Electronic Supplementary Material (ESI) for Dalton Transactions.

Pd(II) Coordinated deprotonated diphenyl phoshino amino pyridine: Reactivity towards Solvent, Base, and Acid

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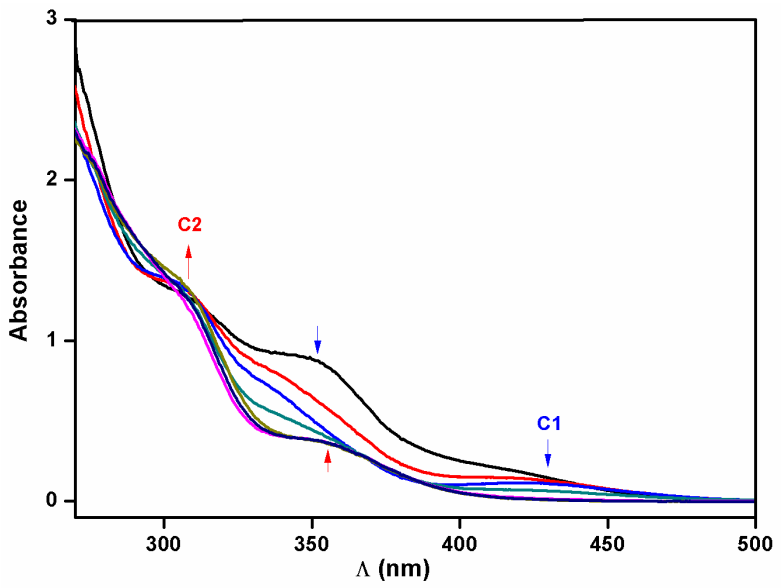


Fig. S1 UV-vis titration of complex C1 with dilute HCl solution.

S1.1 Experimental and calculated transition of complex C1 and C2:

The calculated UV-Vis spectra of **C1** resemble well with the experimentally observed transitions. The experimental transition at 418 nm (calculated = 415 nm) is found to be a π to σ* transition originating from ligand based π occupied molecular orbital to M-$L_{\sigma*}$ orbital. Similarly, the transition at 352 nm (calculated =342 nm), 310 nm (calculated = 317 nm) and 262 nm (calculated = 281 nm) are assigned to ligand based π to π* transition, ligand based π to M-$L_{\sigma*}$ and metal d_z2 orbital to M-$L_{\sigma*}$ transition respectively. The experimental bands at 361 nm (calculated = 373 nm) for **C2** is assigned to be ligand based π molecular orbital to M-$L_{\sigma*}$ transition. The band at 306 nm (calculated = 306 nm) is due to be transition from metal d_z^2 orbital to M-$L_{\sigma*}$ orbital. The other two calculated bands at 382 nm and 283 nm is due to the transition from ligand based π molecular orbital to M-$L_{\sigma*}$ orbital and metal d_{xz} orbital to M-$L_{\sigma*}$ orbital (Table S1).

Table S1. Key transitions in the TD-DFT computations for **C1** and **C2**.

#	Wavelength (nm) calc. (exp.)	Key Transition (Type)	Osc. Strength (f)
C1	415 (418)	HOMO→LUMO (Lπ → M-Lσ*)	0.0382
	398	HOMO-1→LUMO (Lπ → M-Lσ*)	0.0195
	342 (352)	HOMO→LUMO+1 (Lπ → Lπ*)	0.0792
	331	HOMO-1→LUMO+1 (Lπ → Lπ*)	0.030
	317 (310)	HOMO-2→LUMO (Lπ → M-Lσ*)	0.0651
	281 (262)	HOMO-4→LUMO (dz2 → M-Lσ*)	0.1061
C2	382	HOMO→LUMO (Lπ → M-Lσ*)	0.0356
	373 (361)	HOMO-1→LUMO (Lπ → M-Lσ*)	0.0101
	331	HOMO-4→LUMO (Lπ → M-Lσ*)	0.0149
	306 (306)	HOMO-6→LUMO (dz2 → M-Lσ*)	0.0089
	283	HOMO-12→LUMO (dxz → M-Lσ*)	0.0677

