Supplementary information

Catechol and 1,2,4,5-tetrahydroxybenzene functionalized cyclodiphosphazane ligands synthesis, structural studies, and transition metal complexes

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NMR spectra of compounds **1-16**	2–26
HRMS spectra of compounds **1-16**	2–26

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[a]These authors contributed equally to this work

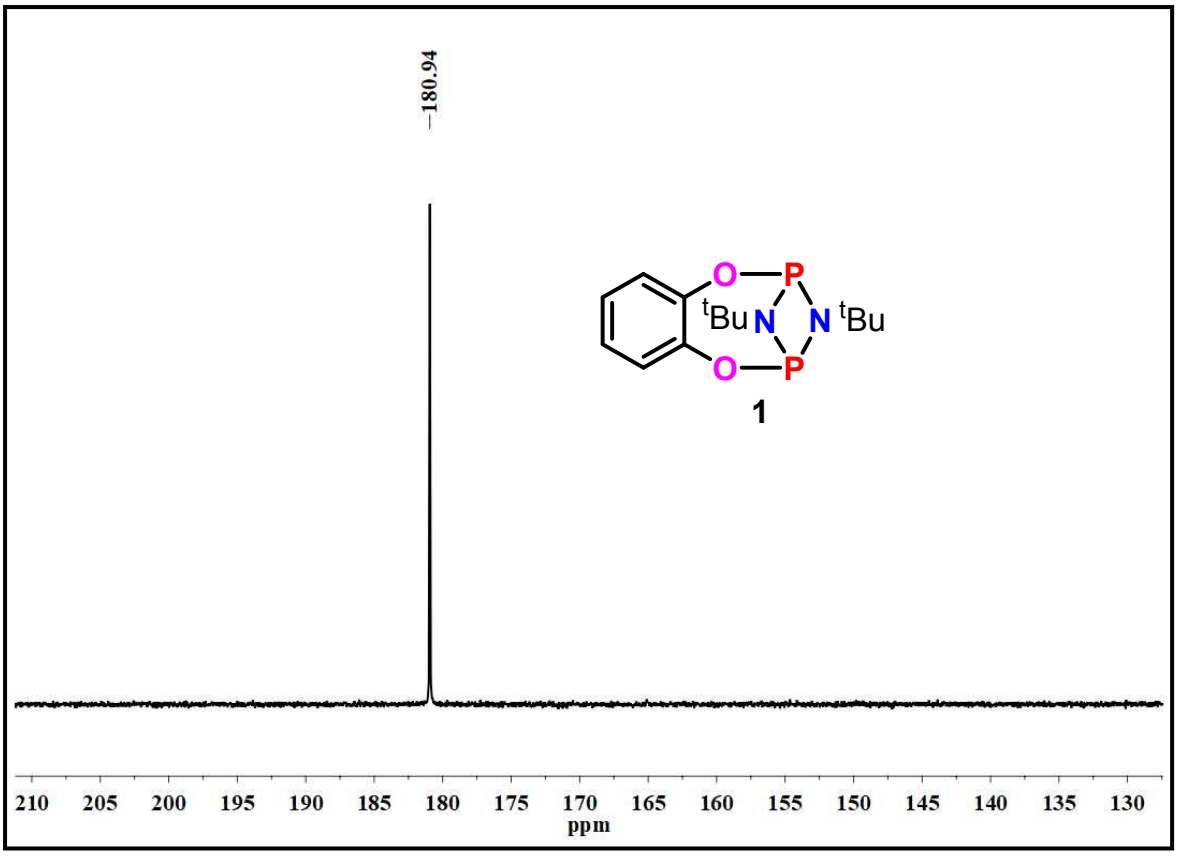

Fig. S1 $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$(162 MHz)

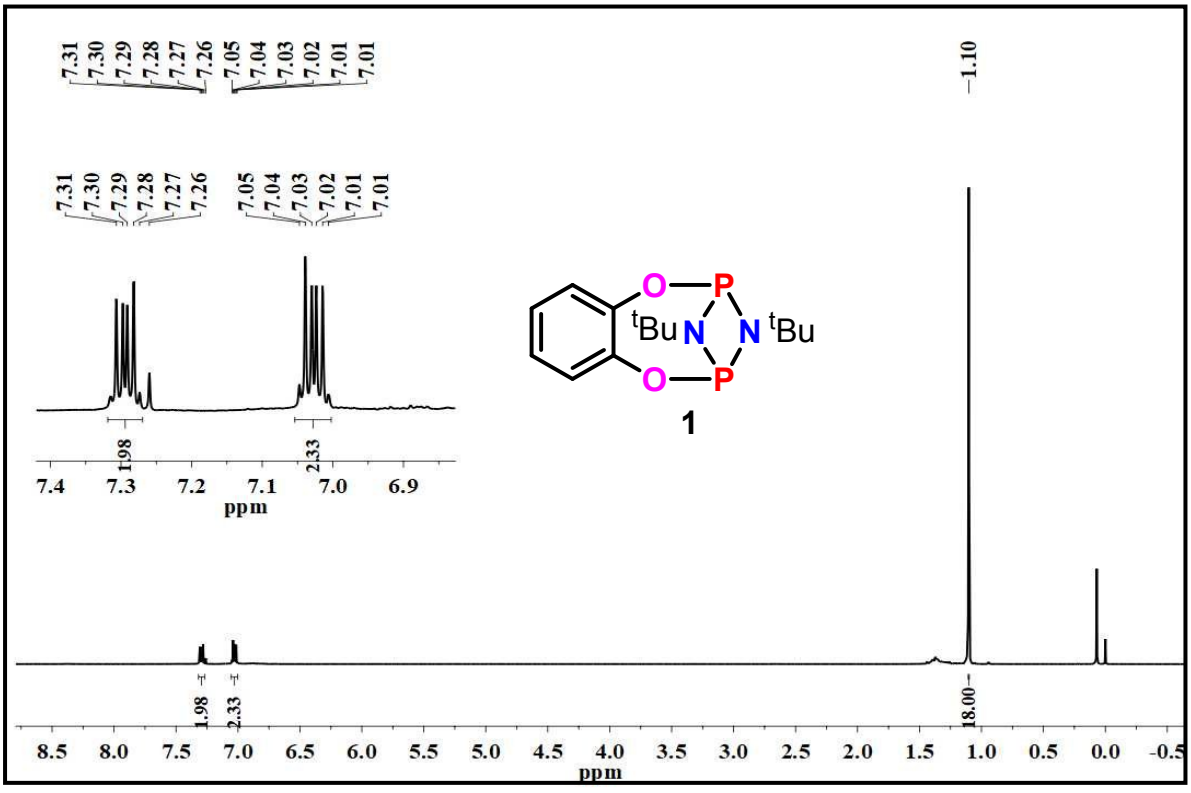

Fig. S2 ^{1}H NMR spectrum of **1** in $CDCl_3$(400 MHz)

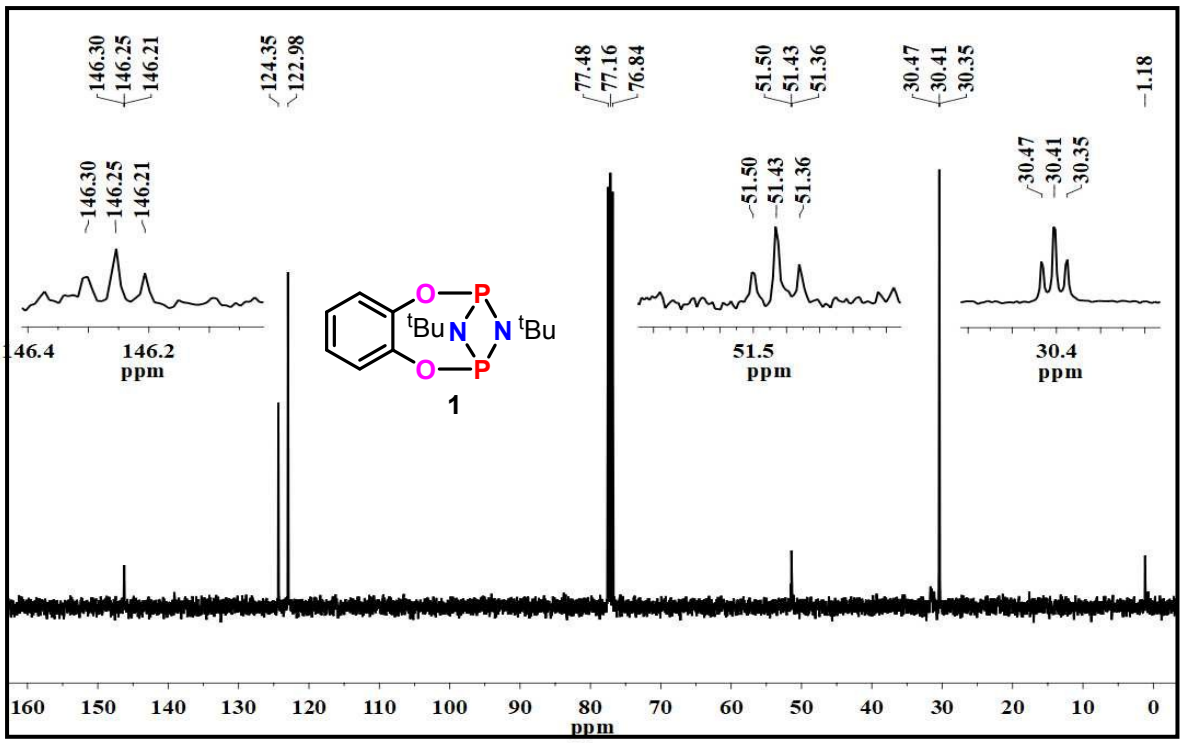

Fig. S3 $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$(101 MHz)

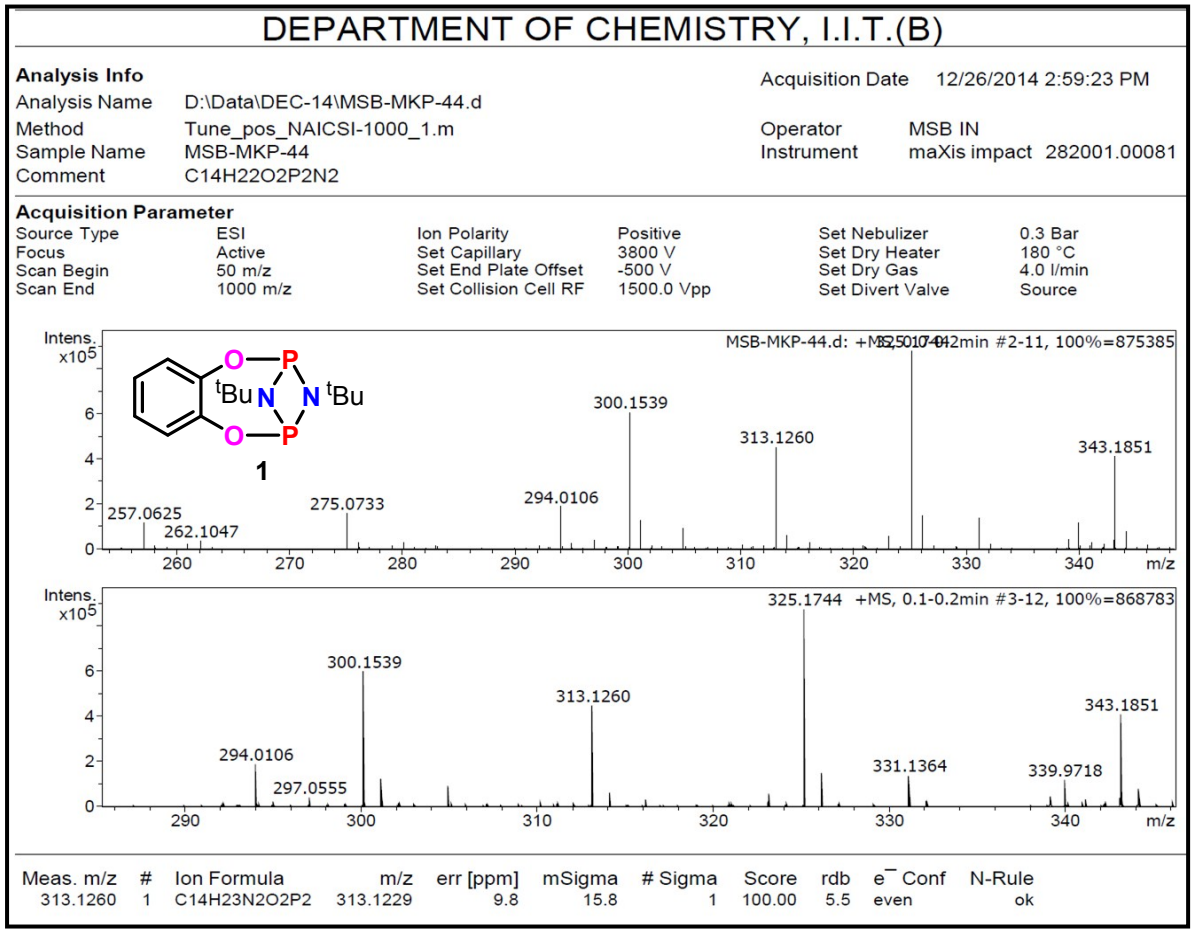

Fig. S4 HRMS spectrum of **1**

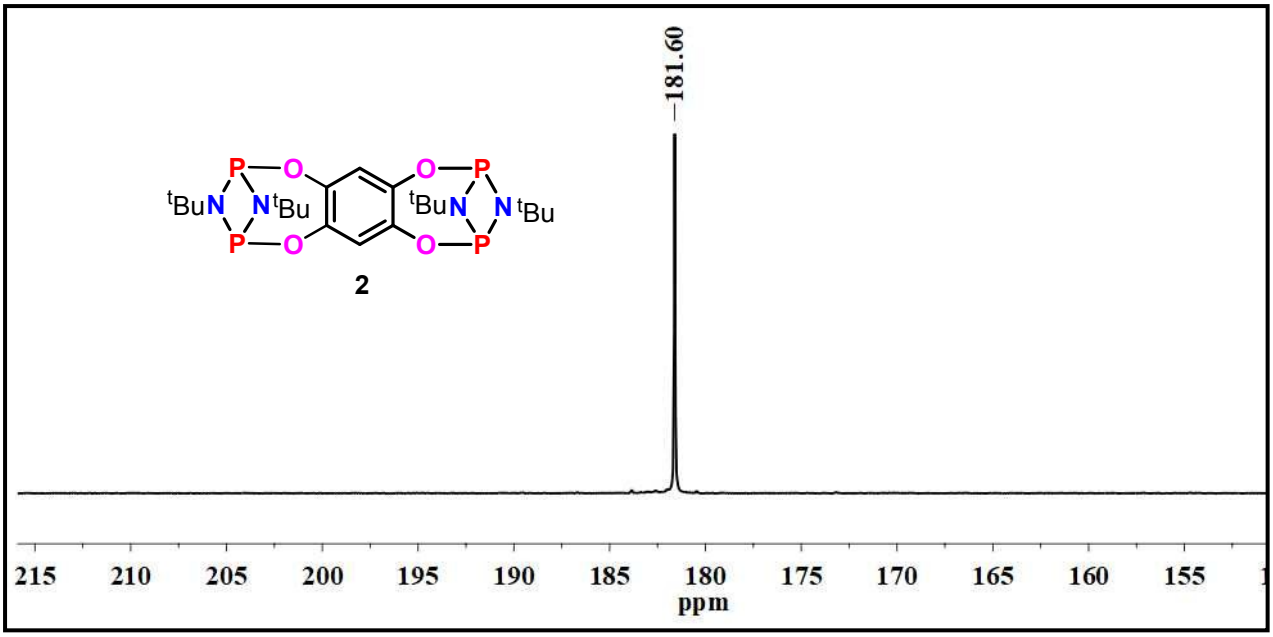

Fig. S5 $^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$(202 MHz)

