Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Coordination chemistry of gold with N-Phosphine Oxide-Substituted Imidazolylidenes (PoxIms)

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Supporting Information

Table S1. Crystal data for compounds **5**, **6-Cl**, **7**, **9-OTf** and **pseudo-10**

Compound	**5**	**6-Cl**	**7**	**9-OTf**	**Pseudo-10**
Formula	C_{23} H_{37} Au Cl N_2 O P	C_{40} H_{62} Au Cl N_4 O_2 P_2	C_{23} H_{37} Au Cl_3 N_2 O P	$C_{41}H_{62}AuBr_2F_3N_4O_5P_2S$	C_{42} H_{65} Au_2 $Br_{3.88}$ $Cl_{2.12}$ N_5 O_2 P_2
Molecular Weight	620.93	925.30	691.84	1198.73	1513.06
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Space group	*P* 2_1/c	*C* 2/c	*P* 2_1/n	*I 2/a*	*Pbcn*
a[Å]	9.9549(18)	16.7669(6)	9.9566(4)	11.5747(3)	22.602(2)
b[Å]	14.877(3)	27.1662(12)	21.0444(8)	28.8162(6)	15.0955(14)
c[Å]	17.809(3)	12.0319(4)	13.5564(6)	14.7781(3)	15.1623(15)
β[°]	96.370(2)	121.124(1)	104.009(2)	99 .269(2)	90
V[Å^3]	2621.2(8)	4691.5(3)	2756.0(2)	4864.69(19)	5173.1(8)
Temperature (K)	273	290	200	303	99.99
Z	4	4	4	4	4
D_{calc}[g·cm^{-3}]	1.574	1.310	1.667	1.637	1.943
μ[cm^{-1}]	5.791	3.294	5.704	4.831	8.872
F(000)	1232.0	1888.0	1368.0	2392.0	2911.0
Reflections collected	40830	24383	52984	10660	62675
Independent reflections	7944	5334	8422	5570	6166
R(int)	0.0899	0.0571	0.0568	0.0226	0.0872
Refined parameters	272	240	290	297	320
R_1 [*I*> 2σ(*I*)]	R_1 = 0.0399 wR_2 = 0.0923	R_1 = 0.0527 wR_2 = 0.1391	R_1 = 0.0303 wR_2 = 0.0851	R_1 = 0.0281 wR_2 = 0.0781	R1 = 0.0327 wR2 = 0.0560
wR_2 [all data]	R_1 = 0.0795 wR_2 = 0.1061	R_1 = 0.0637 wR_2 = 0.1497	R_1 = 0.0401 wR_2 = 0.0932	R_1 = 0.0303 wR_2 = 0.0799	R1 = 0.0532 wR2 = 0.0608
GOF	1.004	0.921	1.005	1.069	1.027
CCDC	1942490	1942489	1942491	1911218	1942492

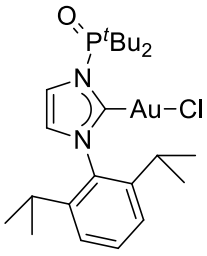
$R_1 = \Sigma|Fo-Fc|/\Sigma(Fo)$; $wR_2 = [\Sigma[w(Fo^2-Fc^2)^2]/\Sigma[w(Fo^2)^2]]^{1/2}$.

Compound 9-OTf refinement details.

Mo Kα (λ = 0.71073) radiation was used for data collection. Structural solution and refinement were carried out as described in the article experimental section. Methyl groups in the phosphanyl oxide moiety were disordered over two sites, the occupancies of which were constrained to sum to 1.0. To better model this disorder, SADI and RIGU restrains coupled to EADP constrains have been applied. The structure has a highly disordered triflate anion close to a two-fold symmetry axis. The anion was successfully modelled using an idealized molecular geometry.[1]

1. I. A. Guzei, *J. Appl. Crystallogr.,* 2014, **47**, 806.

Compound 5 ^{1}H, ^{13}C, ^{31}P NMR characterization



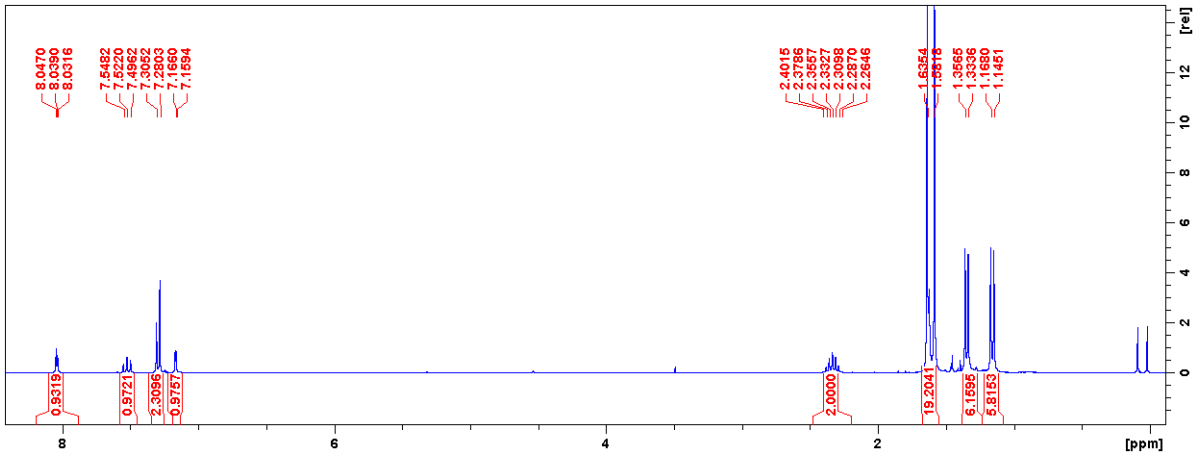


Figure S1. ^{1}H NMR spectrum of compound **5** in $CDCl_3$

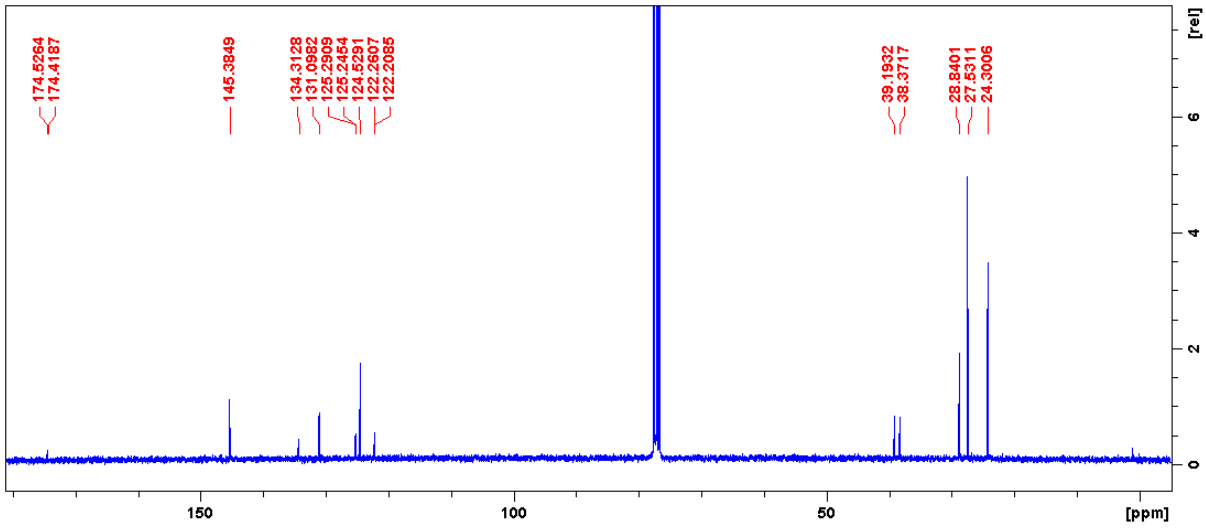


Figure S2. ^{13}C NMR spectrum of compound **5** in $CDCl_3$

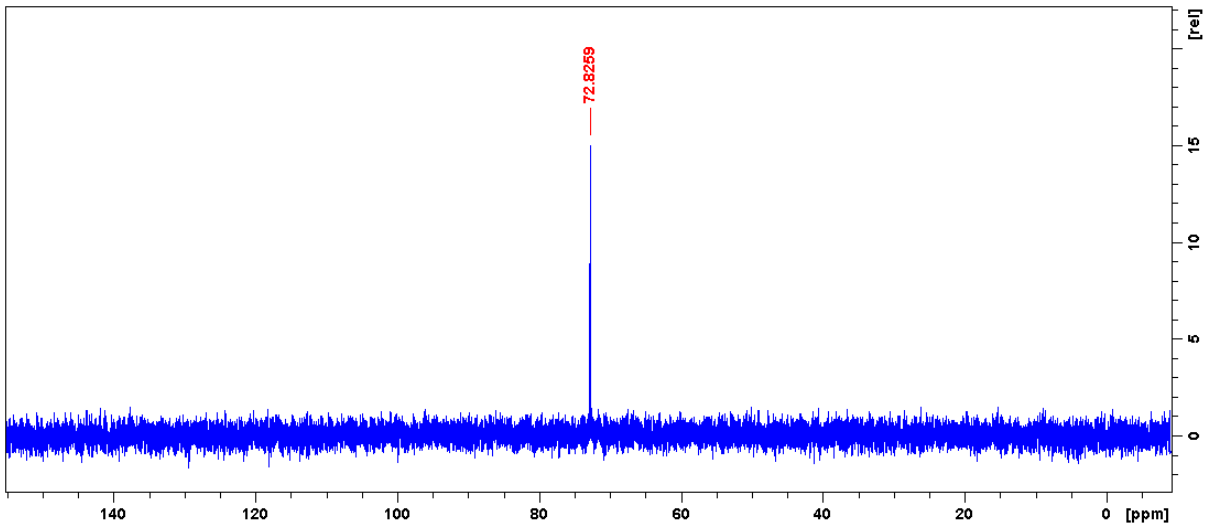
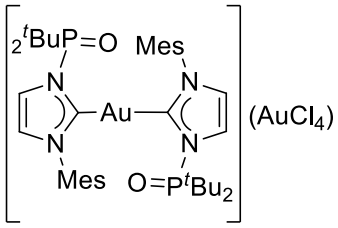