S1.2 Elctrophilicity of Sn(IV) Reagents:

The observed electrophilicity (ω) order is $SnCl_4$ > $PhSnCl_3$ > Me_2SnCl_2 (Fig. S2). The order suggested that substitution of chloride by phenyl increases the electron density at tin centre due to +R and –I effect of phenyl ring, which is further increase in alkyl substituted Me_2SnCl_2 because of the +I effect of Me. So, it was expected that hydrolysis rate of the organotin(IV) reagents will also decrease in the same order $SnCl_4$ > $PhSnCl_3$ > Me_2SnCl_2, as generation of HCl will also depend upon the electron density at tin centre. Gratifyingly, the calculated LUMO energy of the three reagents suggested the faster hydrolysis in case of $SnCl_4$ because of low lying LUMO compared to $PhSnCl_3$ and Me_2SnCl_2 (Fig. S2).

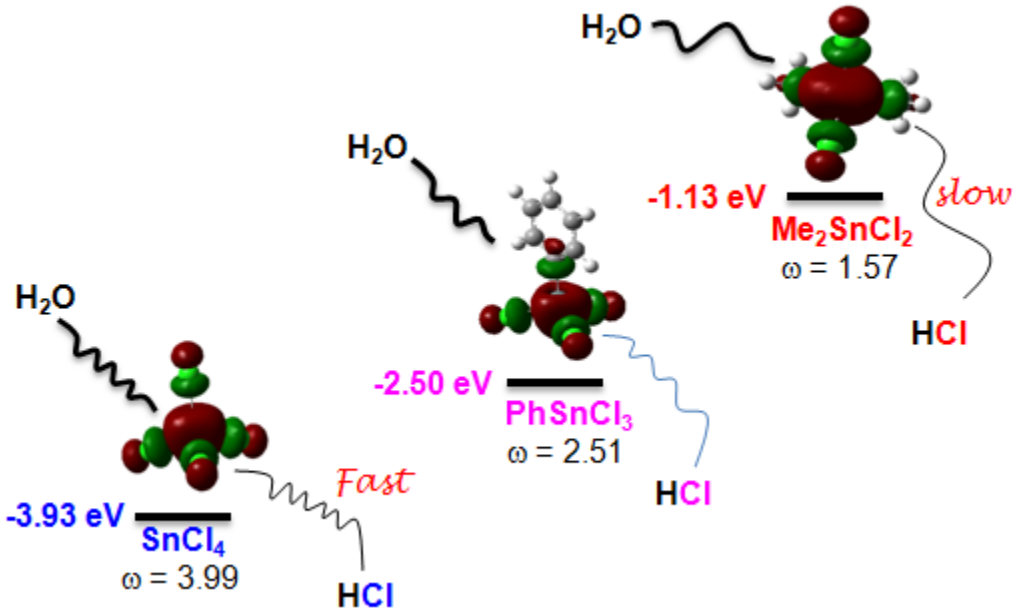


Fig. S2 Relation between the rate of hydrolysis, LUMO, and electrophilicity of three organotin (IV) reagents.

S1.3 Experimental and calculated transition of complex C6 and C7:

The reaction between **C1** and SnI_4 also has been monitored with UV-vis spectroscopy. Upon gradual addition of SnI_4 to **C1** in MeCN, two bands of **C1** at 352, and 310 nm disappeared, while a new peak at 302 nm and 458 nm appeared due to the generation of a new complexes (Fig. 6). To assign the UV-Vis transitions, we have performed TD-DFT calculations on **C6** and **C7**. Table S2 contains the key transitions. The first two transition for **C7** at 459 and 438 nm are assigned to iodine lone pair to M-$L_{\sigma*}$ orbital. The next two transitions at 324 and 312 nm are assigned to π orbital of DPAP ligand to M-$L_{\sigma*}$ orbital. The last two transitions at 282 and 271 nm are assigned to iodine lone pair and π orbital of DPAP to M-$L_{\sigma*}$ orbital. Similarly, the calculated values for **C6** are in close agreement with the experimental observed transitions. The transition at 408 and 374 nm for **C6** are assigned to bromine lone pair to M-$L_{\sigma*}$ transition. The transitions at 313, 303 and 298 nm are assigned to $L_n \rightarrow$ M-$L_{\sigma*}$ transition while the transitions at 287 and 273 nm are assigned to bromine lone pair to ligand based π* orbital of diphenyl phoshino amino pyridine (DPAP) ligand. The other two transition at 265 and 259 nm are assigned to bromine lone pair to M-$L_{\pi*}$ orbital.

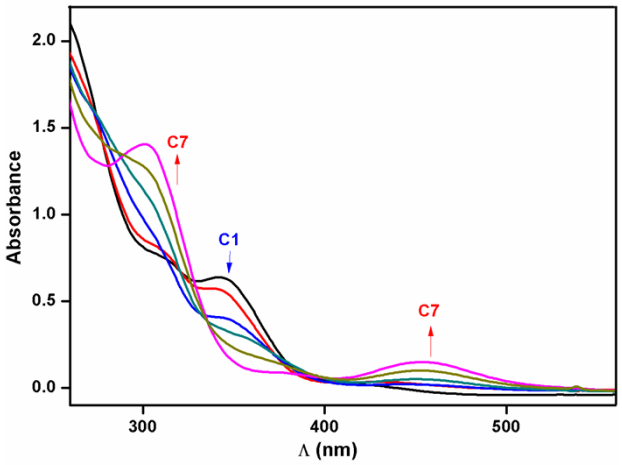


Fig. S3. UV-vis titration of complex C1 with SnI4 in MeCN solution.

Table S2. Key transitions in the TD-DFT computations for **C6** and **C7**.

Complex	Wavelength (nm) calculated (Experimental)	Key Transition (Type)	Osc. Strength (*f*)
C6	408	HOMO-3→LUMO ($Br_{(lp)}$ → M-L_{σ^*})	0.0175
	374 (372)	HOMO-2→LUMO ($Br_{(lp)}$ → M-L_{σ^*})	0.0152
	313 (310)	HOMO-6→LUMO (L_{π} → M-L_{σ^*})	0.1236
	303	HOMO-7→LUMO (L_{π} → M-L_{σ^*})	0.0633
	298	HOMO-8→LUMO (L_{π} → M-L_{σ^*})	0.0147
	287 (278)	HOMO→LUMO+1 ($Br_{(lp)}$ → L_{π^*})	0.0856
	273	HOMO-1→LUMO+1 ($Br_{(lp)}$ → L_{π^*})	0.0613
	265	HOMO→LUMO+2 ($Br_{(lp)}$ → M-L_{π^*})	0.0382
	259	HOMO-3→LUMO+2 ($Br_{(lp)}$ → M-L_{π^*})	0.0254
C7	459 (458)	HOMO→LUMO (L_n → M-L_{σ^*})	0.0201
	438	HOMO-3→LUMO (L_n → M-L_{σ^*})	0.0135
	324	HOMO-6→LUMO (L_{π} → M-L_{σ^*})	0.208
	312 (306)	HOMO-8→LUMO (L_{π} → M-L_{σ^*})	0.0503
	282	HOMO→LUMO+2 ($I_{(lp)}$ → M-L_{π^*})	0.1112
	271	HOMO-12→LUMO ($I_{(\pi)}$ → M-L_{σ^*})	0.0856