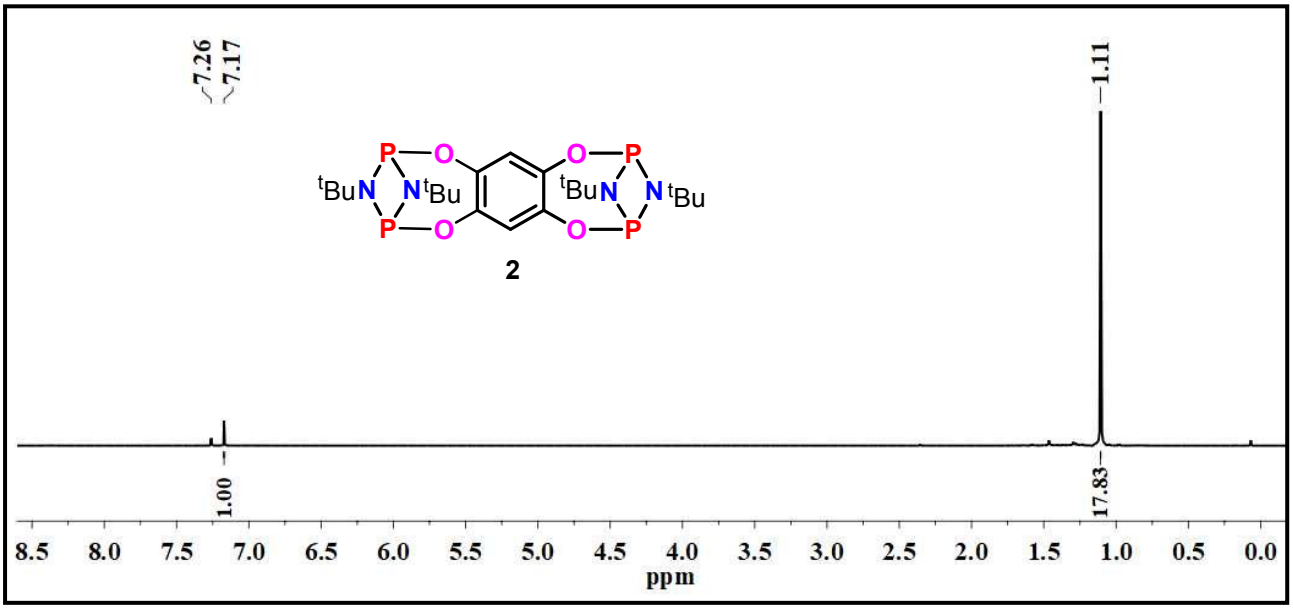

Fig. S6 ^{1}H NMR spectrum of **2** in $CDCl_3$(500 MHz)

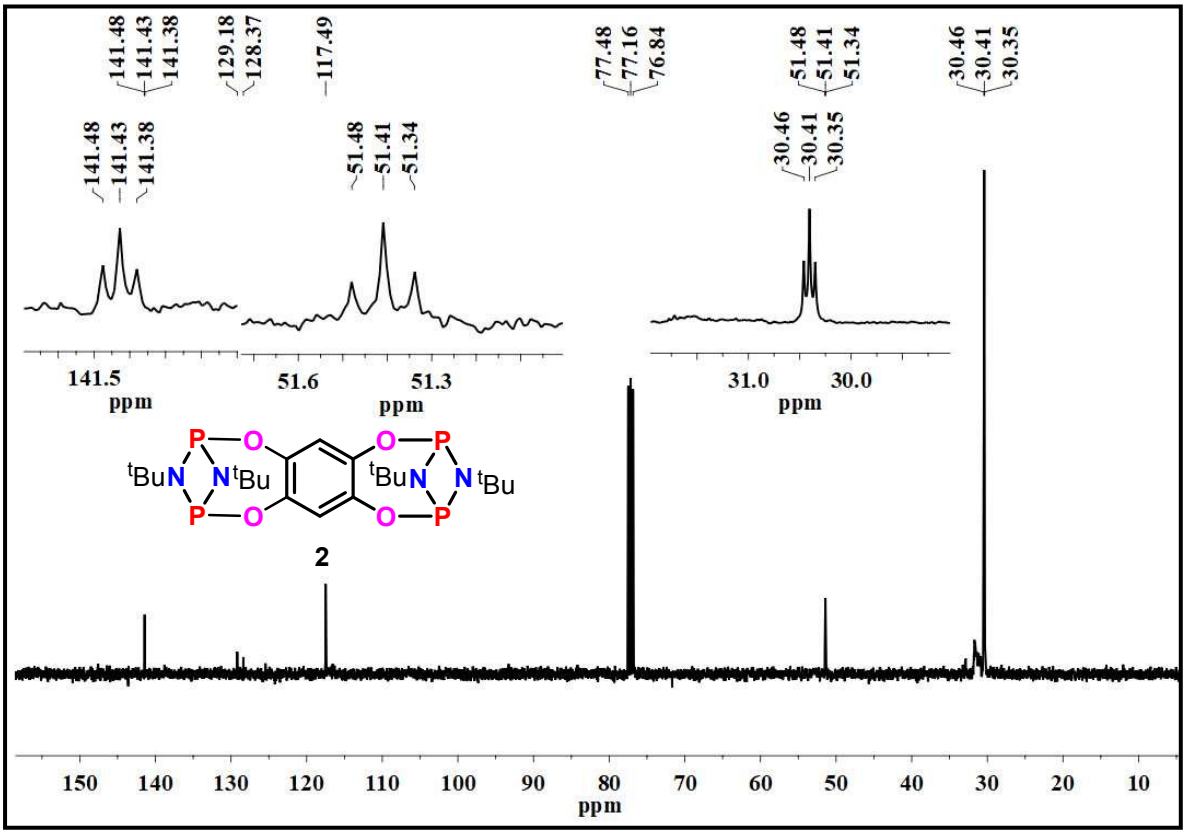

Fig. S7 $^{13}C\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$(126 MHz)

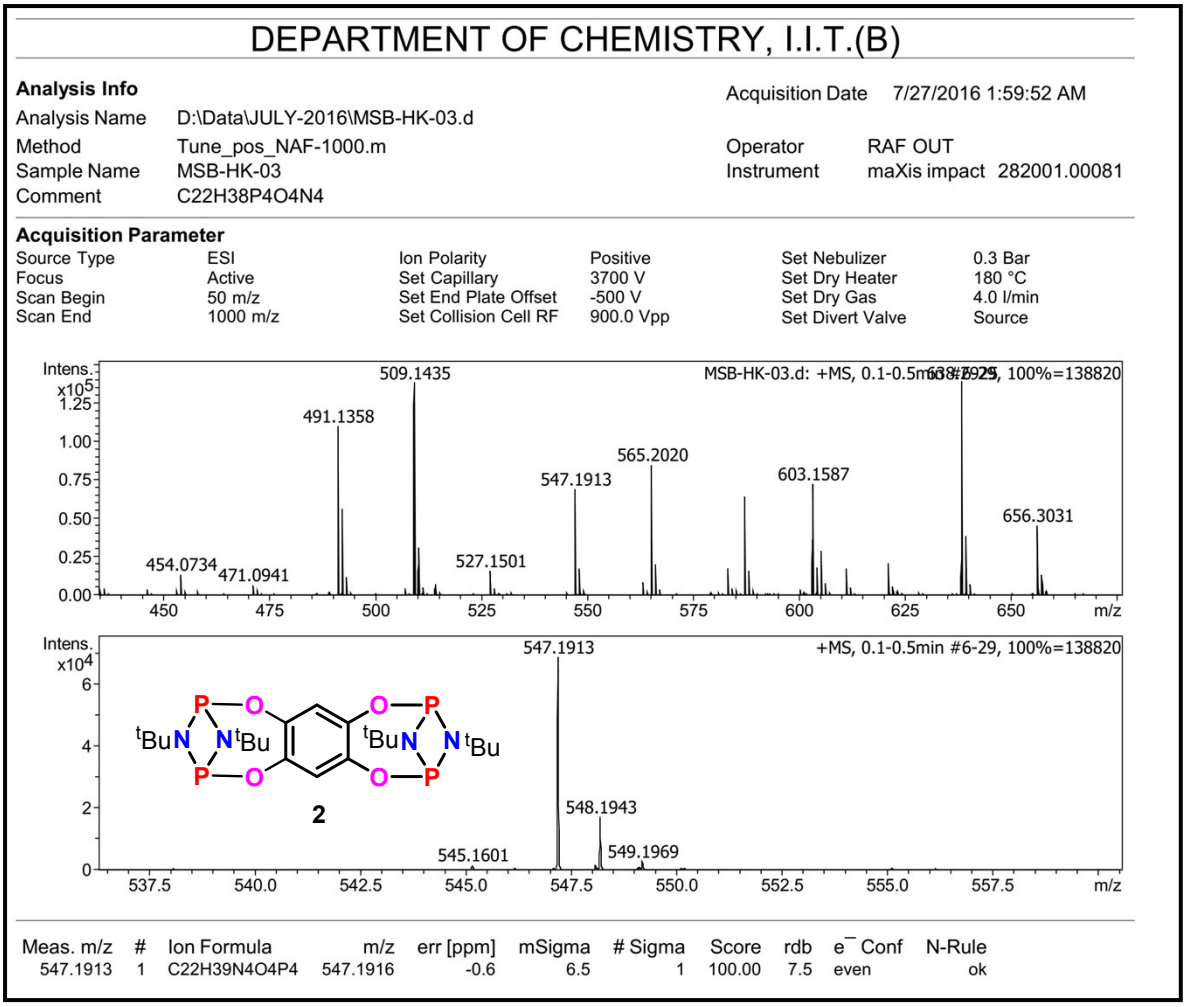

Fig. S8 HRMS spectrum of **2**

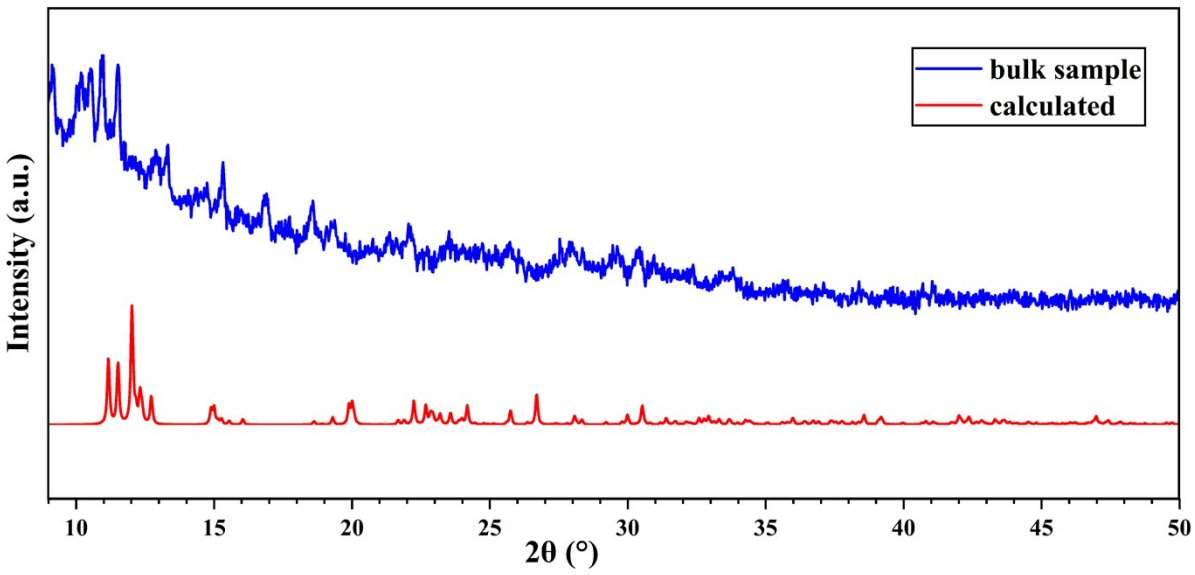

Fig. S9. The powder-XRD patterns of compound **3.** Experimental in blue and simulated in red.

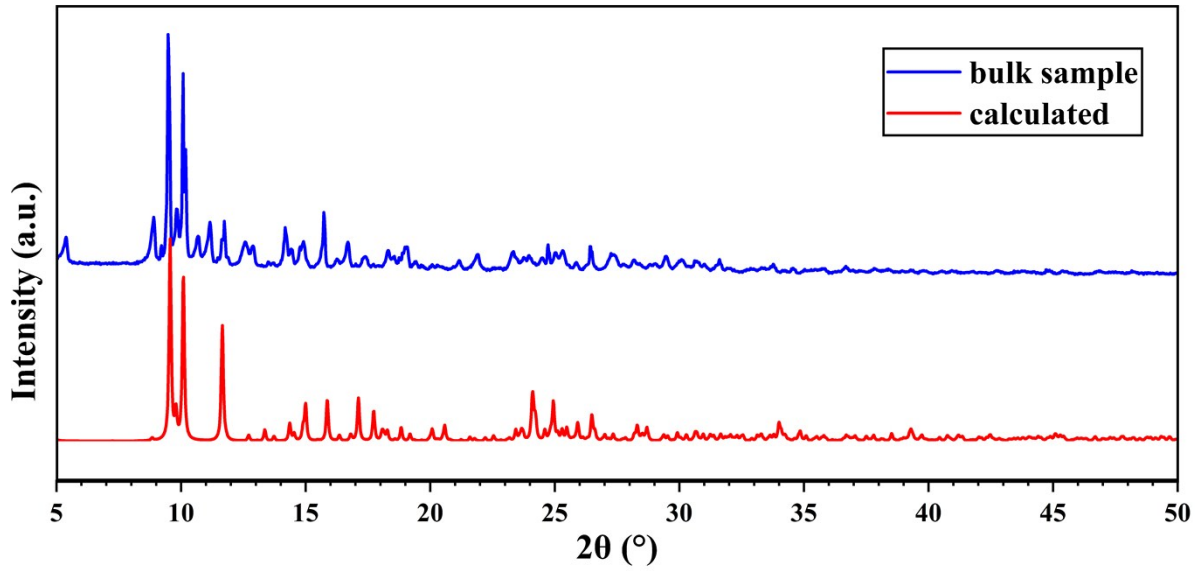

Fig. S10. The powder-XRD patterns of compound **4.** Experimental in blue and simulated in red.

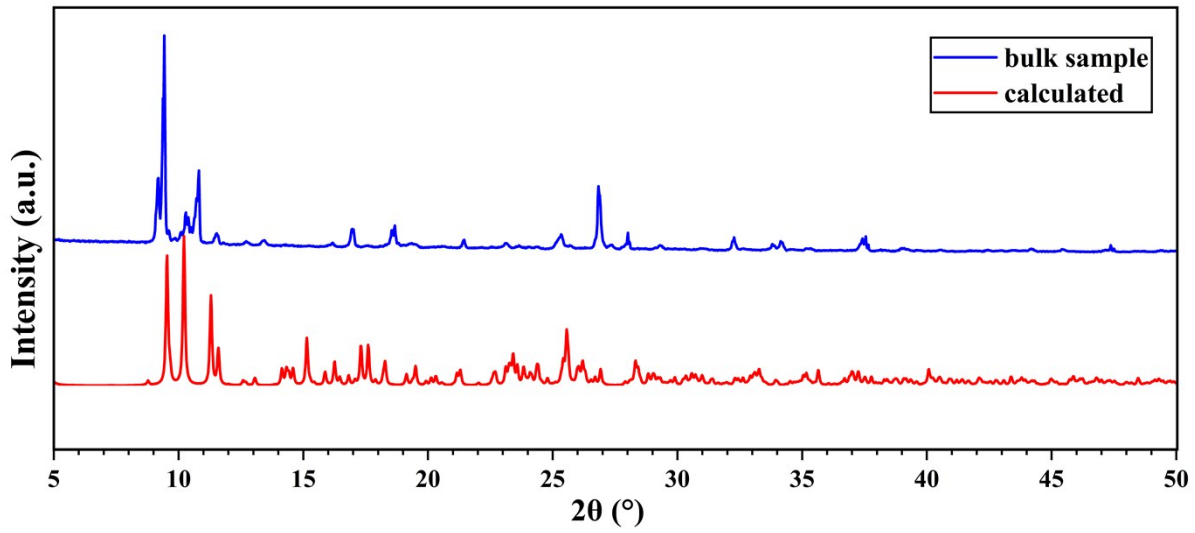

Fig. S11. The powder-XRD patterns of compound **5.** Experimental in blue and simulated in red. (Some extra peaks observed may be due to the presence of some non-identified material).

