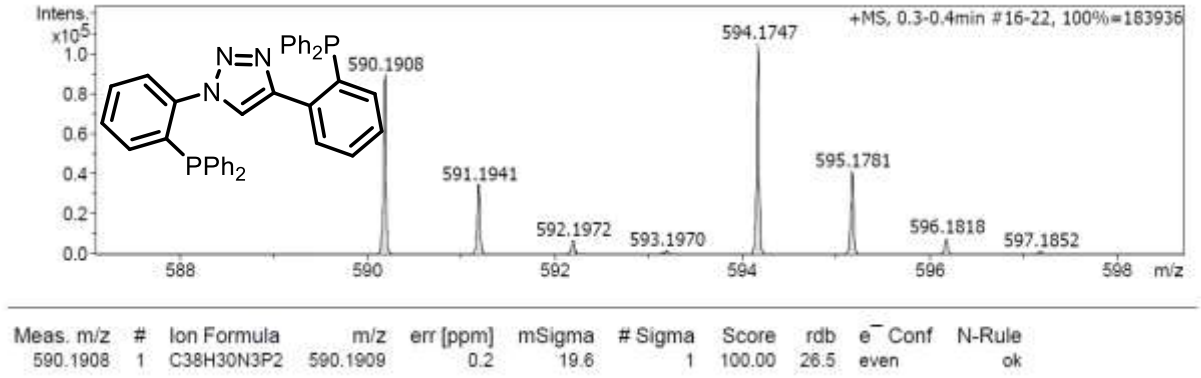


Fig. S12 ^{13}C NMR spectrum of **6** in $CDCl_3$ (101 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
590.1908	1	C38H30N3P2	590.1909	0.2	19.6	1	100.00	26.5	even	ok

Fig. S13 EI mass spectrum of **6**

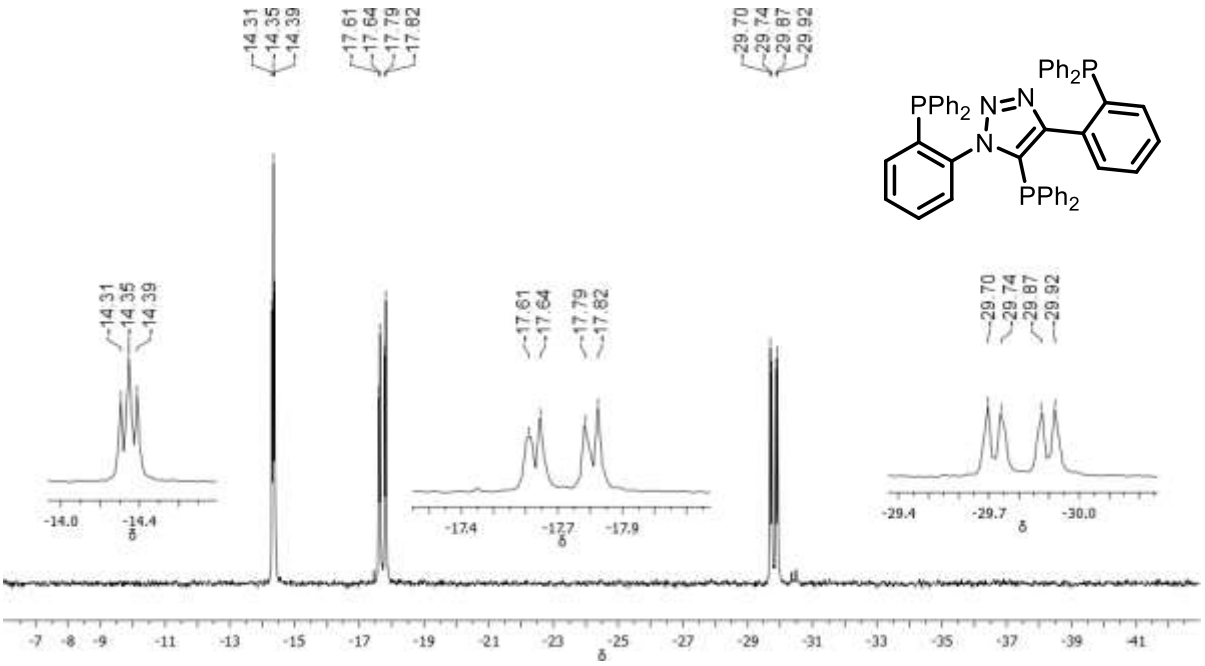


Fig. S14 $^{31}P\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$ (162 MHz)

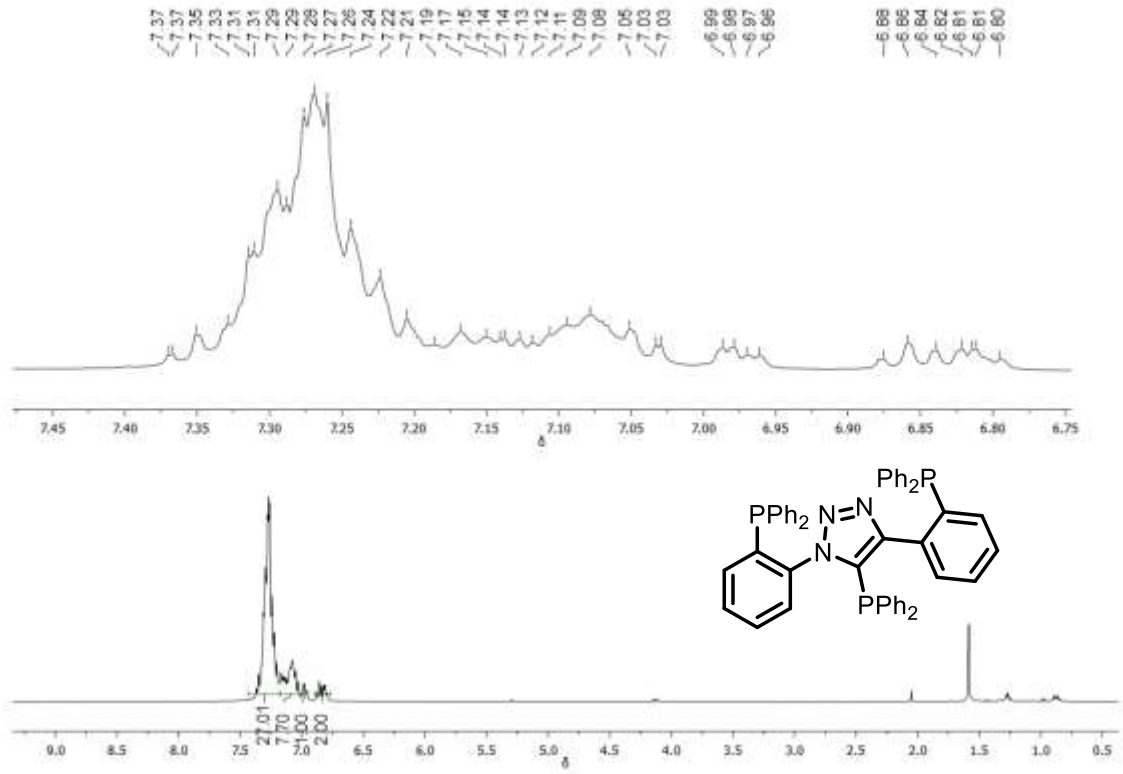


Fig. S15 ^{1}H NMR spectrum of **7** in $CDCl_3$ (400 MHz)

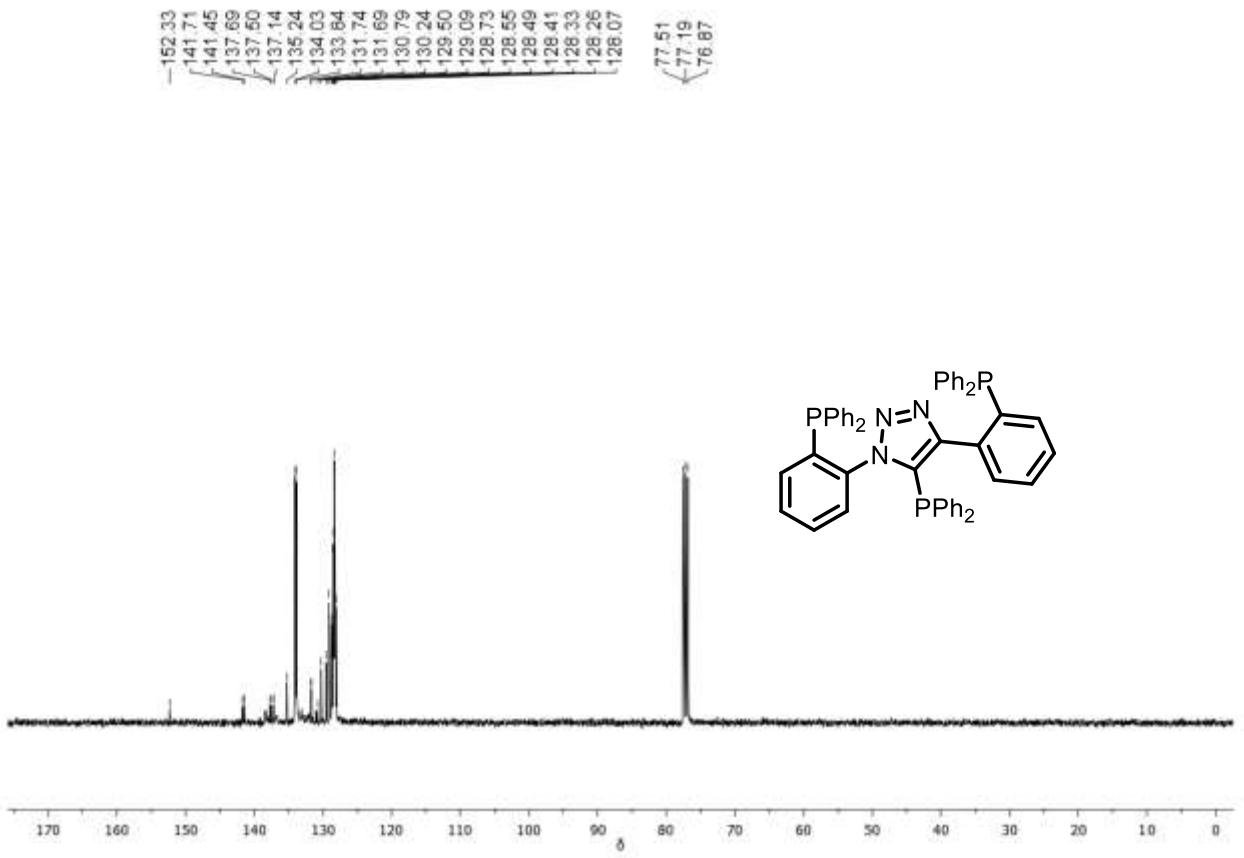
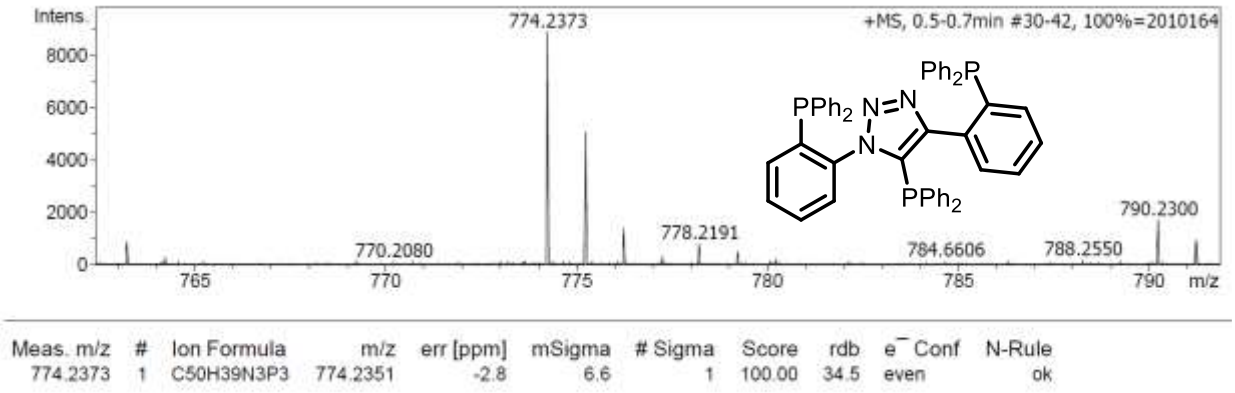


Fig. S16 ^{13}C NMR spectrum of **7** in $CDCl_3$ (101 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
774.2373	1	C50H39N3P3	774.2351	-2.8	6.6	1	100.00	34.5	even	ok

Fig. S17 EI mass spectrum of **7**

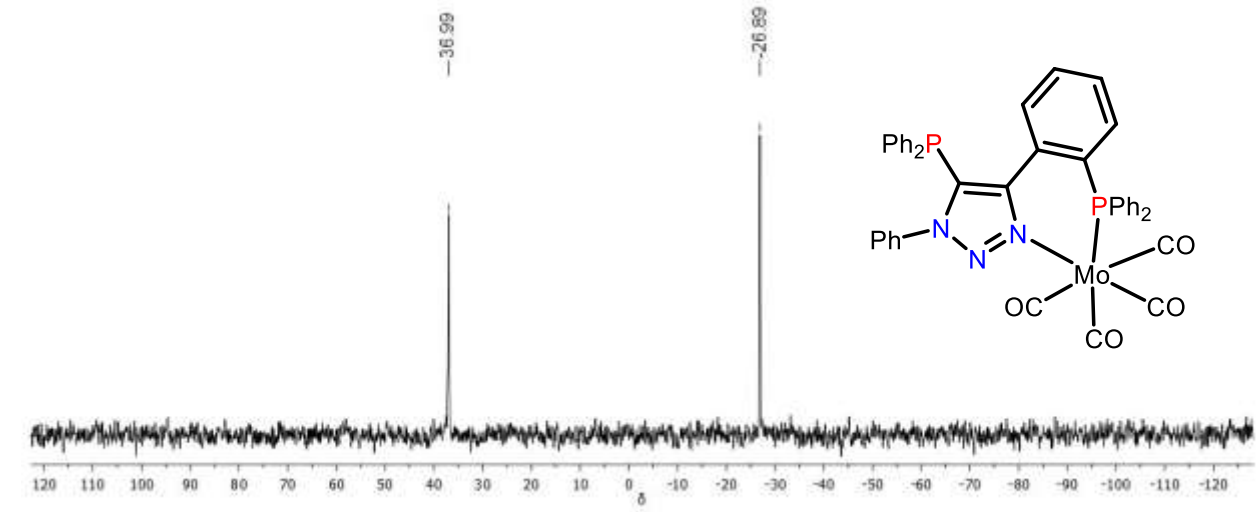


Fig. S18 $^{31}P\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$ (202 MHz)

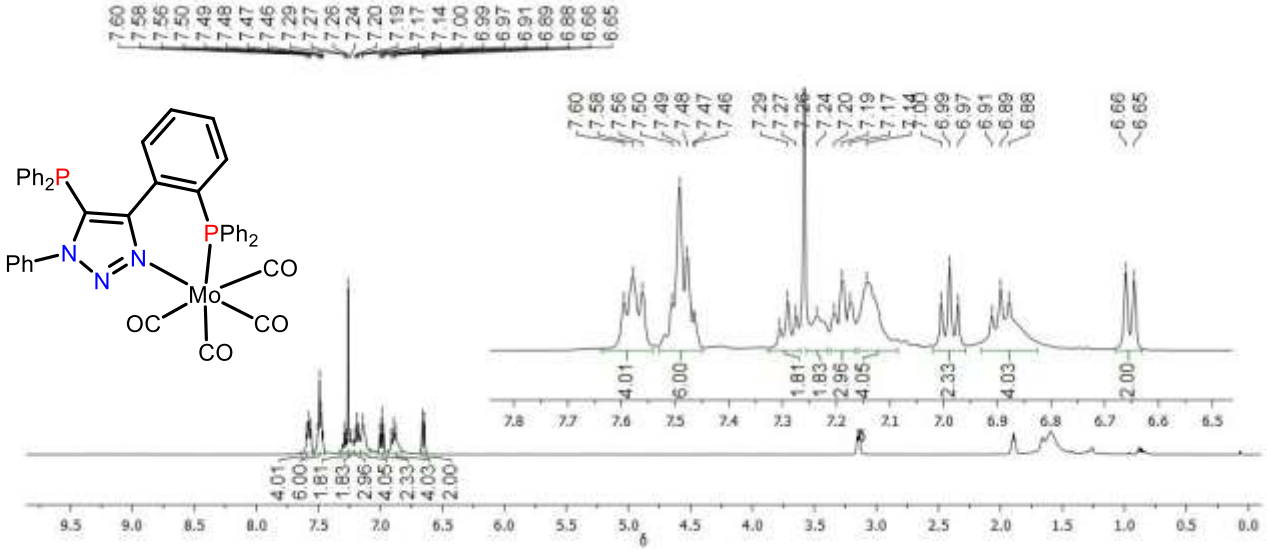


Fig. S19 ^{1}H NMR spectrum of **8** in $CDCl_3$ (500 MHz)

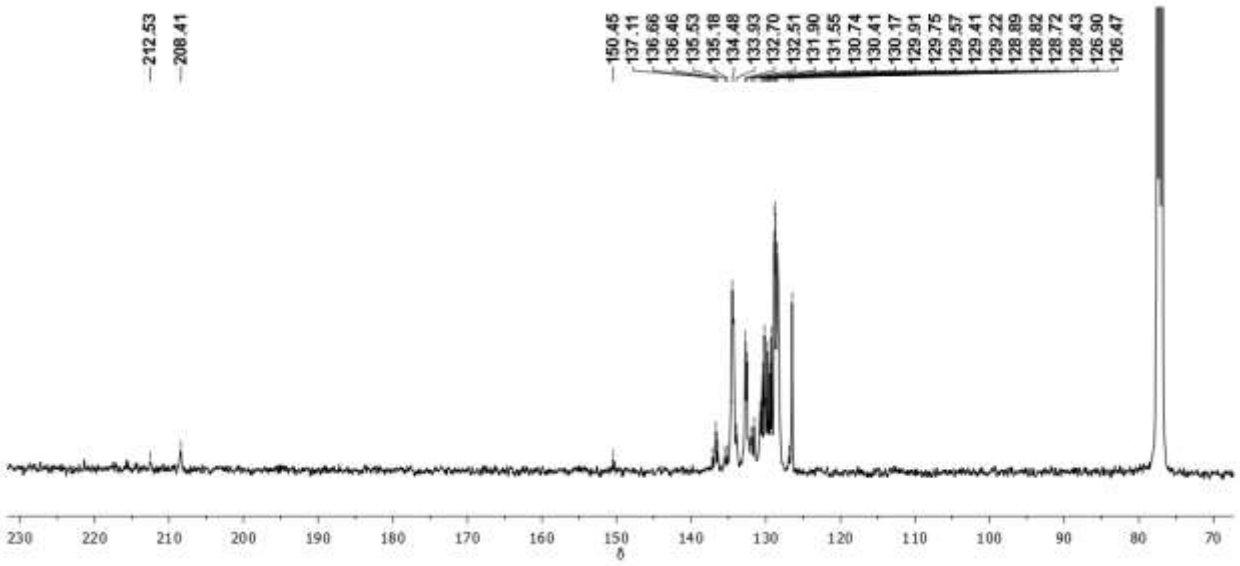


Fig. S20 $^{13}C\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$ (101 MHz)

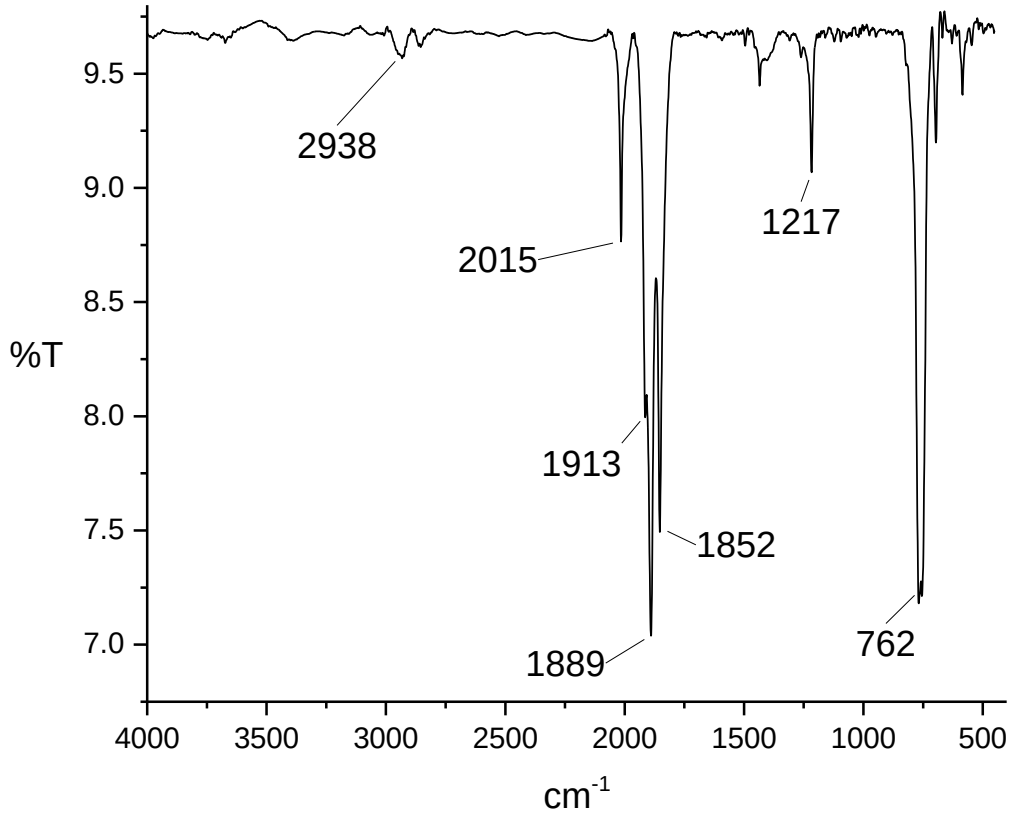


Fig. S21 IR spectrum of **8**

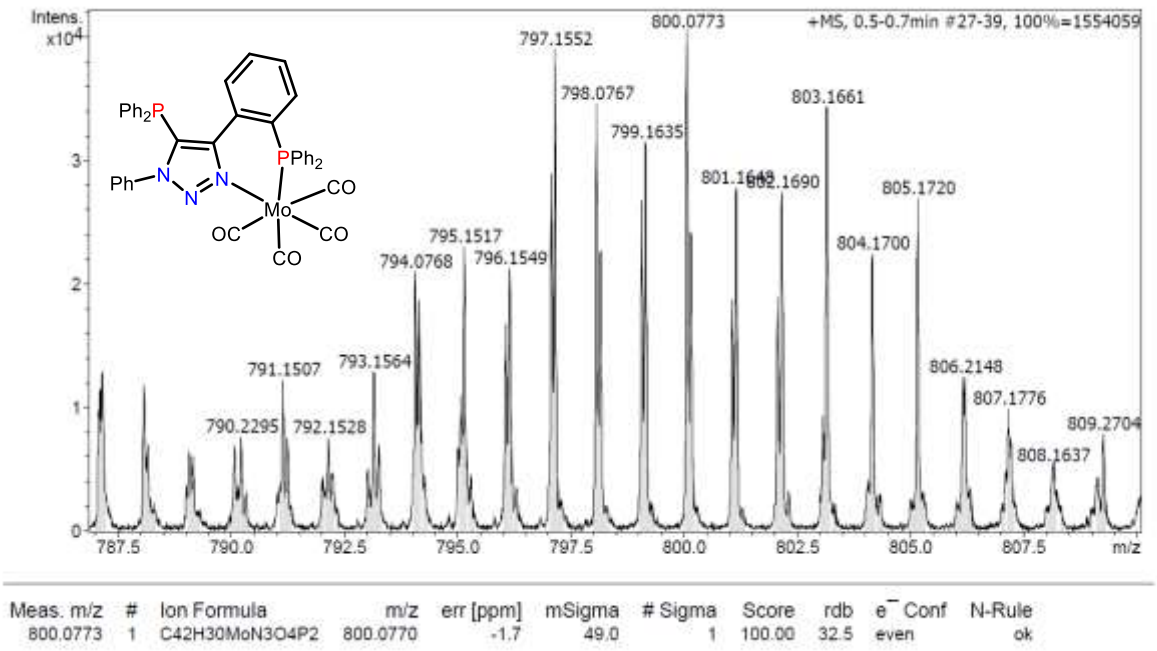


Fig. S22 EI mass spectrum of **8**

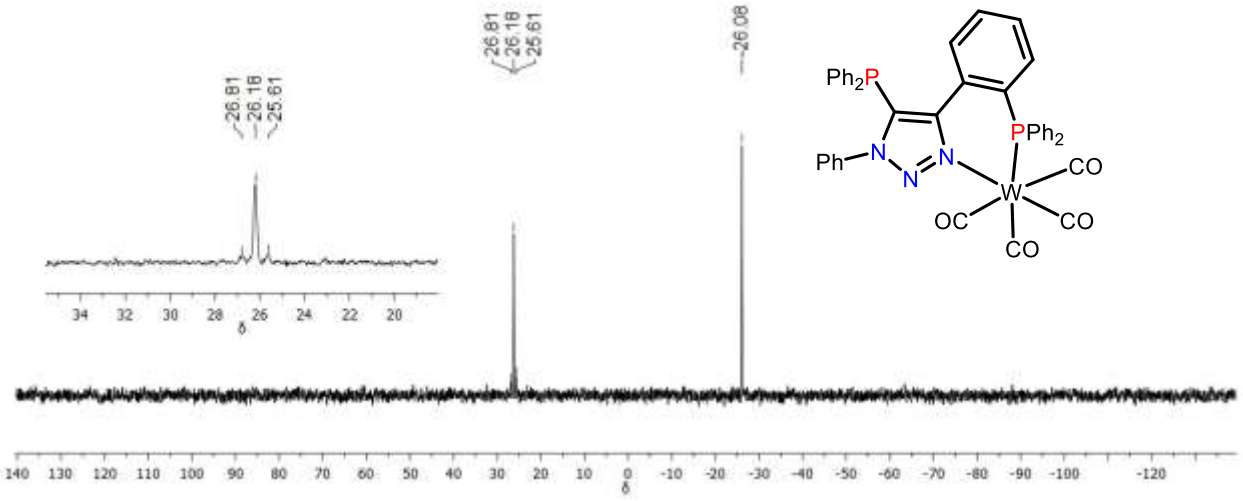


Fig. S23 $^{31}P\{^{1}H\}$NMR spectrum of **9** in $CDCl_3$ (202 MHz)