Figure S3. ^{31}P NMR spectrum of compound **5** in $CDCl_3$

Compound 6-$AuCl_4$ ^{1}H, ^{13}C, ^{31}P NMR characterization



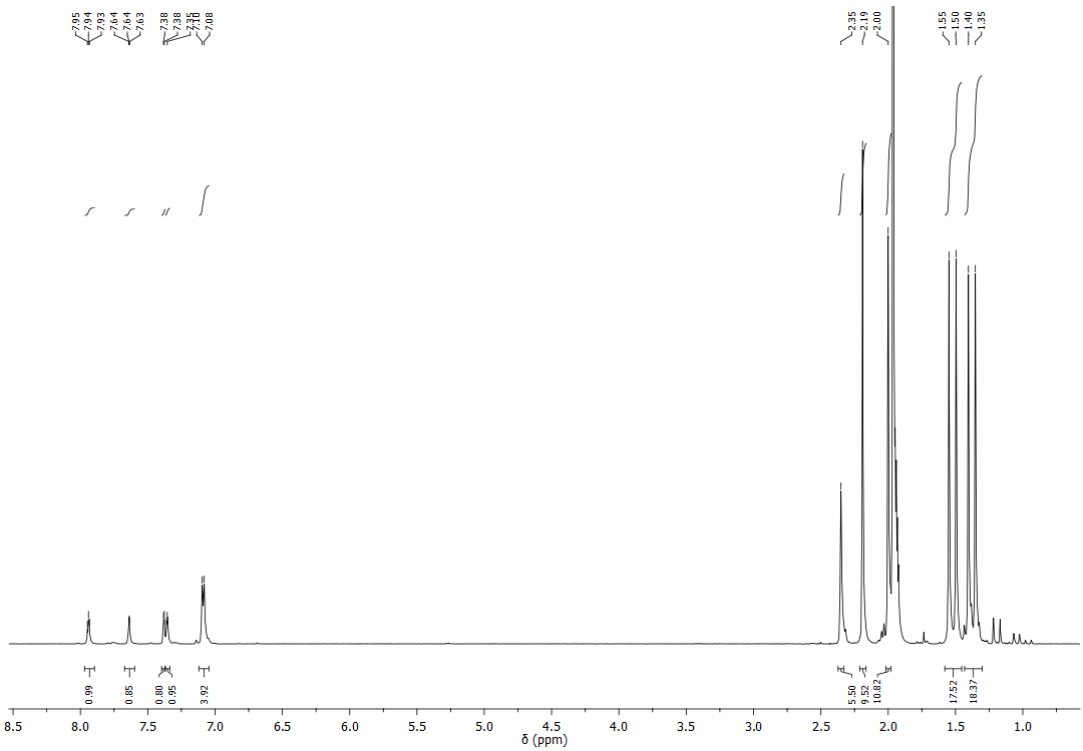


Figure S4. ^{1}H NMR spectrum of compound **6-$AuCl_4$** in CD_3CN

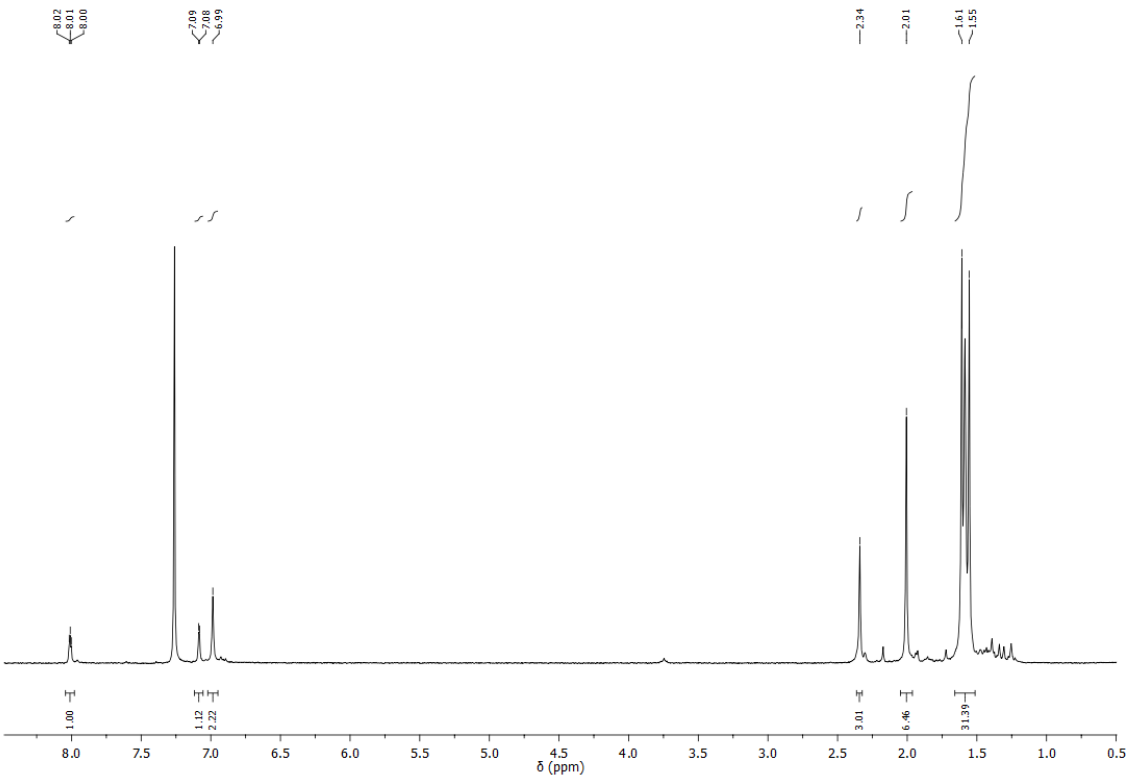


Figure S5. ^{1}H NMR spectrum of compound **6-AuCl4** in $CDCl_3$

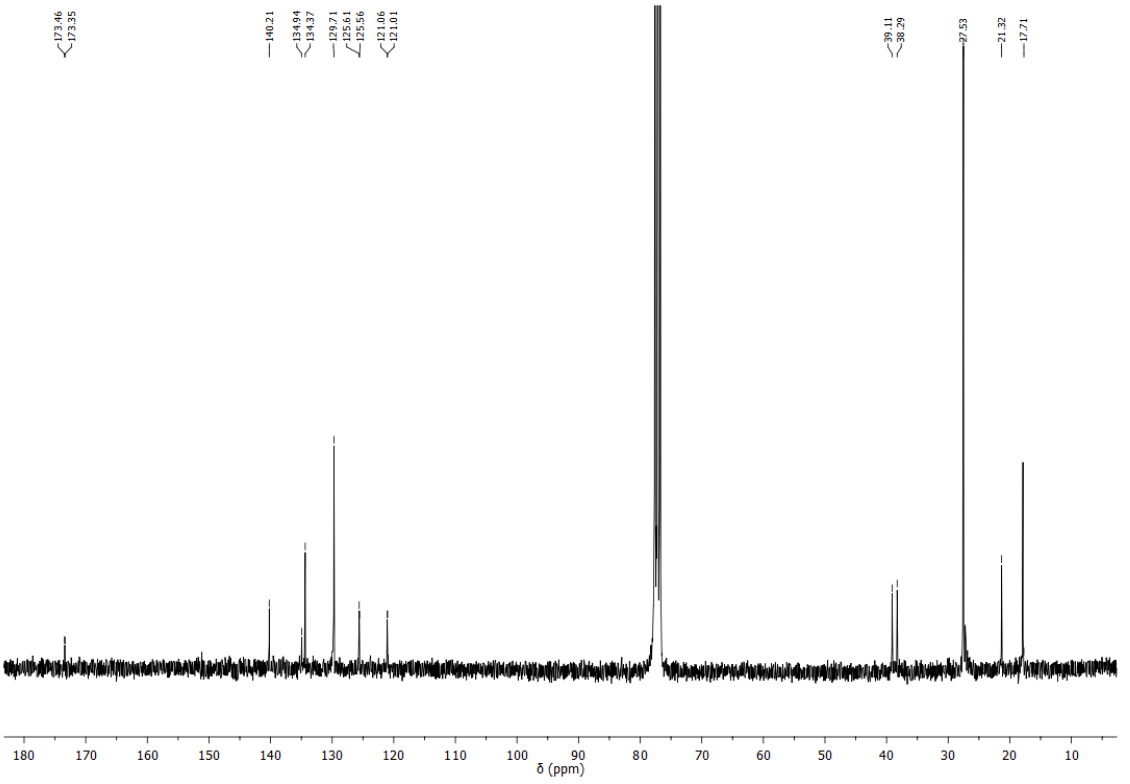


Figure S6. ^{13}C NMR spectrum of compound **6-AuCl$_4$** in $CDCl_3$

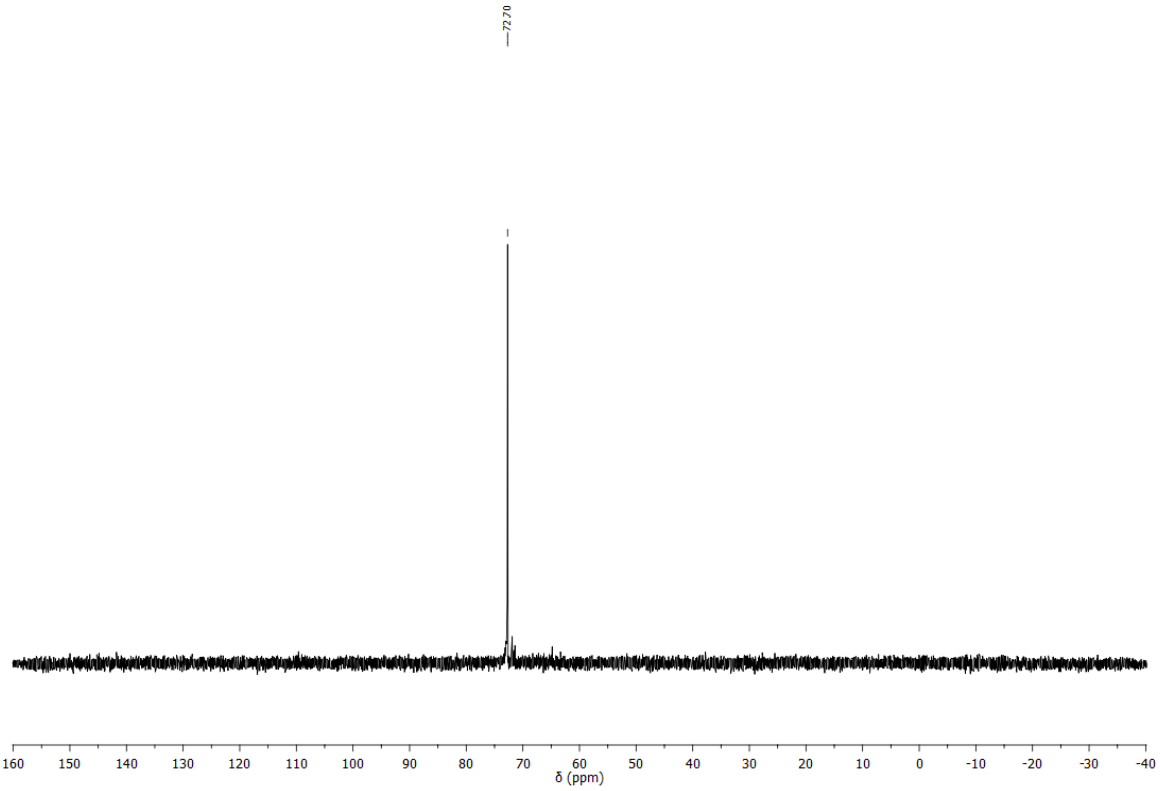
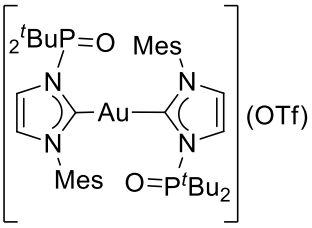