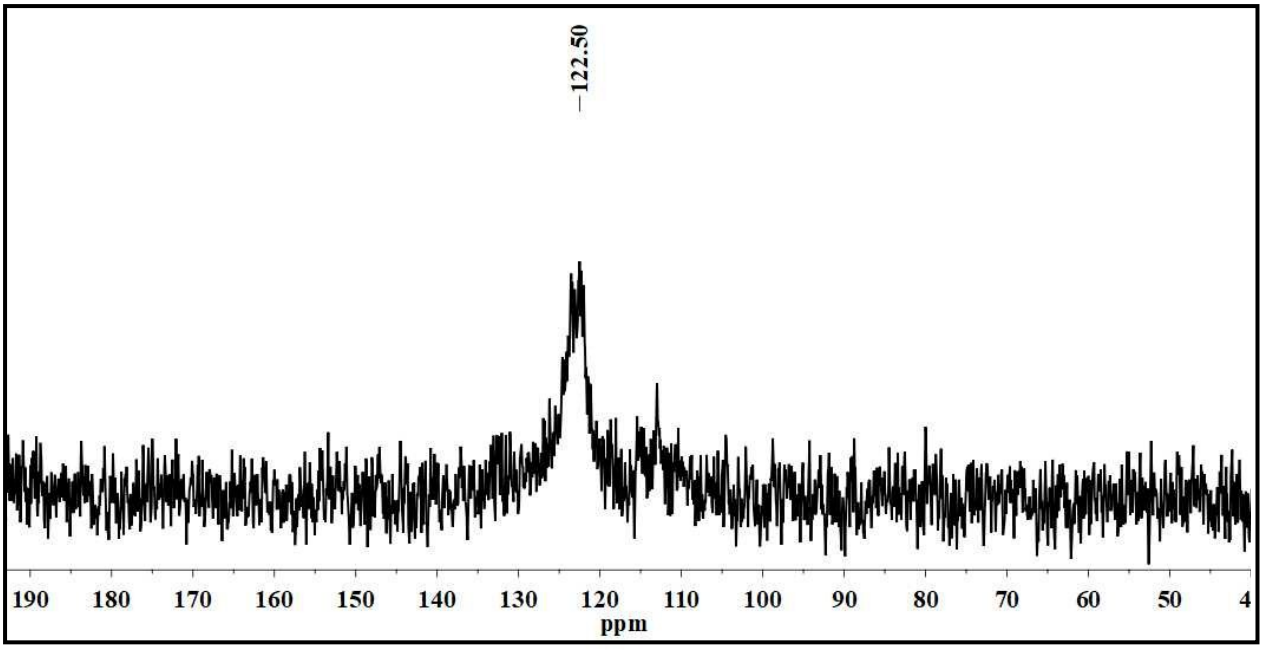

Fig. S12 $^{31}P\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$(162 MHz)

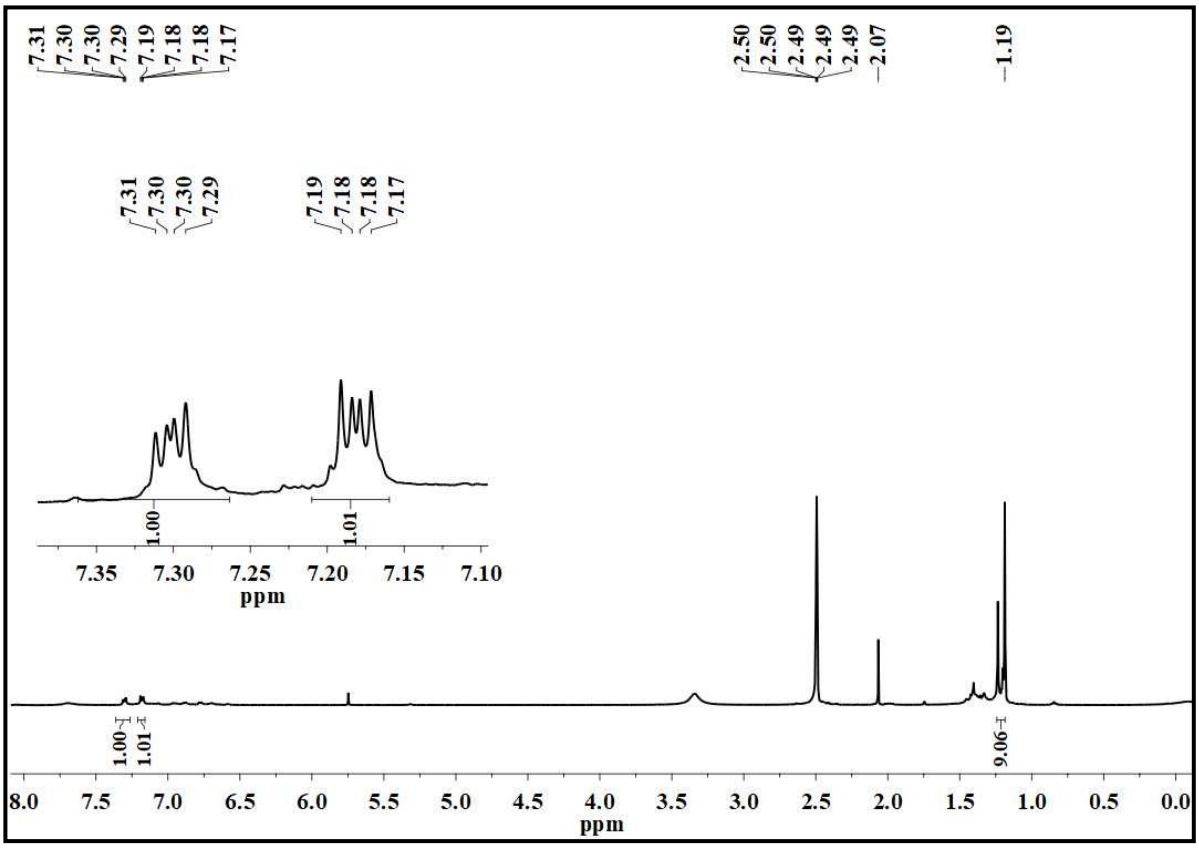

Fig. S13 ^{1}H NMR spectrum of **6** in $CDCl_3$(500 MHz)

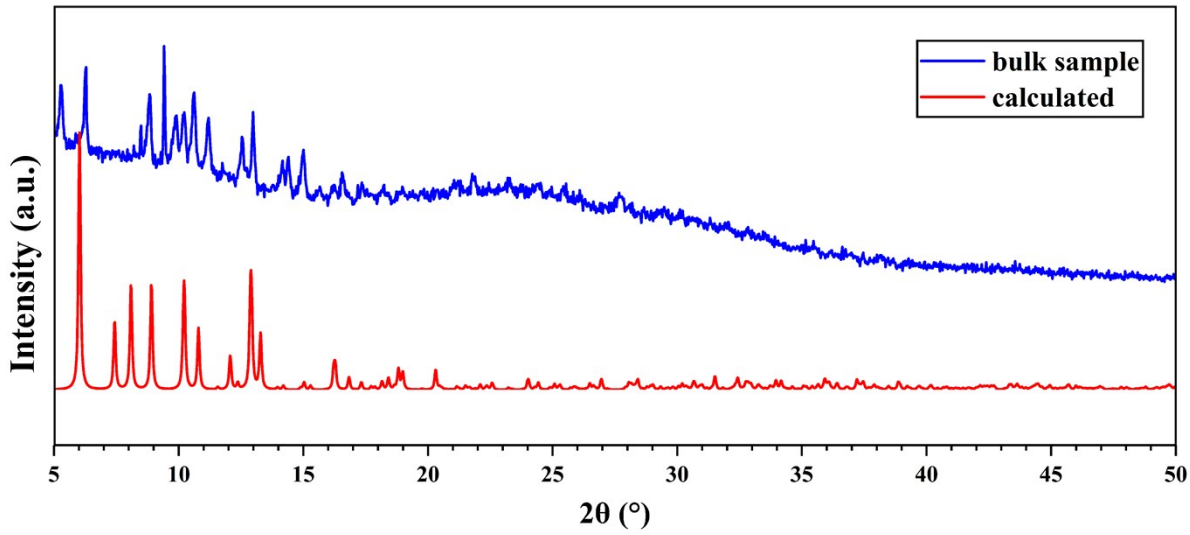

Fig. S14. The powder-XRD patterns of compound **6.** Experimental in blue and simulated in red.

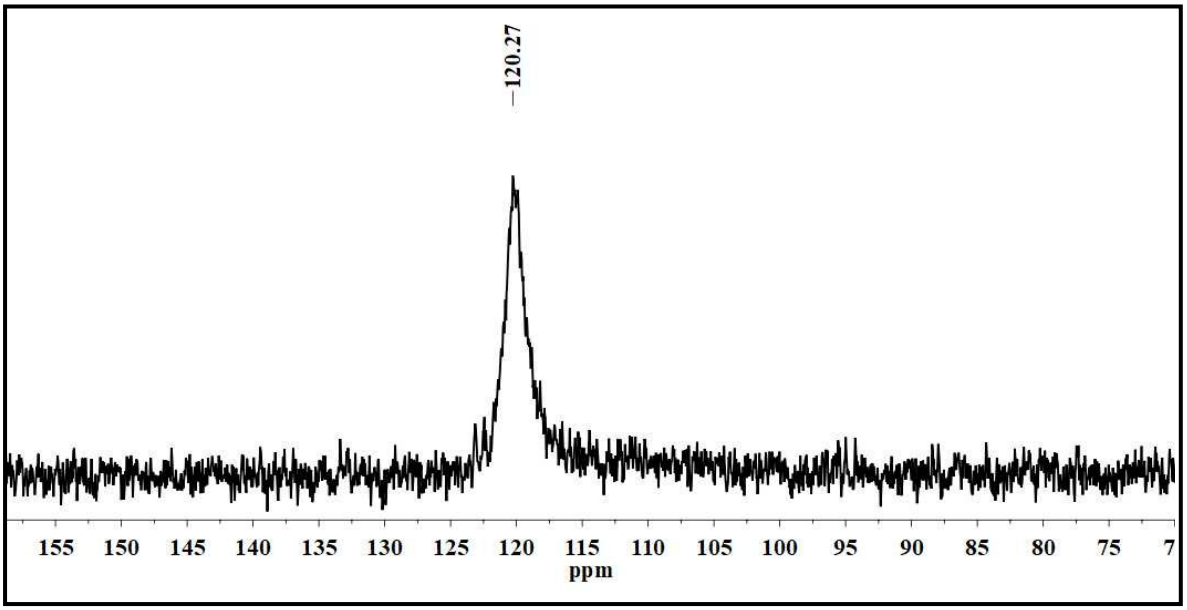

Fig. S15 $^{31}P\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$(162 MHz)

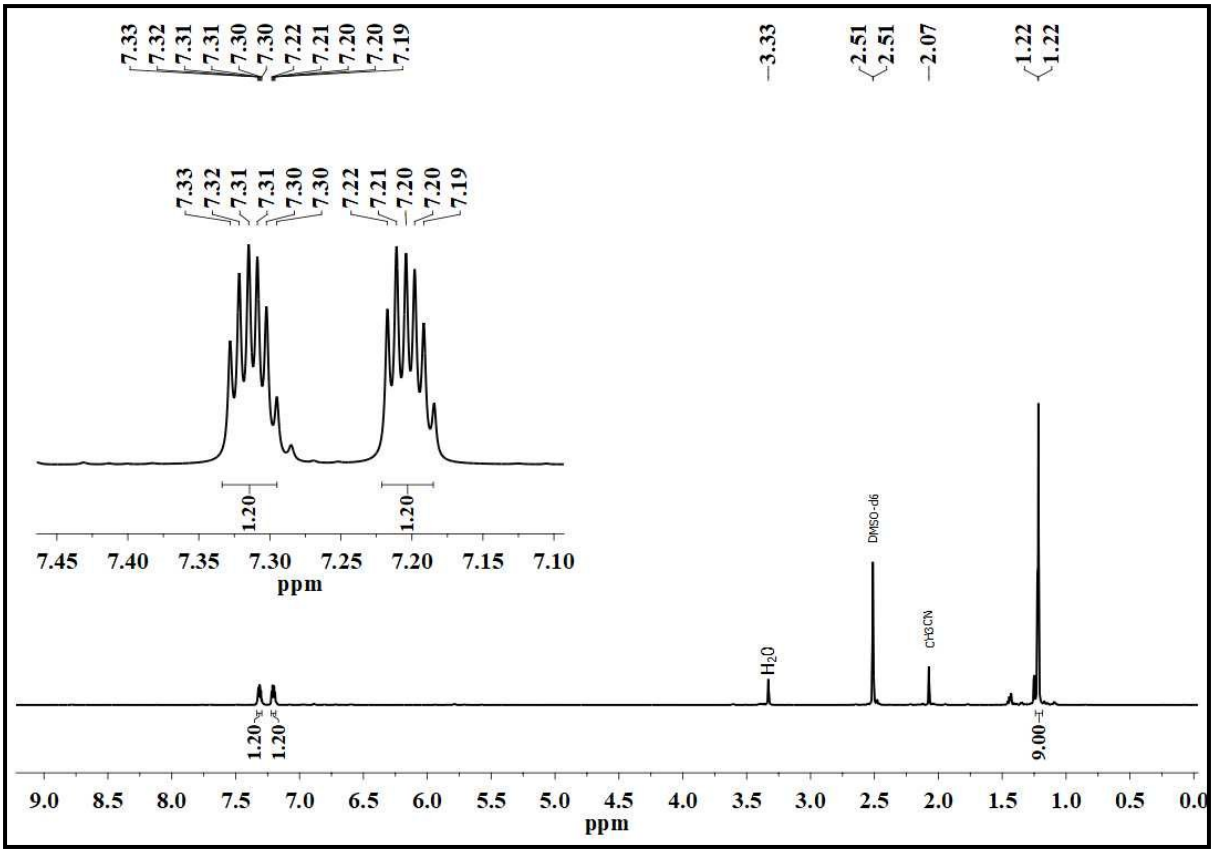

Fig. S16 ^{1}H NMR spectrum of **7** in $CDCl_3$(500 MHz)

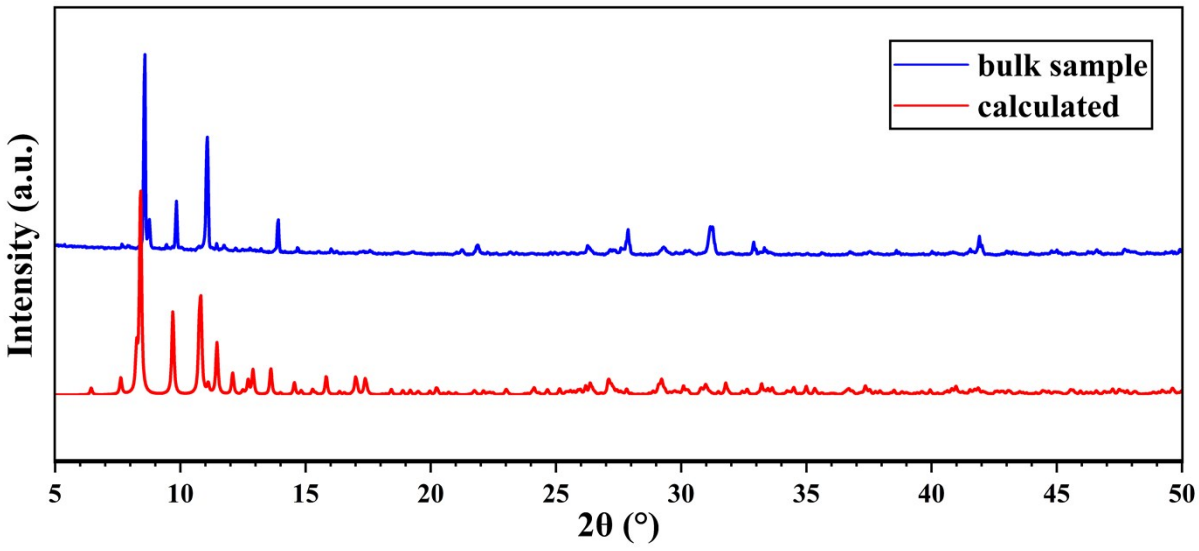

Fig. S17. The powder-XRD patterns of compound **7.** Experimental in blue and simulated in red.