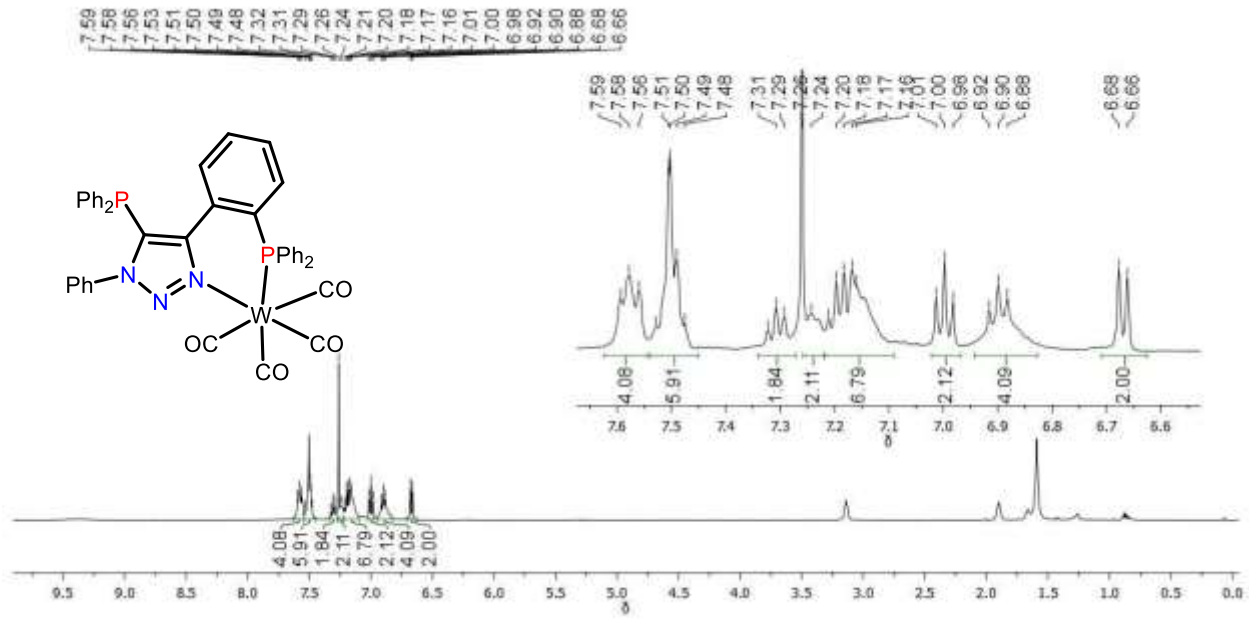


Fig. S24 ^{1}H NMR spectrum of **9** in $CDCl_3$ (500 MHz)

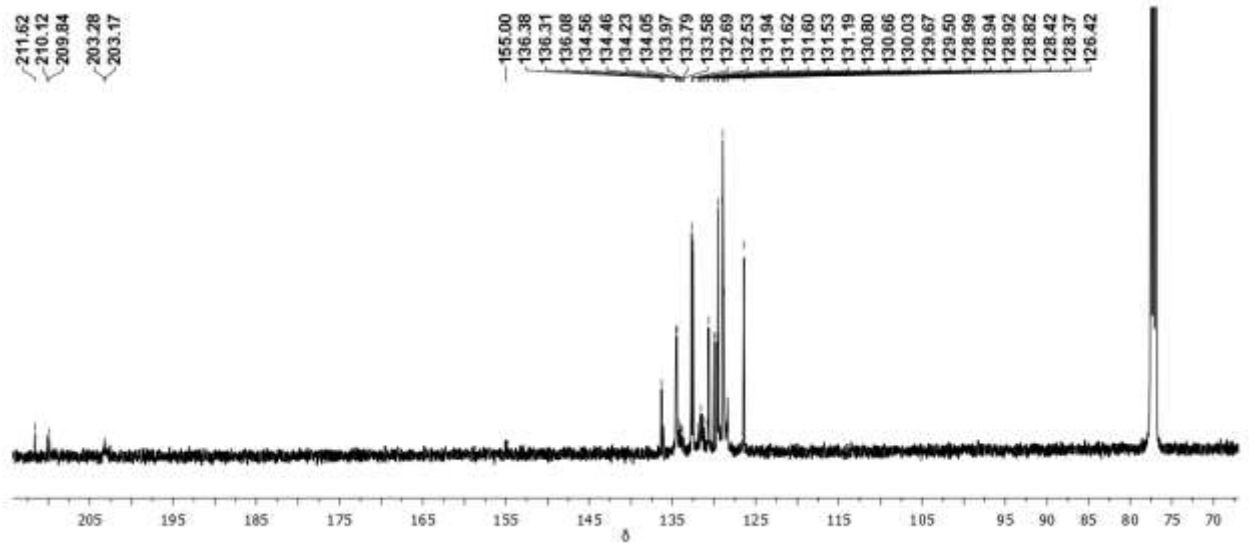


Fig. S25 $^{13}C\{^{1}H\}$ NMR spectrum of **9** in $CDCl_3$ (126 MHz)

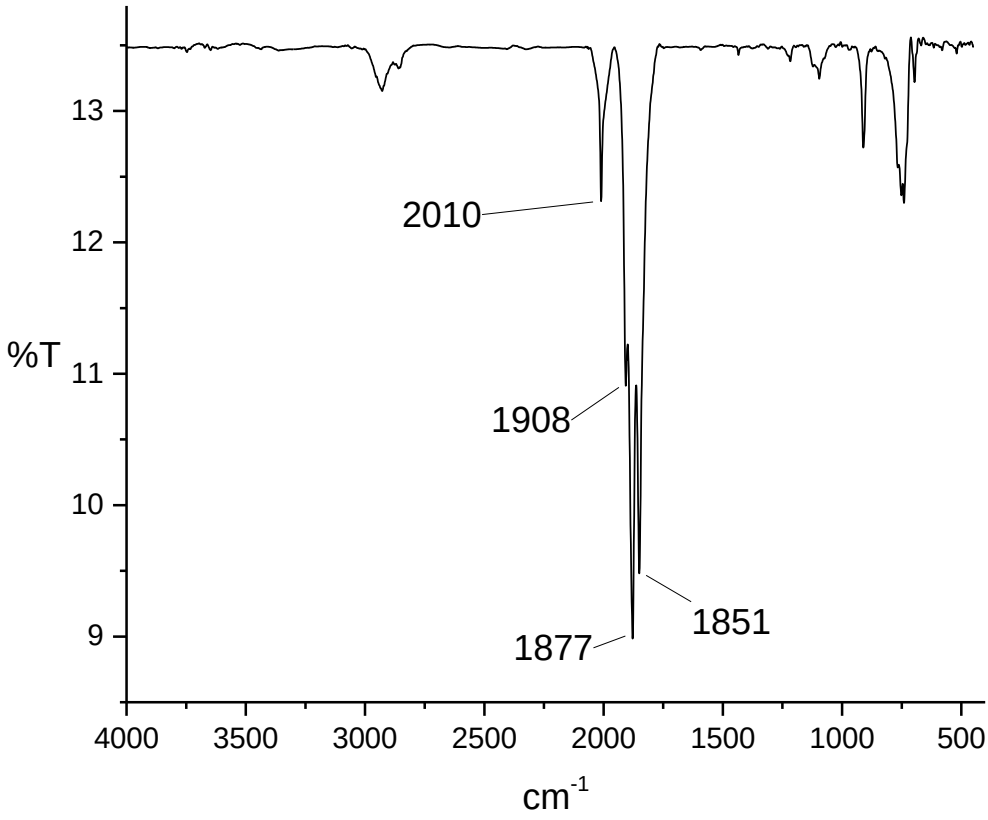


Fig. S26 IR spectrum of **9**

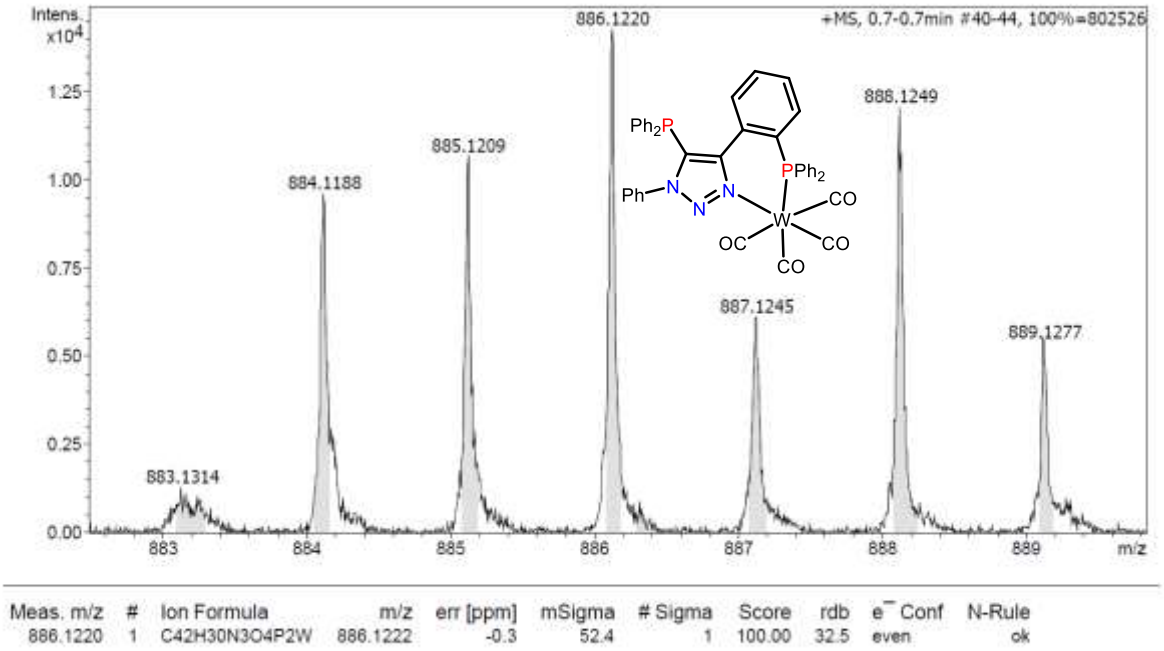


Fig. S27 EI mass spectrum of **9**

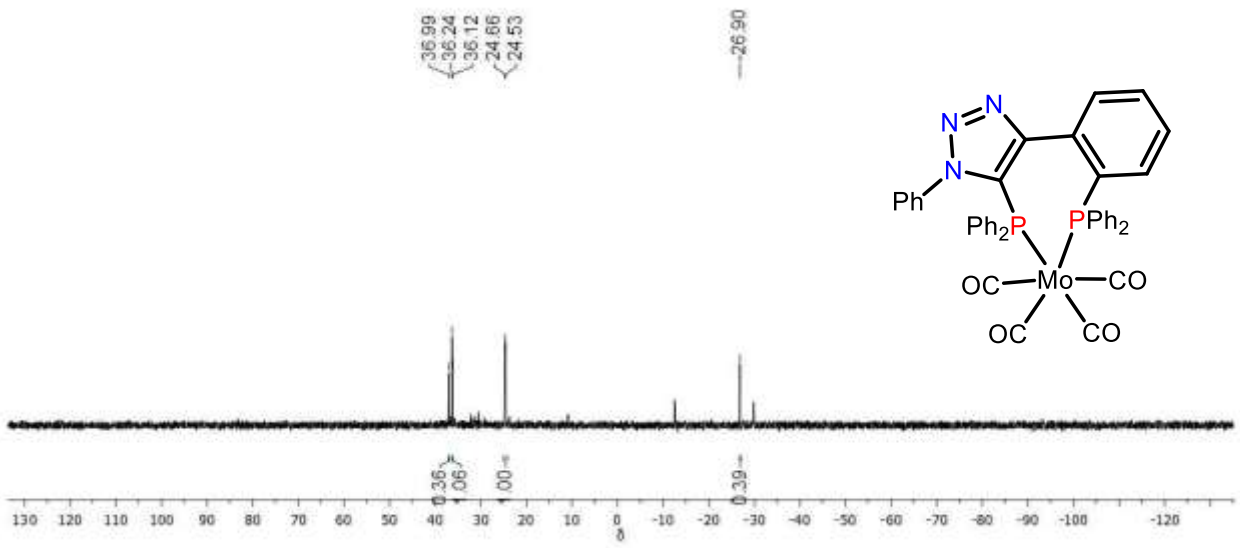


Fig. S28 $^{31}P\{^{1}H\}$ NMR spectrum of **10** in $CDCl_3$ (162 MHz)

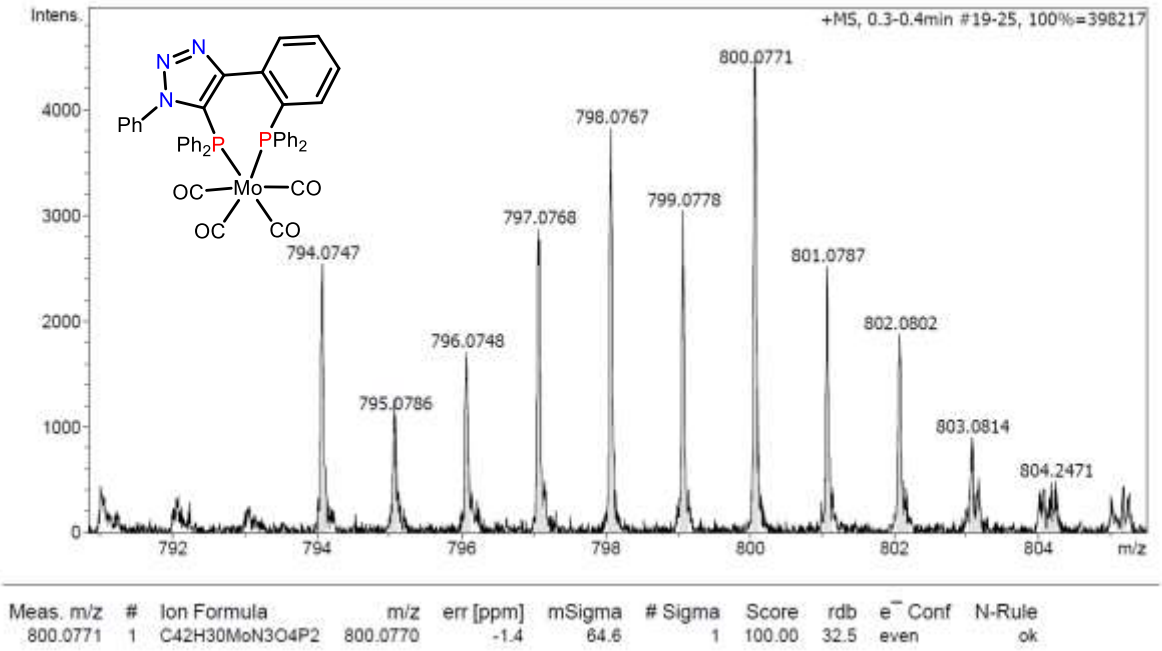


Fig. S29 EI mass spectrum of **10**

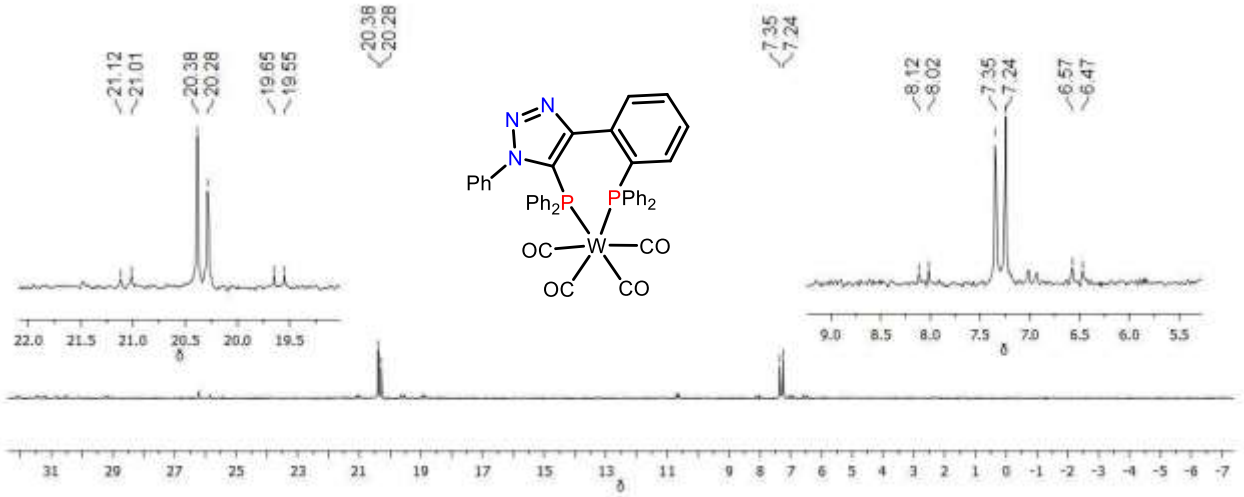


Fig. S30 $^{31}P\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$ (162 MHz)

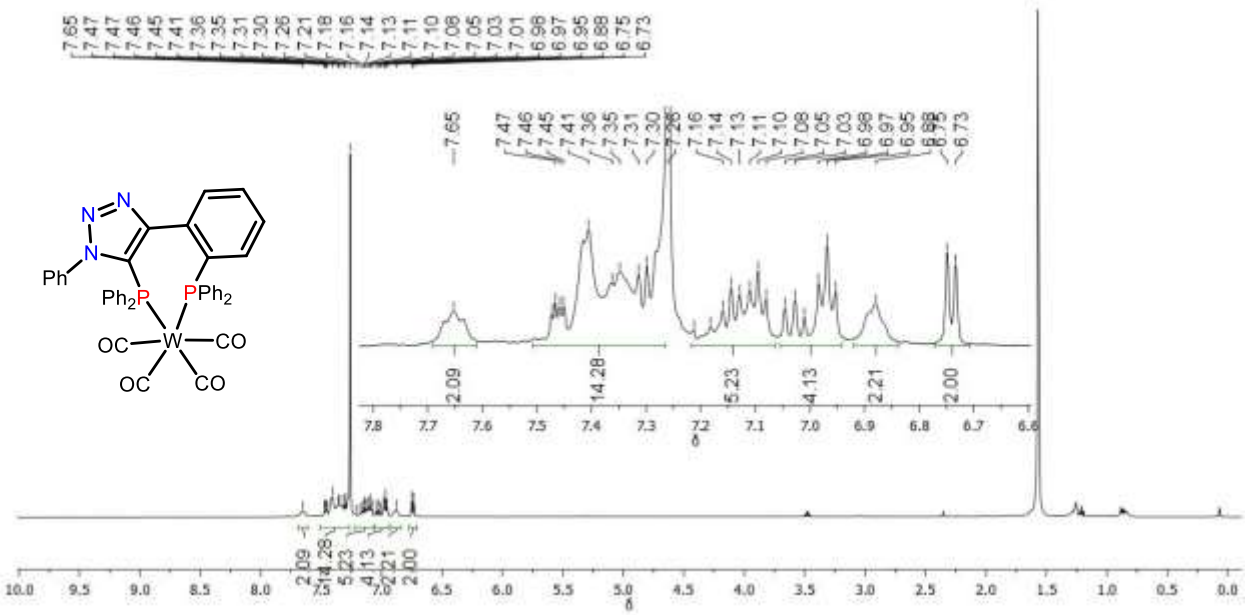


Fig. S31 ^{1}H NMR spectrum of **11** in $CDCl_3$ (500 MHz)

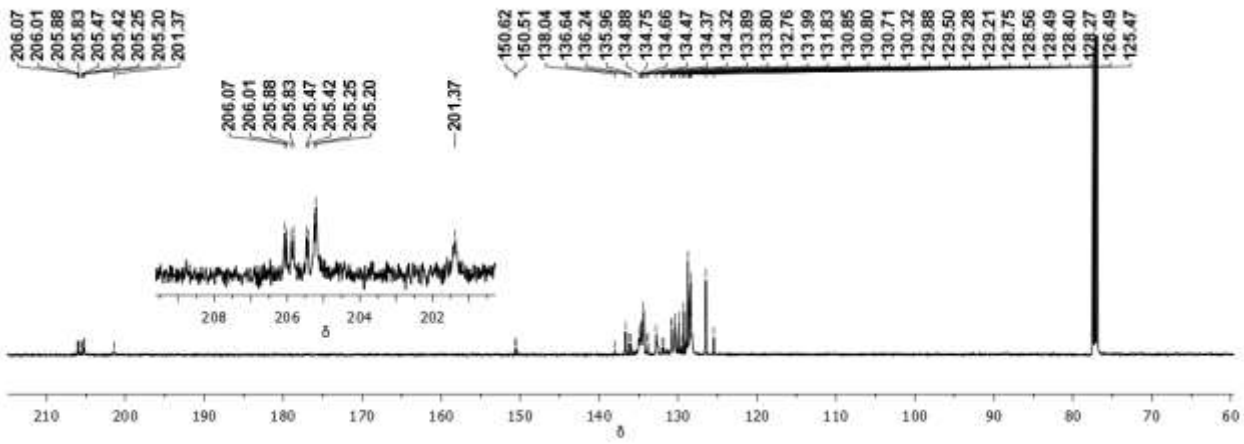


Fig. S32 $^{13}C\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$ (126 MHz)

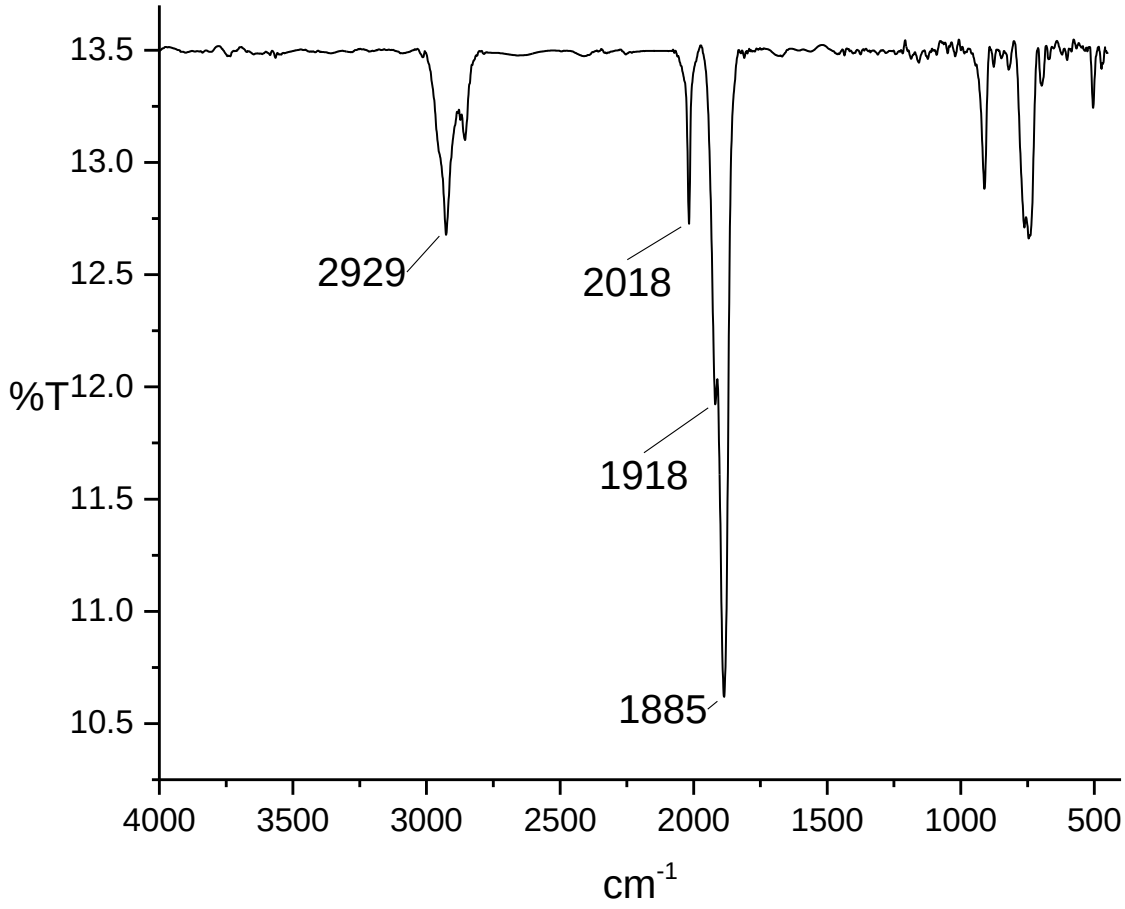


Fig. S33 IR spectrum of **11**

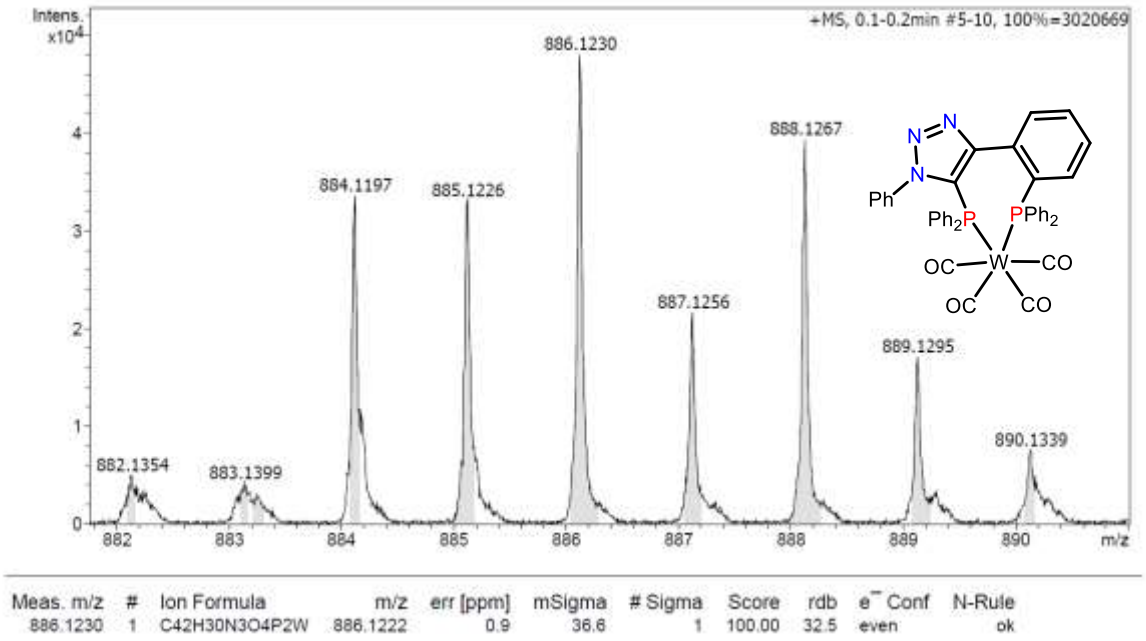


Fig. S34 EI mass spectrum of **11**

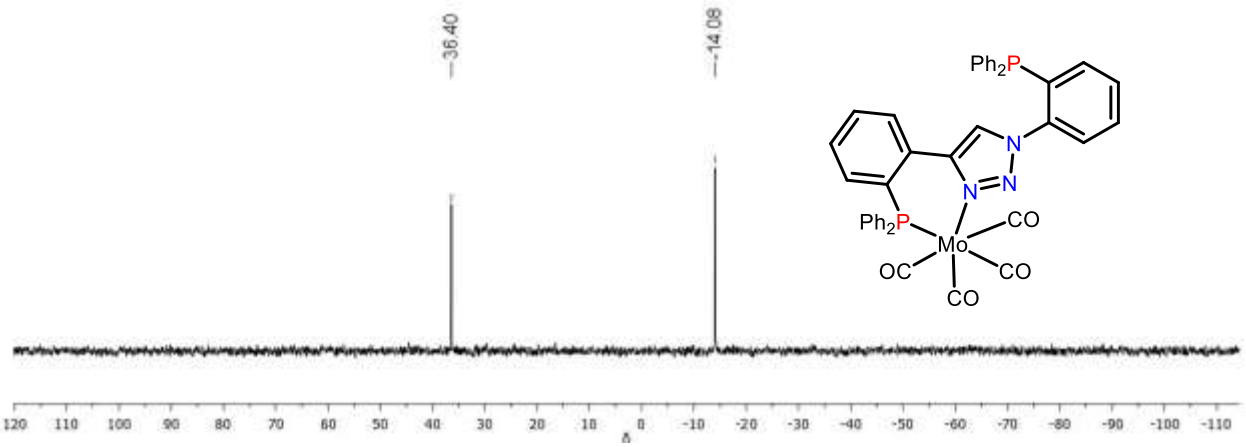


Fig. S35 $^{31}P\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$ (162 MHz)