Figure S7. ^{31}P NMR spectrum of compound **6-AuCl$_4$** in $CDCl_3$

Compound 6-OTf ^{1}H, ^{13}C, ^{31}P NMR characterization



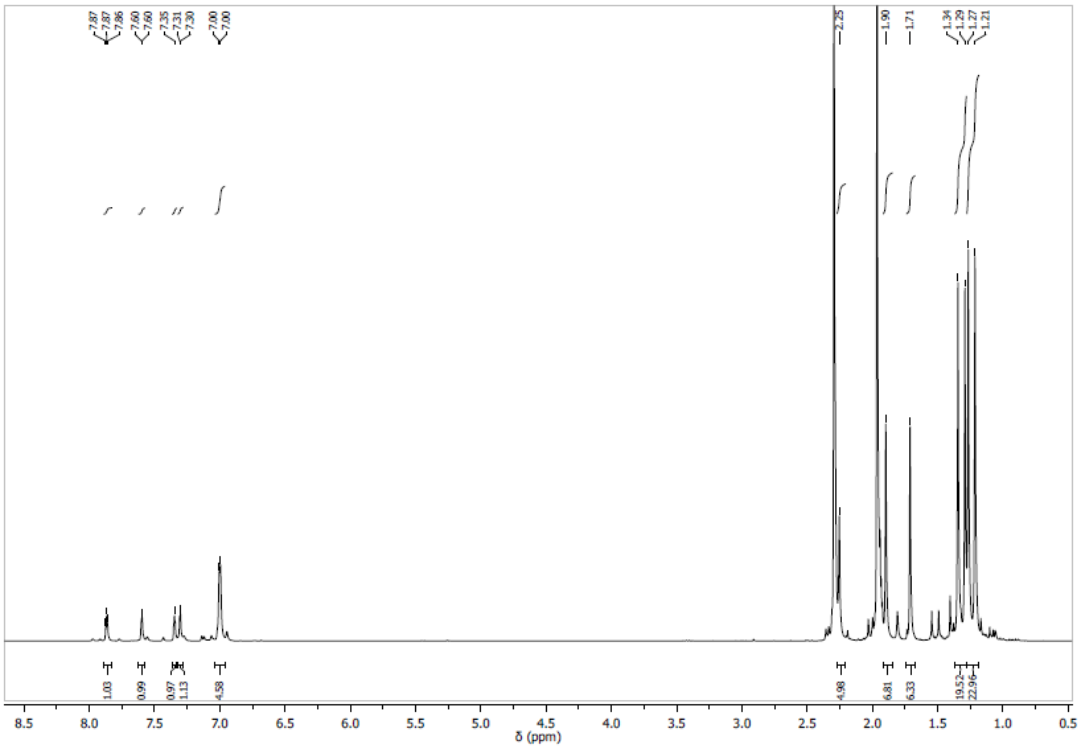


Figure S8. ^{1}H NMR spectrum of compound **6-OTf** in CD_3CN

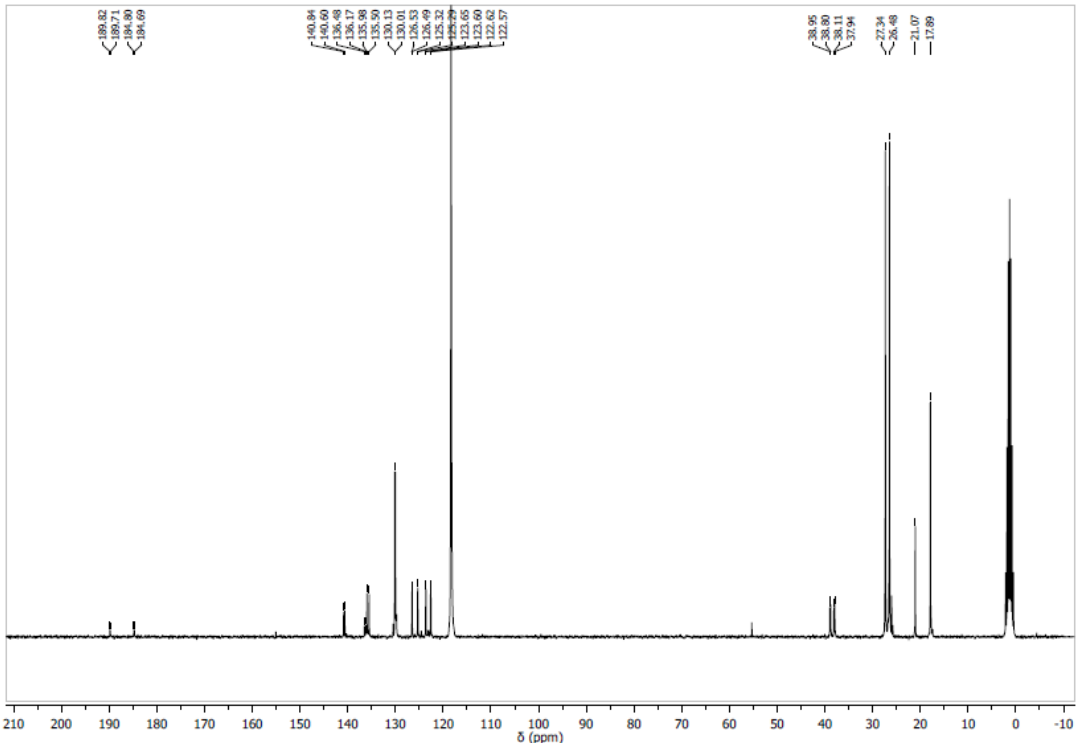


Figure S9. ^{13}C NMR spectrum of compound **6-OTf** in CD_3CN

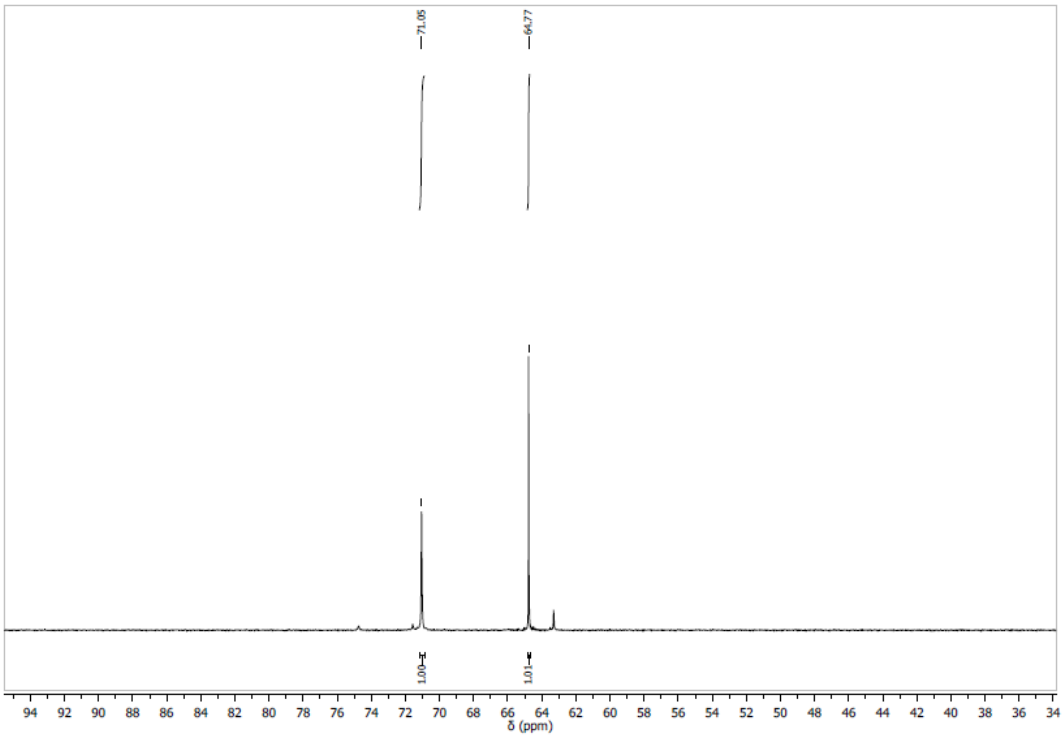


Figure S10. ^{31}P NMR spectrum of compound **6-OTf** in CD_3CN

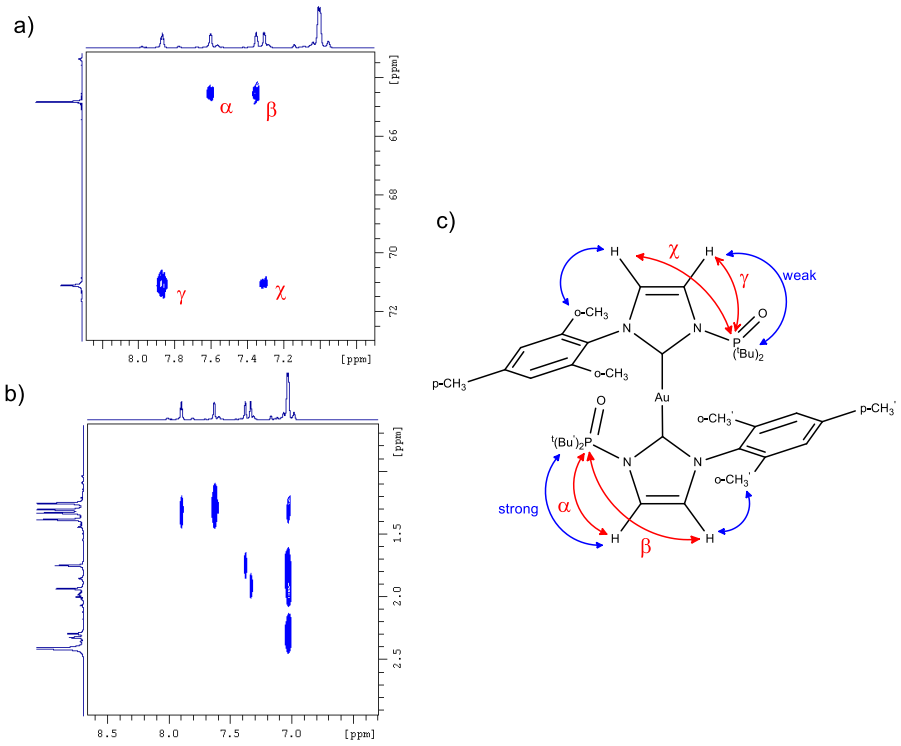


Figure S11. ^{1}H-^{31}P HMBC (a) and NOESY (b) NMR spectra of compound **6-OTf** in CD_3CN and the resulting magnetization transfers (c).