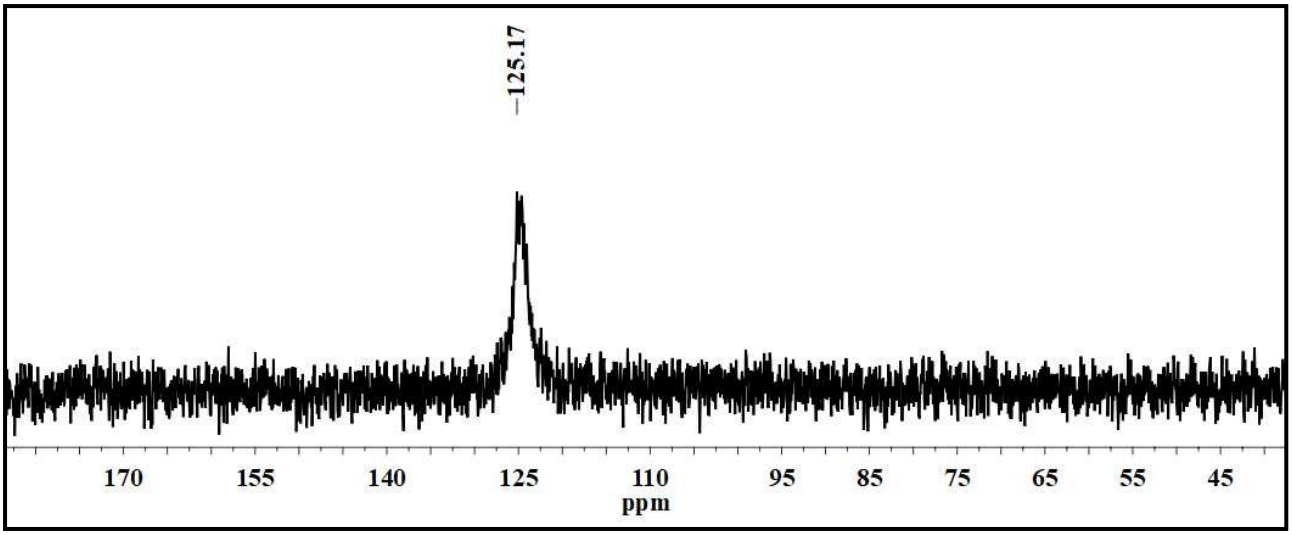

Fig. S18 $^{31}P\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$(162 MHz)

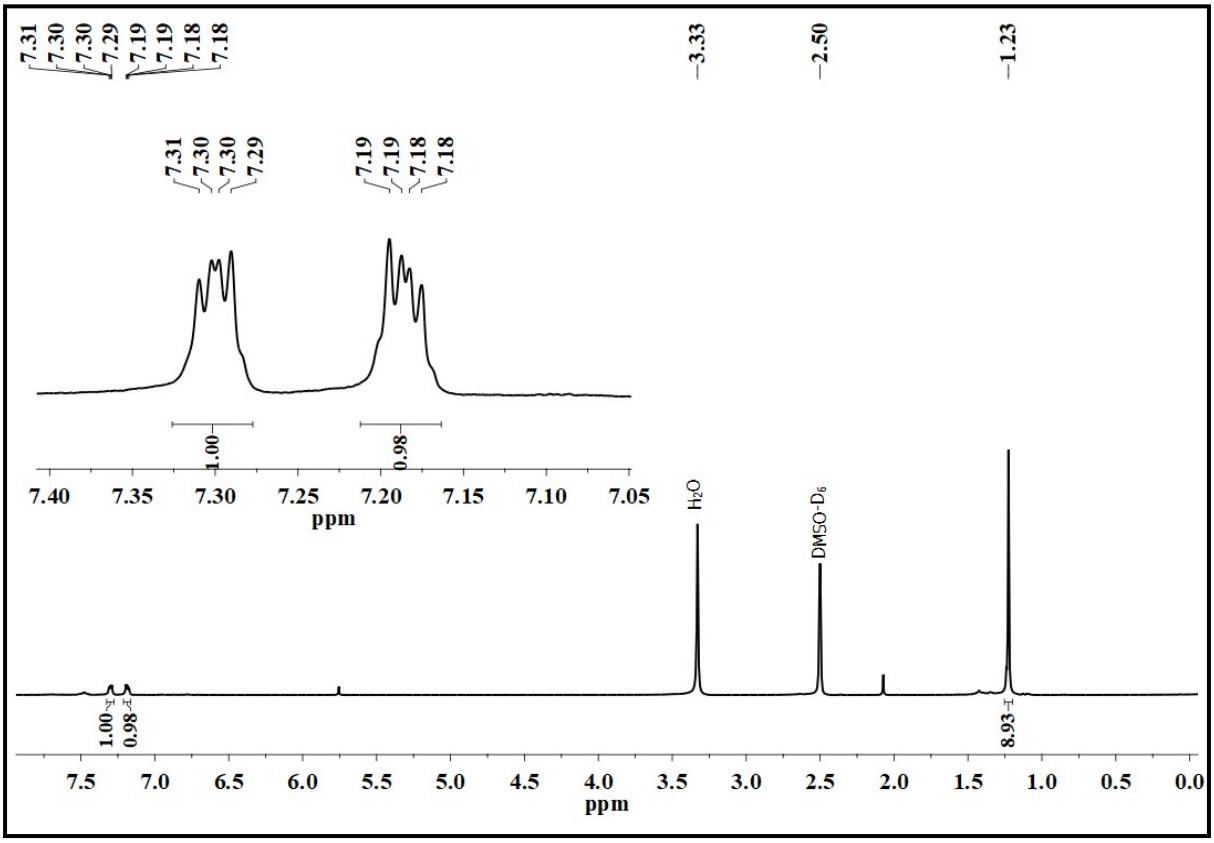

Fig. S19 ^{1}H NMR spectrum of **8** in $CDCl_3$(500 MHz)

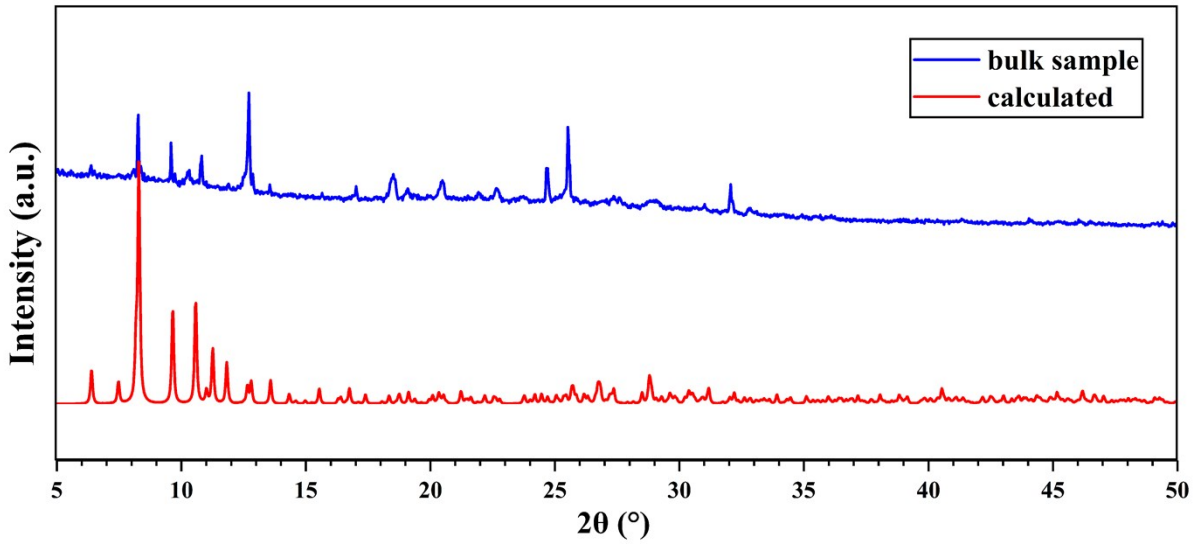

Fig. S20. The powder-XRD patterns of compound **8.** Experimental in black and simulated in red. (Some extra peaks observed may be due to the presence of some non-identified material).

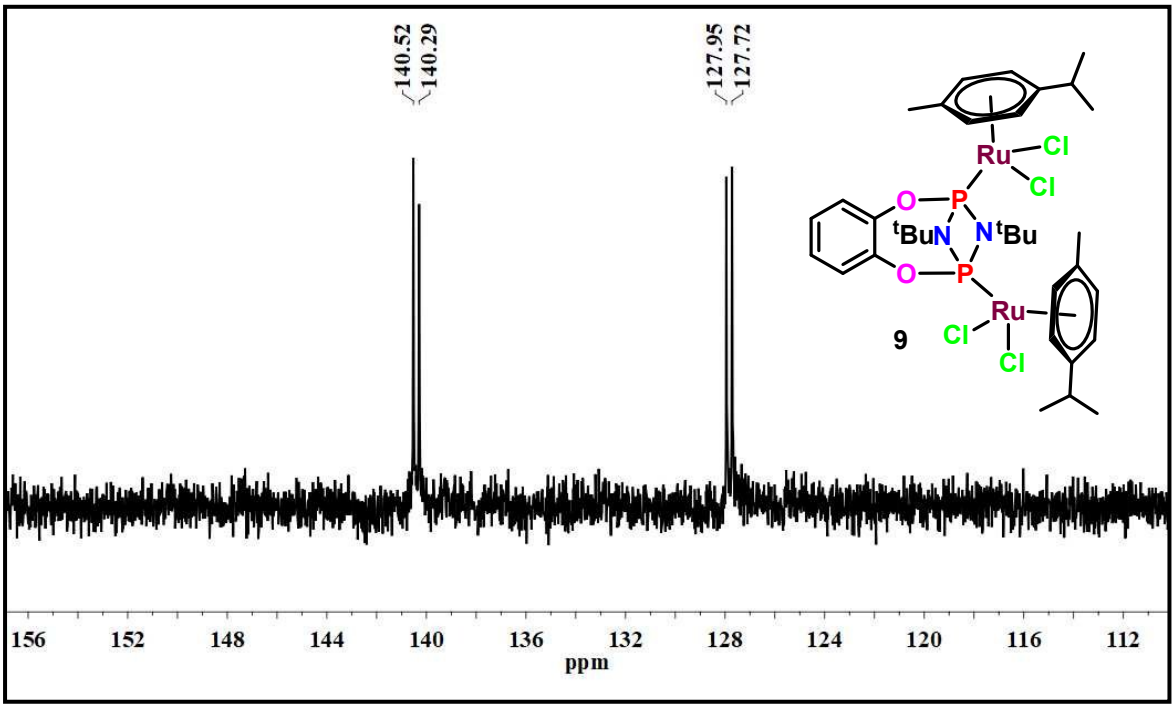

Fig. S21 $^{31}P\{^{1}H\}$ NMR spectrum of **9** in $CDCl_3$(202 MHz)

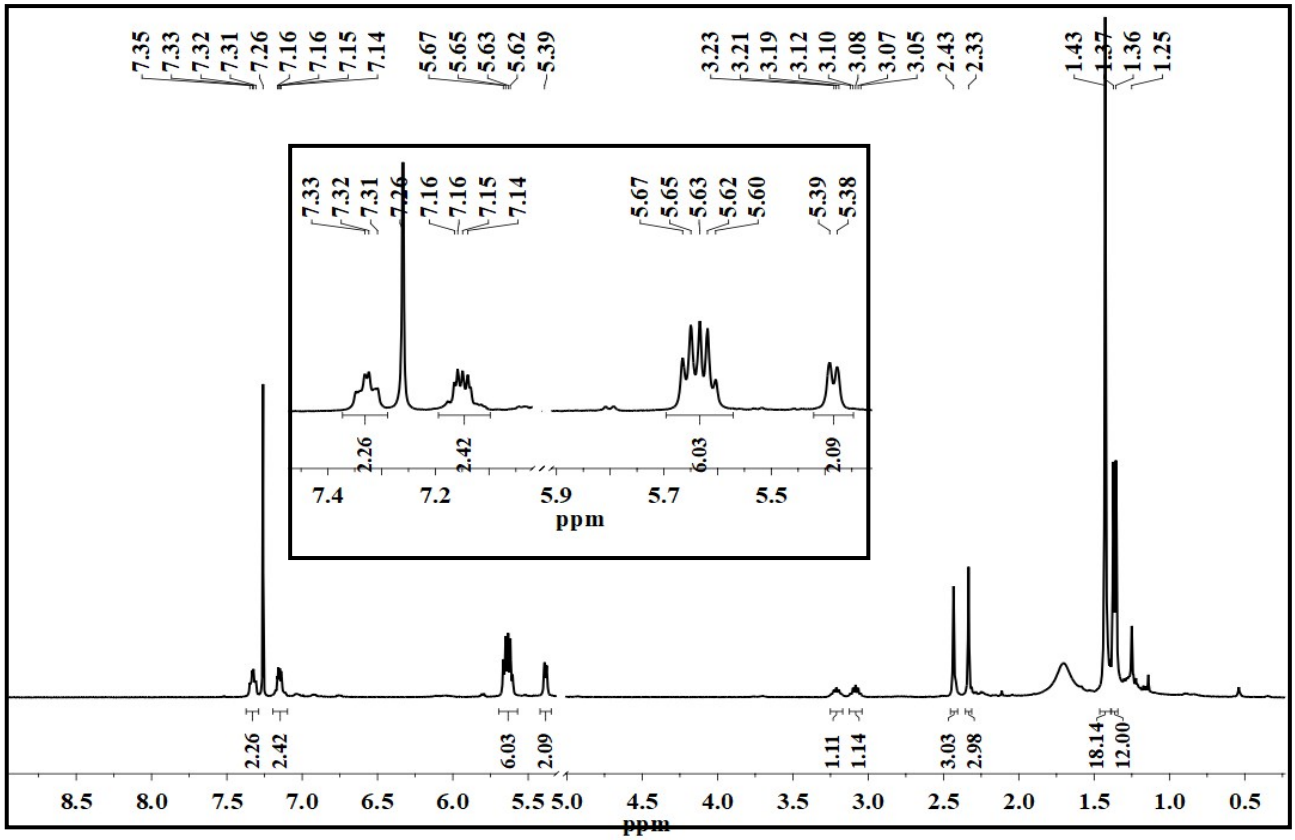

Fig. S22 ^{1}H NMR spectrum of **9** in $CDCl_3$(400 MHz)