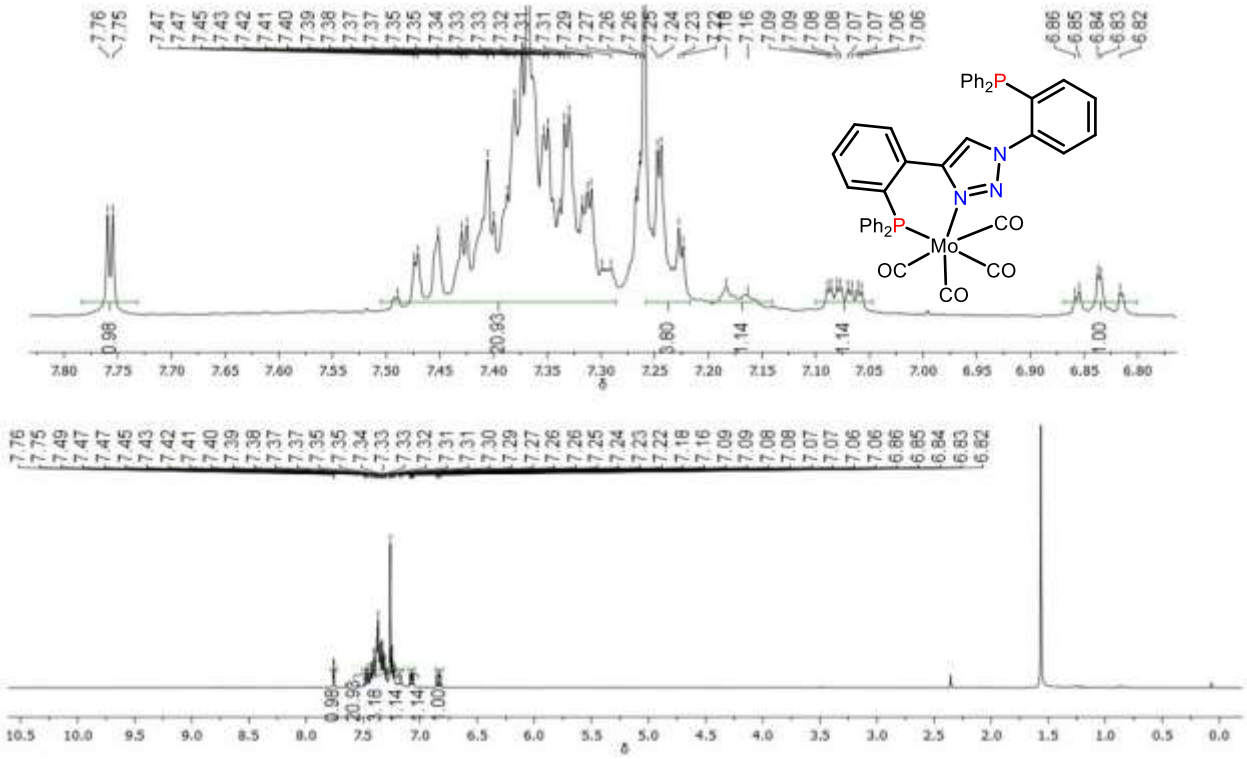


Fig. S36 ^{1}H NMR spectrum of **12** in $CDCl_3$ (400 MHz)

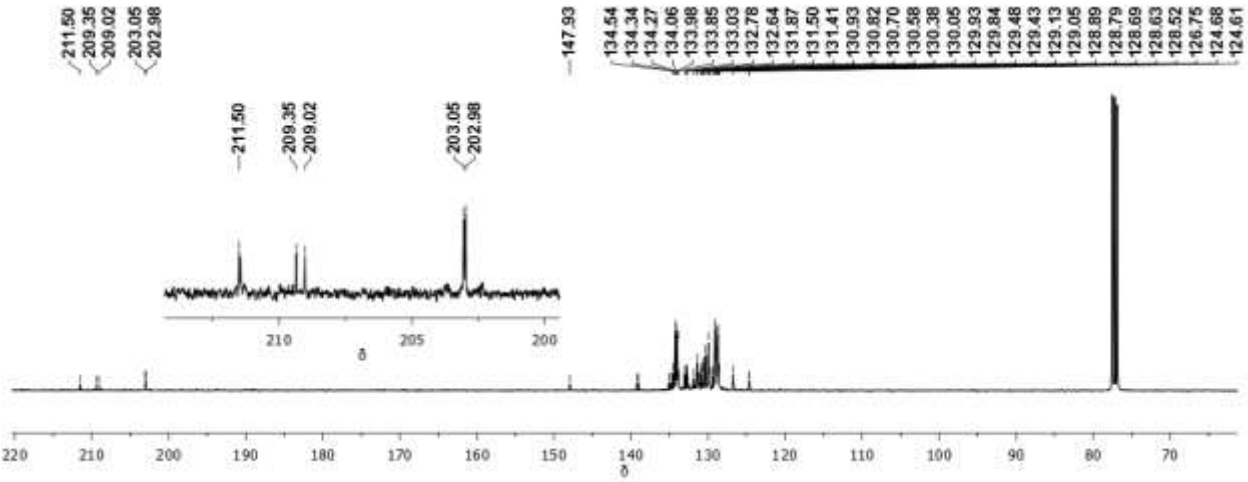


Fig. S37 $^{13}C\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$ (101 MHz)

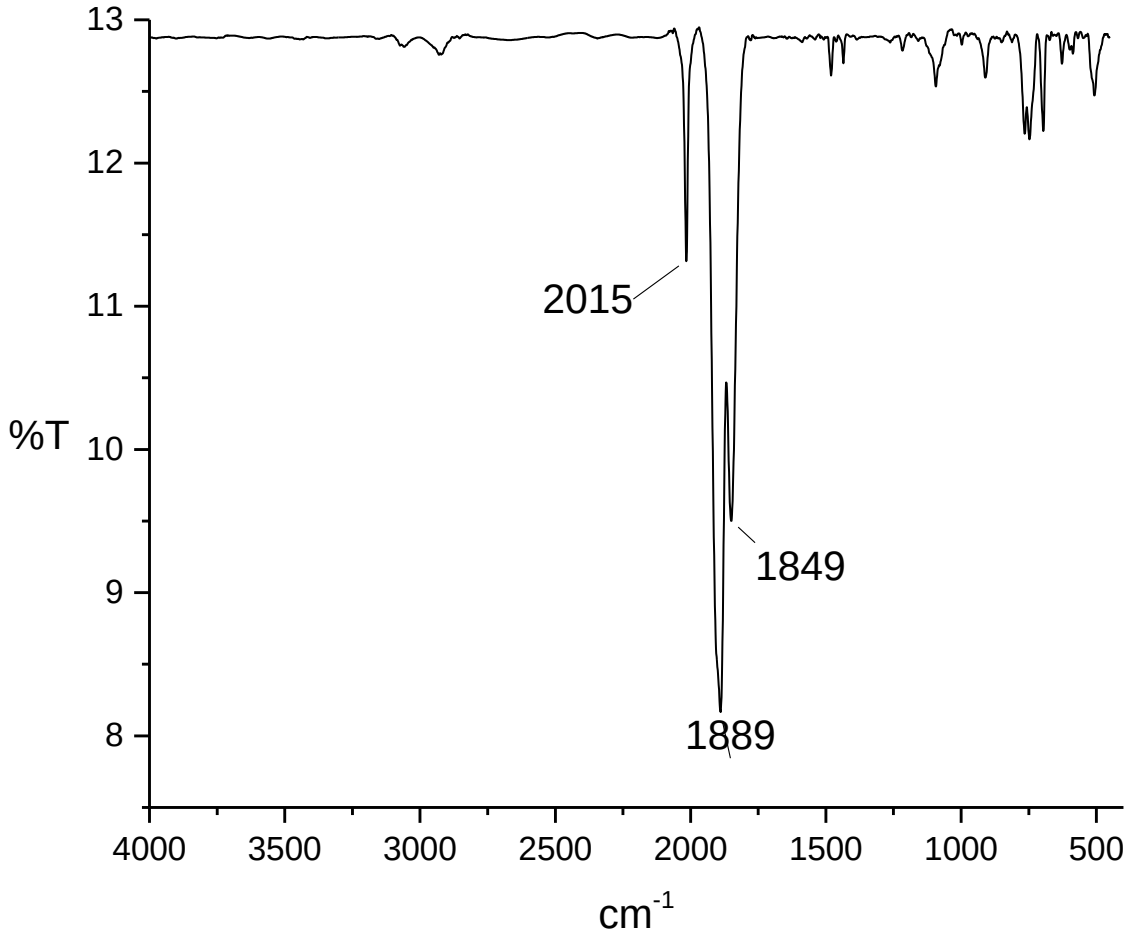
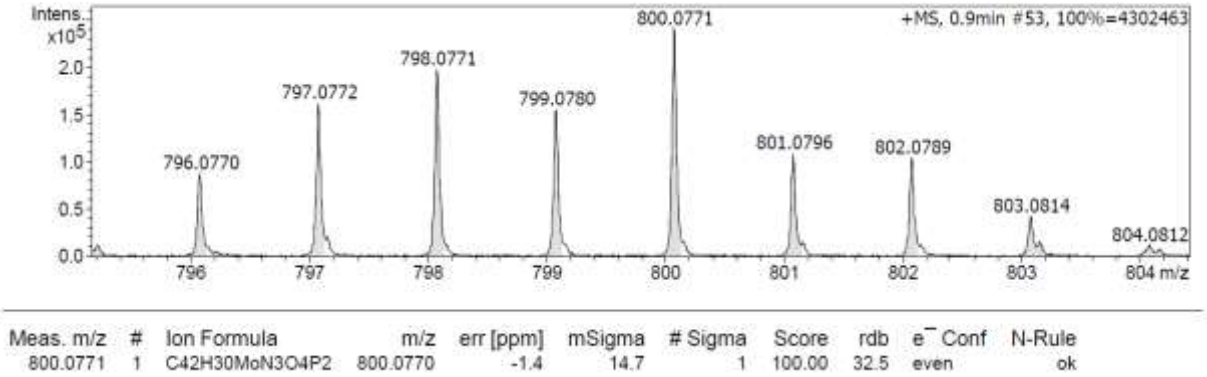


Fig. S38 IR spectrum of **12**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
800.0771	1	C42H30MoN3O4P2	800.0770	-1.4	14.7	1	100.00	32.5	even	ok

Fig. S39 EI mass spectrum of **12**

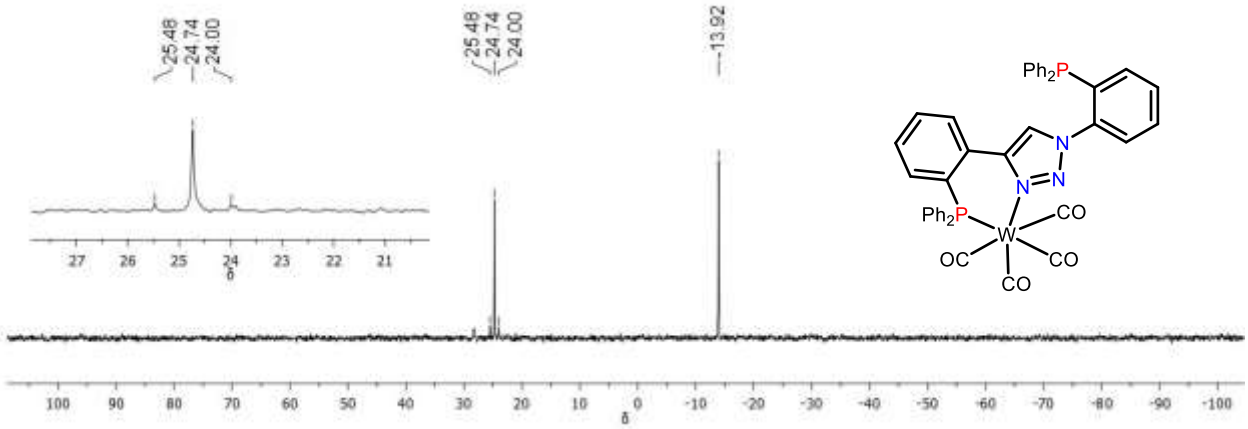


Fig. S40 $^{31}P\{^{1}H\}$ NMR spectrum of **13** in $CDCl_3$ (162 MHz)

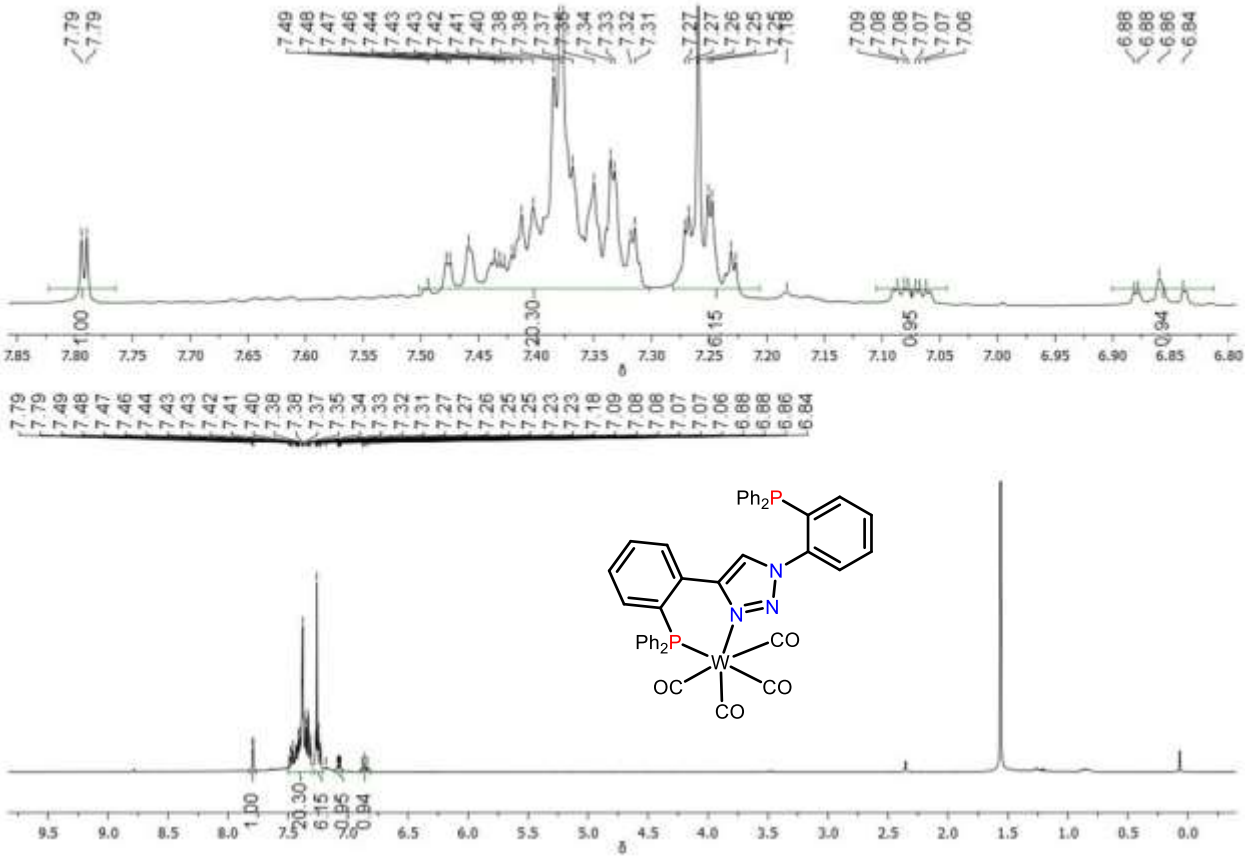


Fig. S41 ^{1}H NMR spectrum of **13** in $CDCl_3$ (400 MHz)

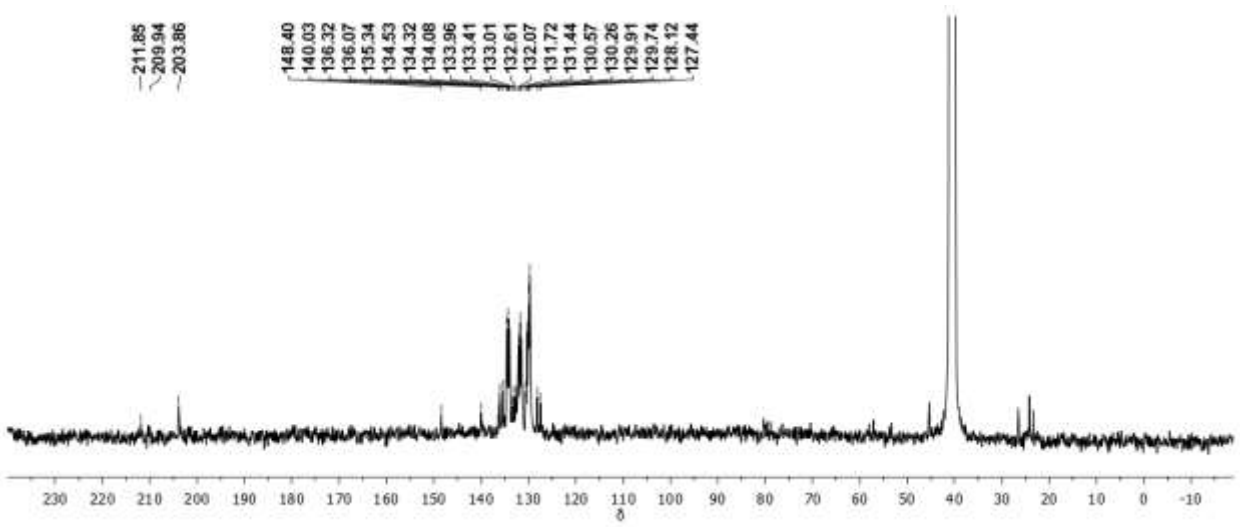


Fig. S42 $^{13}C\{^{1}H\}$ NMR spectrum of **13** in DMSO-d_6 (101 MHz)

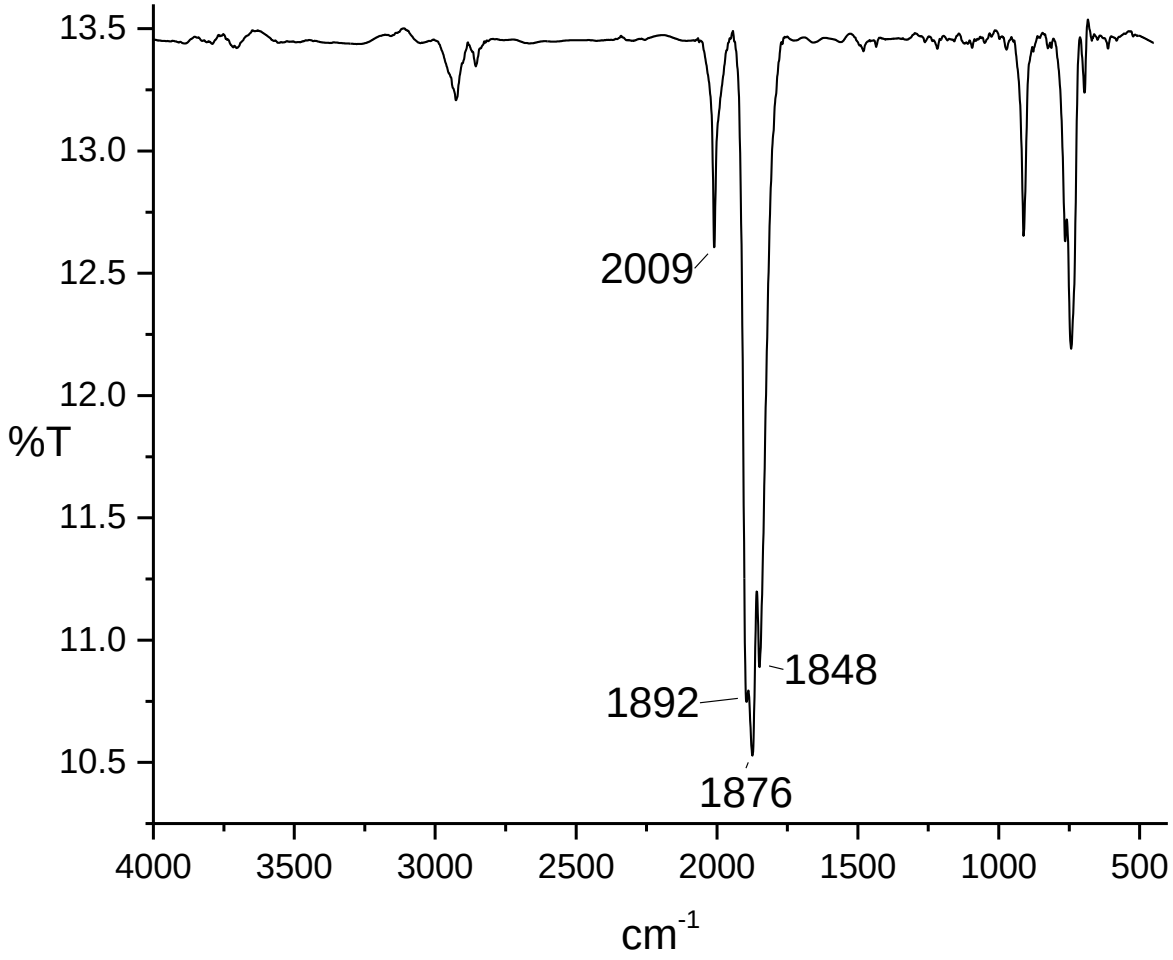
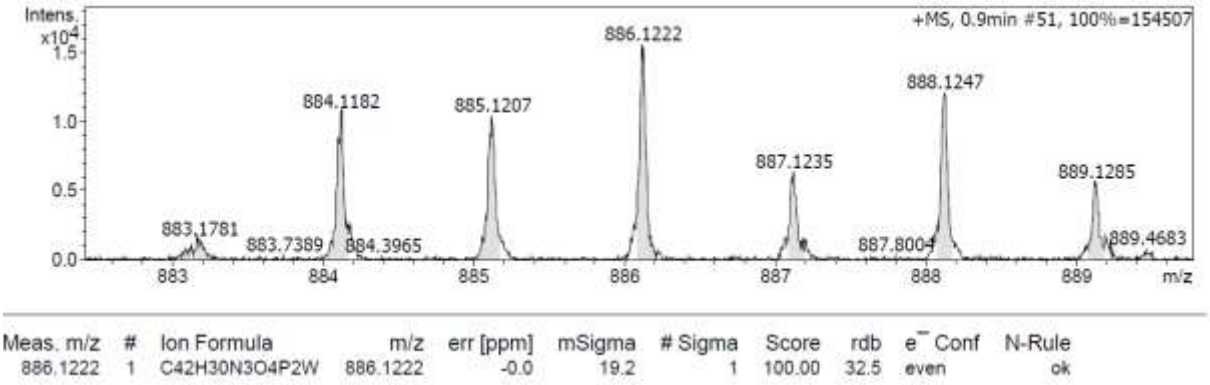


Fig. S43 IR spectrum of **13**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
886.1222	1	C42H30N3O4P2W	886.1222	-0.0	19.2	1	100.00	32.5	even	ok