Compound 7 ^{1}H, ^{13}C, ^{31}P NMR characterization

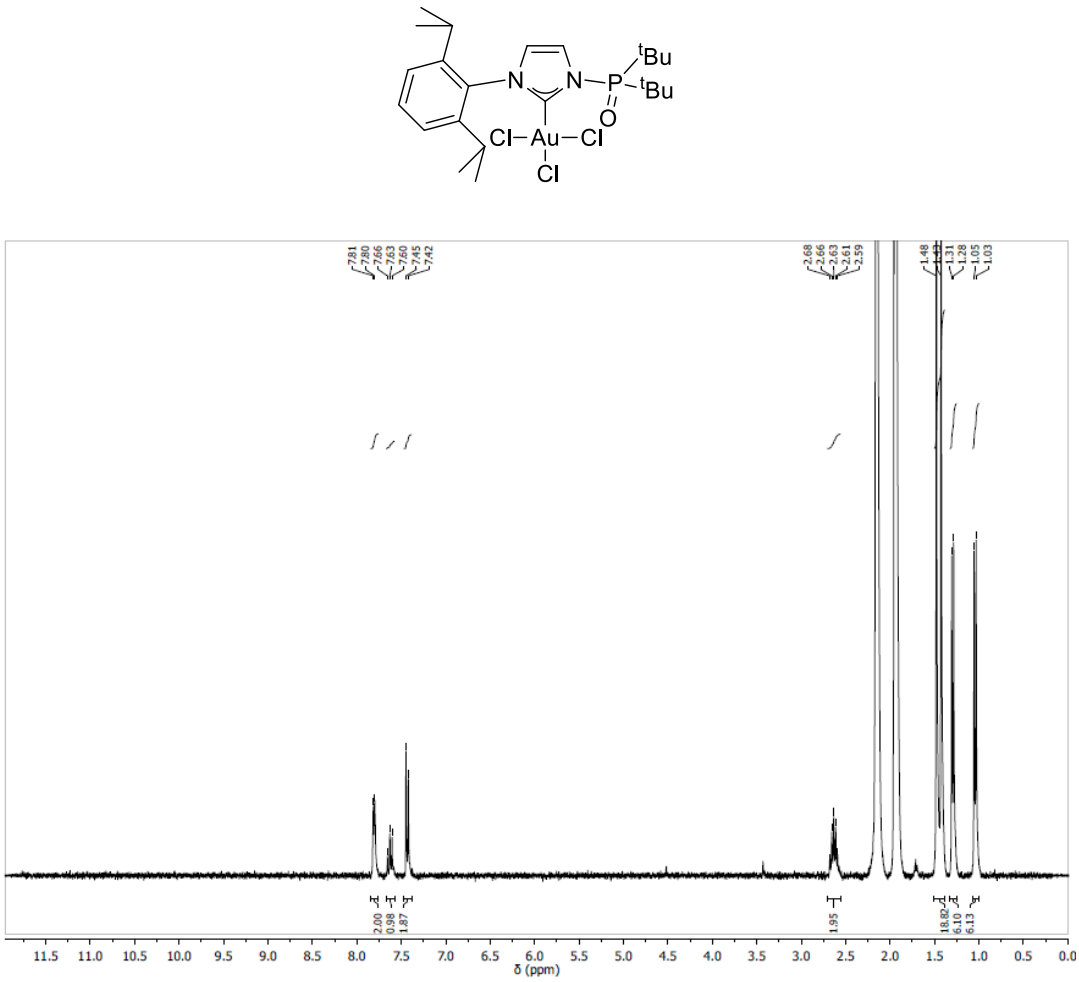


Figure S12. ^{1}H NMR spectrum of compound **7** in CD_3CN

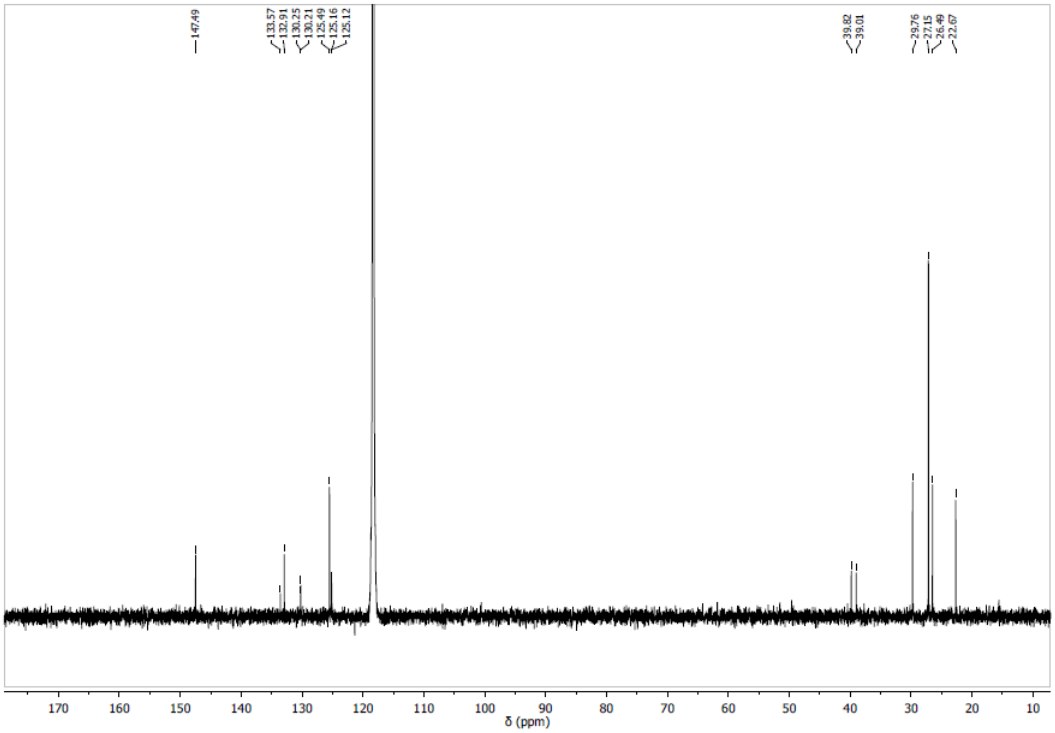


Figure S13. ^{13}C NMR spectrum of compound **7** in CD_3CN

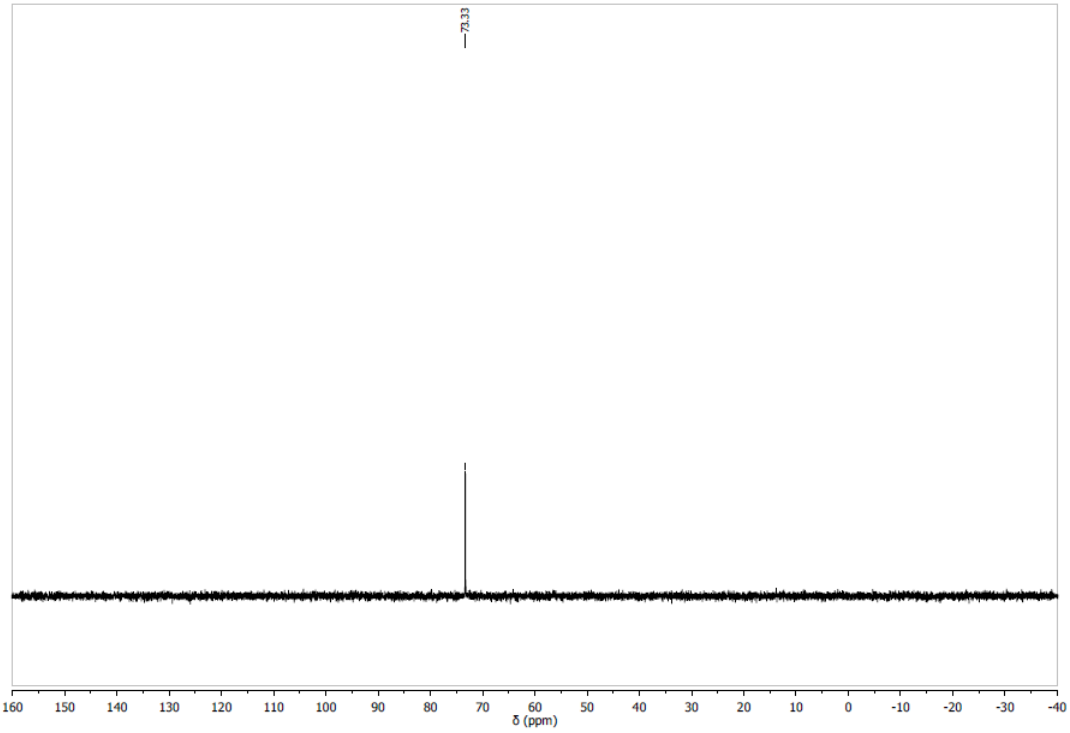
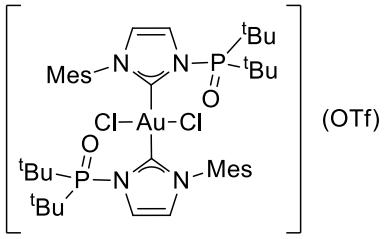