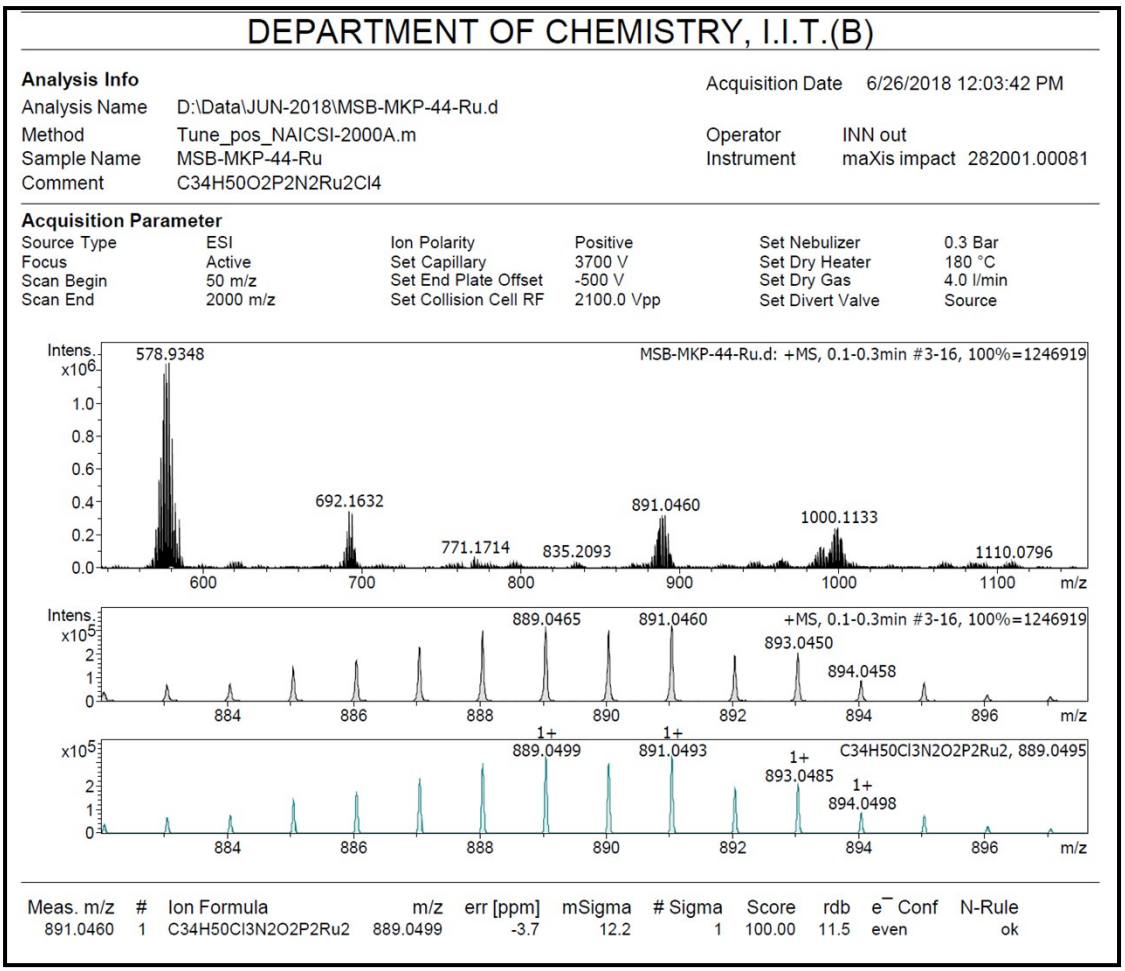

Fig. S23 HRMS spectrum of **9**

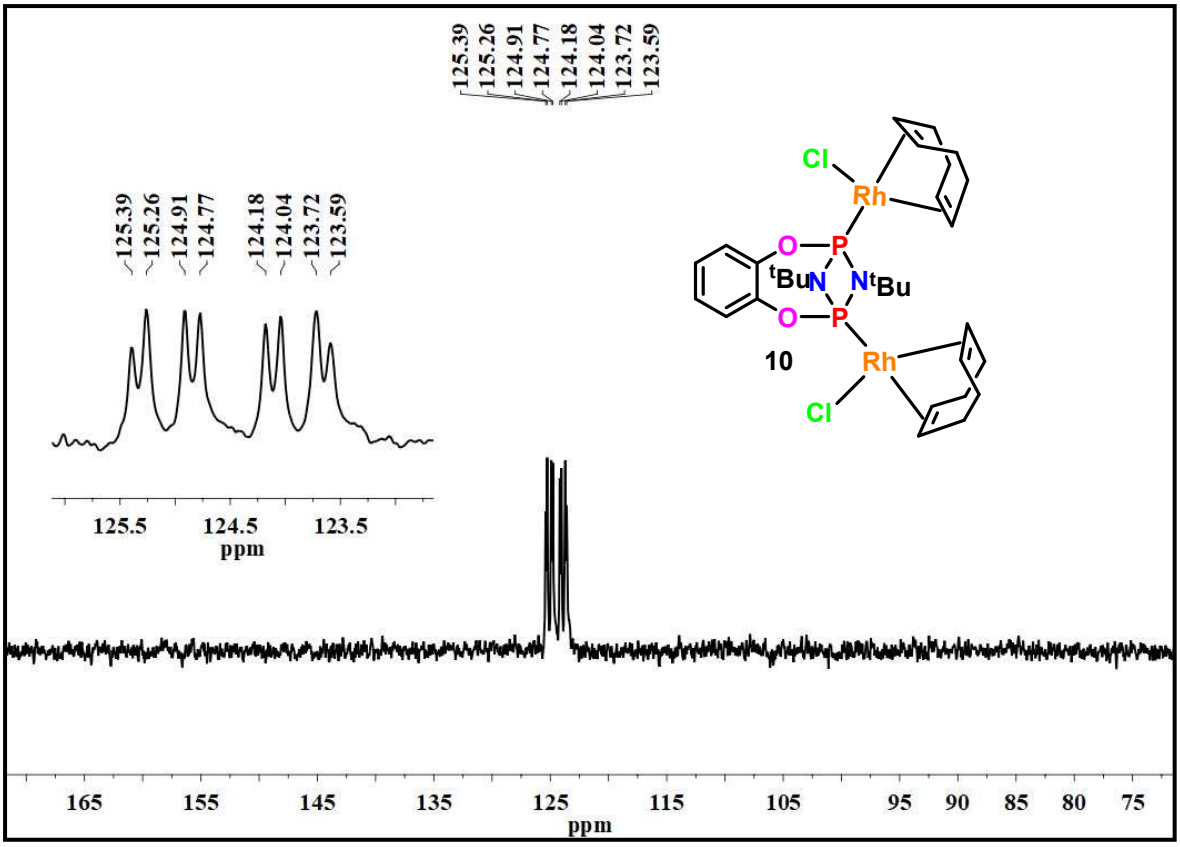

Fig. S24 $^{31}P\{^{1}H\}$ NMR spectrum of **10** in $CDCl_3$(202 MHz)

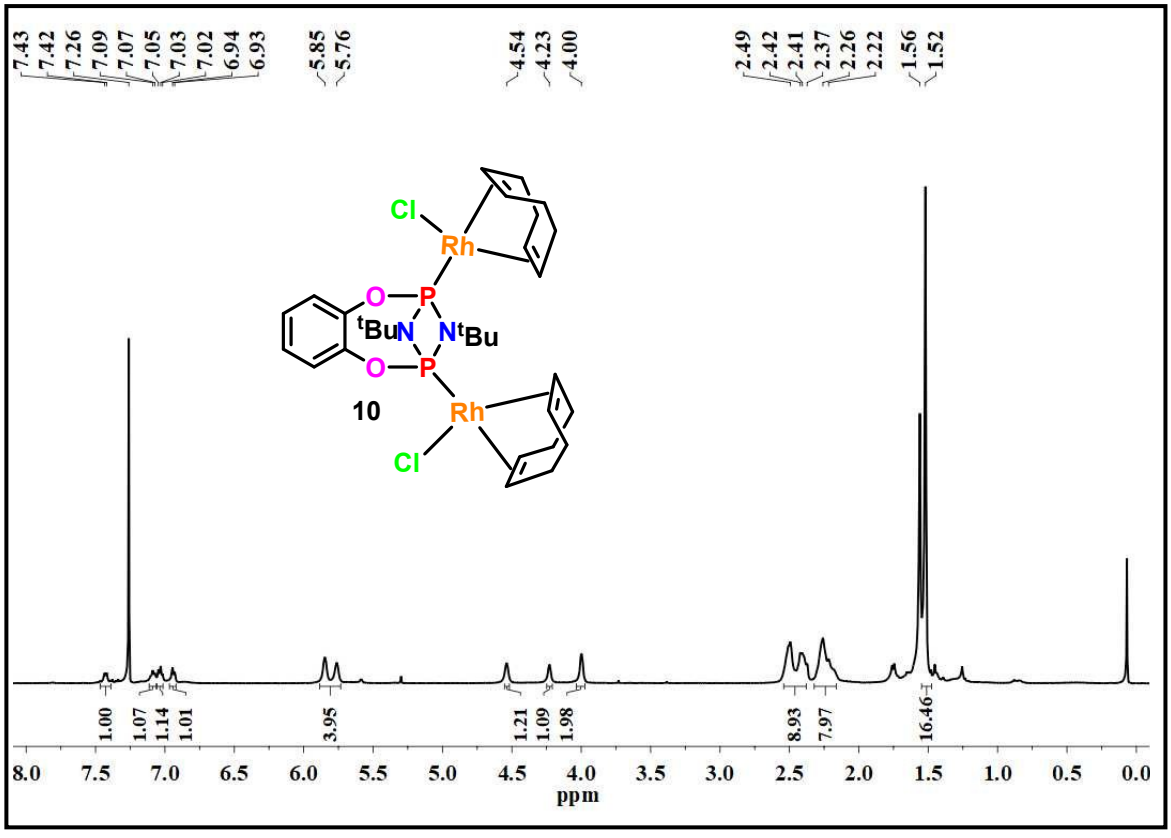

Fig. S25 ^{1}H NMR spectrum of **10** in $CDCl_3$(500 MHz)

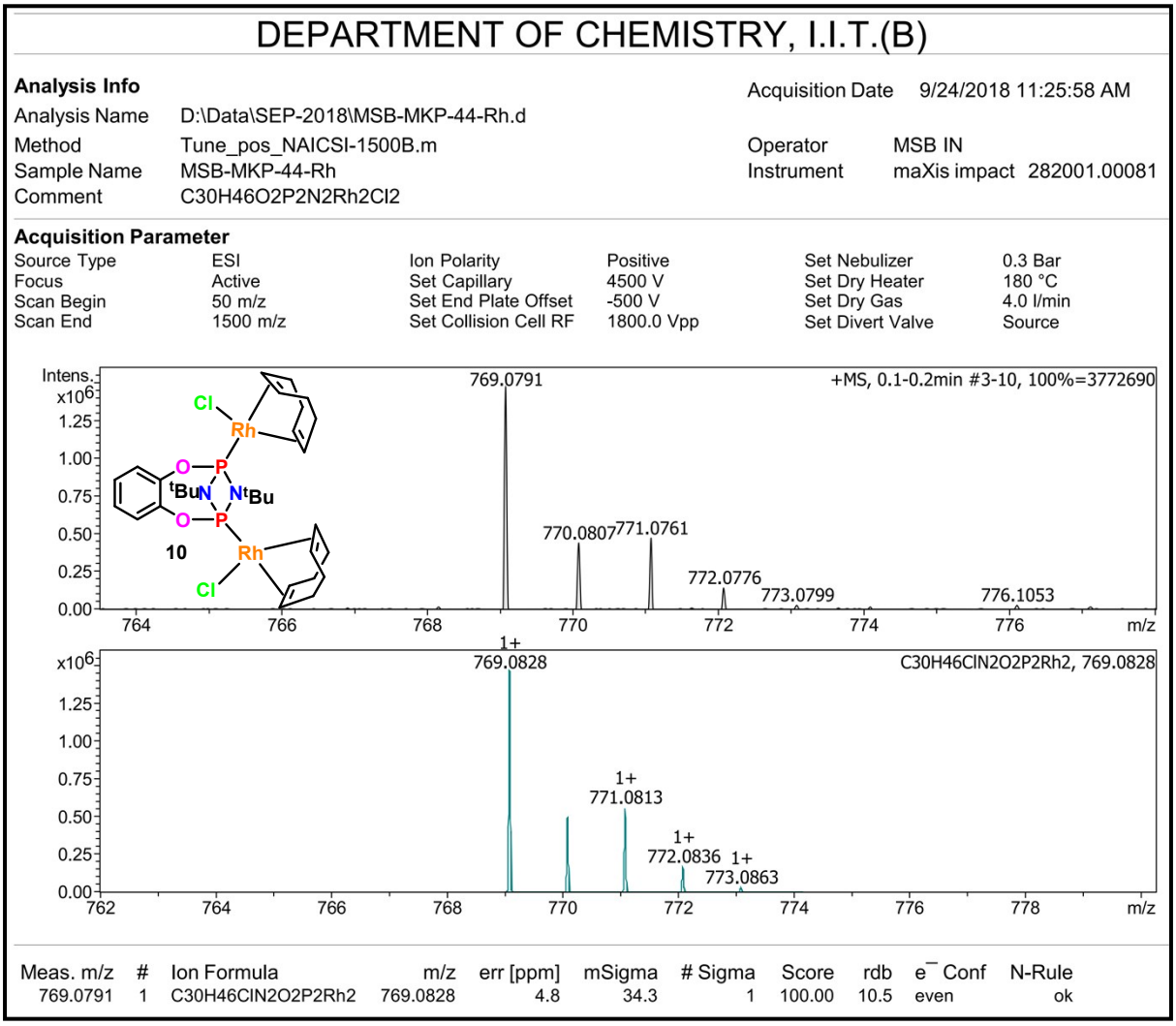

Fig. S26 HRMS spectrum of **10**

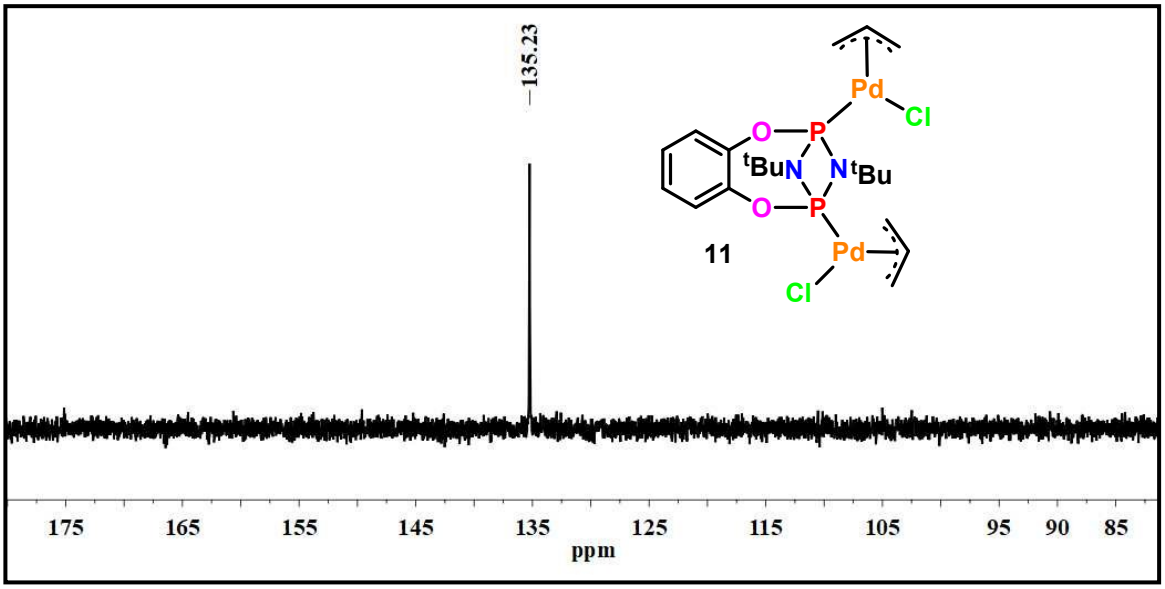

Fig. S27 $^{31}P\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$(202 MHz)