Fig. S44 EI mass spectrum of **13**

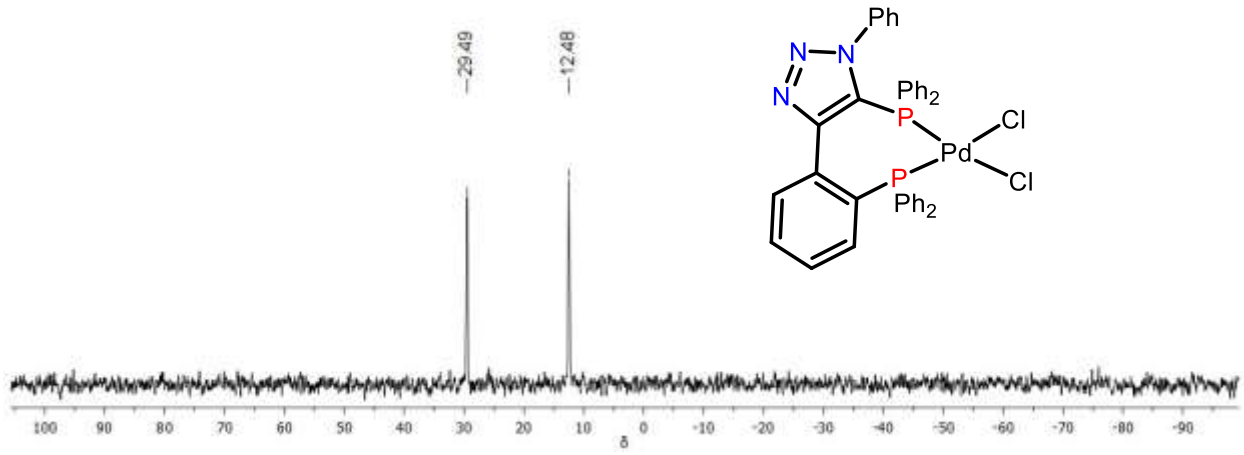


Fig. S45 $^{31}P\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$ (202 MHz)

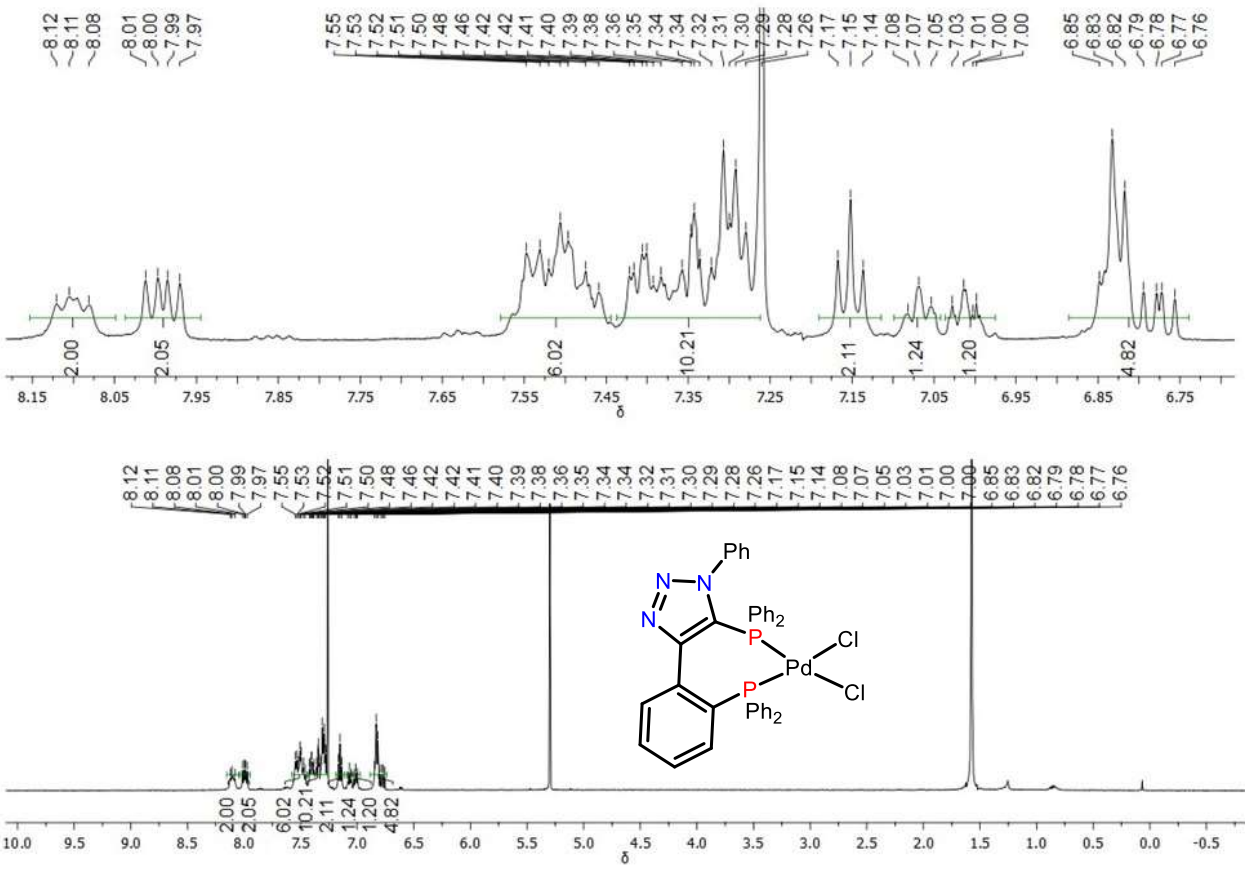


Fig. S46 ^{1}H NMR spectrum of **14** in $CDCl_3$ (500 MHz)

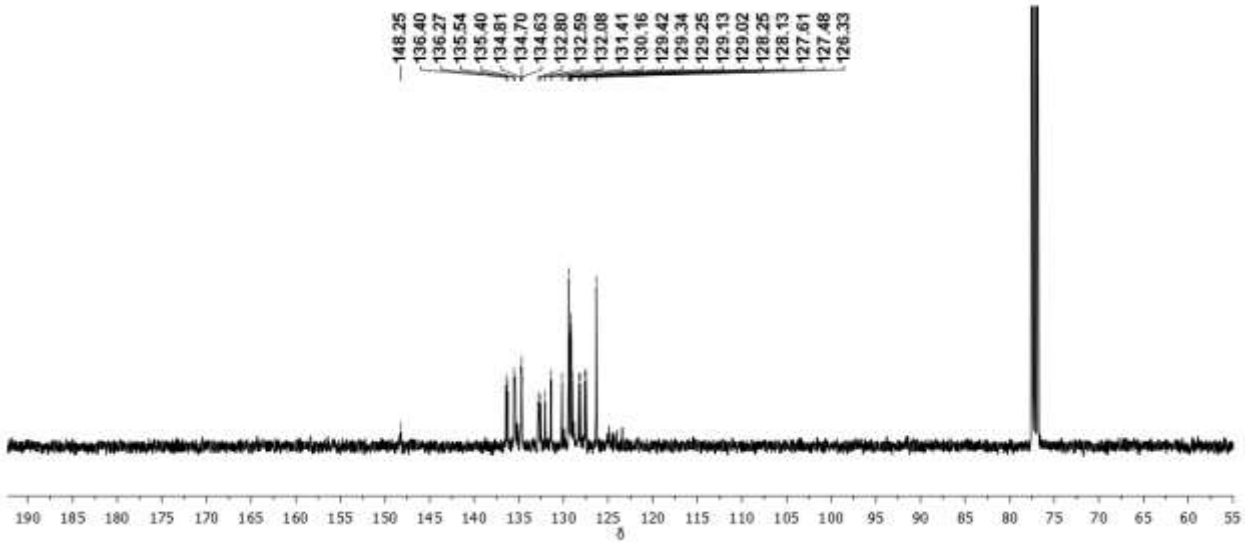


Fig. S47 $^{13}C\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$ (101 MHz)

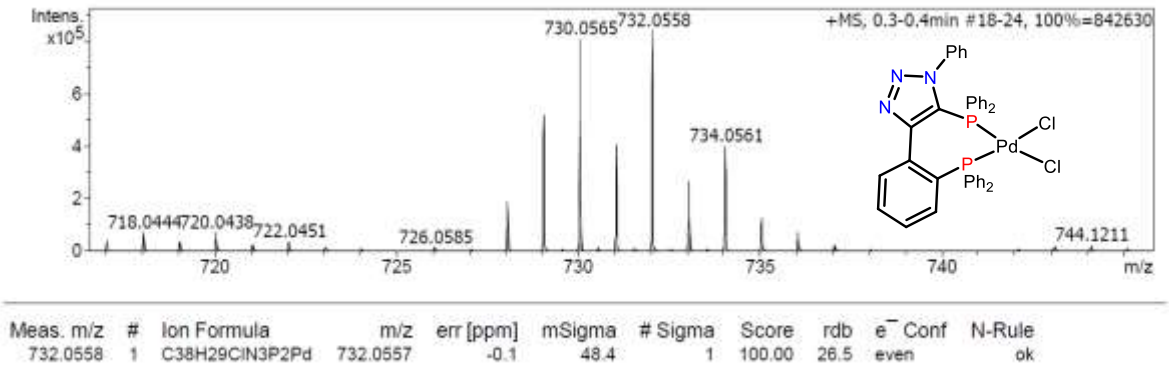


Fig. S48 EI mass spectrum of **14**

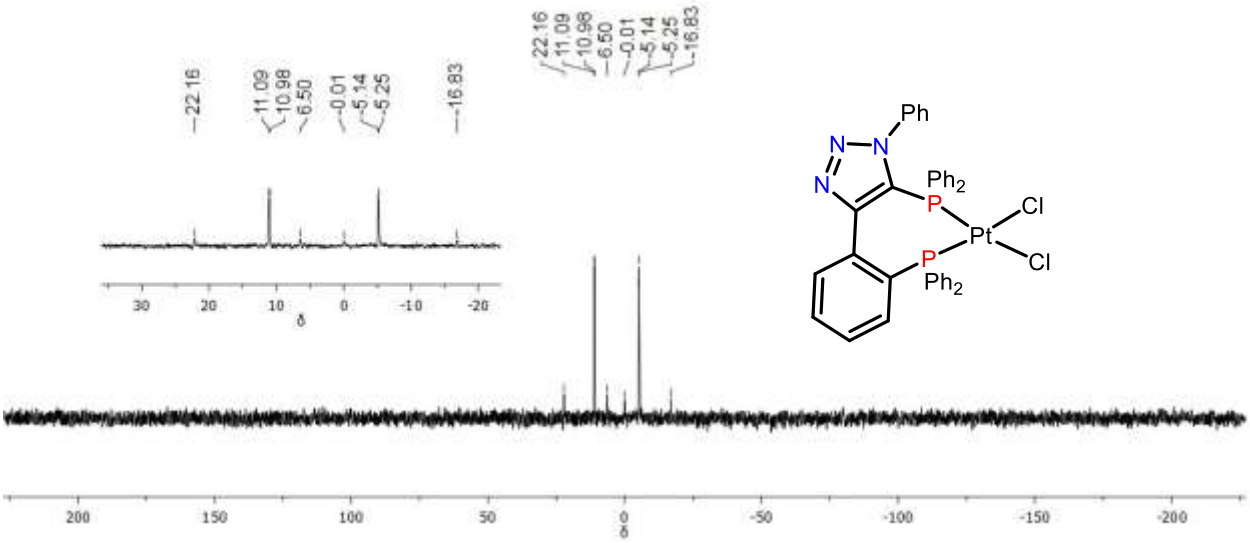


Fig. S49 $^{31}P\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$ (162 MHz)

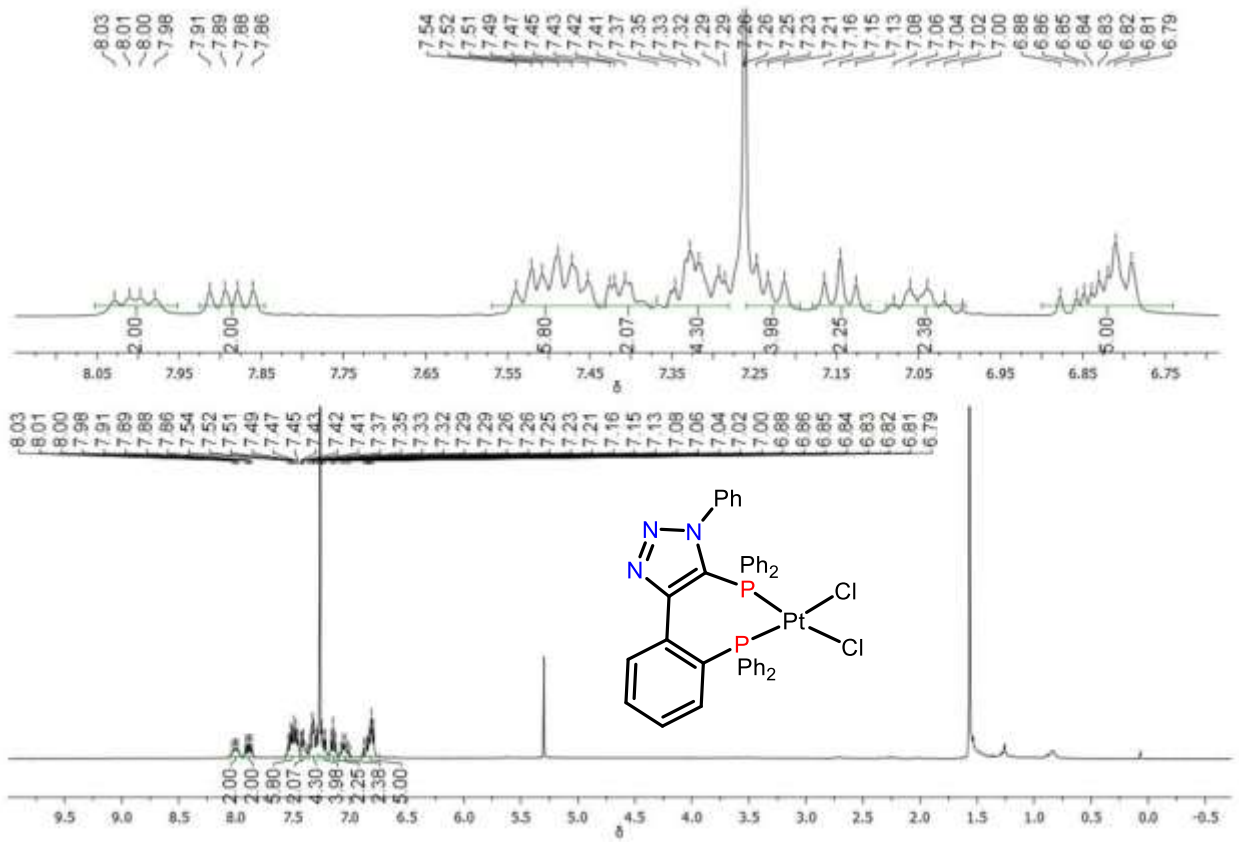


Fig. S50 ^{1}H NMR spectrum of **15** in $CDCl_3$ (400 MHz)

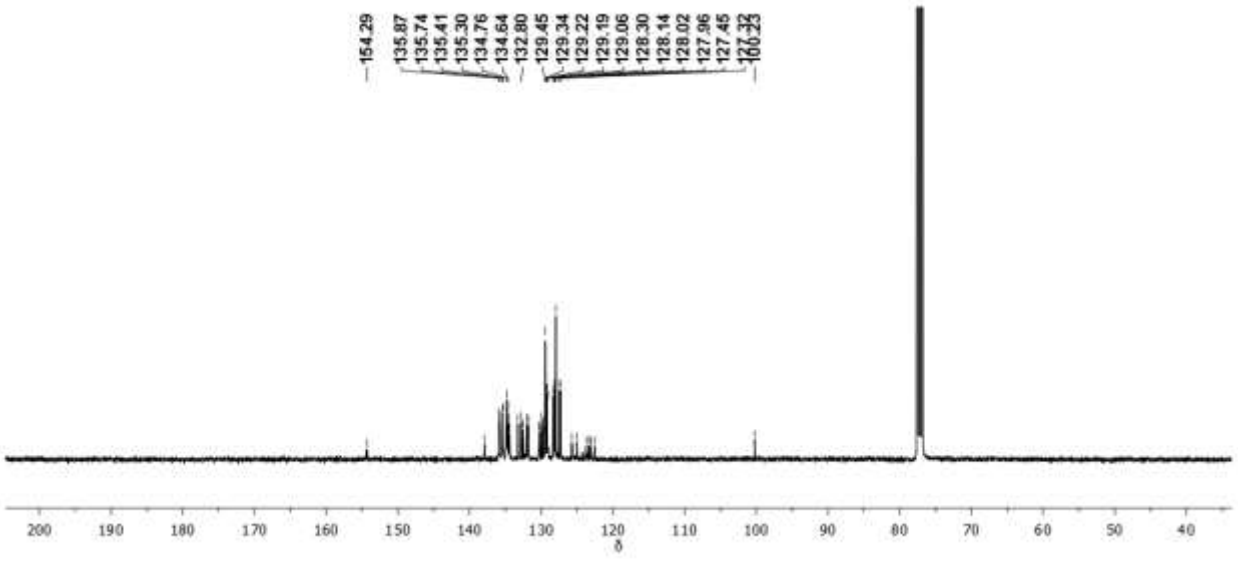


Fig. S51 $^{13}C\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$ (101 MHz)

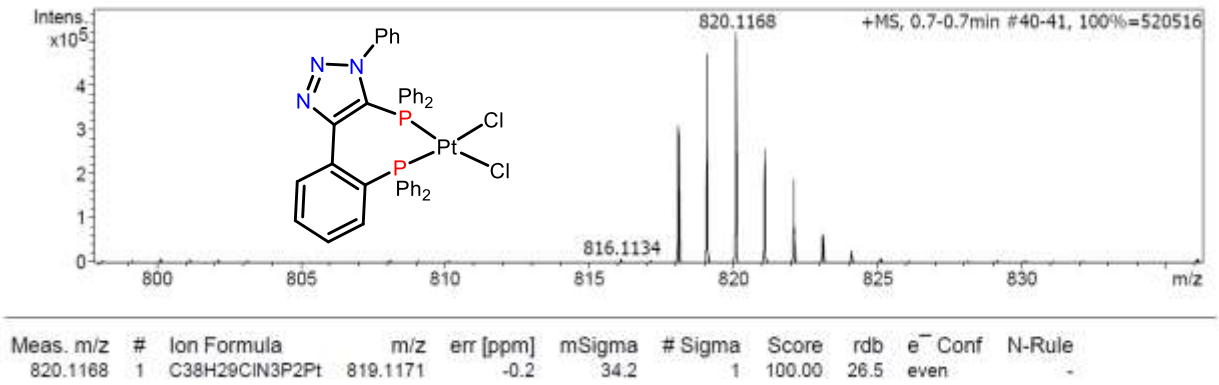


Fig. S52 EI mass spectrum of **15**

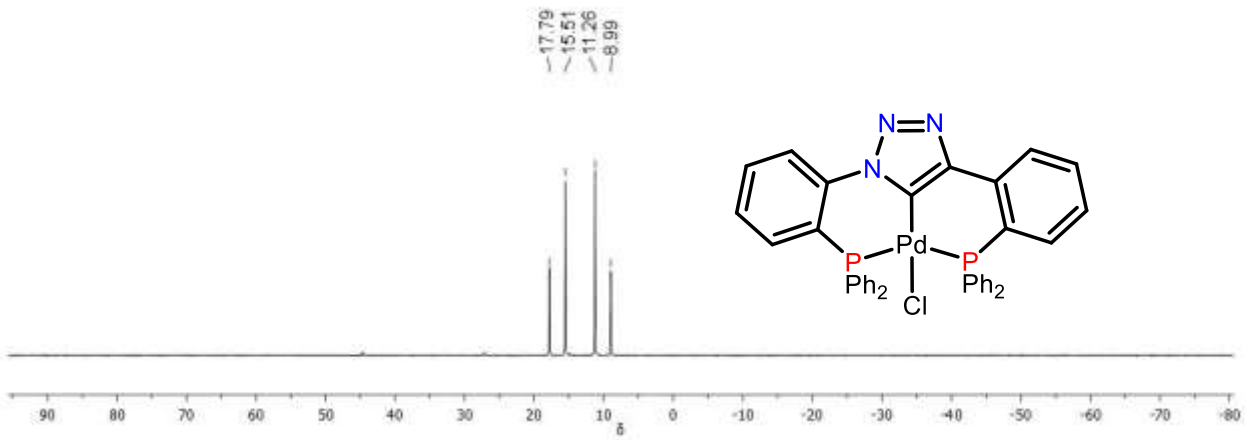


Fig. S53 $^{31}P\{^{1}H\}$ NMR spectrum of **16** in $CDCl_3$ (202 MHz)

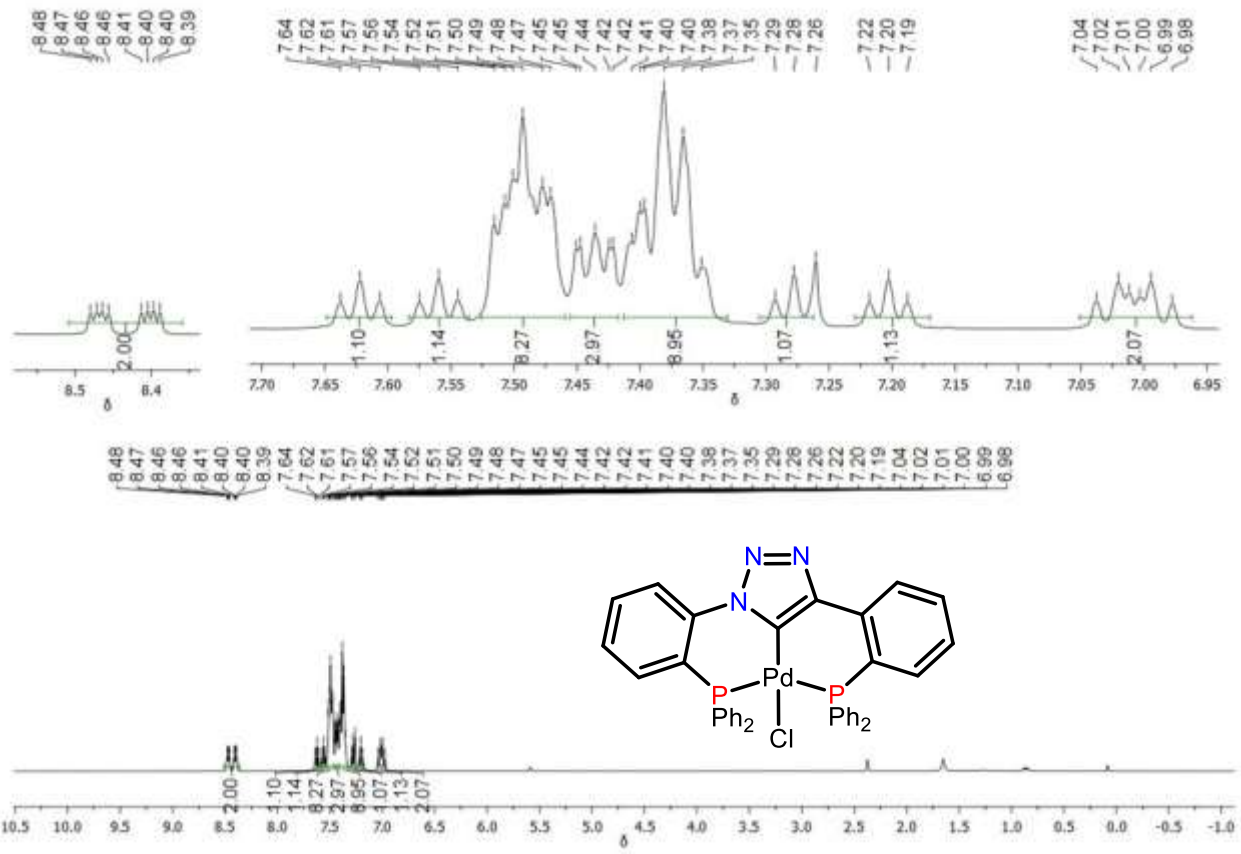


Fig. S54 ^{1}H NMR spectrum of **16** in $CDCl_3$ (500 MHz)

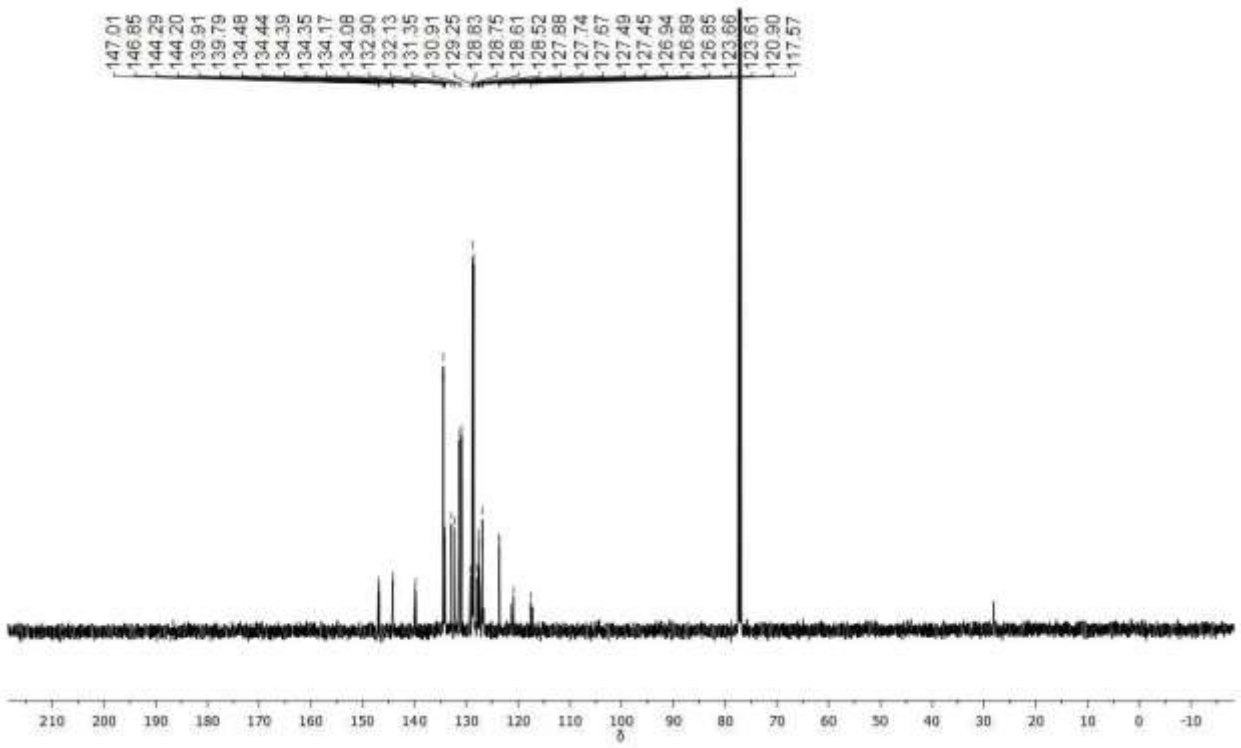
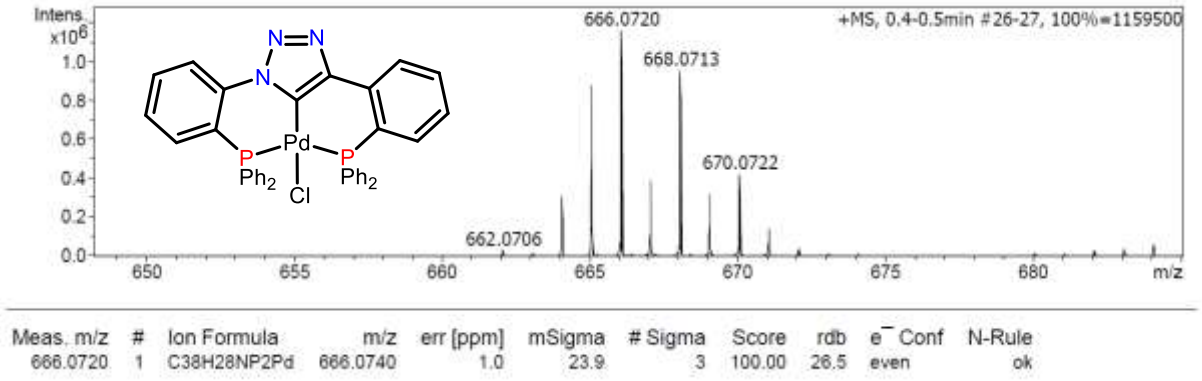