Figure S14. ^{31}P NMR spectrum of compound **7** in CD_3CN

Compound 8 ^{1}H, ^{13}C, ^{31}P NMR characterization



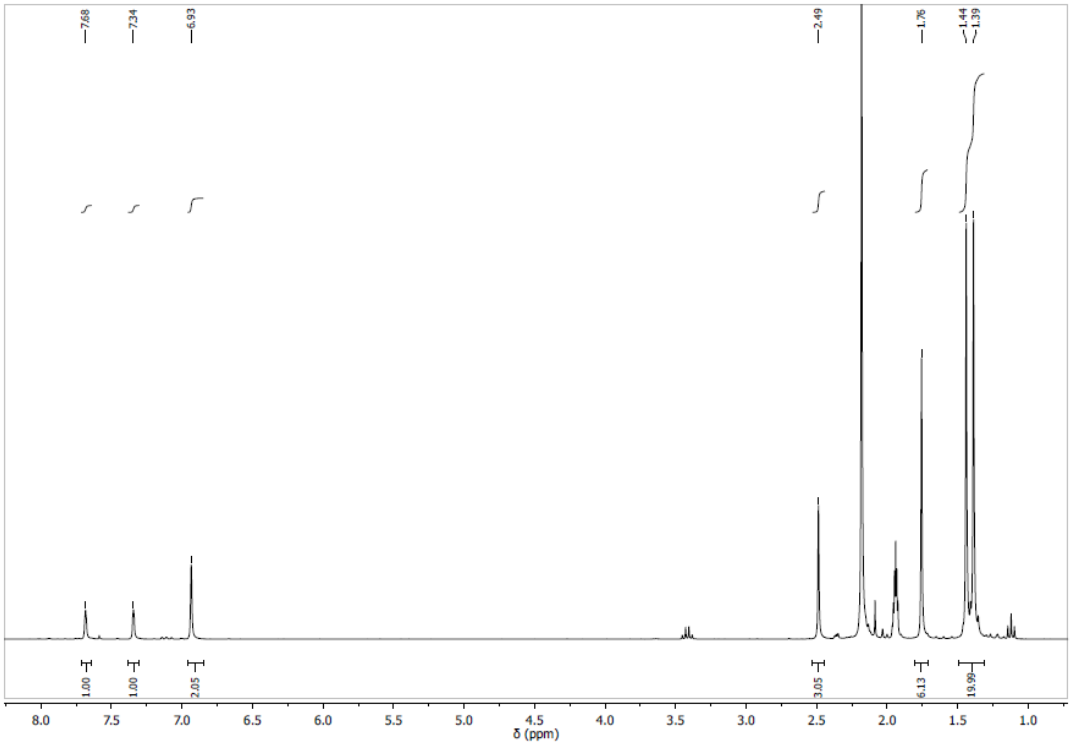


Figure S15. ^{1}H NMR spectrum of compound **8** in CD_3CN

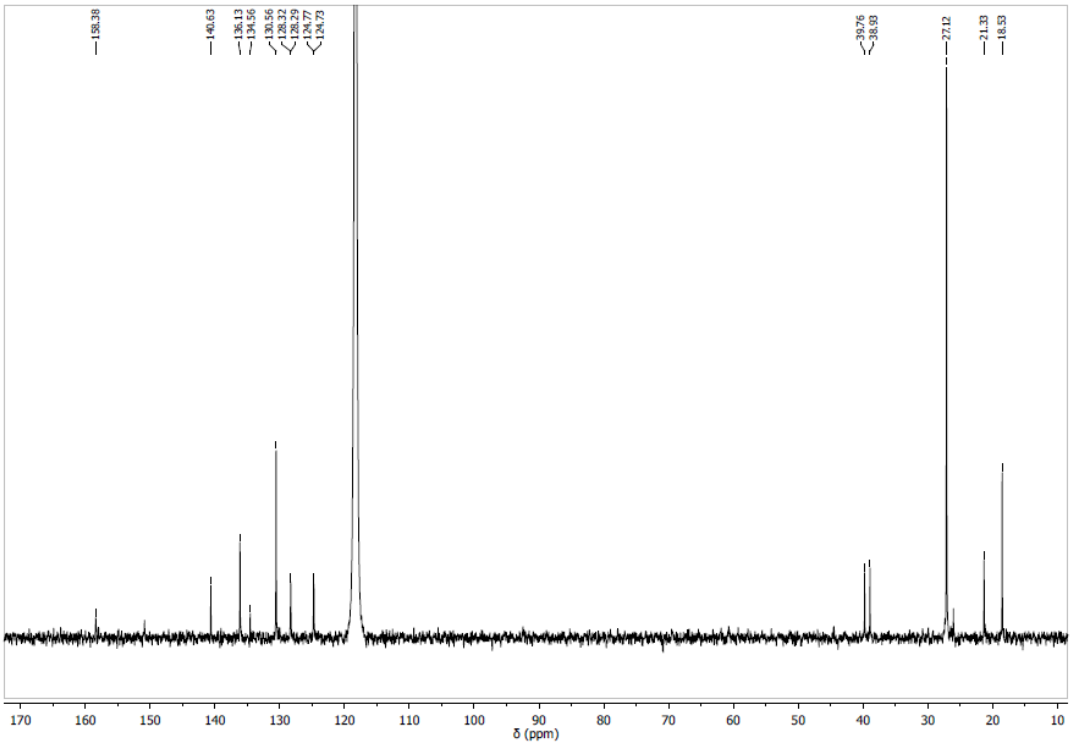


Figure S16. ^{13}C NMR spectrum of compound **8** in CD_3CN

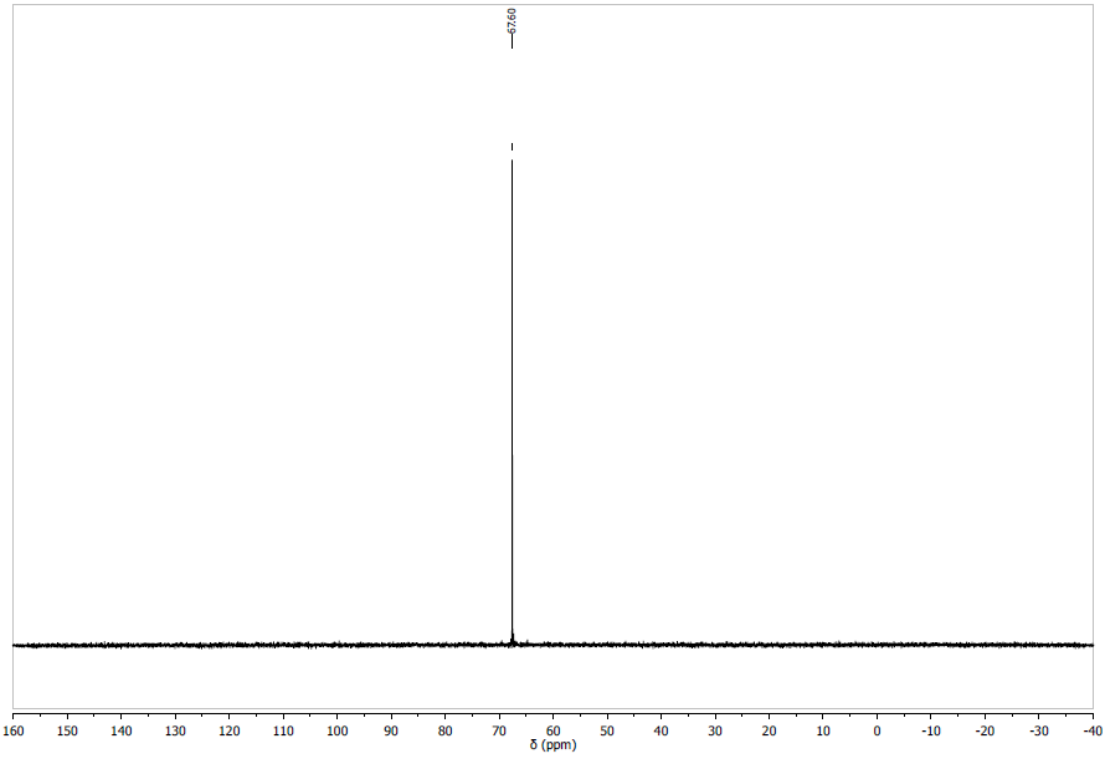
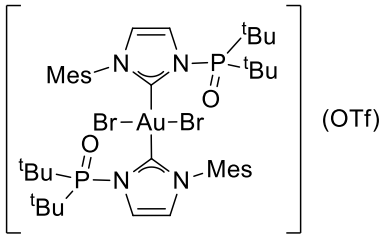