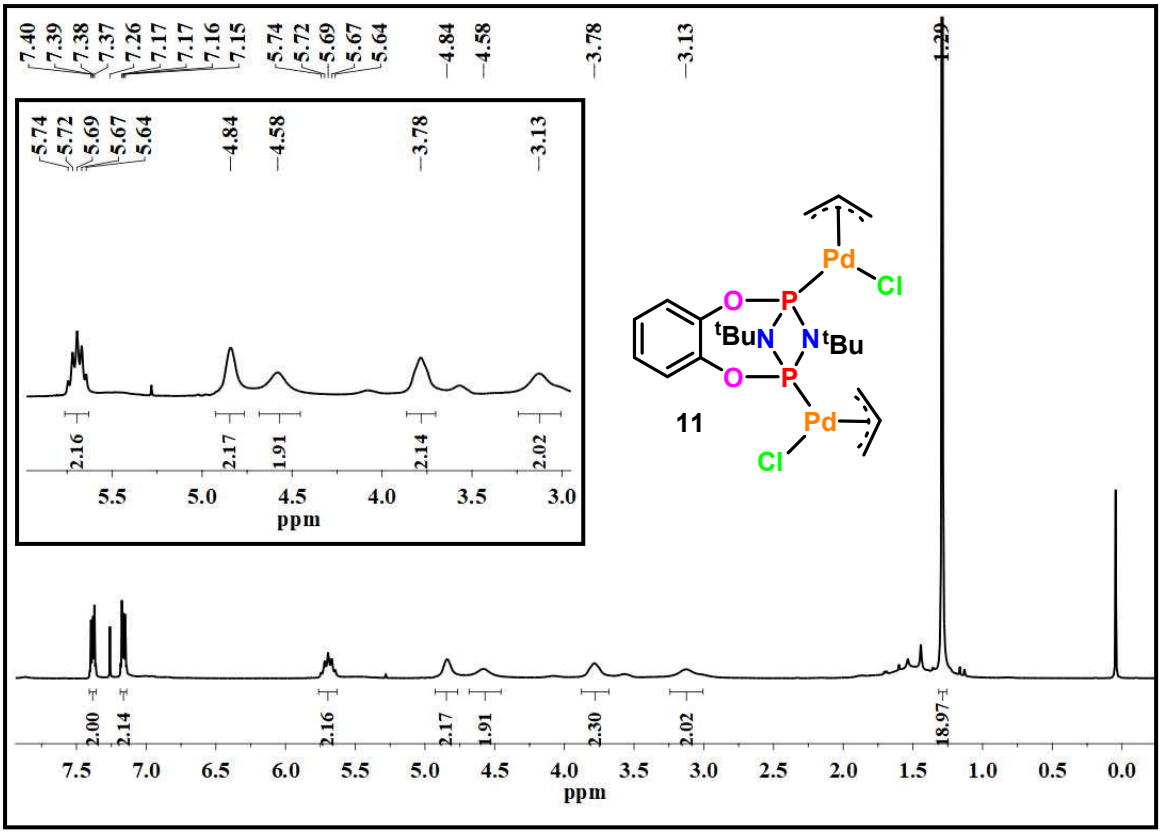

Fig. S28 ^{1}H NMR spectrum of **11** in $CDCl_3$(400 MHz)

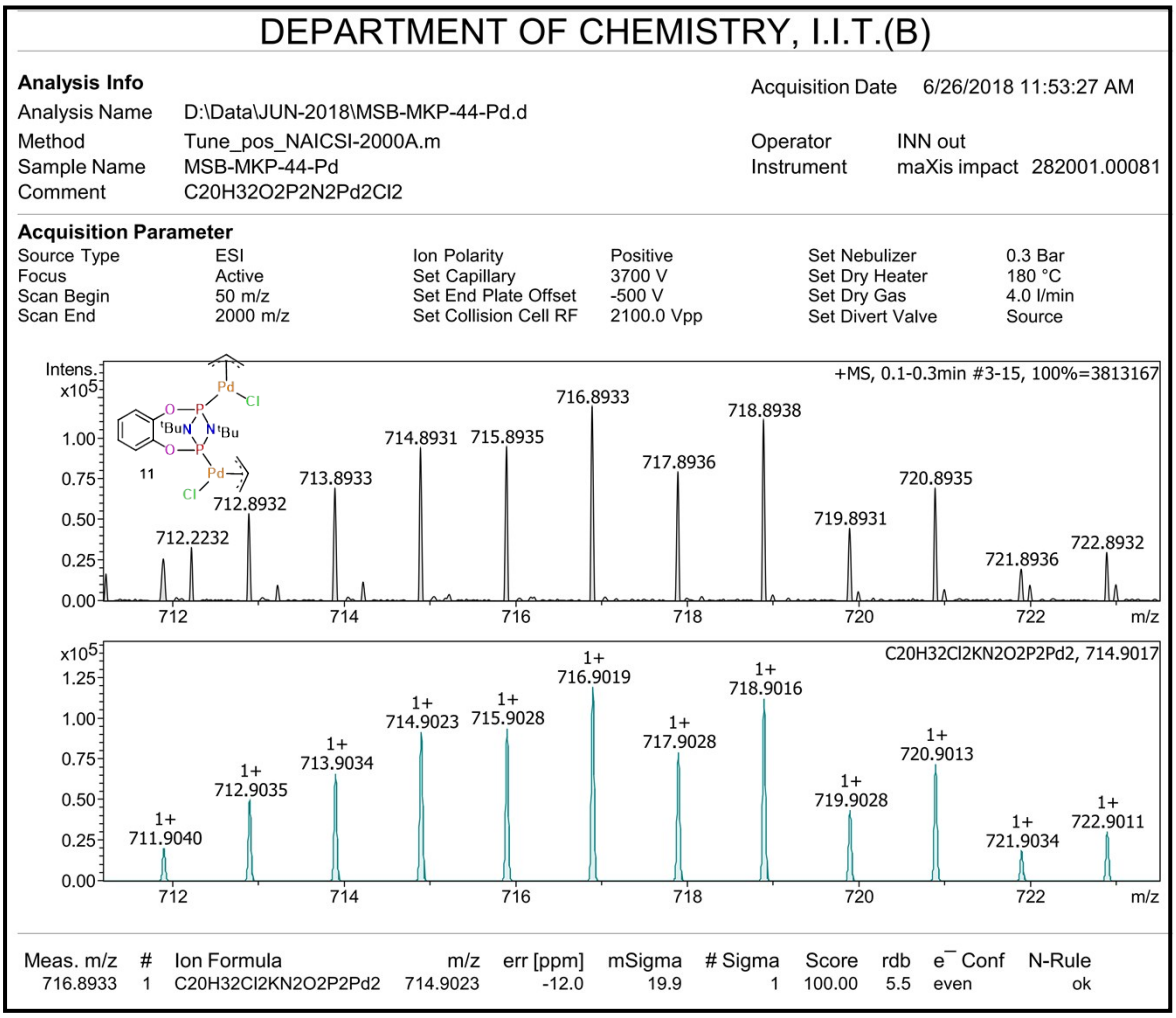

Fig. S29 HRMS spectrum of **11**

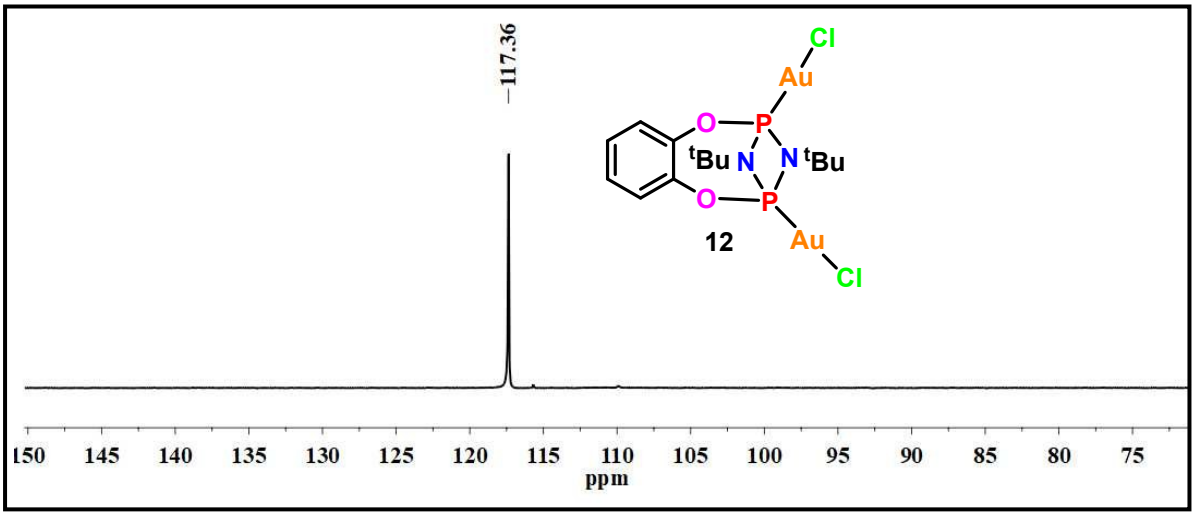

Fig. S30 $^{31}P\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$(202 MHz)

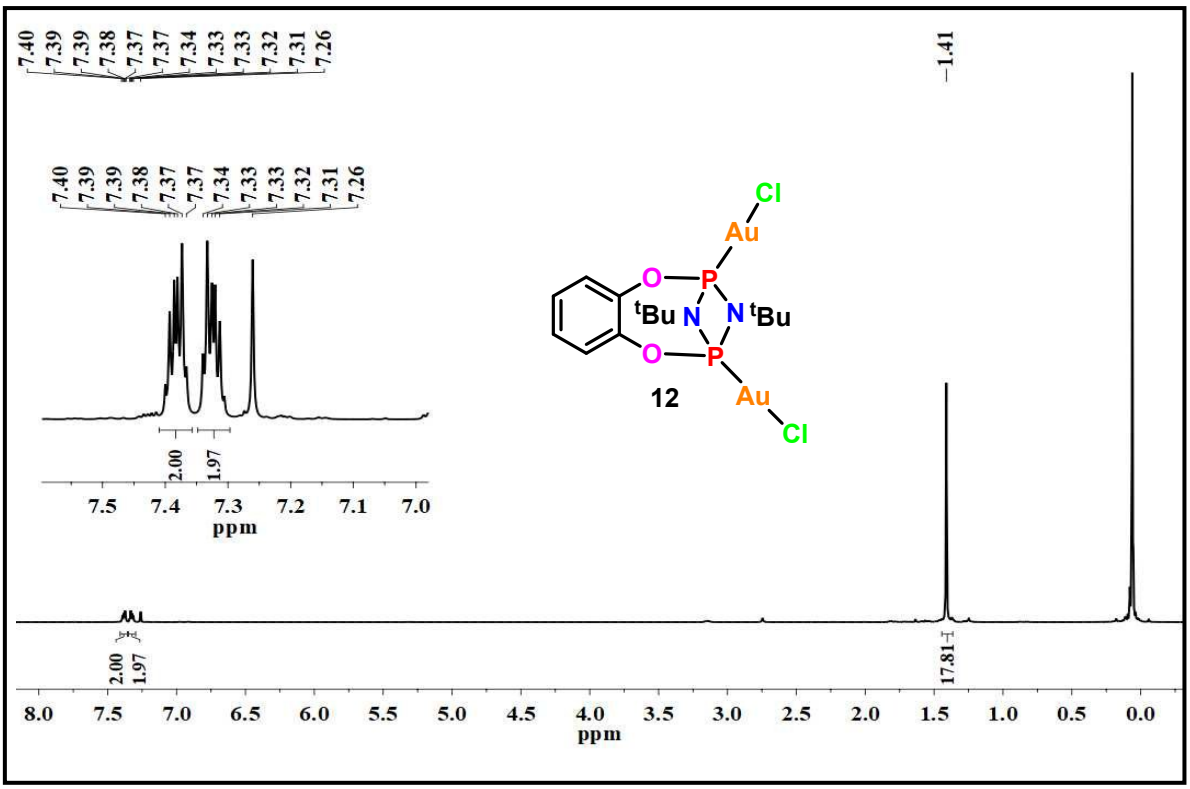

Fig. S31 ^{1}H NMR spectrum of **12** in $CDCl_3$(500 MHz)

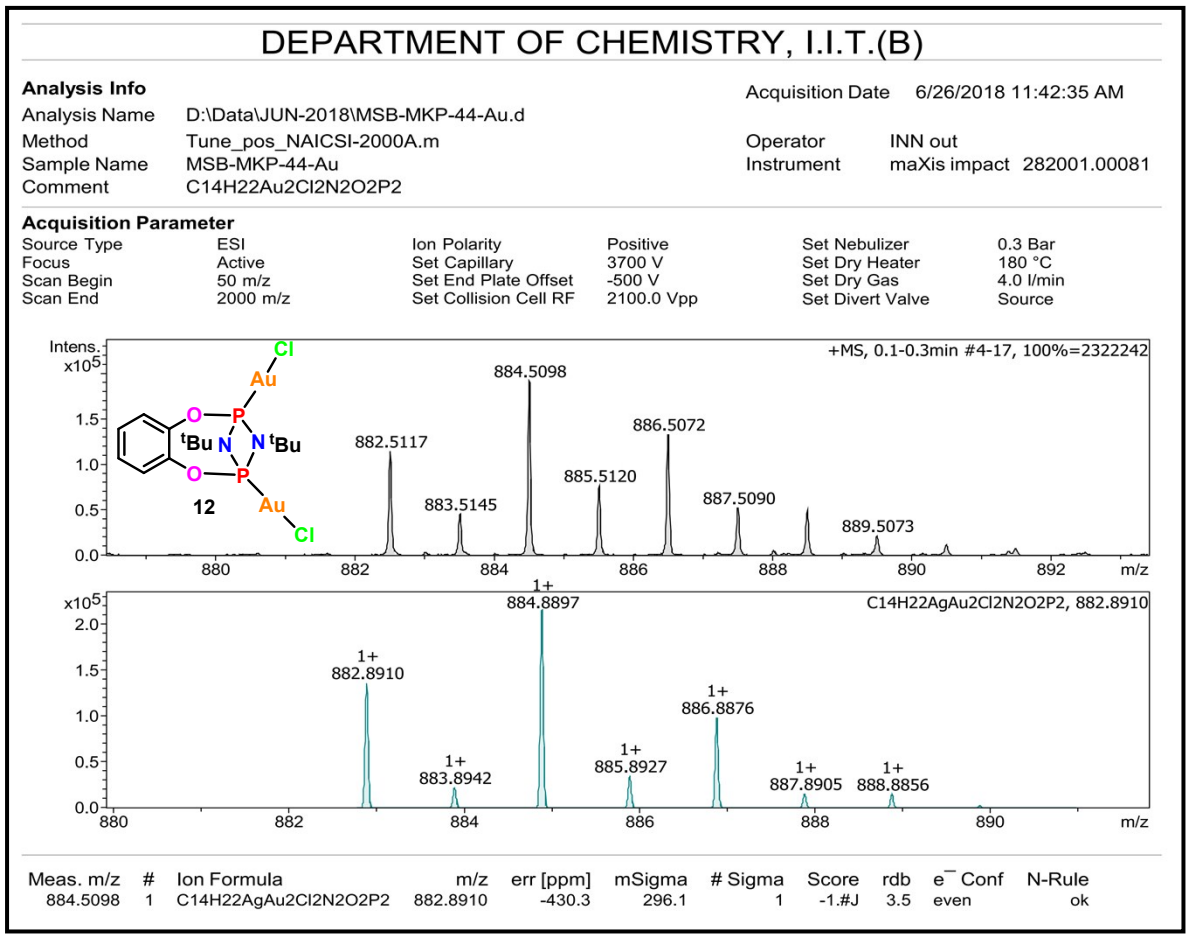

Fig. S32 HRMS spectrum of **12**

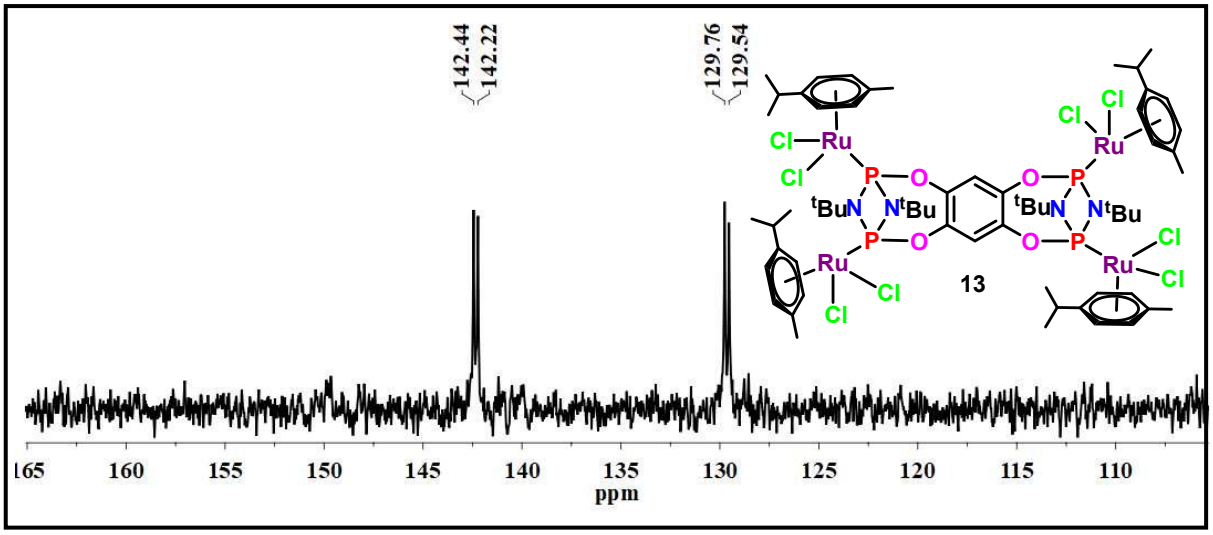

Fig. S33 $^{31}P\{^{1}H\}$ NMR spectrum of **13** in $CDCl_3$(202 MHz)