Fig. S55 ^{13}C NMR spectrum of **16** in $CDCl_3$ (126 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
666.0720	1	C38H28NP2Pd	666.0740	1.0	23.9	3	100.00	26.5	even	ok

Fig. S56 EI mass spectrum of **16**

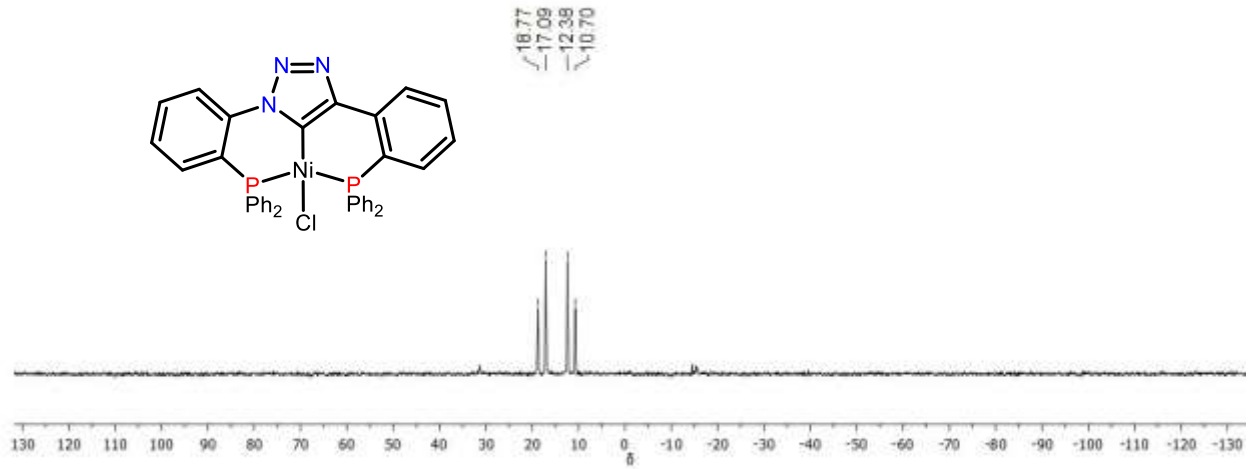


Fig. S57 $^{31}P\{^{1}H\}$ NMR spectrum of **17** in $CDCl_3$ (202 MHz)

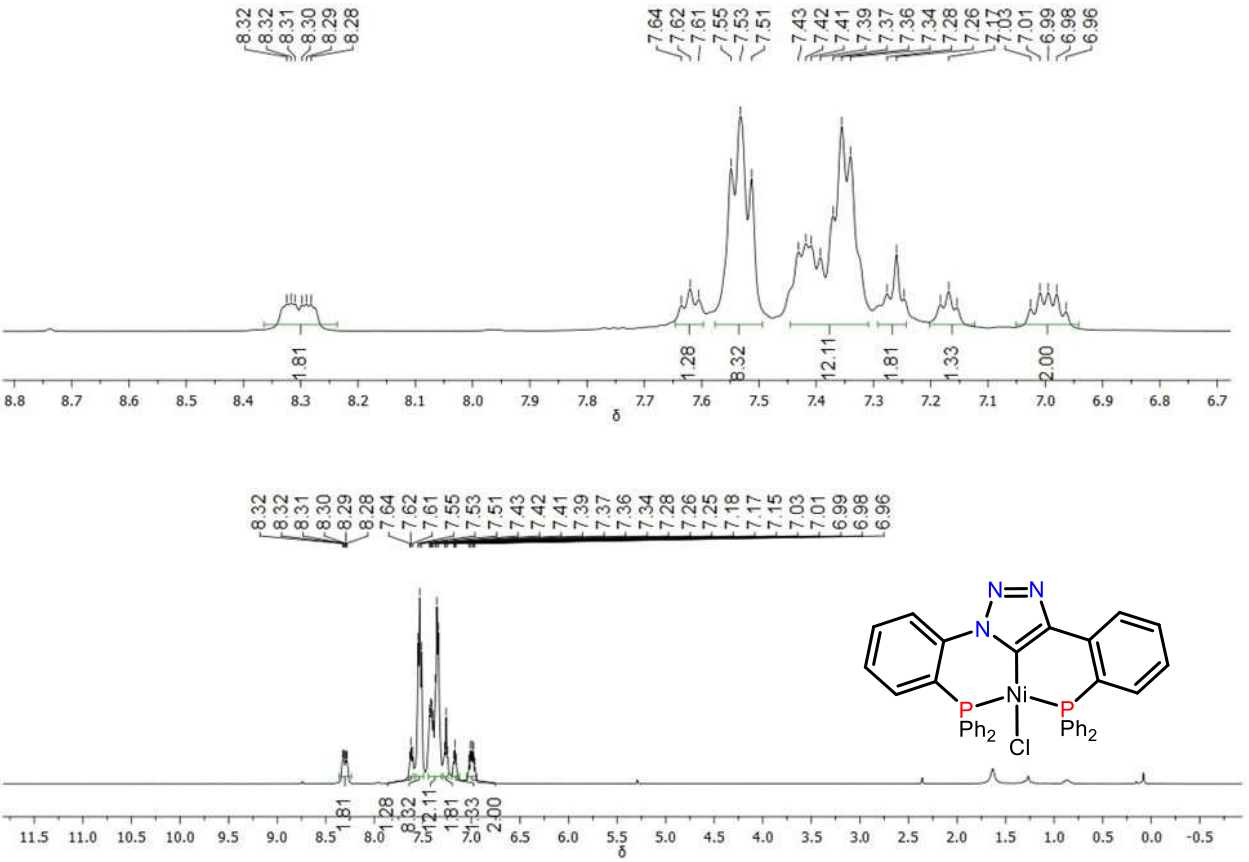


Fig. S58 ^{1}H NMR spectrum of **17** in $CDCl_3$ (500 MHz)

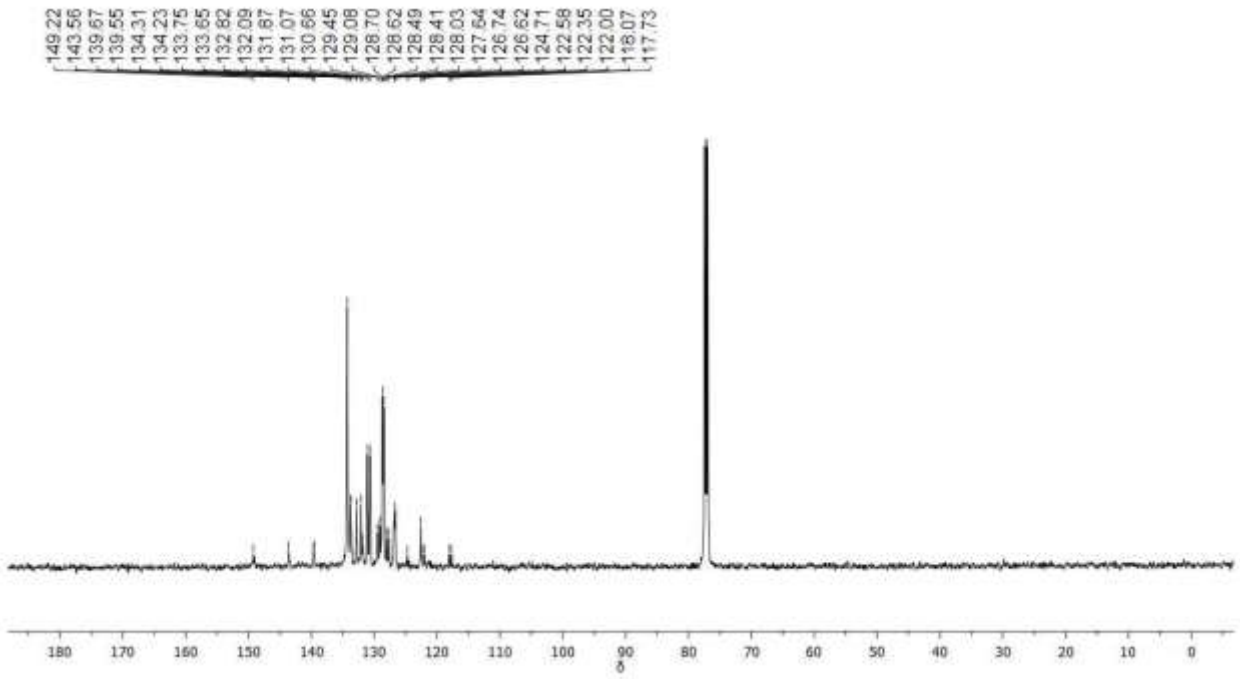
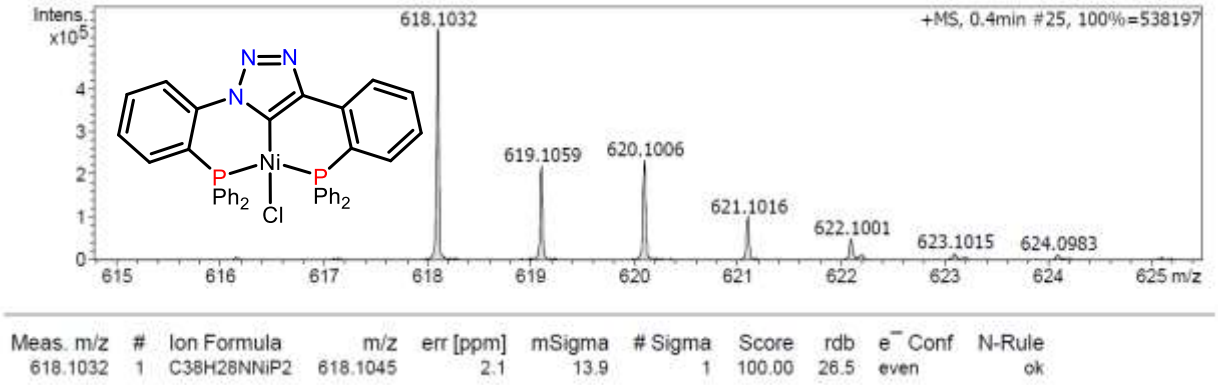


Fig. S59 ^{13}C NMR spectrum of **17** in $CDCl_3$ (126 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
618.1032	1	C38H28NNiP2	618.1045	2.1	13.9	1	100.00	26.5	even	ok

Fig. S60 EI mass spectrum of **17**

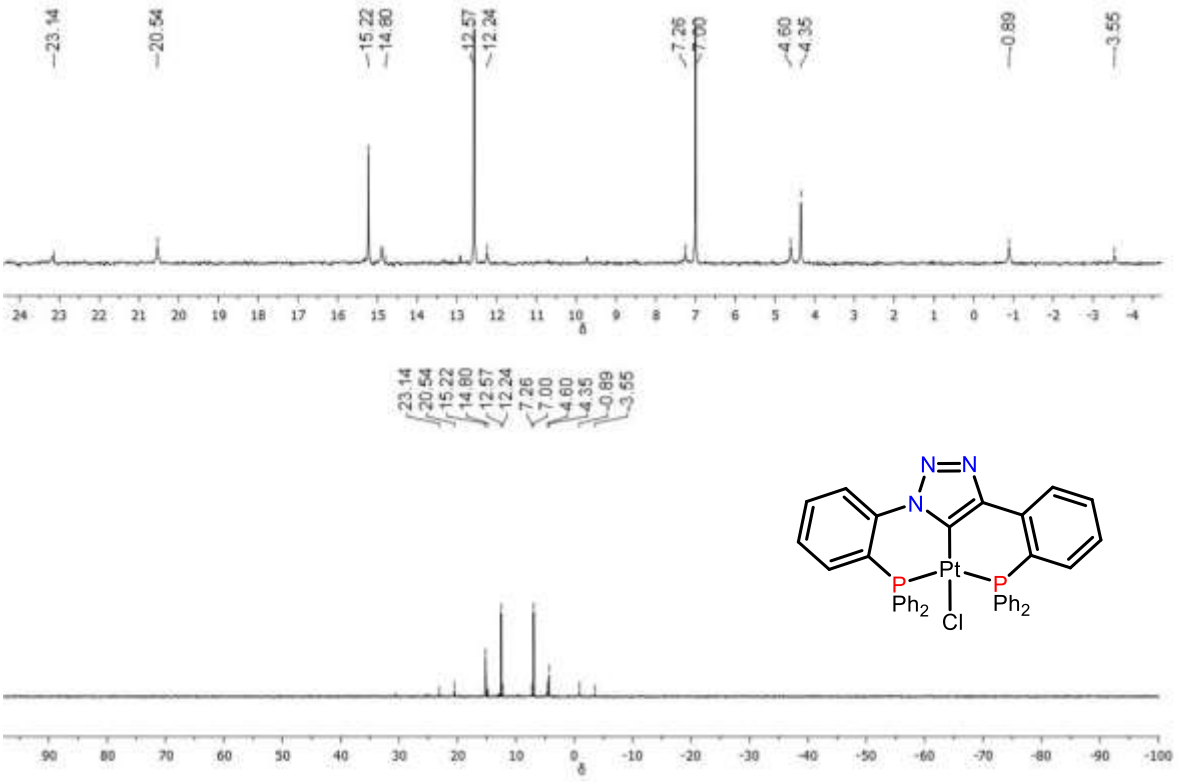


Fig. S61 $^{31}P\{^{1}H\}$ NMR spectrum of **18** in $CDCl_3$ (162 MHz)

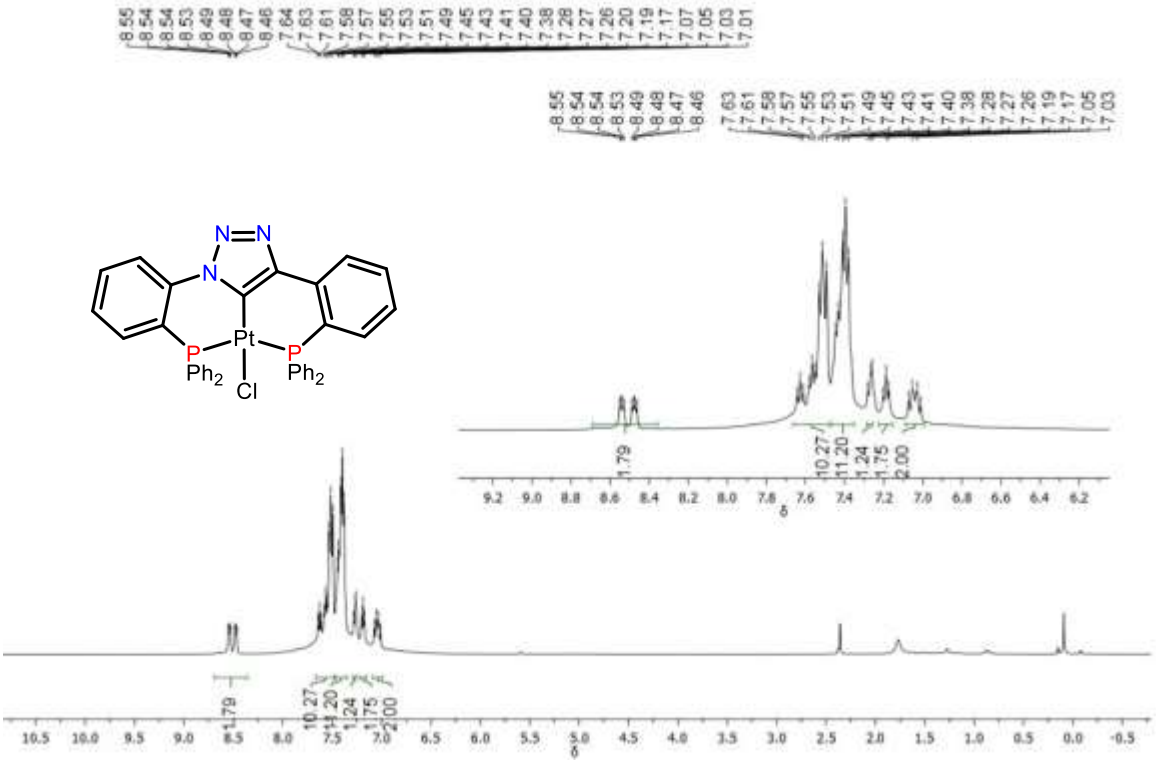


Fig. S62 ^{1}H NMR spectrum of **18** in $CDCl_3$ (500 MHz)

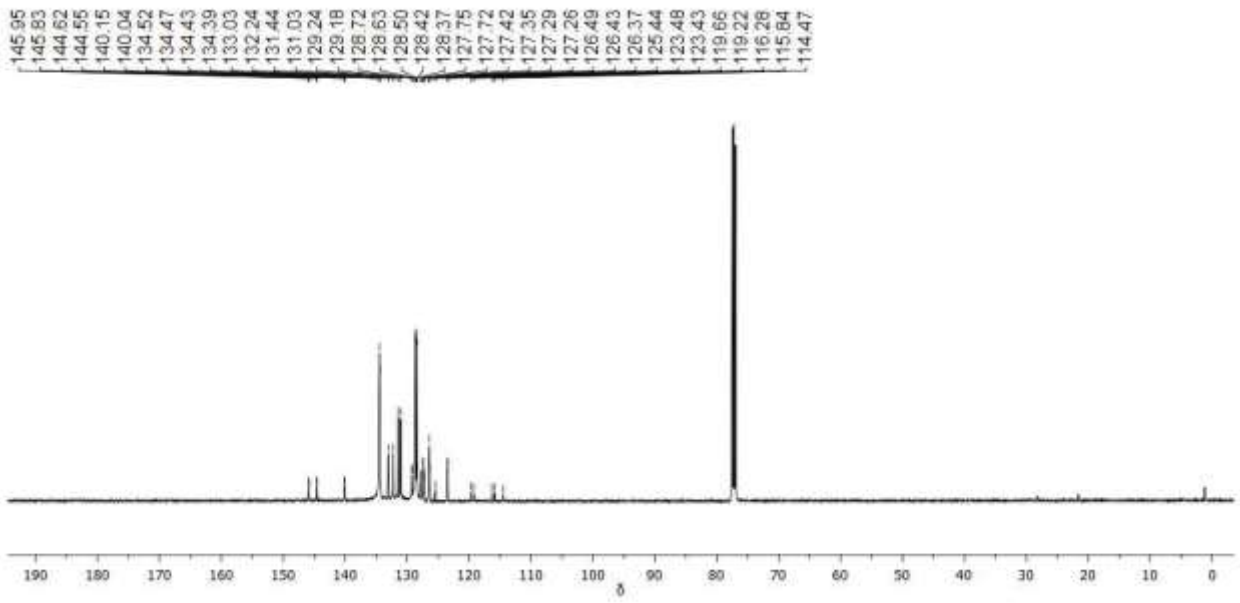
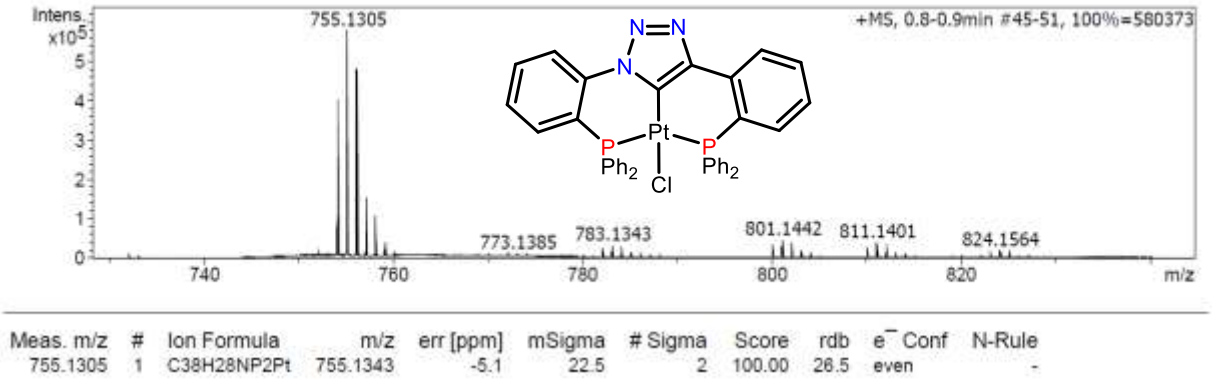


Fig. S63 ^{13}C NMR spectrum of **18** in $CDCl_3$ (126 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
755.1305	1	C38H28NP2Pt	755.1343	-5.1	22.5	2	100.00	26.5	even	-

Fig. S64 EI mass spectrum of **18**

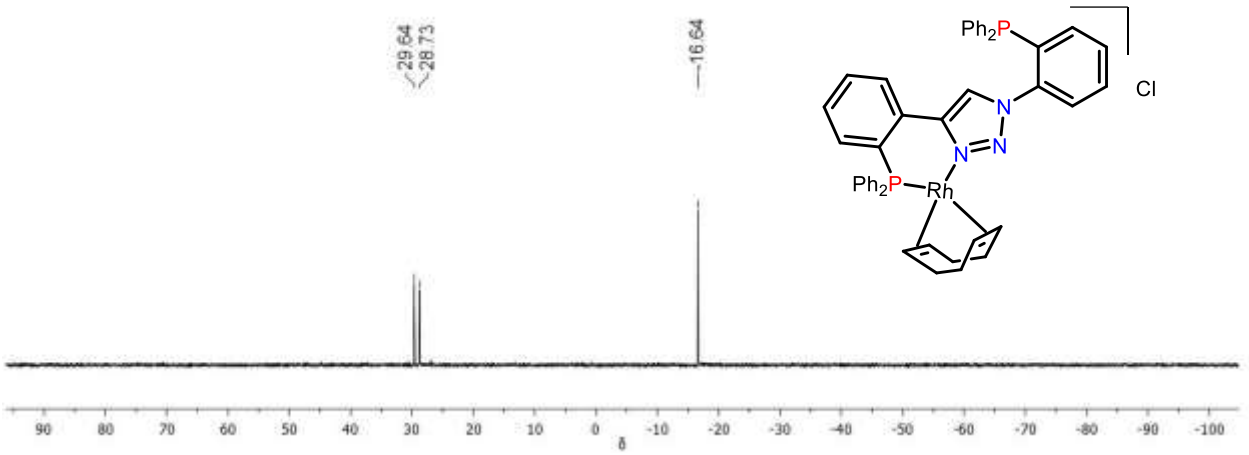


Fig. S65 $^{31}P\{^{1}H\}$ NMR spectrum of **19** in $CDCl_3$ (162 MHz)

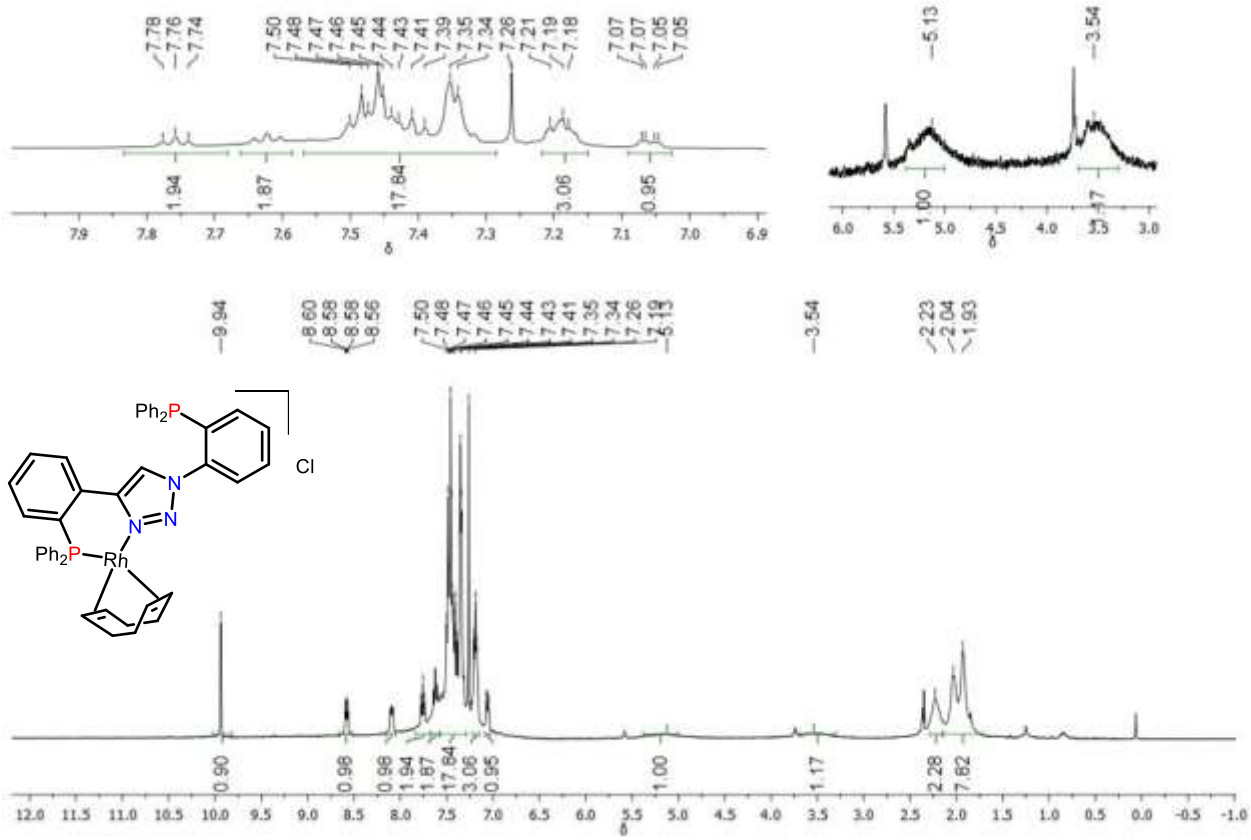


Fig. S66 ^{1}H NMR spectrum of **19** in $CDCl_3$ (400 MHz)