Figure S17. ^{31}P NMR spectrum of compound **8** in CD_3CN

Compound 9-OTf ^{1}H, ^{13}C, ^{31}P NMR characterization



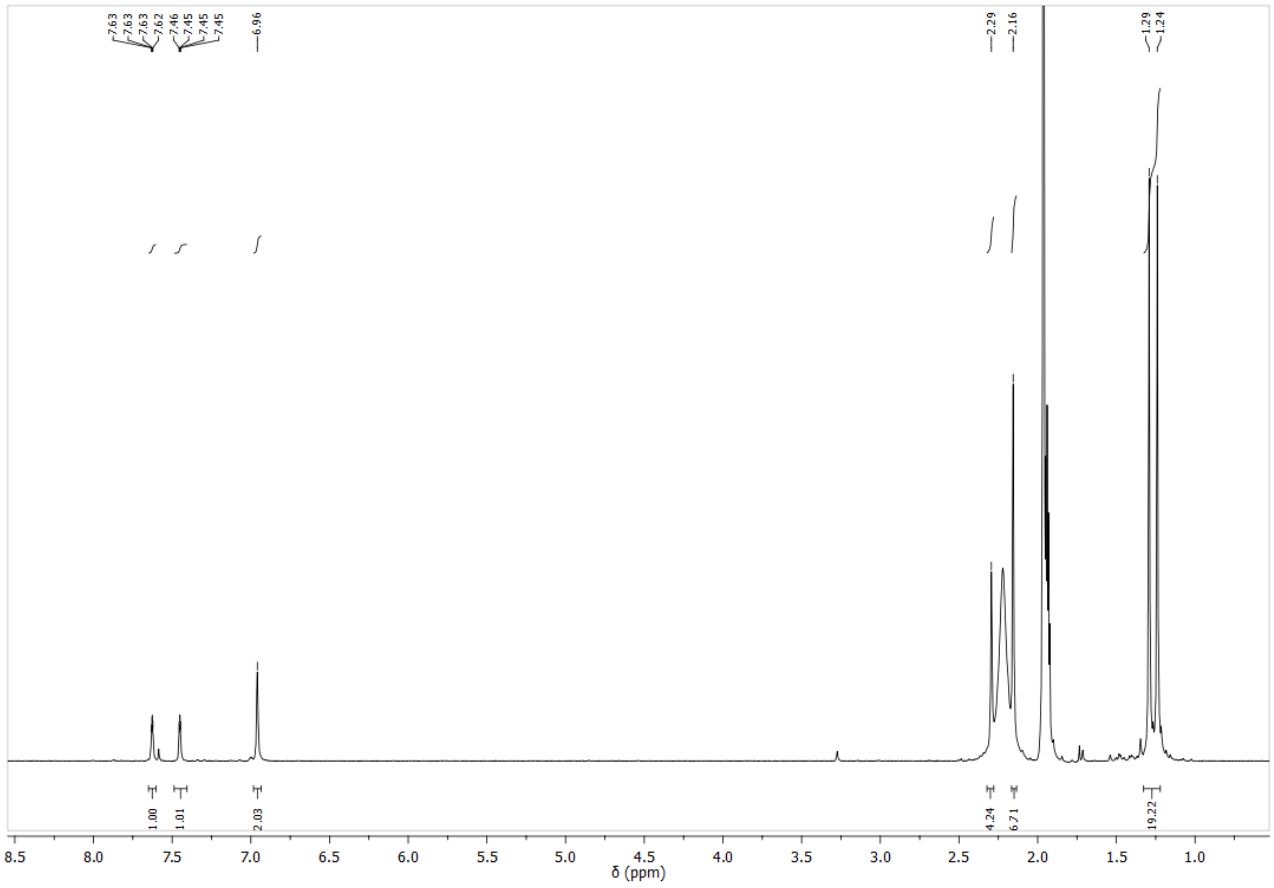


Figure S18. ^{1}H NMR spectrum of compound **9-OTf** in CD_3CN

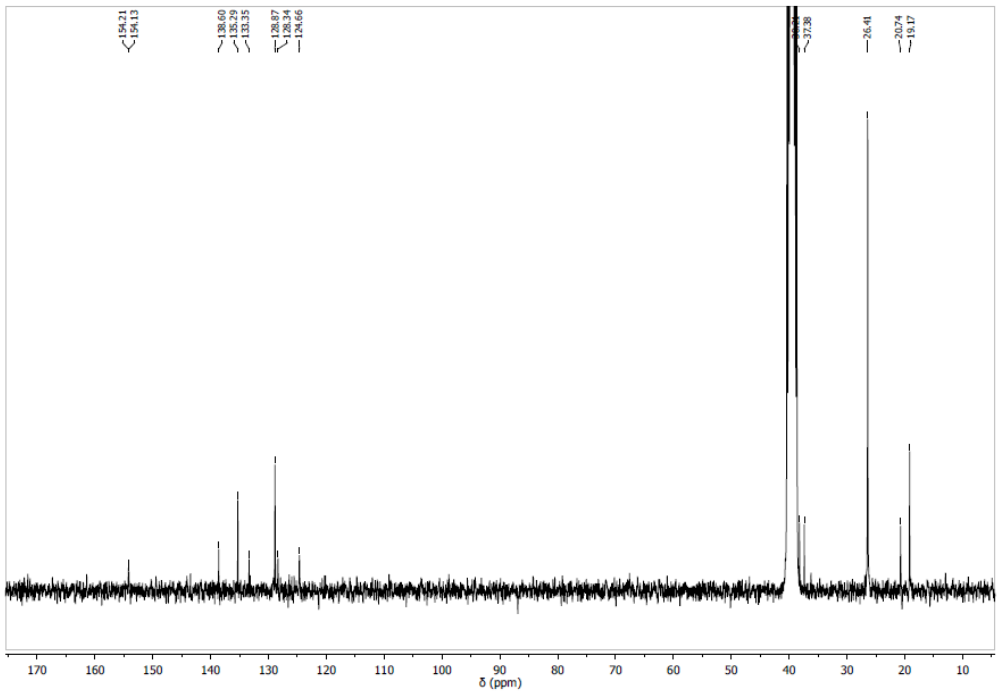


Figure S19. ^{13}C NMR spectrum of compound **9-OTf** in DMSO-d_6

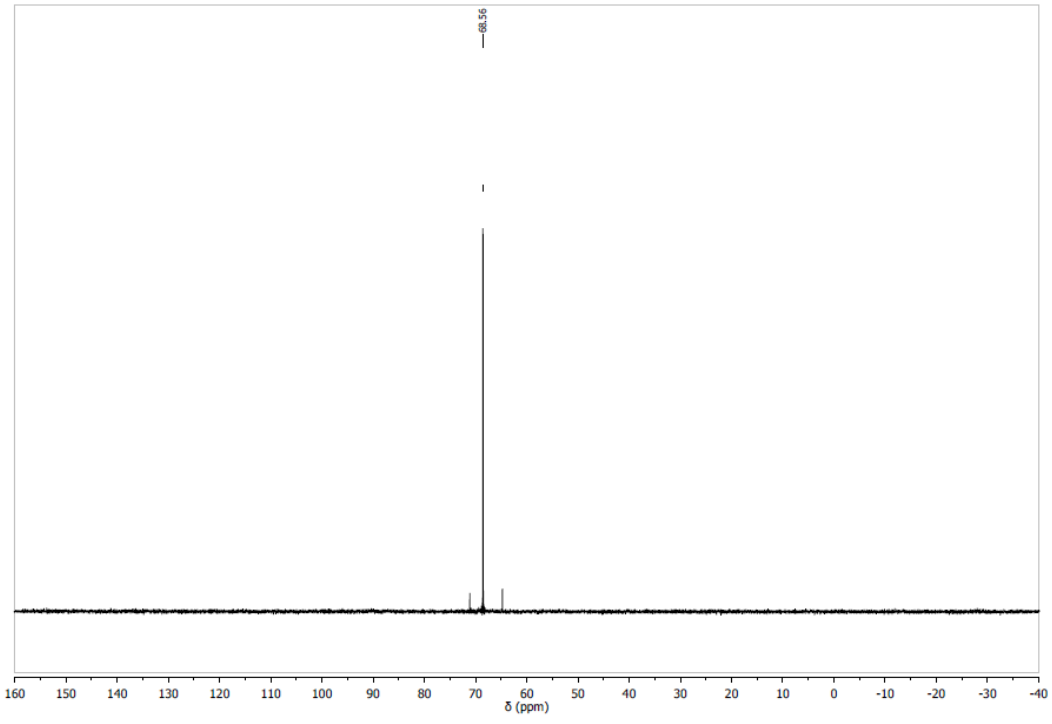
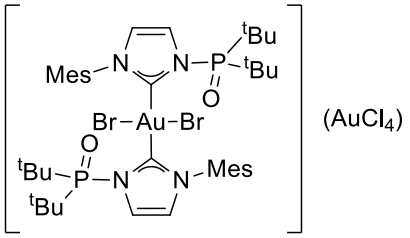