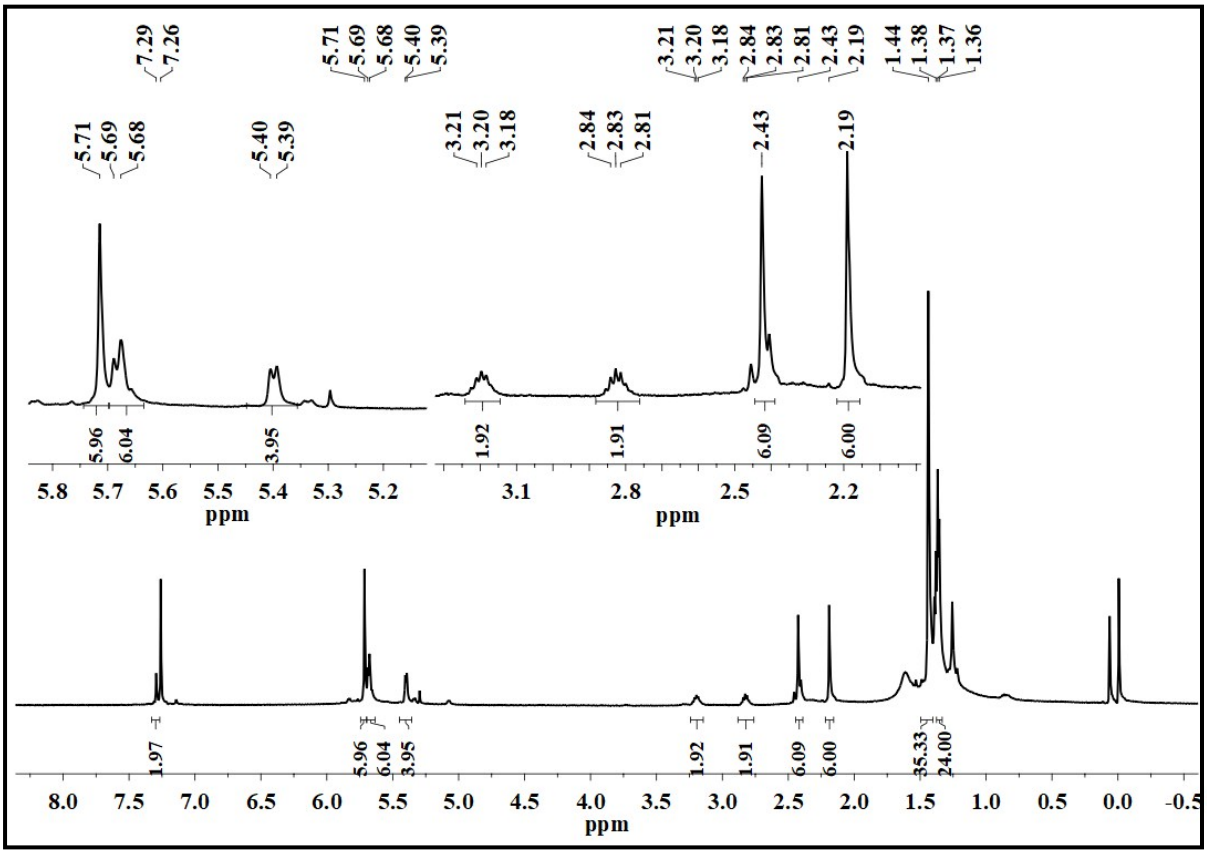

Fig. S34 ^{1}H NMR spectrum of **13** in $CDCl_3$(500 MHz)

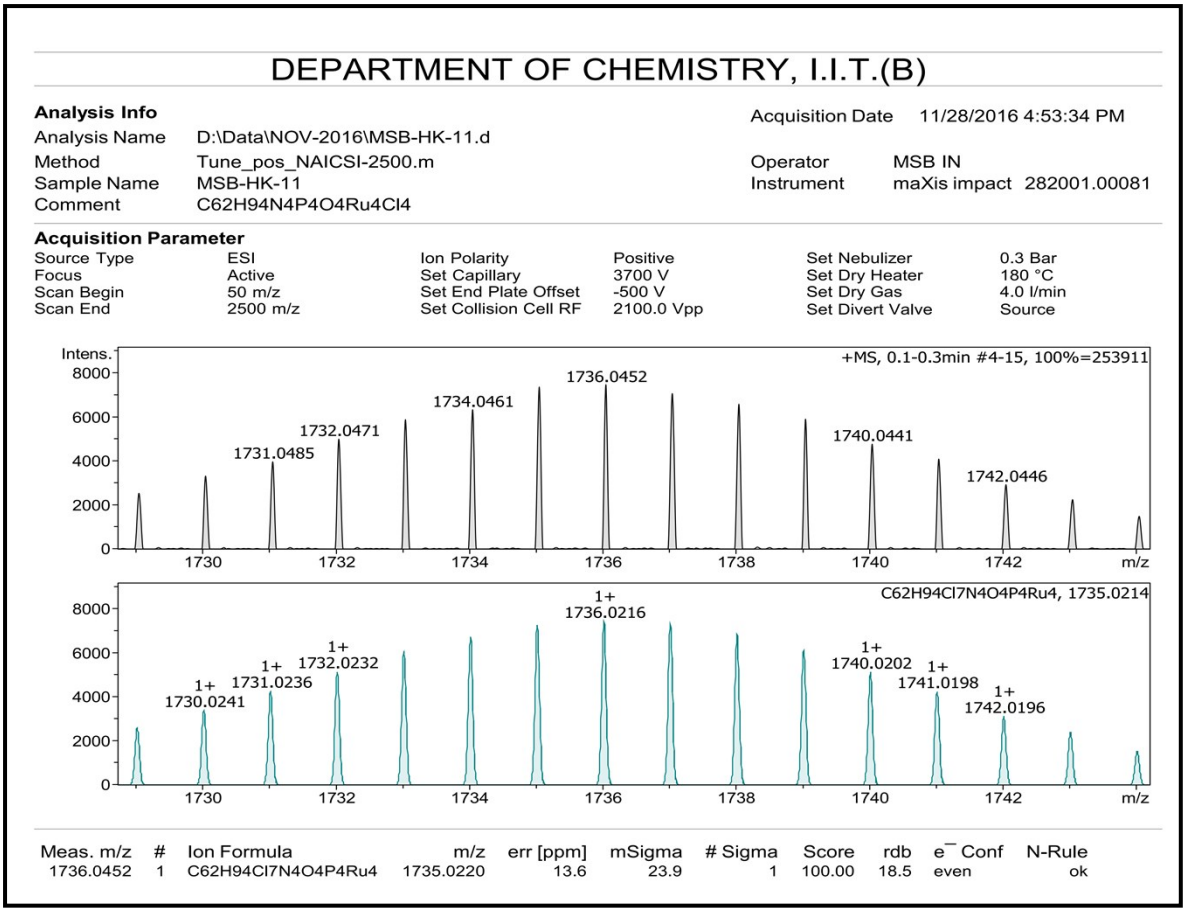

Fig. S35 HRMS spectrum of **13**

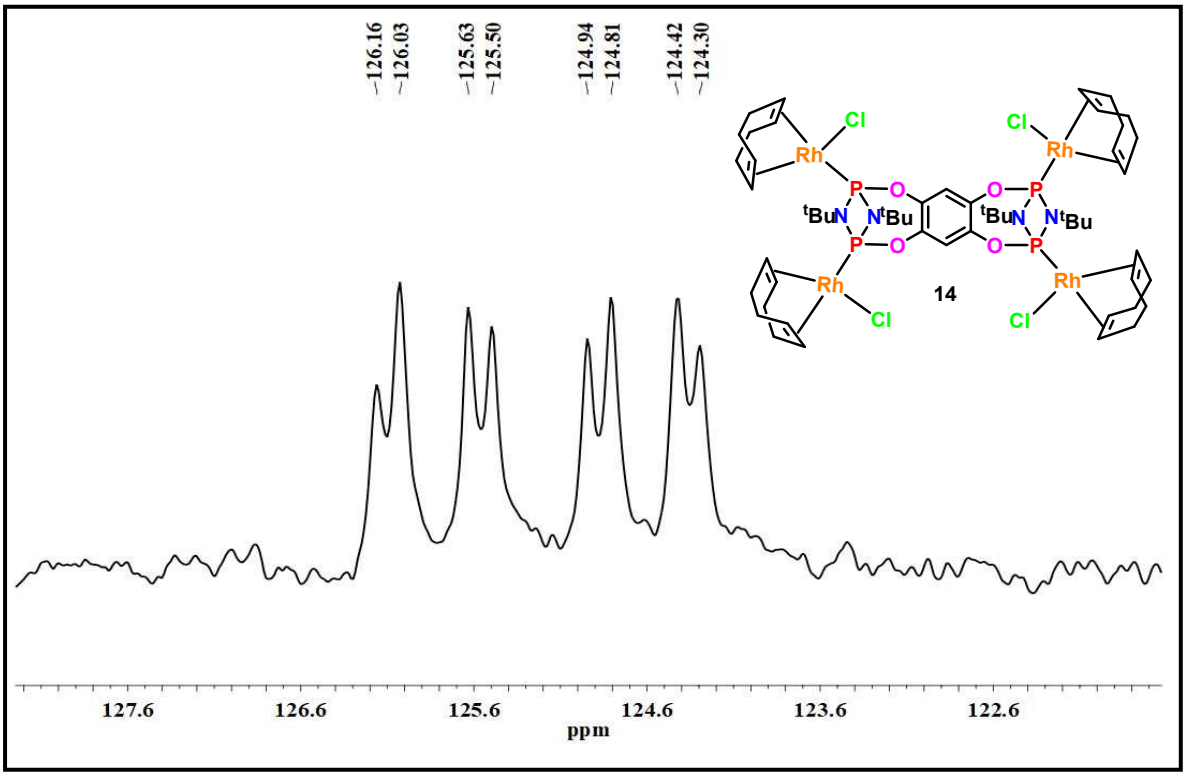

Fig. S36 $^{31}P\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$(202 MHz)

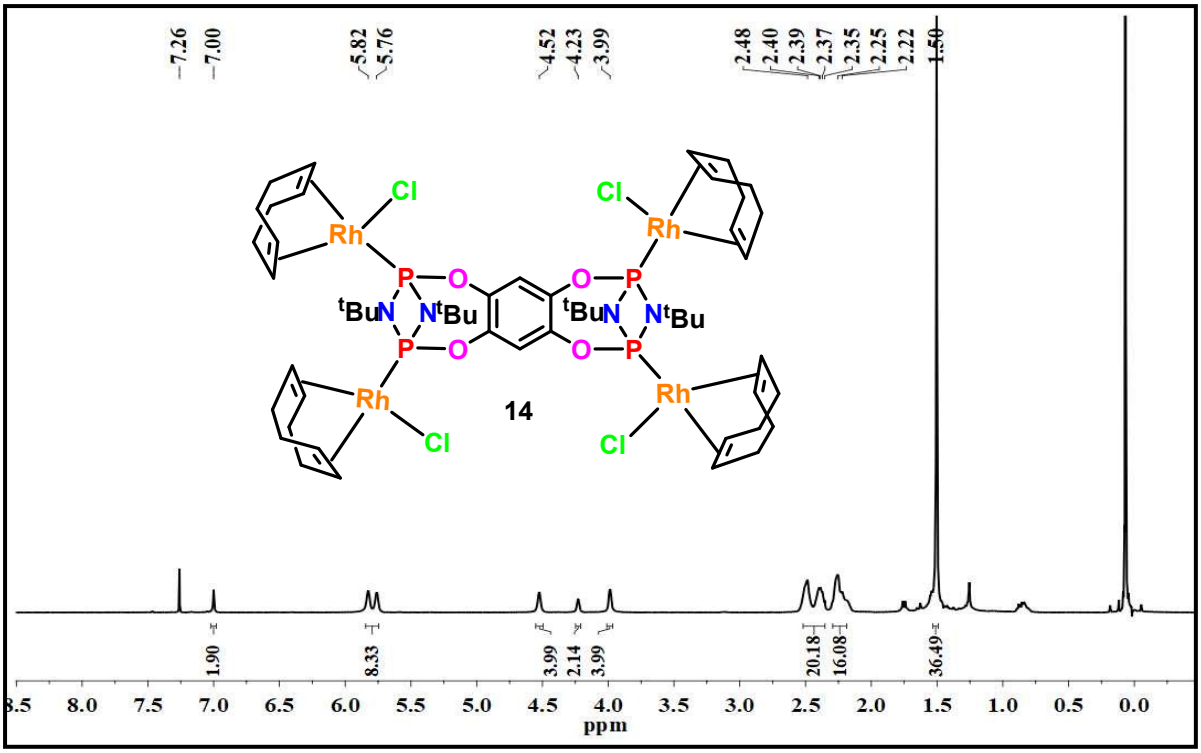

Fig. S37 ^{1}H NMR spectrum of **14** in $CDCl_3$(500 MHz)