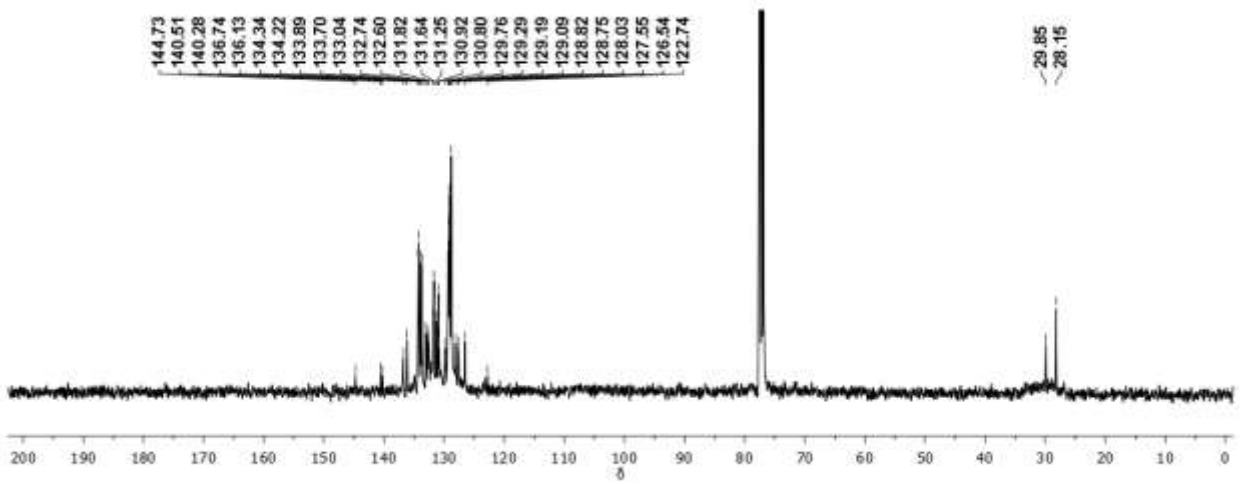
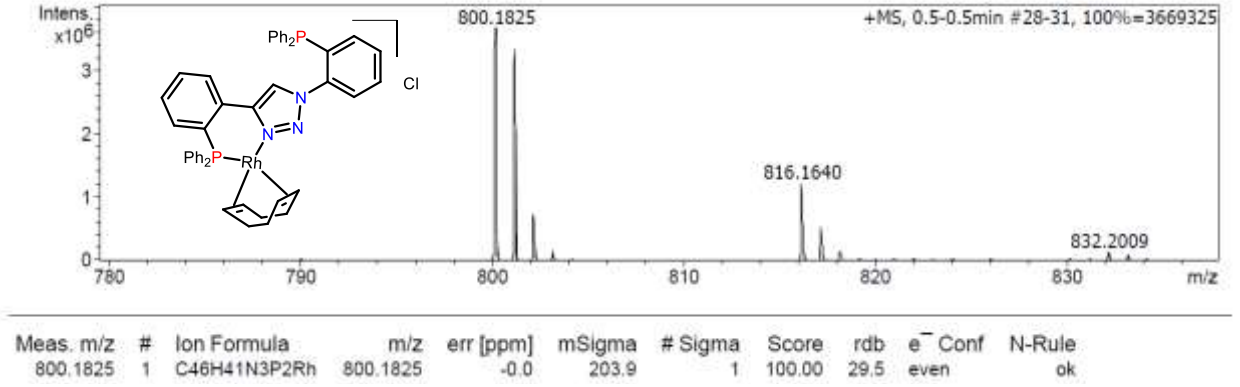


Fig. S67 $^{13}C\{^{1}H\}$ NMR spectrum of **19** in $CDCl_3$ (101 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
800.1825	1	C46H41N3P2Rh	800.1825	-0.0	203.9	1	100.00	29.5	even	ok

Fig. S68 EI mass spectrum of **19**

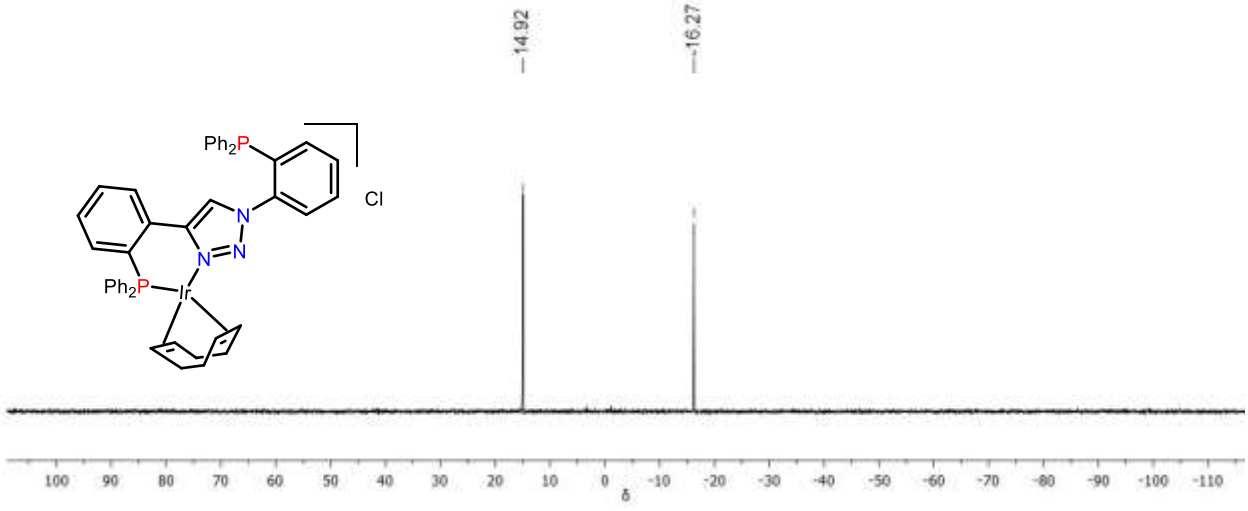


Fig. S69 $^{31}P\{^{1}H\}$ NMR spectrum of **20** in $CDCl_3$ (162 MHz)

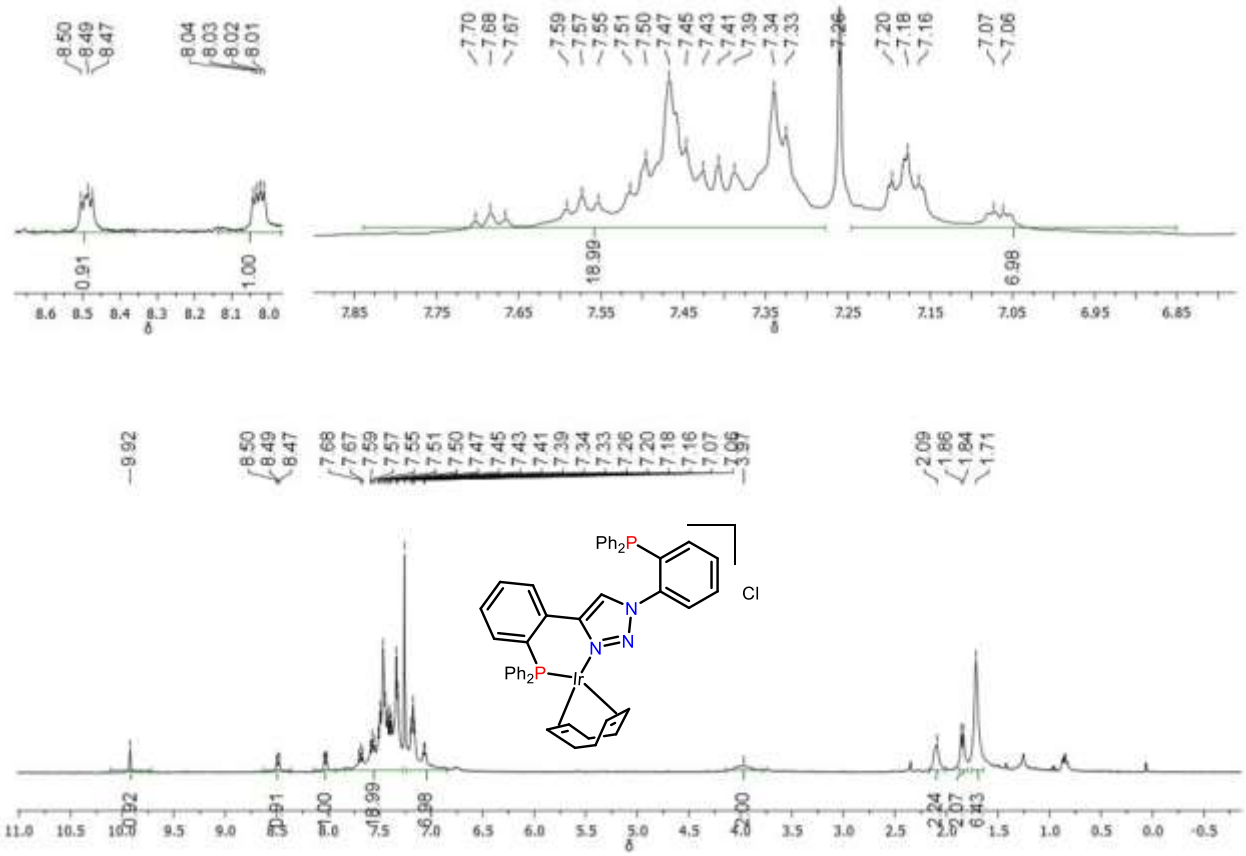


Fig. S70 ^{1}H NMR spectrum of **20** in $CDCl_3$ (400 MHz)

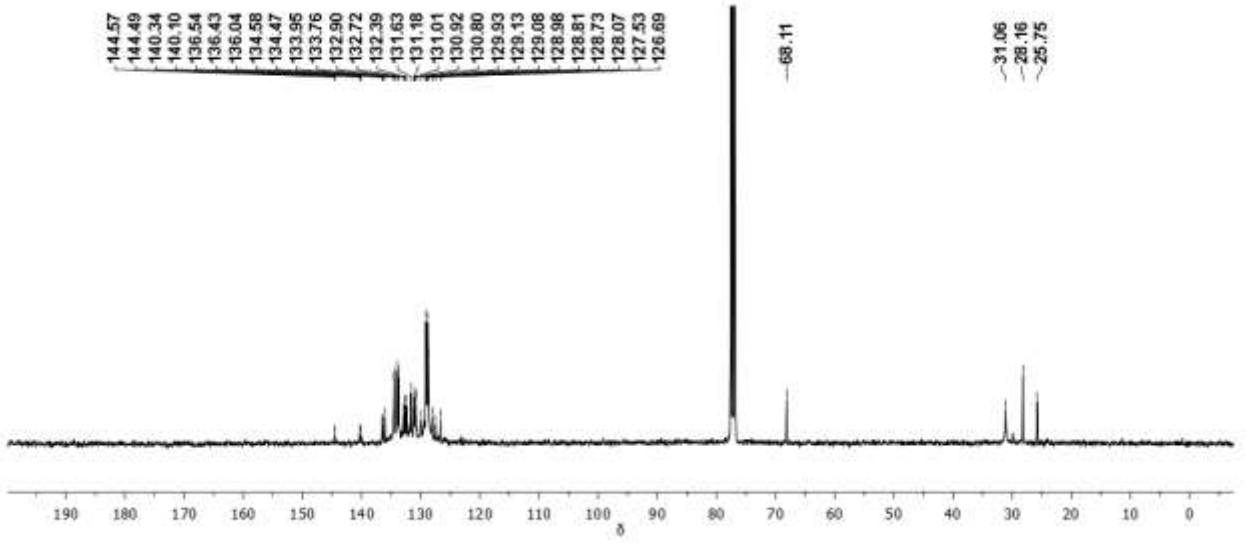
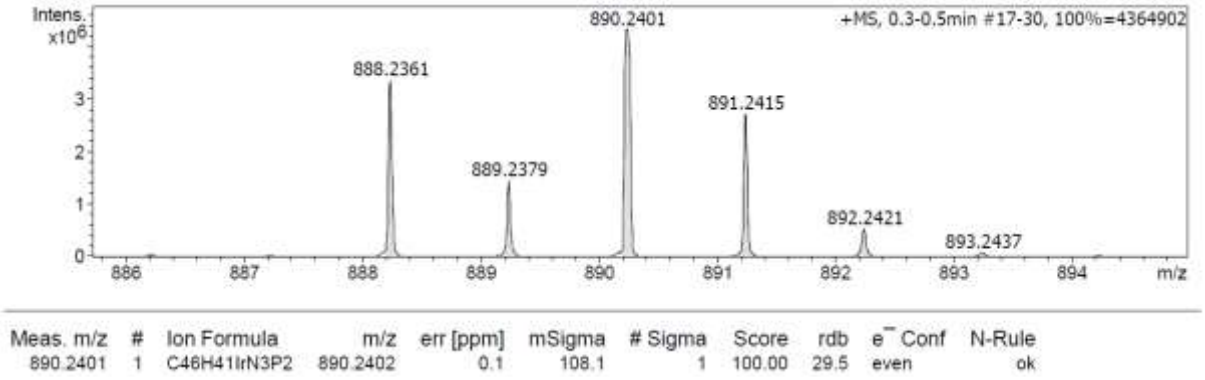


Fig. S71 $^{13}C\{^{1}H\}$ NMR spectrum of **20** in $CDCl_3$ (101 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
890.2401	1	C46H41IrN3P2	890.2402	0.1	108.1	1	100.00	29.5	even	ok

Fig. S72 EI mass spectrum of **20**

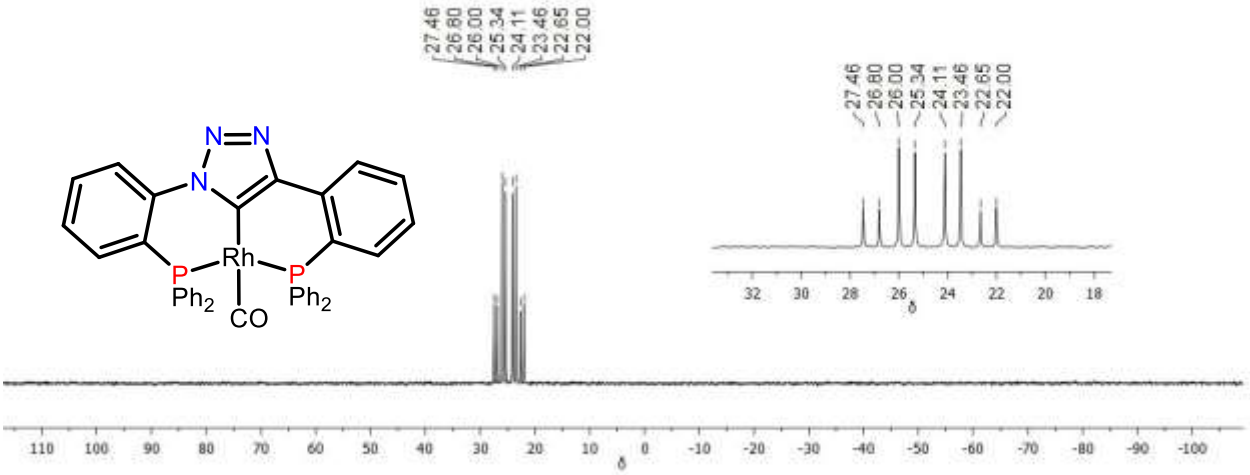


Fig. S73 $^{31}P\{^{1}H\}$ NMR spectrum of **21** in $CDCl_3$ (202 MHz)

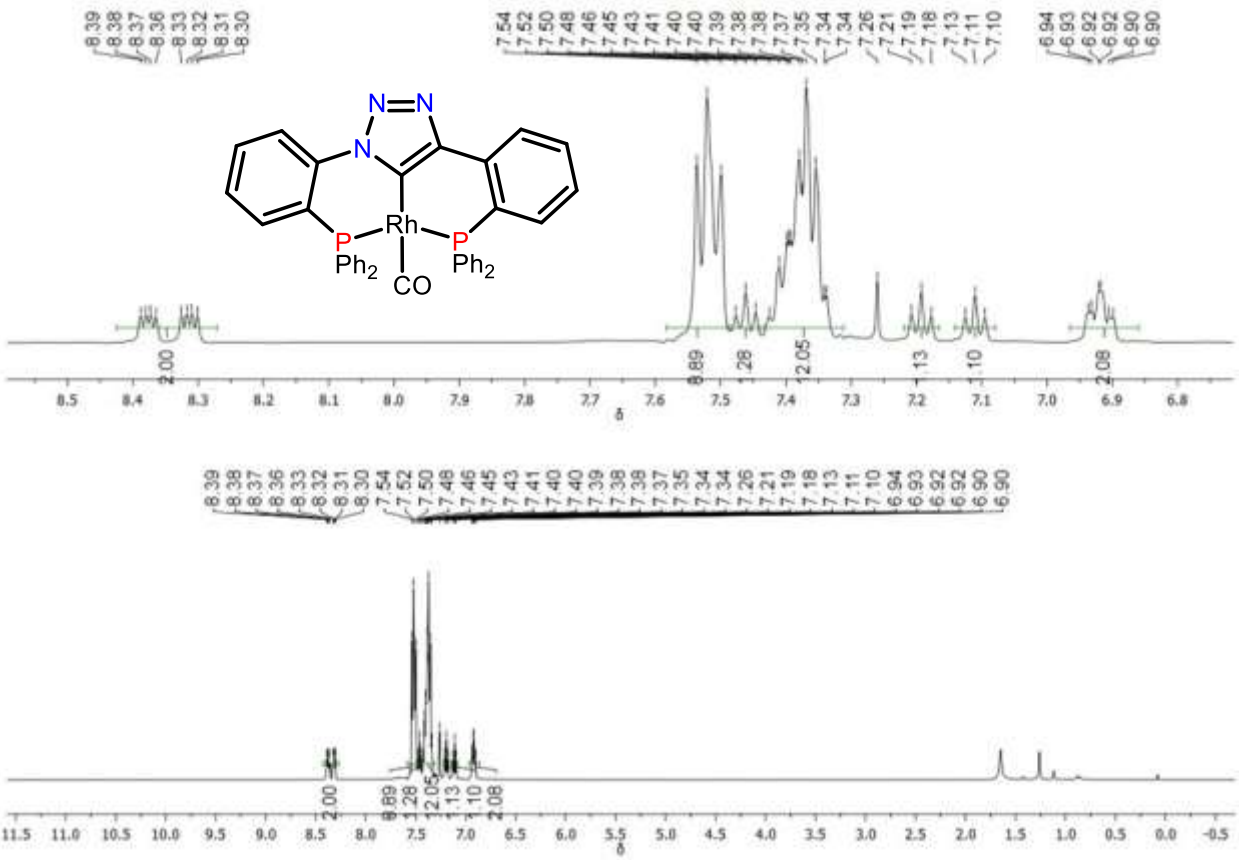


Fig. S74 ^{1}H NMR spectrum of **21** in $CDCl_3$ (500 MHz)

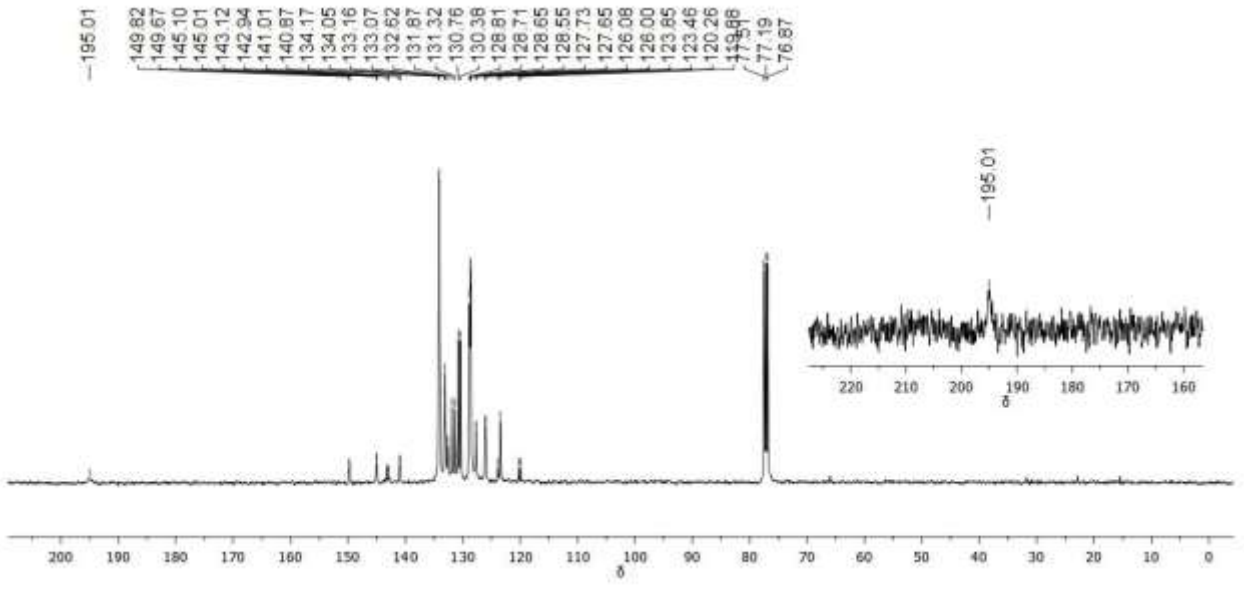


Fig. S75 ^{13}C NMR spectrum of **21** in $CDCl_3$ (101 MHz)

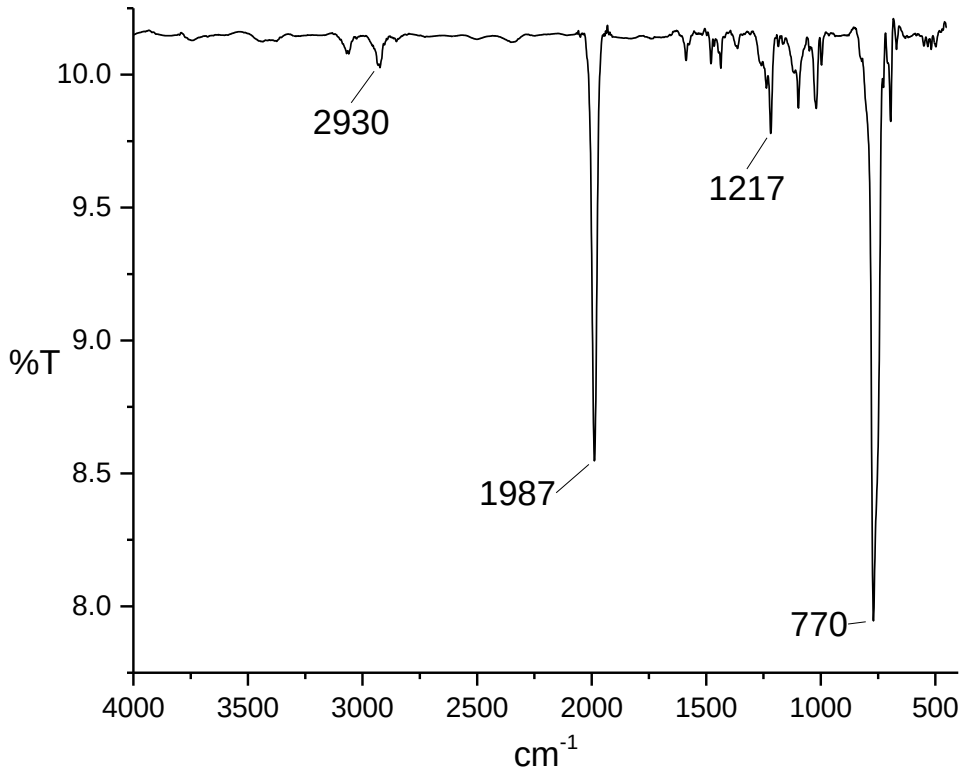


Fig. S76 IR spectrum of **21**

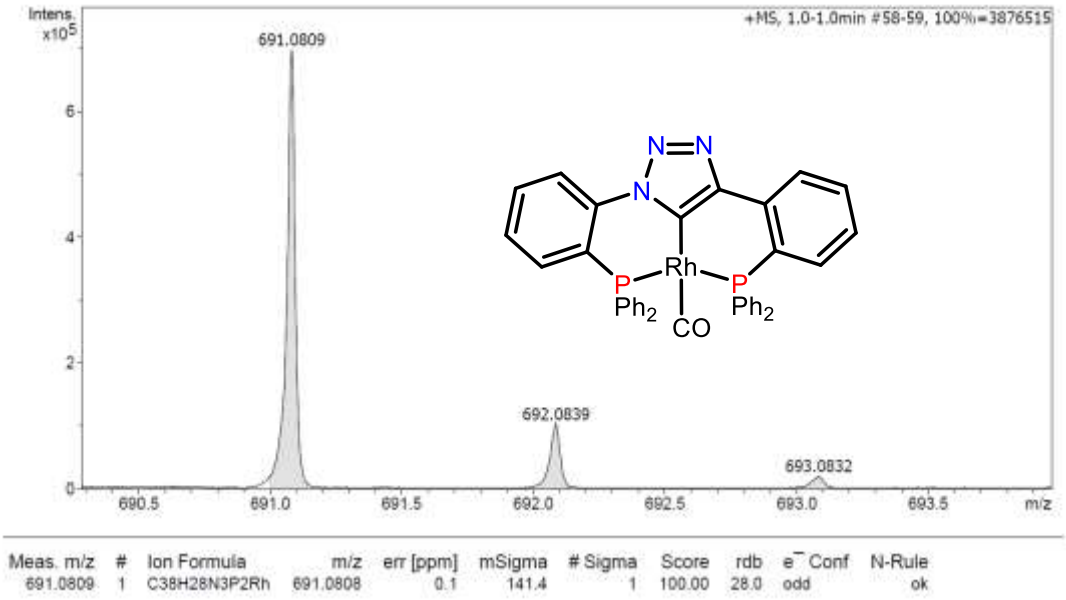


Fig. S77 EI mass spectrum of **21**

NMR spectra of a-i

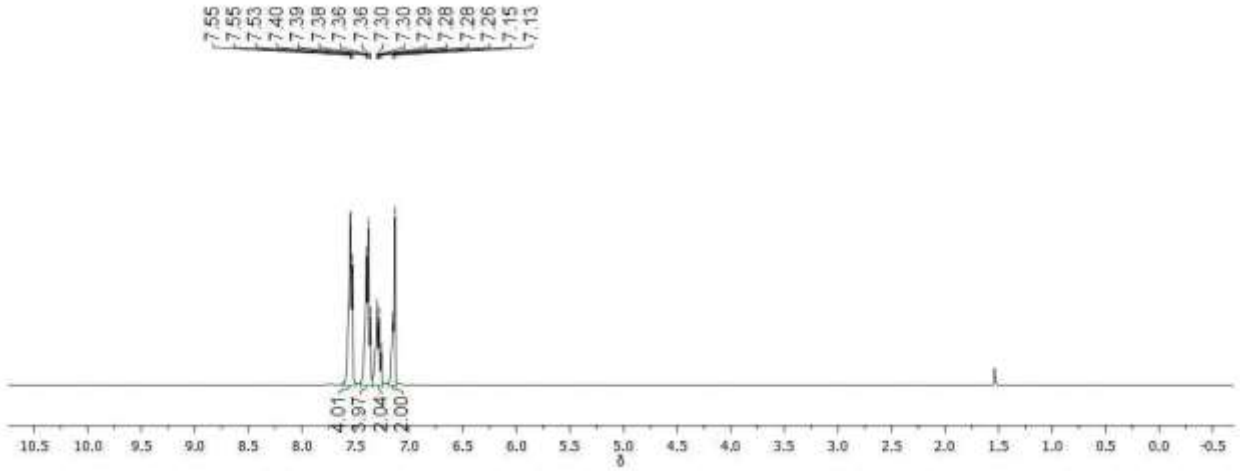


Fig. S78 ^{1}H NMR spectrum of **a** in $CDCl_3$ (400 MHz)