Figure S20. ^{31}P NMR spectrum of compound **9-OTf** in CD_3CN

Compound 9-$AuCl_4$ ^{1}H, ^{13}C, ^{31}P NMR characterization



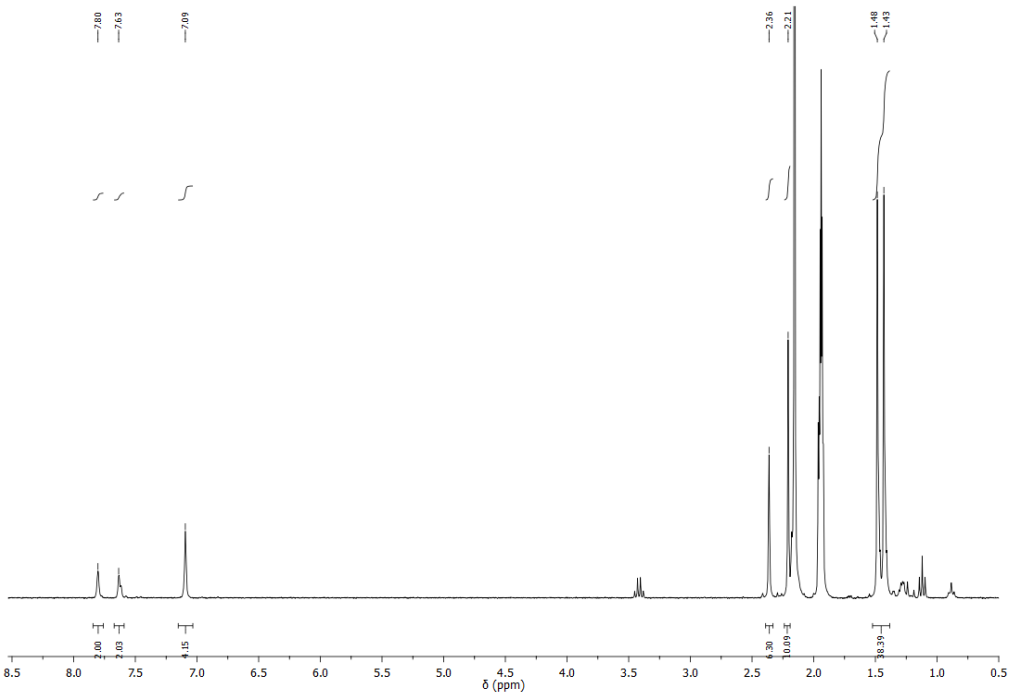


Figure S21. ^{1}H NMR spectrum of compound **9-$AuCl_4$** in CD_3CN

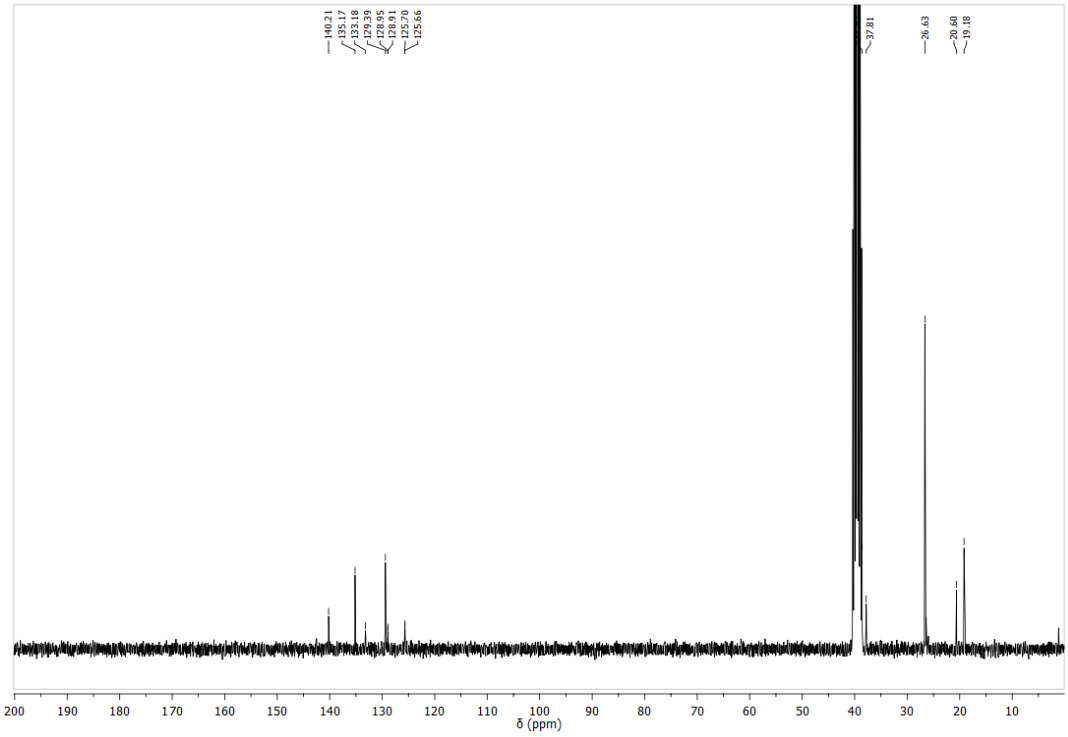


Figure S22. ^{13}C NMR spectrum of compound **9-AuCl₄** in DMSO-d_6

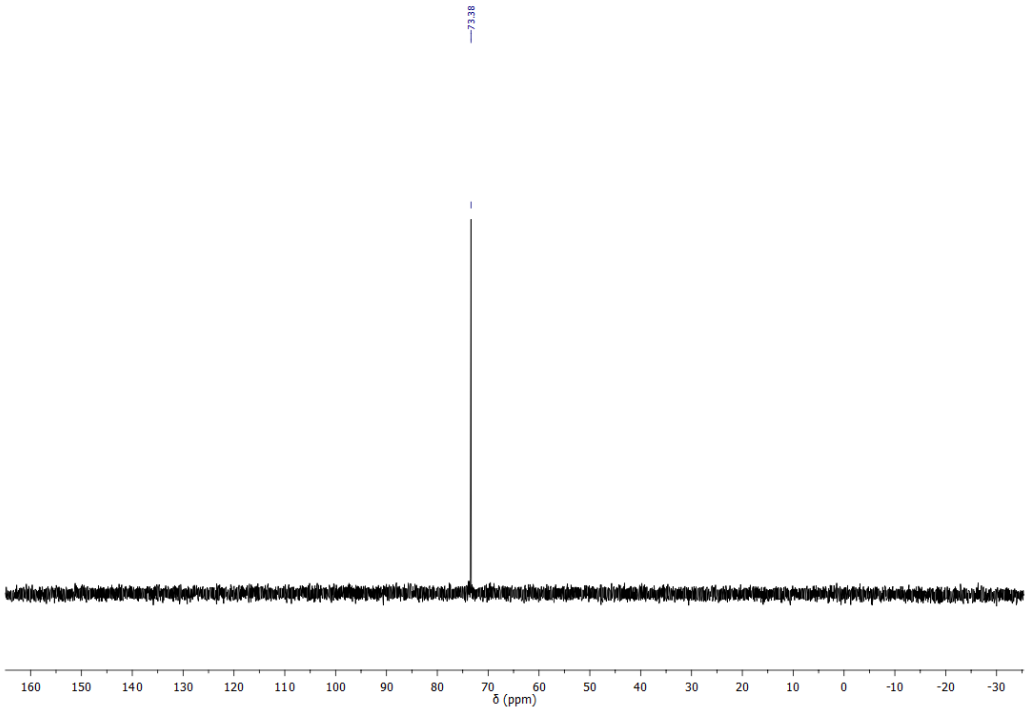
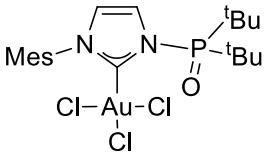