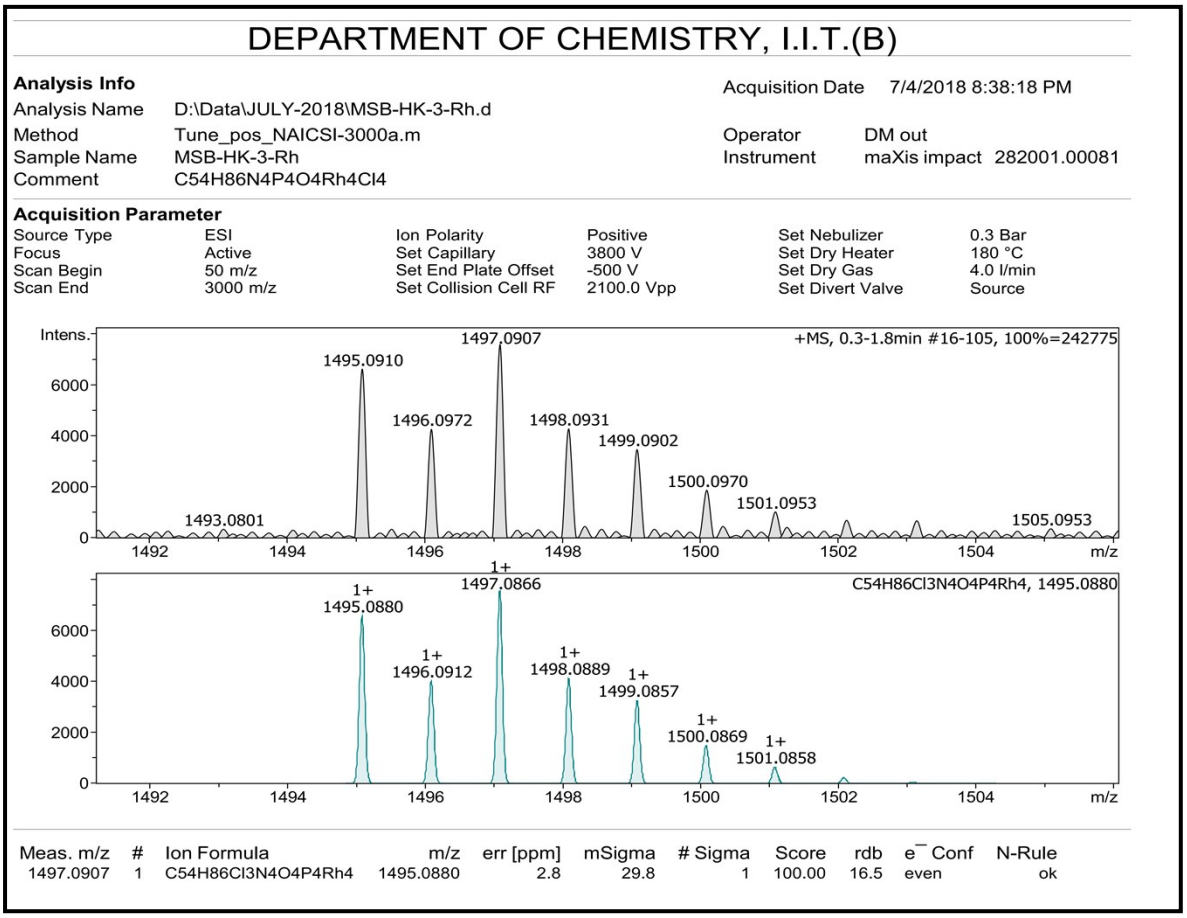

Fig. S38 HRMS spectrum of **14**

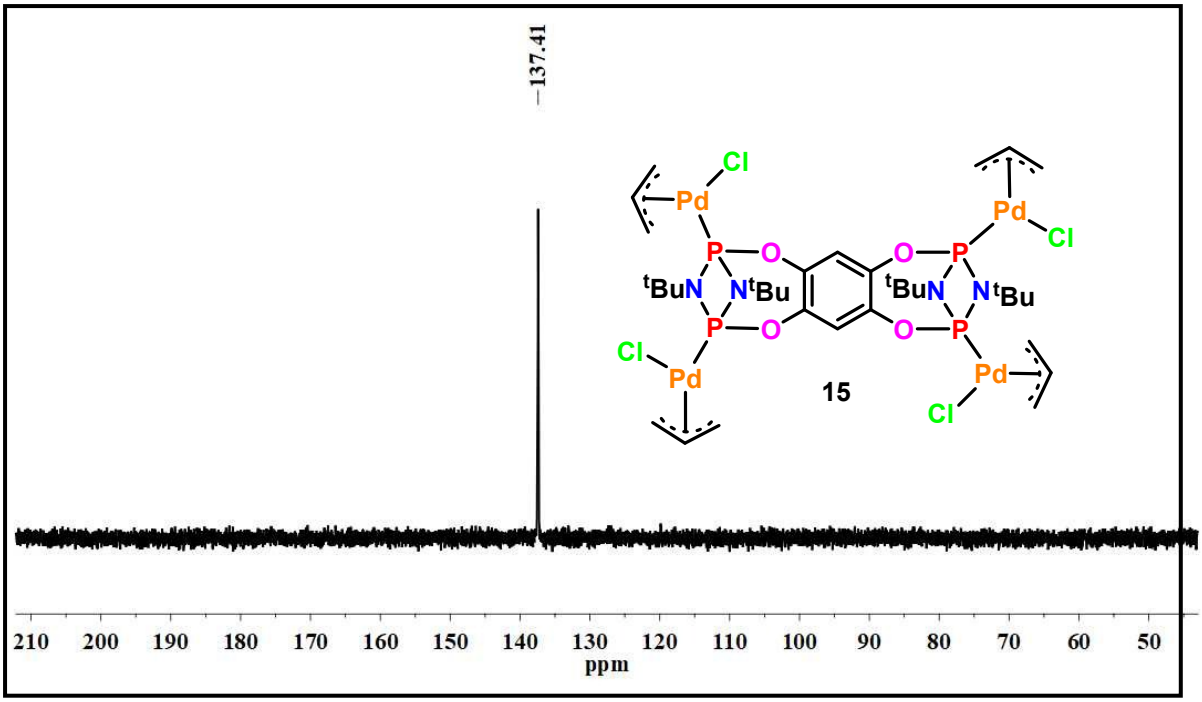

Fig. S39 $^{31}P\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$(202 MHz)

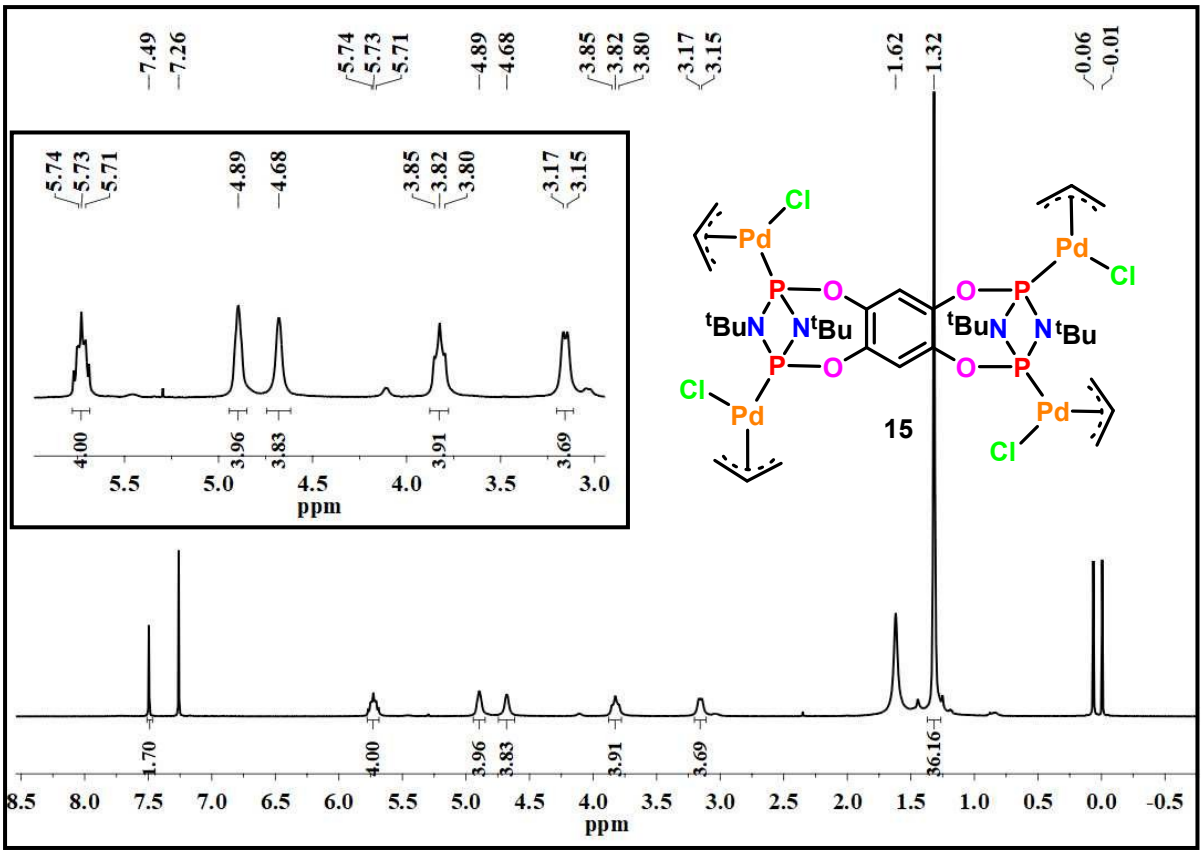

Fig. S40 ^{1}H NMR spectrum of **15** in $CDCl_3$(500 MHz)

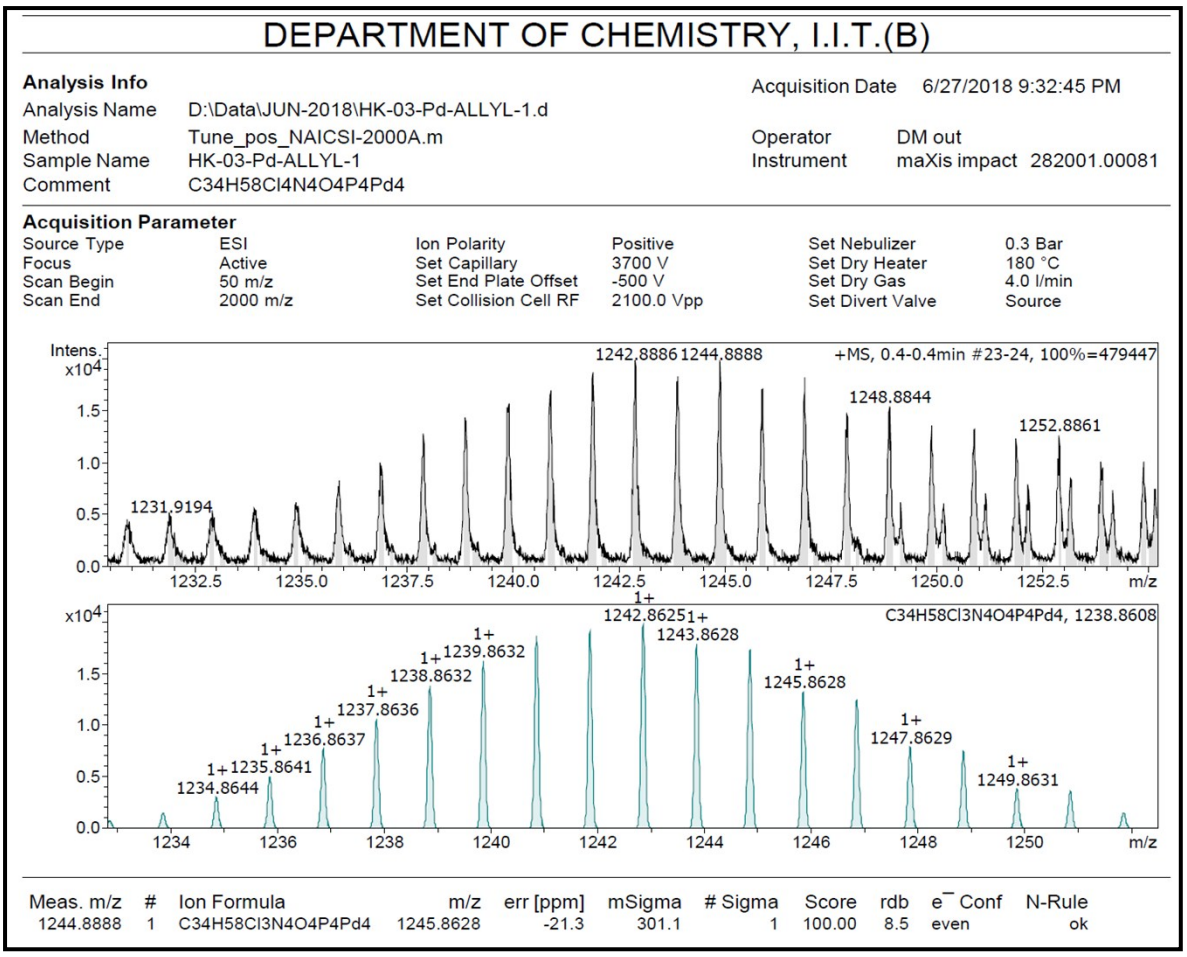

Fig. S41 HRMS spectrum of **15**

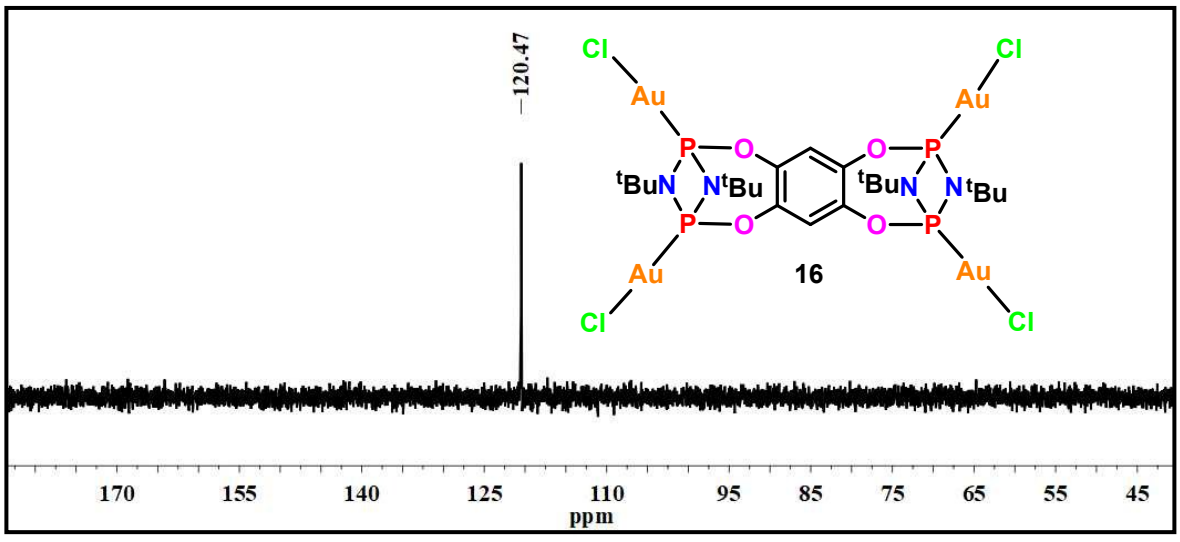

Fig. S42 $^{31}P\{^{1}H\}$ NMR spectrum of **16** in $CDCl_3$(202 MHz)

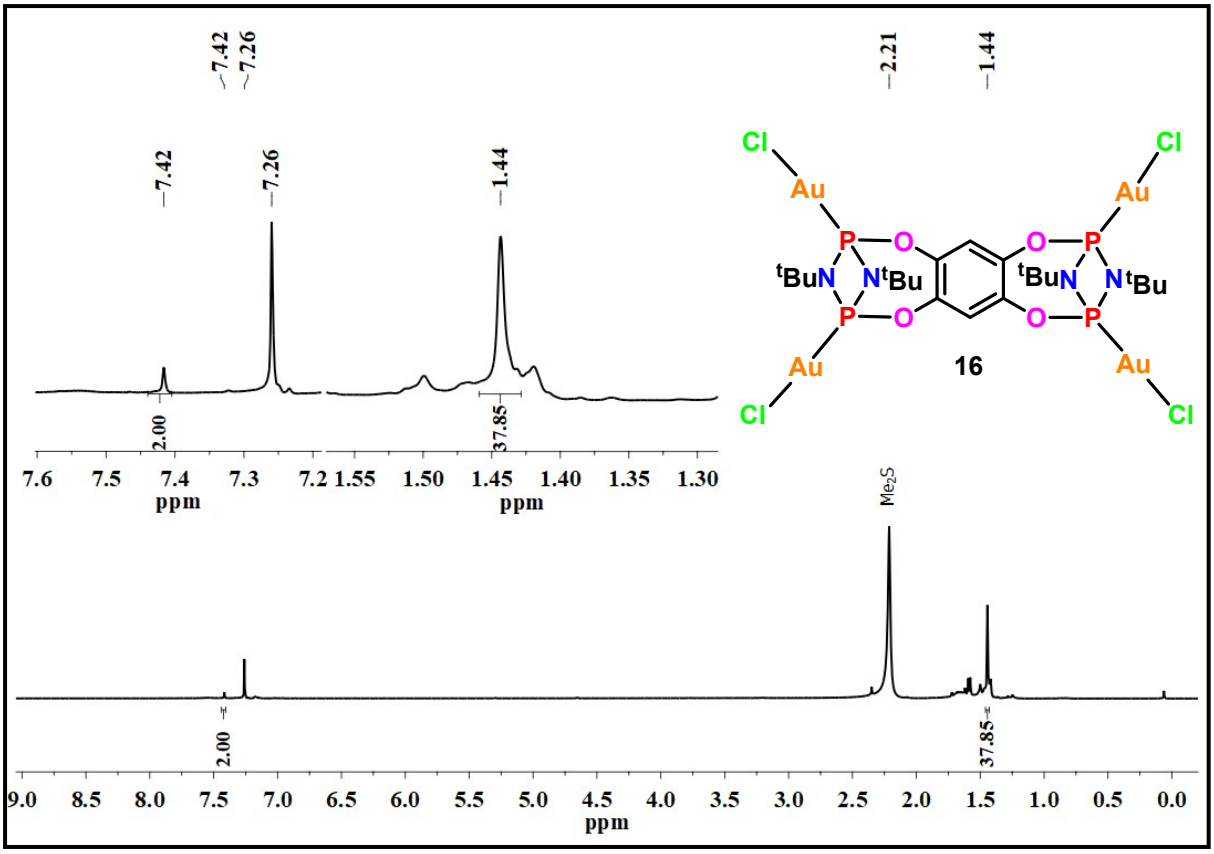

Fig. S43 ^{1}H NMR spectrum of **16** in $CDCl_3$(500 MHz)