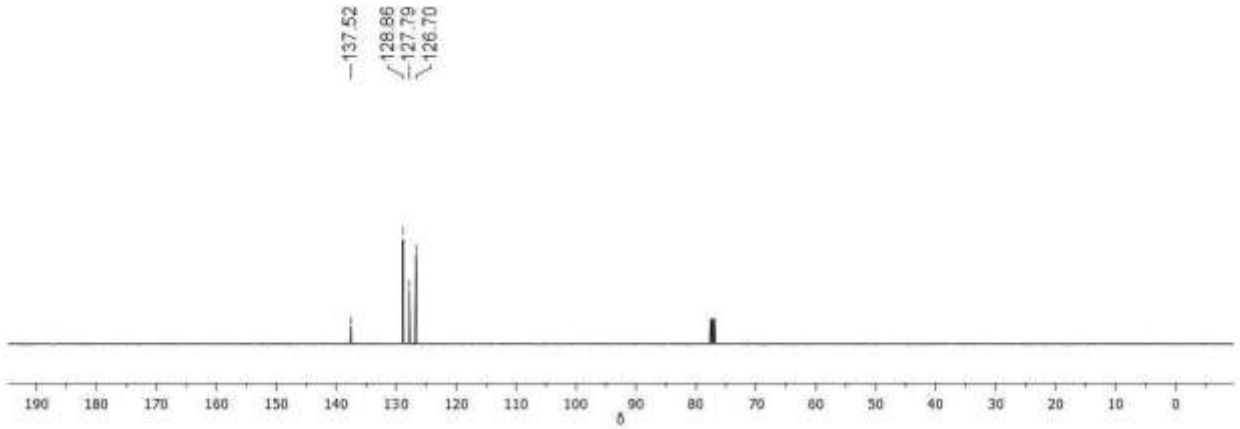


Fig. S79 ^{13}C NMR spectrum of **a** in $CDCl_3$ (101 MHz)

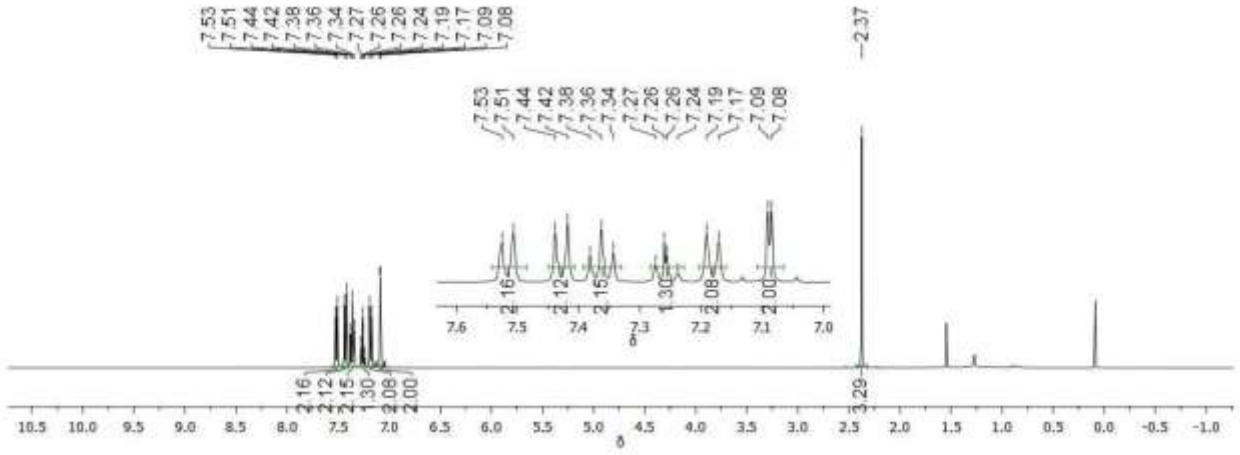


Fig. S80 ^{1}H NMR spectrum of **b** in $CDCl_3$ (400 MHz)

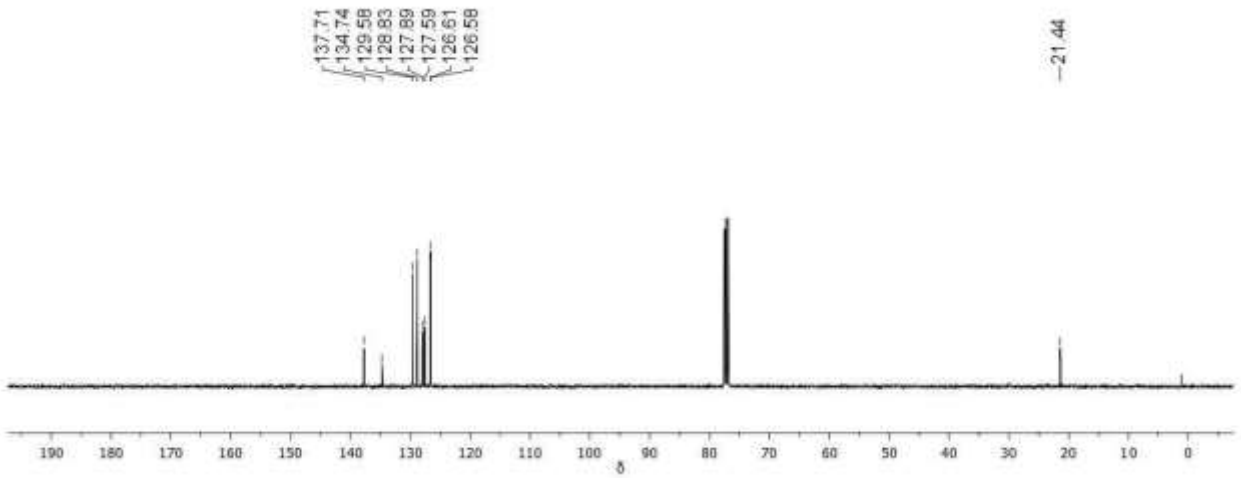


Fig. S81 ^{13}C NMR spectrum of **b** in $CDCl_3$ (101 MHz)

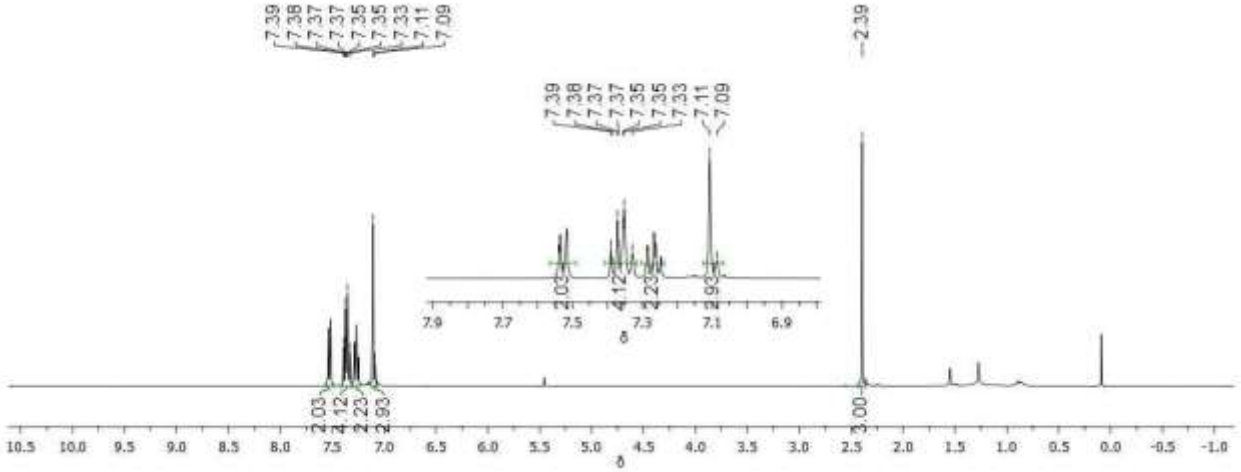


Fig. S82 ^{1}H NMR spectrum of **c** in $CDCl_3$ (400 MHz)

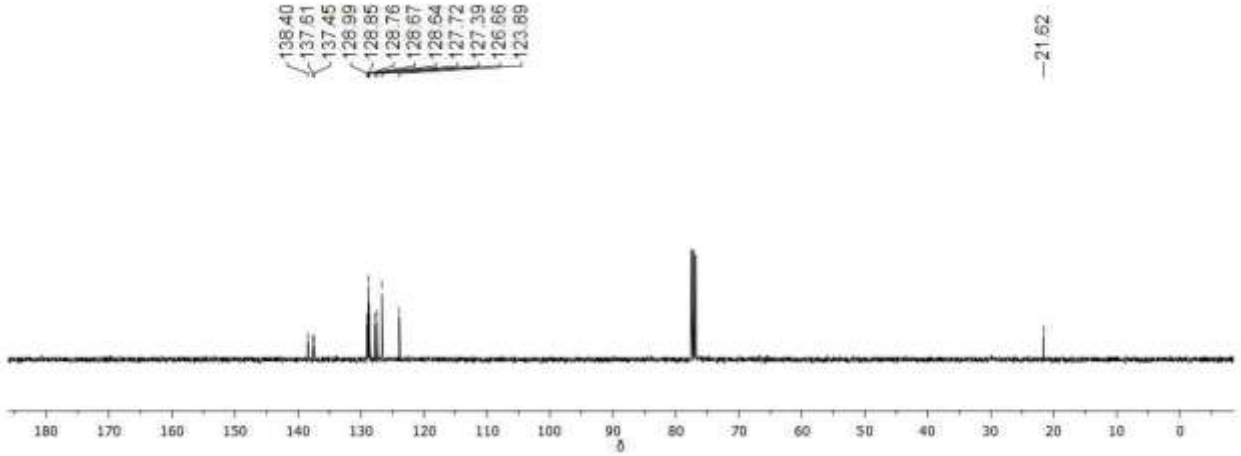


Fig. S83 ^{13}C NMR spectrum of **c** in $CDCl_3$ (101 MHz)

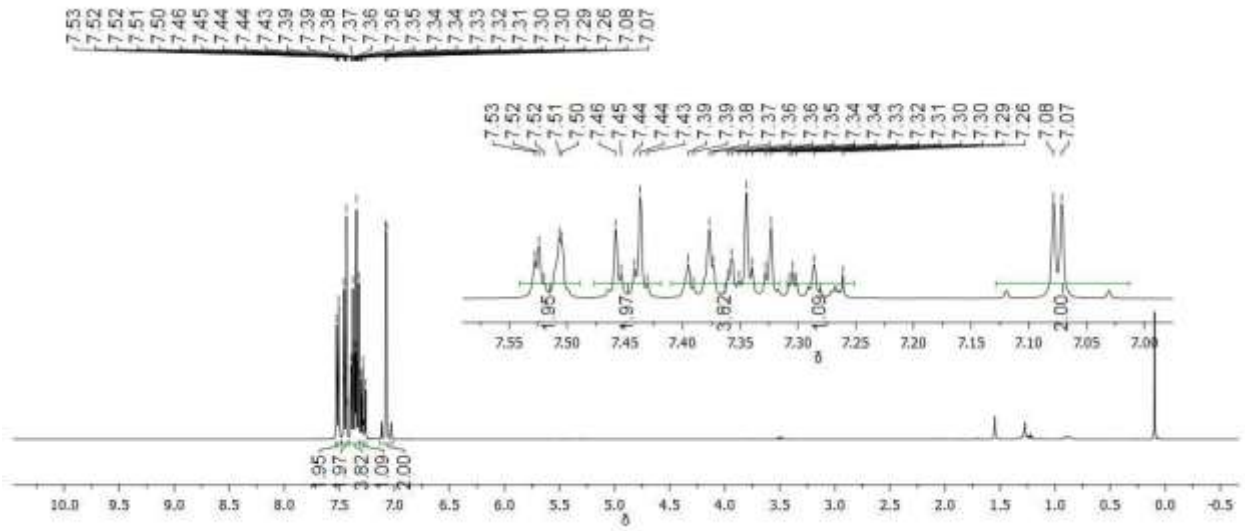


Fig. S84 ^{1}H NMR spectrum of **d** in $CDCl_3$ (400 MHz)

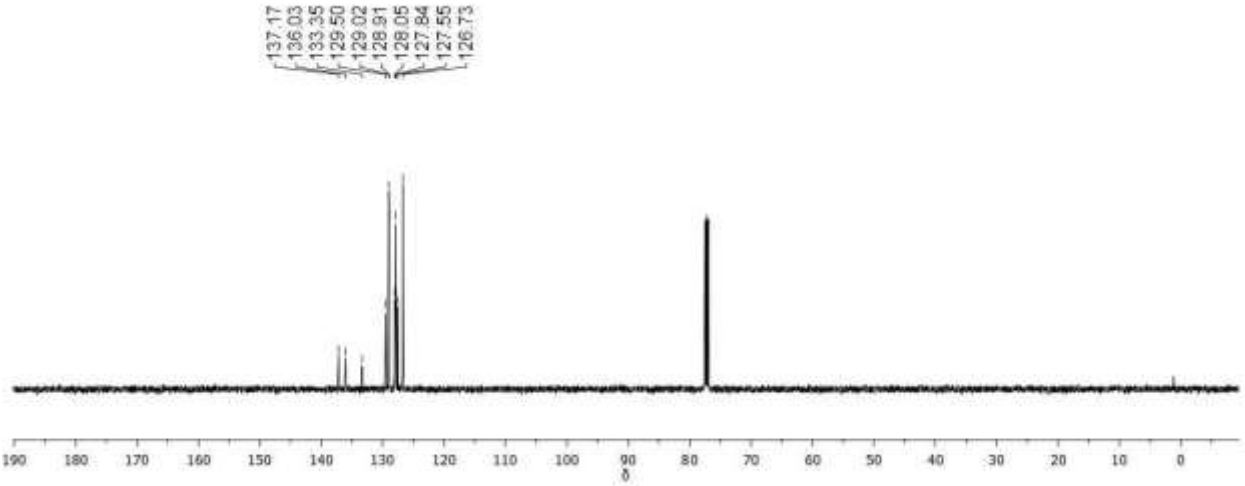


Fig. S85 ^{13}C NMR spectrum of **d** in $CDCl_3$ (126 MHz)

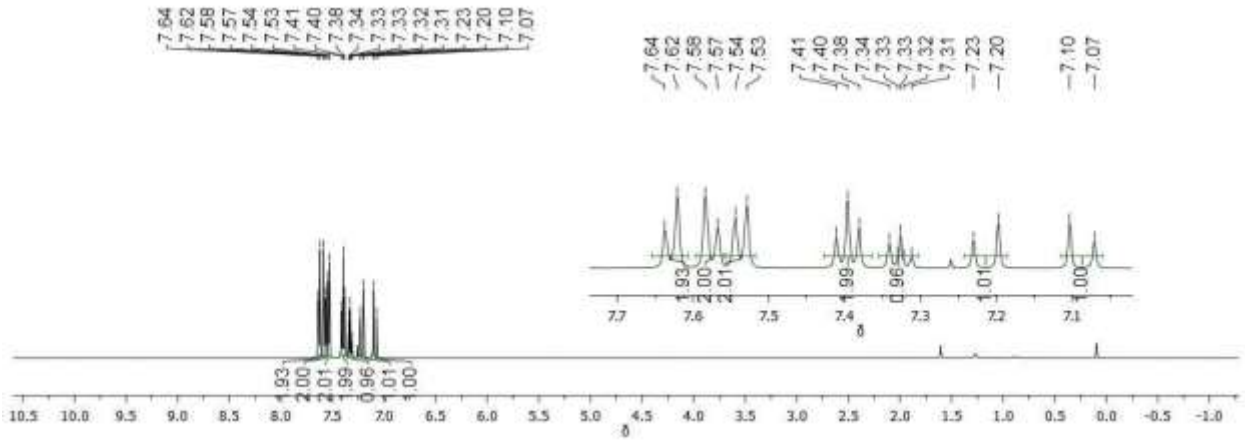


Fig. S86 ^{1}H NMR spectrum of **e** in $CDCl_3$ (500 MHz)

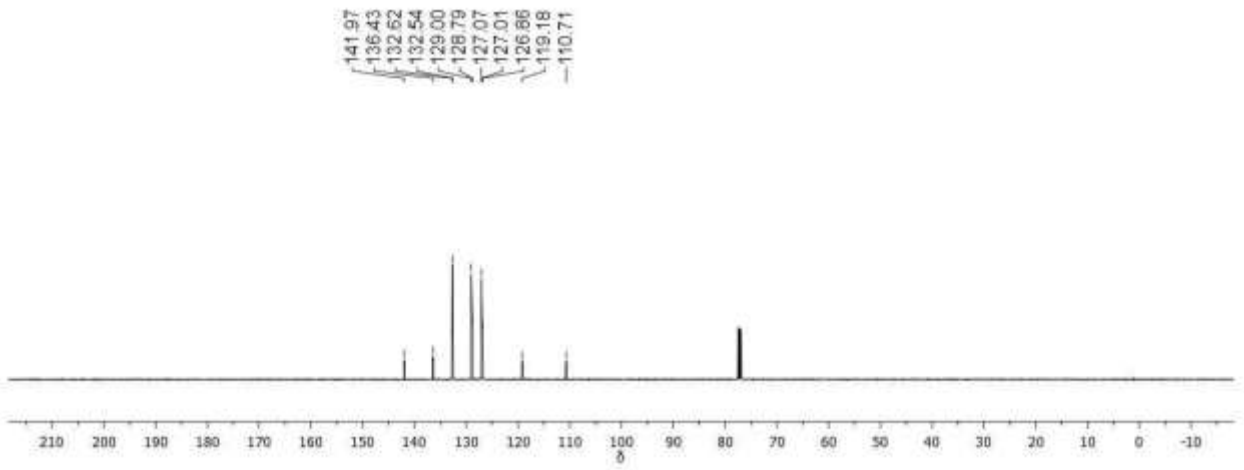


Fig. S87 ^{13}C NMR spectrum of **e** in $CDCl_3$ (126 MHz)

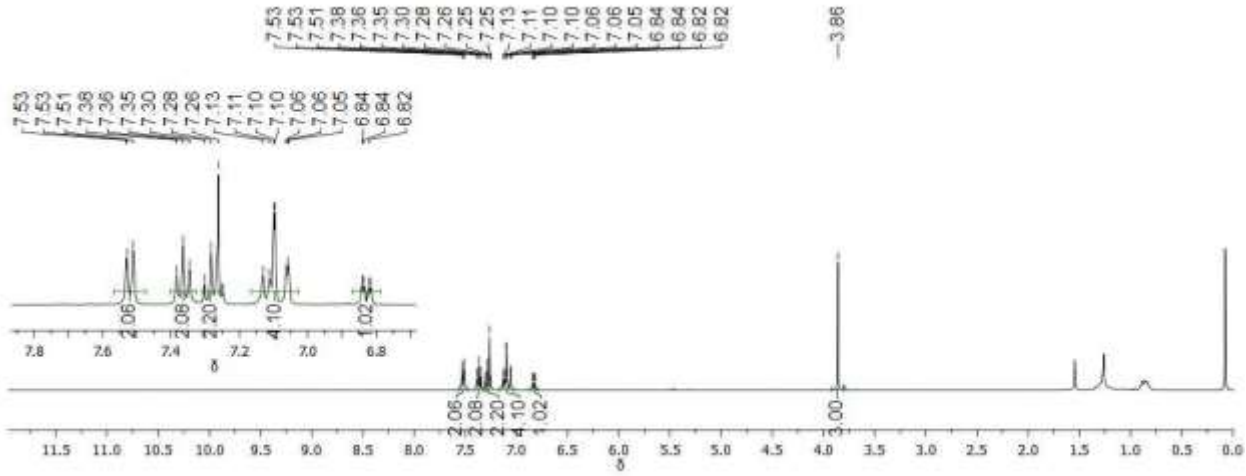


Fig. S88 ^{1}H NMR spectrum of **f** in $CDCl_3$ (400 MHz)

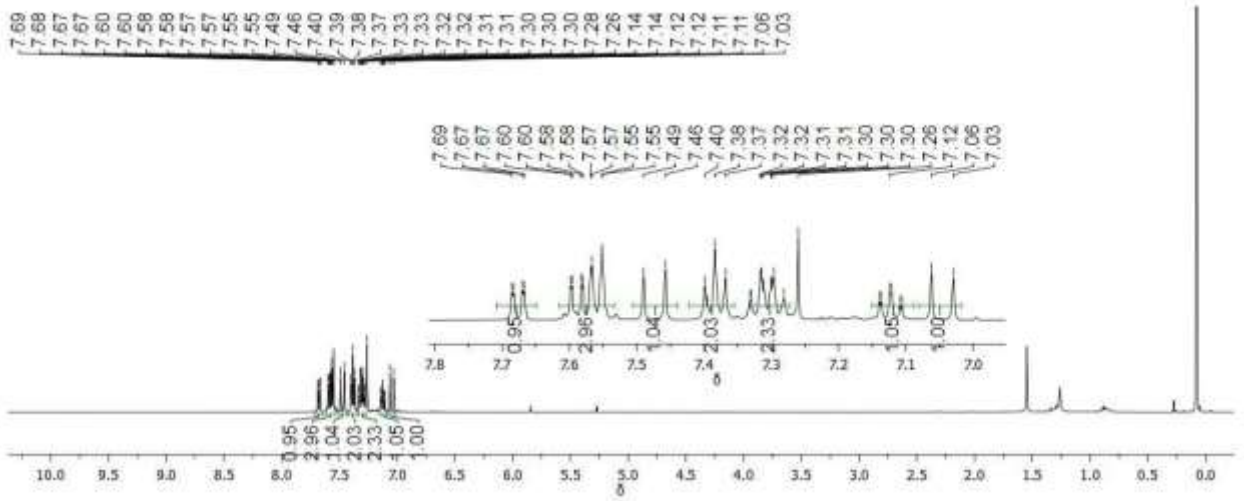


Fig. S89 ^{1}H NMR spectrum of **g** in $CDCl_3$ (500 MHz)

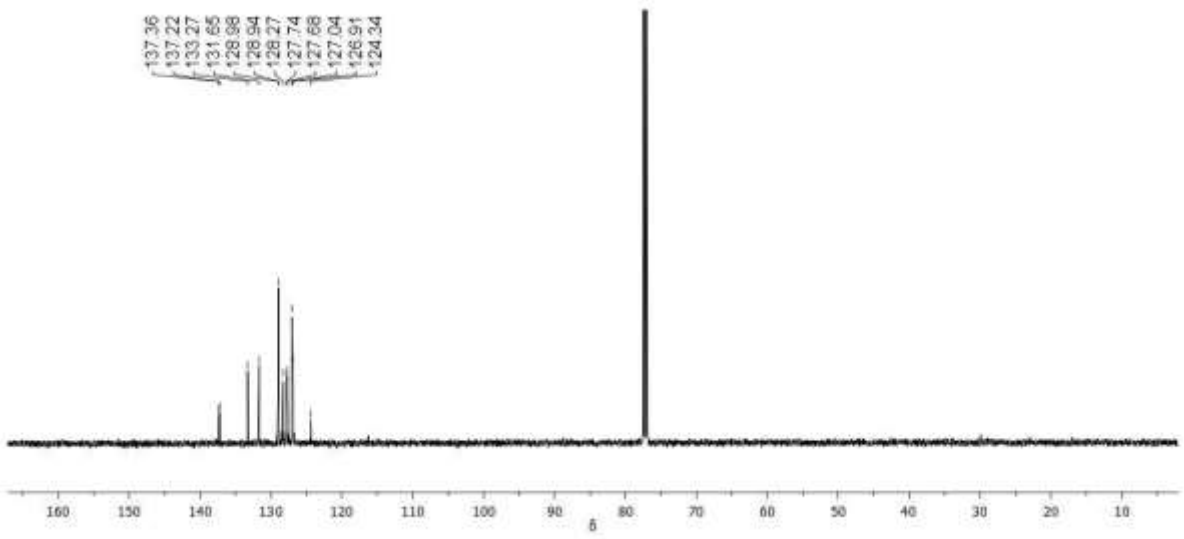


Fig. S90 ^{13}C NMR spectrum of **g** in $CDCl_3$ (126 MHz)