Figure S23. ^{31}P NMR spectrum of compound **9-AuCl₄** in CD_3CN

Compound 10 ^{1}H, ^{13}C, ^{31}P NMR characterization



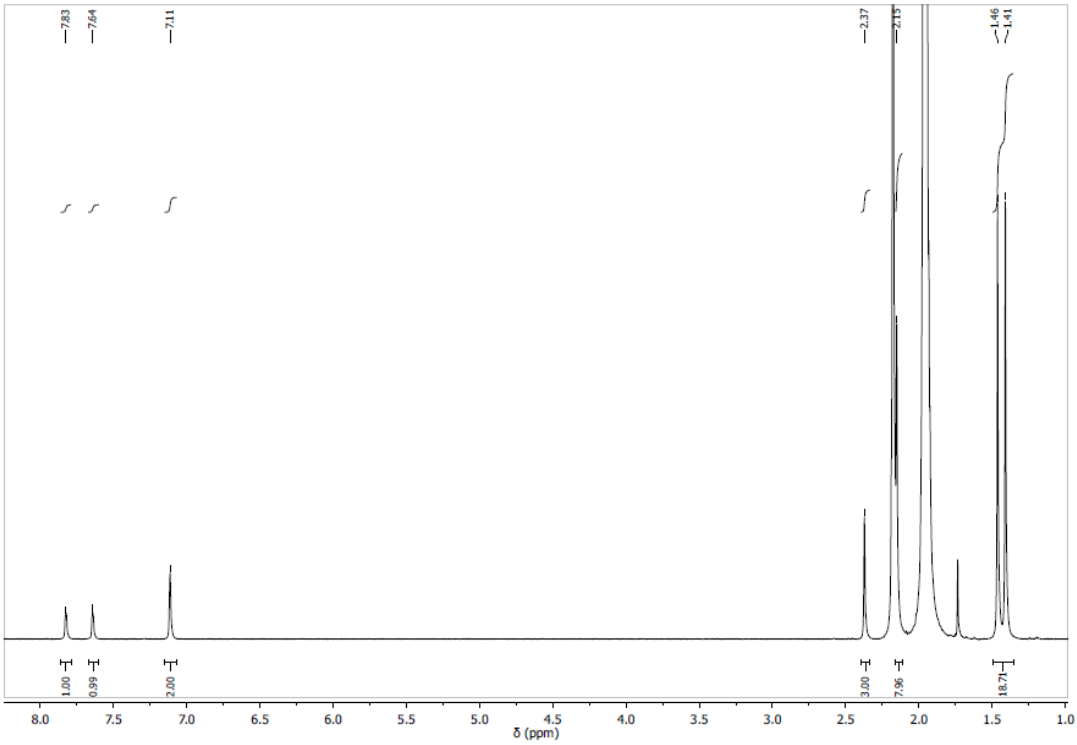


Figure S24. ^{1}H NMR spectrum of compound **10** in CD_3CN

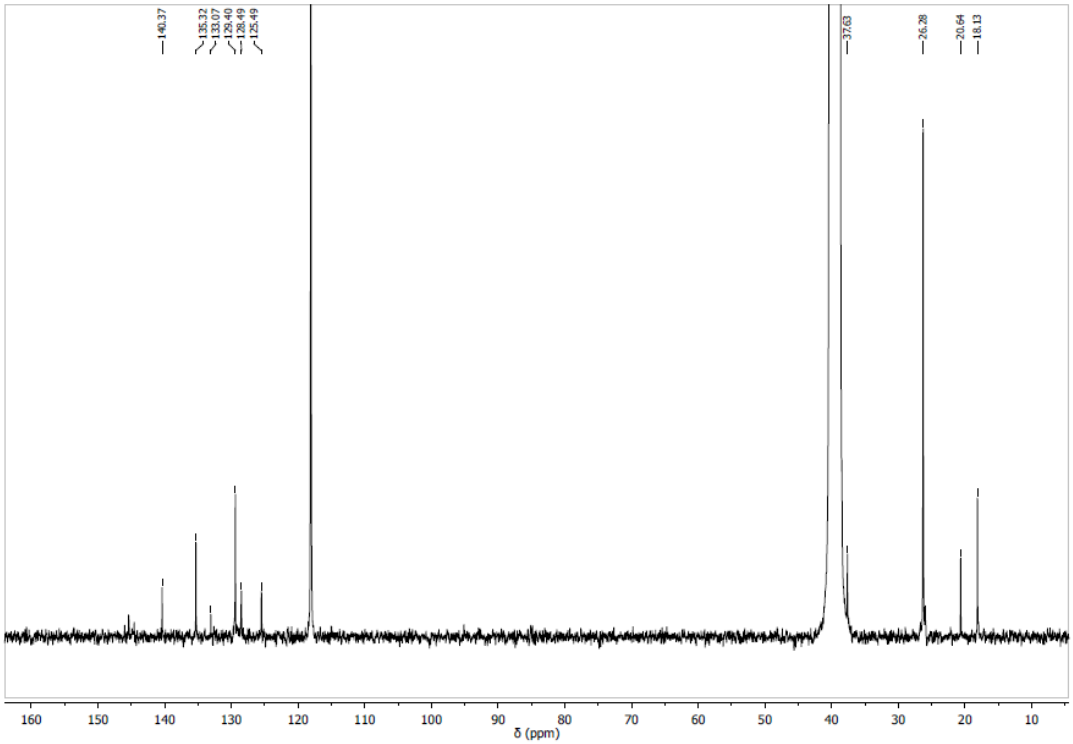


Figure S25. ^{13}C NMR spectrum of compound **10** in CD_3CN

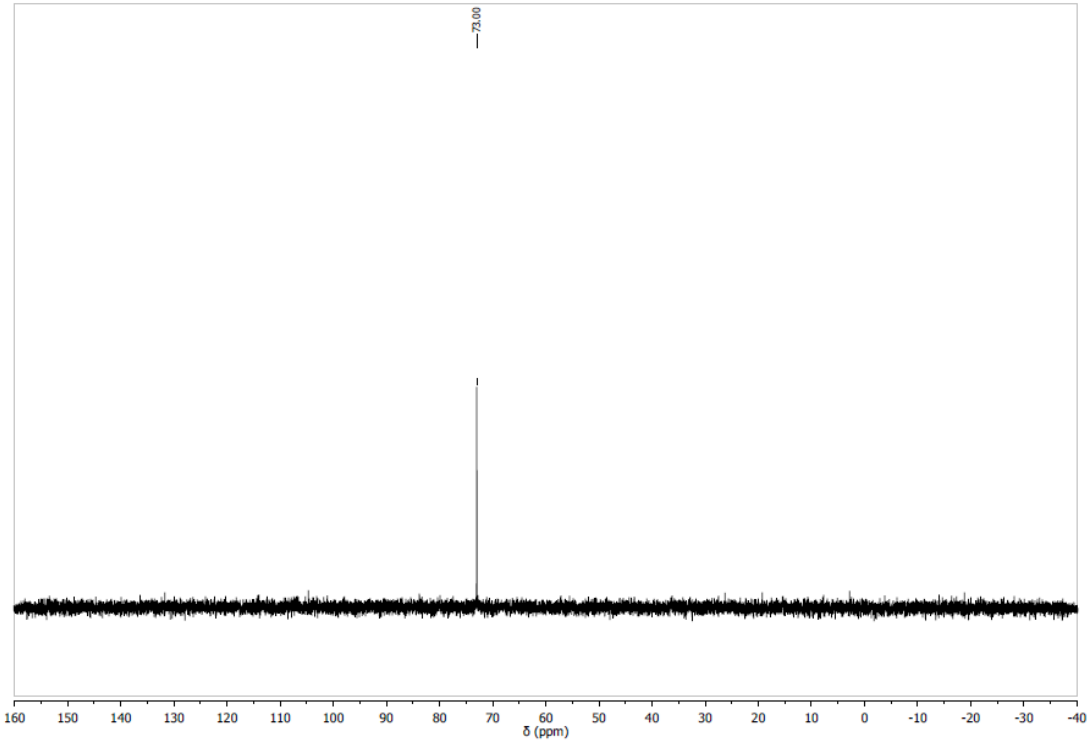


Figure S26. ^{31}P NMR spectrum of compound **10** in CD_3CN