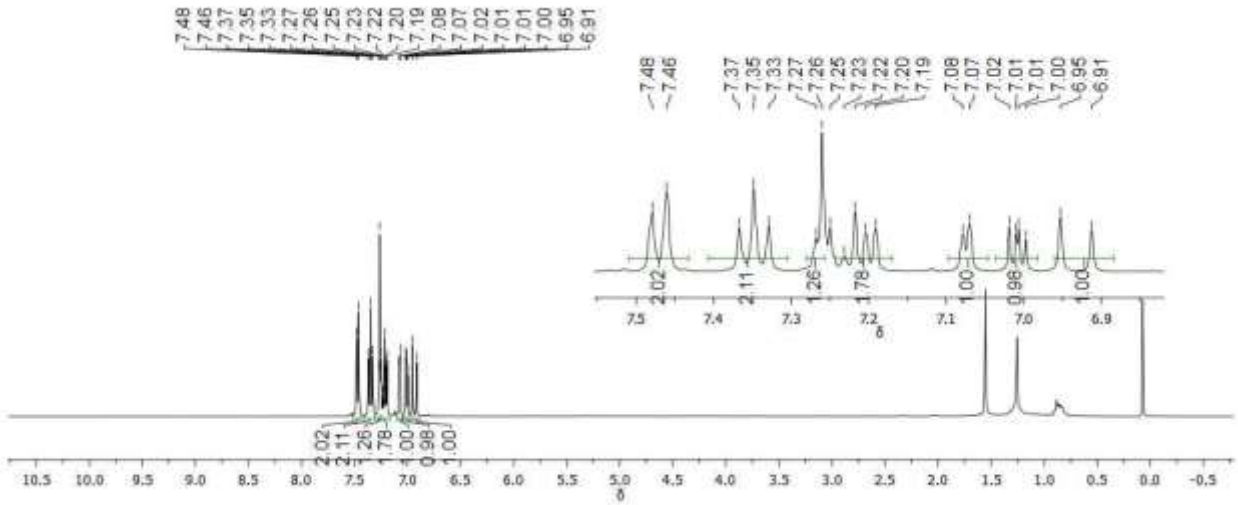


Fig. S91 ^{1}H NMR spectrum of **h** in $CDCl_3$ (500 MHz)

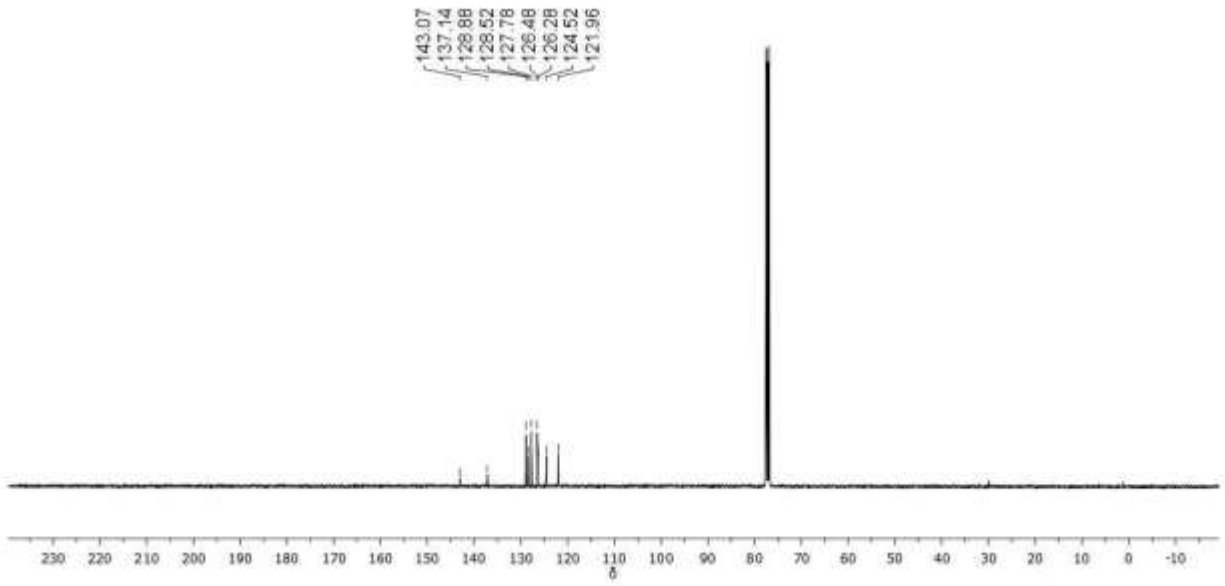


Fig. S92 ^{13}C NMR spectrum of **h** in $CDCl_3$ (101 MHz)

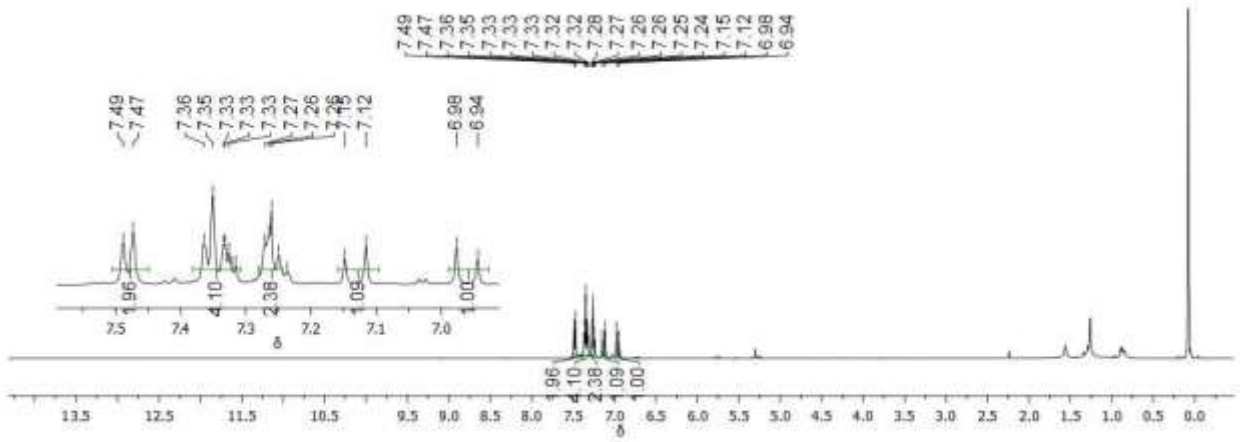


Fig. S93 ^{1}H NMR spectrum of **i** in $CDCl_3$ (500 MHz)

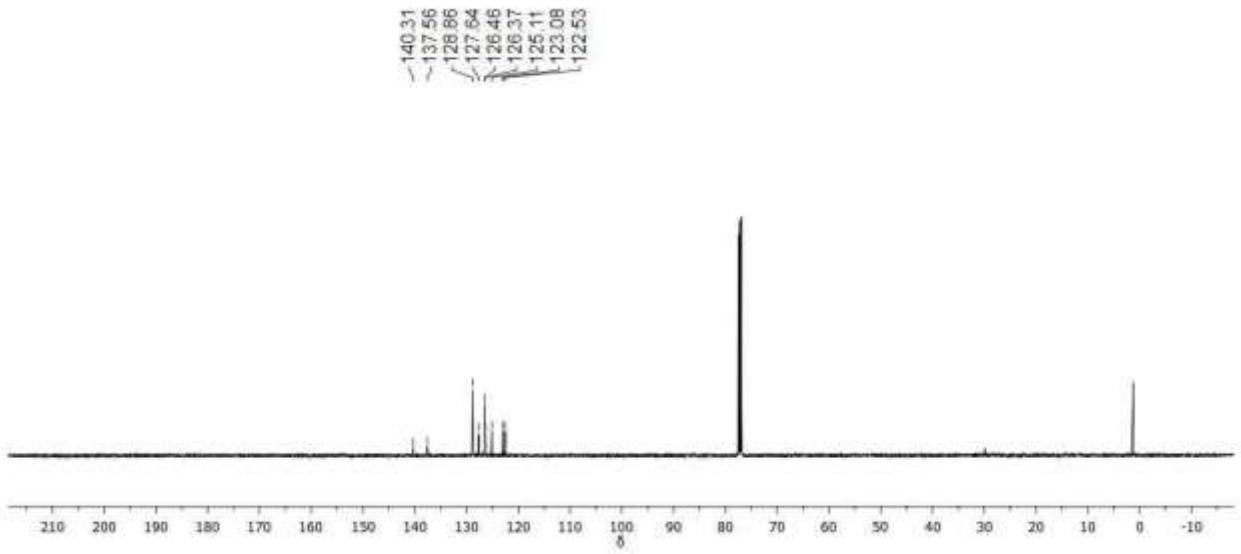


Fig. S94 ^{13}C NMR spectrum of **i** in $CDCl_3$ (126 MHz)

Cartesian coordinates of optimized geometries of 8-11

Total electronic energies and Gibbs free energies (in a.u) and Cartesian coordinates of optimized geometries of **8-11** at the M06/6-31G**, lanl2dz (Mo, W) level of theory.

8			
Zero-point correction=	0.601658		
Thermal correction to Energy=	0.647805		
Thermal correction to Enthalpy=	0.648749		
Thermal correction to Gibbs Free Energy=	0.519545		
Sum of electronic and zero-point Energies=	-2831.260530		
Sum of electronic and thermal Energies=	-2831.214383		
Sum of electronic and thermal Enthalpies=	-2831.213439		
Sum of electronic and thermal Free Energies=	-2831.342643		
15	0.347379000	6.630002000	11.740414000
15	-0.075147000	1.726460000	13.796422000
8	1.991453000	-0.582073000	9.020753000
8	3.578975000	0.355550000	13.115539000
8	-2.146273000	0.445217000	10.207587000

8	0.149102000	-2.388390000	12.757275000
6	2.853999000	3.954564000	15.691380000
1	3.316847000	3.979448000	16.674996000
7	0.416206000	3.079375000	9.887016000
7	0.318497000	4.411952000	9.861780000
6	1.853462000	3.024075000	15.423361000
1	1.540941000	2.337421000	16.207482000
6	-1.135884000	1.212117000	16.386752000
1	-1.785758000	2.071806000	16.234627000
6	-2.739855000	2.314014000	13.204777000
1	-2.730748000	1.340294000	12.717609000
6	-1.132460000	0.489719000	10.764081000
6	-1.570988000	2.802429000	13.794064000
6	1.241482000	2.962890000	14.172004000
6	1.513631000	-0.183504000	9.998202000
6	3.254778000	4.845081000	14.705930000
1	4.036955000	5.573530000	14.903061000
6	2.553710000	0.447849000	12.586127000
6	-1.595918000	4.055145000	14.418772000
1	-0.692440000	4.448380000	14.883571000
6	-0.247649000	0.817733000	15.381718000
6	3.654222000	9.453180000	10.142305000
1	4.437705000	10.129906000	9.810275000
7	0.867876000	2.745041000	11.063460000
6	-1.212838000	7.009892000	10.836552000
6	2.806931000	7.211938000	10.421426000
1	2.942403000	6.136380000	10.301948000
6	-0.172949000	5.013999000	8.662178000
6	-2.771957000	4.797883000	14.459816000
1	-2.777884000	5.771600000	14.944703000
6	1.494326000	9.092510000	11.151831000

1	0.599871000	9.497864000	11.625438000
6	-1.377441000	8.015512000	9.883466000
1	-0.525127000	8.619048000	9.574594000
6	1.660445000	3.857932000	13.163646000
6	0.091533000	6.531217000	6.828121000
1	0.673322000	7.287823000	6.307980000
6	0.576742000	-0.291714000	15.596787000
1	1.265406000	-0.613211000	14.816704000
6	-3.934863000	4.297141000	13.879812000
1	-4.854158000	4.877905000	13.915911000
6	-1.195197000	0.508513000	17.585184000
1	-1.893586000	0.820382000	18.358553000
6	0.579349000	5.982465000	8.008366000
1	1.536276000	6.298109000	8.415403000
6	-1.127861000	6.105956000	6.311043000
1	-1.504637000	6.535004000	5.385705000
6	2.659730000	4.792150000	13.450958000
1	2.999218000	5.466392000	12.666053000
6	1.628050000	7.707484000	10.989250000
6	2.491419000	9.957753000	10.717926000
1	2.364669000	11.030941000	10.840380000
6	-1.862699000	5.123573000	6.969426000
1	-2.812060000	4.785211000	6.562567000
6	0.704288000	4.967783000	11.055804000
6	3.812316000	8.078530000	10.002545000
1	4.721556000	7.674649000	9.563132000
6	-2.316358000	6.229415000	11.201775000
1	-2.201337000	5.440439000	11.947451000
6	-3.916309000	3.056284000	13.249031000
1	-4.820891000	2.660284000	12.793287000
6	0.358946000	-1.318041000	12.349840000

6	-1.387388000	4.568634000	8.150531000
1	-1.938949000	3.797196000	8.682163000
6	-2.624372000	8.233758000	9.304776000
1	-2.740720000	9.017468000	8.559243000
6	-3.556235000	6.440130000	10.612592000
1	-4.400269000	5.816416000	10.900704000
6	-3.713980000	7.447517000	9.664415000
1	-4.685355000	7.619391000	9.206368000
6	1.083675000	3.866408000	11.813710000
6	0.522218000	-0.986428000	16.799579000
1	1.169319000	-1.846209000	16.954058000
6	-0.365747000	-0.588449000	17.794264000
1	-0.414801000	-1.137342000	18.731964000
42	0.700957000	0.521202000	11.698901000

9

Zero-point correction= 0.601666

Thermal correction to Energy= 0.647469

Thermal correction to Enthalpy= 0.648413

Thermal correction to Gibbs Free Energy= 0.522809

Sum of electronic and zero-point Energies= -2831.265531

Sum of electronic and thermal Energies= -2831.219728

Sum of electronic and thermal Enthalpies= -2831.218784

Sum of electronic and thermal Free Energies= -2831.344388

15	1.784446000	4.738888000	8.076203000
15	2.224754000	6.226072000	11.309194000
6	-2.059707000	3.902054000	6.984737000
1	-2.733897000	3.063159000	7.138536000
6	-0.785978000	3.871122000	7.539365000
1	-0.472024000	3.000638000	8.114790000
6	-0.073693000	4.133174000	10.769934000
8	5.020427000	3.064198000	9.956778000

6	3.715863000	7.228687000	10.922010000
8	-1.194648000	4.300807000	10.989144000
7	3.536407000	8.288719000	7.247711000
6	4.934556000	6.577100000	10.725989000
1	4.982657000	5.491507000	10.779738000
6	0.094370000	4.942436000	7.358866000
7	2.537391000	8.679425000	7.967541000
8	2.247715000	2.547858000	13.346493000
6	3.678220000	8.626044000	10.871612000
1	2.735459000	9.150724000	11.021358000
6	3.915102000	3.365177000	10.144563000
6	4.833469000	9.350932000	10.606463000
1	4.785407000	10.435499000	10.550289000
6	0.759413000	7.773079000	9.393568000
8	1.154139000	0.914928000	9.388940000
6	-2.469737000	5.004676000	6.242092000
1	-3.469478000	5.034129000	5.815214000
6	2.965512000	7.240714000	13.868112000
1	3.702016000	7.851858000	13.351968000
6	-1.596785000	6.069209000	6.047396000
1	-1.908636000	6.933440000	5.464943000
6	4.611172000	6.268160000	6.595593000
6	5.020170000	6.657880000	5.324867000
1	4.498872000	7.469665000	4.824519000
6	6.081229000	5.990570000	4.726294000
1	6.408266000	6.284022000	3.731855000
6	1.945400000	6.538724000	15.940082000
1	1.878973000	6.594936000	17.024011000
6	-0.235644000	7.587774000	11.582882000
1	-0.207823000	7.240863000	12.612918000
6	5.263519000	5.254542000	7.286845000

1	4.959599000	5.006736000	8.302093000
6	2.128496000	6.385933000	13.145294000
6	-0.319374000	6.037645000	6.598159000
1	0.350869000	6.881288000	6.442510000
6	6.091273000	7.303403000	10.458677000
1	7.030150000	6.779679000	10.293793000
6	1.202827000	5.604766000	13.848340000
1	0.549020000	4.921908000	13.308454000
6	2.874851000	7.312181000	15.255309000
1	3.539705000	7.977468000	15.801419000
6	0.824023000	7.294555000	10.721069000
6	6.040507000	8.691076000	10.394288000
1	6.940170000	9.260192000	10.172650000
6	-0.328253000	8.551480000	8.993724000
1	-0.334825000	8.943206000	7.978166000
6	2.452827000	6.444152000	7.921734000
6	1.105140000	5.685294000	15.231522000
1	0.378578000	5.069295000	15.755694000
6	2.128971000	3.022701000	12.296724000
6	3.073983000	3.559412000	4.345052000
1	3.026923000	3.946336000	3.329688000
6	6.304330000	4.574788000	6.667571000
1	6.795439000	3.761034000	7.196212000
6	2.488819000	4.271993000	5.381460000
1	1.977821000	5.210998000	5.169011000
6	-1.329815000	8.334807000	11.159353000
1	-2.138976000	8.540926000	11.855768000
6	1.463023000	1.964919000	9.778988000
6	3.714595000	2.349177000	4.604747000
1	4.168765000	1.789694000	3.790131000
6	6.710376000	4.938205000	5.387180000

1	7.527176000	4.406389000	4.905218000
6	3.194710000	2.580907000	6.945190000
1	3.248366000	2.196465000	7.960344000
6	-1.375873000	8.826277000	9.862014000
1	-2.219538000	9.424616000	9.527361000
6	2.562251000	3.798451000	6.695929000
6	3.764148000	1.855826000	5.901900000
1	4.251158000	0.906257000	6.110020000
7	3.512532000	6.936167000	7.205586000
6	1.863546000	7.590548000	8.436176000
42	1.936714000	3.789163000	10.444770000

10

Zero-point correction= 0.602064 (Hartree/Particle)

Thermal correction to Energy= 0.648043

Thermal correction to Enthalpy= 0.648987

Thermal correction to Gibbs Free Energy= 0.520144

Sum of electronic and zero-point Energies= -2831.539181

Sum of electronic and thermal Energies= -2831.493202

Sum of electronic and thermal Enthalpies= -2831.492258

Sum of electronic and thermal Free Energies= -2831.621101

74	0.701203000	0.545233000	11.710194000
15	0.357541000	6.632005000	11.740051000
15	-0.071908000	1.734505000	13.800479000
8	1.978322000	-0.511709000	9.012821000
8	3.579319000	0.425173000	13.111416000
8	-2.161474000	0.421905000	10.274168000
8	0.206090000	-2.368783000	12.785287000
6	2.846242000	3.972047000	15.698010000
1	3.308366000	4.001930000	16.681792000
7	0.382347000	3.074267000	9.902289000
7	0.303198000	4.406386000	9.870562000

6	1.844576000	3.041408000	15.434110000
1	1.529611000	2.357800000	16.220038000
6	-1.156400000	1.183479000	16.368340000
1	-1.821076000	2.030611000	16.210248000
6	-2.735319000	2.309271000	13.185135000
1	-2.716566000	1.341841000	12.686144000
6	-1.132973000	0.482886000	10.807198000
6	-1.574167000	2.799770000	13.788050000
6	1.236335000	2.975075000	14.181907000
6	1.505101000	-0.130678000	10.002079000
6	3.250393000	4.855546000	14.707517000
1	4.034342000	5.582885000	14.901539000
6	2.550670000	0.500081000	12.580381000
6	-1.609049000	4.048641000	14.419859000
1	-0.709696000	4.445212000	14.889966000
6	-0.245359000	0.811404000	15.375454000
6	3.676506000	9.432712000	10.128846000
1	4.463255000	10.104159000	9.793868000
7	0.835780000	2.740628000	11.080613000
6	-1.202983000	7.016785000	10.839422000
6	2.816375000	7.197146000	10.413331000
1	2.945358000	6.120664000	10.295320000
6	-0.186672000	5.007220000	8.669536000
6	-2.789317000	4.784762000	14.458195000
1	-2.803985000	5.755205000	14.949342000
6	1.517158000	9.086816000	11.144719000
1	0.626372000	9.498229000	11.620023000
6	-1.364272000	8.020658000	9.883965000
1	-0.509454000	8.619079000	9.572071000
6	1.656224000	3.863987000	13.169175000
6	0.083164000	6.517974000	6.831338000

1	0.667900000	7.270463000	6.308569000
6	0.598239000	-0.282454000	15.596202000
1	1.305090000	-0.585761000	14.825229000
6	-3.945528000	4.281160000	13.867362000
1	-4.868494000	4.856164000	13.902029000
6	-1.220274000	0.471862000	17.561816000
1	-1.936572000	0.765160000	18.325941000
6	0.569549000	5.970606000	8.012779000
1	1.528219000	6.283286000	8.417944000
6	-1.138364000	6.096335000	6.316331000
1	-1.513901000	6.524263000	5.389988000
6	2.657179000	4.797607000	13.451745000
1	2.999654000	5.466789000	12.663860000
6	1.642162000	7.700793000	10.983737000
6	2.518482000	9.945265000	10.706991000
1	2.398710000	11.019360000	10.828344000
6	-1.876876000	5.118832000	6.977901000
1	-2.827681000	4.783046000	6.572329000
6	0.703266000	4.965266000	11.058311000
6	3.825841000	8.056946000	9.990429000
1	4.731342000	7.646945000	9.549013000
6	-2.309640000	6.242890000	11.209380000
1	-2.197437000	5.455245000	11.957065000
6	-3.915573000	3.045664000	13.226554000
1	-4.814427000	2.648832000	12.760399000
6	0.394130000	-1.295726000	12.368008000
6	-1.403240000	4.565090000	8.160196000
1	-1.957037000	3.796852000	8.694077000
6	-2.611196000	8.243645000	9.307136000
1	-2.725211000	9.026103000	8.559949000
6	-3.549334000	6.457882000	10.621380000

1	-4.396019000	5.838983000	10.911995000
6	-3.703798000	7.463436000	9.670715000
1	-4.675092000	7.638553000	9.213761000
6	1.075238000	3.865626000	11.821577000
6	0.538116000	-0.984821000	16.794076000
1	1.199333000	-1.832763000	16.953816000
6	-0.373011000	-0.610051000	17.776983000
1	-0.425824000	-1.165687000	18.710487000

11

Zero-point correction= 0.602090

Thermal correction to Energy= 0.647722

Thermal correction to Enthalpy= 0.648666

Thermal correction to Gibbs Free Energy= 0.523357

Sum of electronic and zero-point Energies= -2831.545714

Sum of electronic and thermal Energies= -2831.500082

Sum of electronic and thermal Enthalpies= -2831.499138

Sum of electronic and thermal Free Energies= -2831.624447

74	1.932286000	3.802878000	10.441595000
15	1.786183000	4.743299000	8.083303000
15	2.219285000	6.224218000	11.303967000
6	-2.050721000	3.884735000	6.981880000
1	-2.719504000	3.040572000	7.130086000
6	-0.777871000	3.858677000	7.538595000
1	-0.459836000	2.986198000	8.108474000
6	-0.065785000	4.153740000	10.757691000
8	5.010546000	3.092875000	9.950832000
6	3.713507000	7.221204000	10.916257000
8	-1.188518000	4.334012000	10.968505000
7	3.532124000	8.292634000	7.242970000
6	4.932996000	6.569800000	10.725448000
1	4.983002000	5.484745000	10.782093000

6	0.095489000	4.937054000	7.365309000
7	2.532569000	8.684065000	7.961835000
8	2.234817000	2.569123000	13.341594000
6	3.675155000	8.618575000	10.865987000
1	2.732093000	9.143182000	11.013785000
6	3.900647000	3.384278000	10.142202000
6	4.830614000	9.343936000	10.603177000
1	4.782042000	10.428432000	10.546576000
6	0.757968000	7.779172000	9.392260000
8	1.147011000	0.938424000	9.373737000
6	-2.466406000	4.988154000	6.243520000
1	-3.465481000	5.013146000	5.814828000
6	2.974565000	7.223228000	13.862018000
1	3.716425000	7.827141000	13.345216000
6	-1.599678000	6.058639000	6.054752000
1	-1.915404000	6.923210000	5.474950000
6	4.609460000	6.272871000	6.593500000
6	5.014371000	6.661923000	5.321241000
1	4.490451000	7.472266000	4.821312000
6	6.075134000	5.995885000	4.720711000
1	6.399149000	6.288860000	3.725143000
6	1.952003000	6.529004000	15.935159000
1	1.888369000	6.584694000	17.019276000
6	-0.236953000	7.589992000	11.581760000
1	-0.210183000	7.238617000	12.610251000
6	5.264913000	5.260917000	7.284163000
1	4.963960000	5.012253000	8.299948000
6	2.127624000	6.377189000	13.140502000
6	-0.323105000	6.032613000	6.607941000
1	0.342371000	6.880440000	6.455511000
6	6.089600000	7.296904000	10.459871000

1	7.029214000	6.773491000	10.298497000
6	1.195699000	5.604063000	13.844198000
1	0.534461000	4.927763000	13.305305000
6	2.887394000	7.294280000	15.249427000
1	3.559798000	7.952516000	15.794770000
6	0.820837000	7.296076000	10.718145000
6	6.038270000	8.684464000	10.393679000
1	6.938178000	9.253762000	10.173568000
6	-0.326846000	8.563181000	8.995737000
1	-0.332263000	8.959098000	7.981811000
6	2.452367000	6.448717000	7.923089000
6	1.102367000	5.684045000	15.227640000
1	0.371308000	5.074290000	15.752750000
6	2.120691000	3.039450000	12.286917000
6	3.076513000	3.553504000	4.359766000
1	3.028398000	3.939200000	3.344014000
6	6.305461000	4.582527000	6.662972000
1	6.798687000	3.769937000	7.191387000
6	2.491726000	4.266906000	5.395701000
1	1.979279000	5.204836000	5.182047000
6	-1.328895000	8.341814000	11.160939000
1	-2.137532000	8.547568000	11.857996000
6	1.456437000	1.987557000	9.772765000
6	3.718017000	2.344041000	4.620761000
1	4.171642000	1.783465000	3.806604000
6	6.707864000	4.945473000	5.381287000
1	7.524528000	4.414701000	4.897940000
6	3.200385000	2.578671000	6.961800000
1	3.254631000	2.194300000	7.976676000
6	-1.373186000	8.838241000	9.865488000
1	-2.214970000	9.440491000	9.533142000

6	2.566980000	3.795279000	6.710827000
6	3.768984000	1.852748000	5.918614000
1	4.256411000	0.903663000	6.127740000
7	3.510953000	6.940254000	7.205008000
6	1.860829000	7.595556000	8.433962000

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