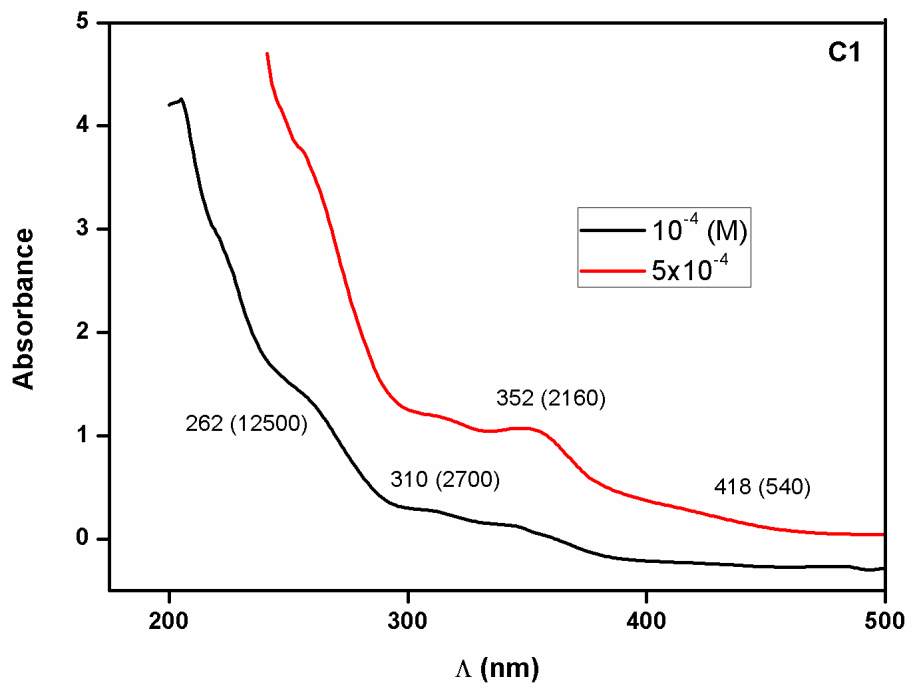


Fig. S4. UV-Vis spectra of **C1**

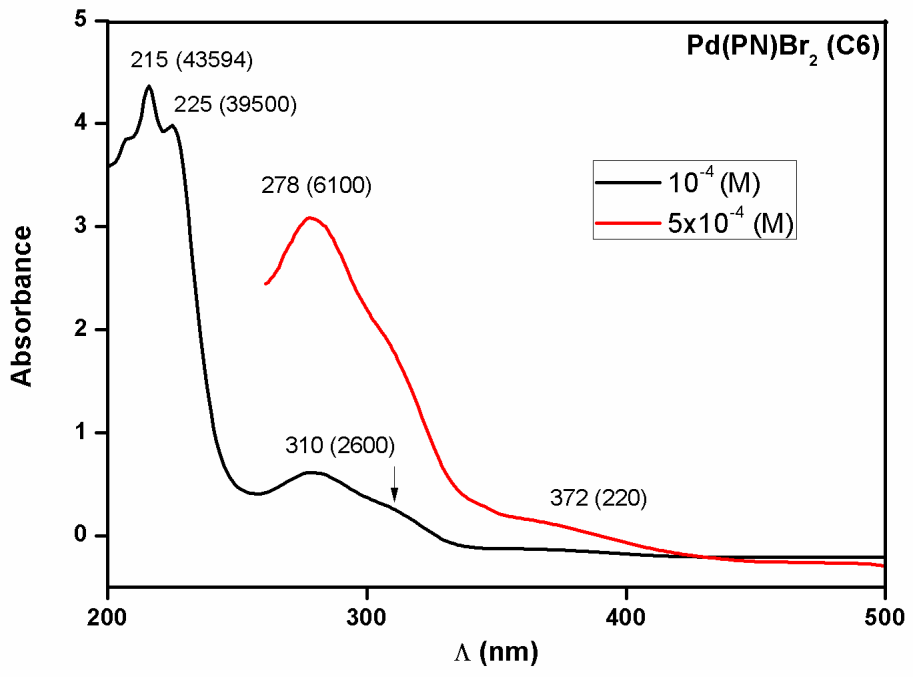
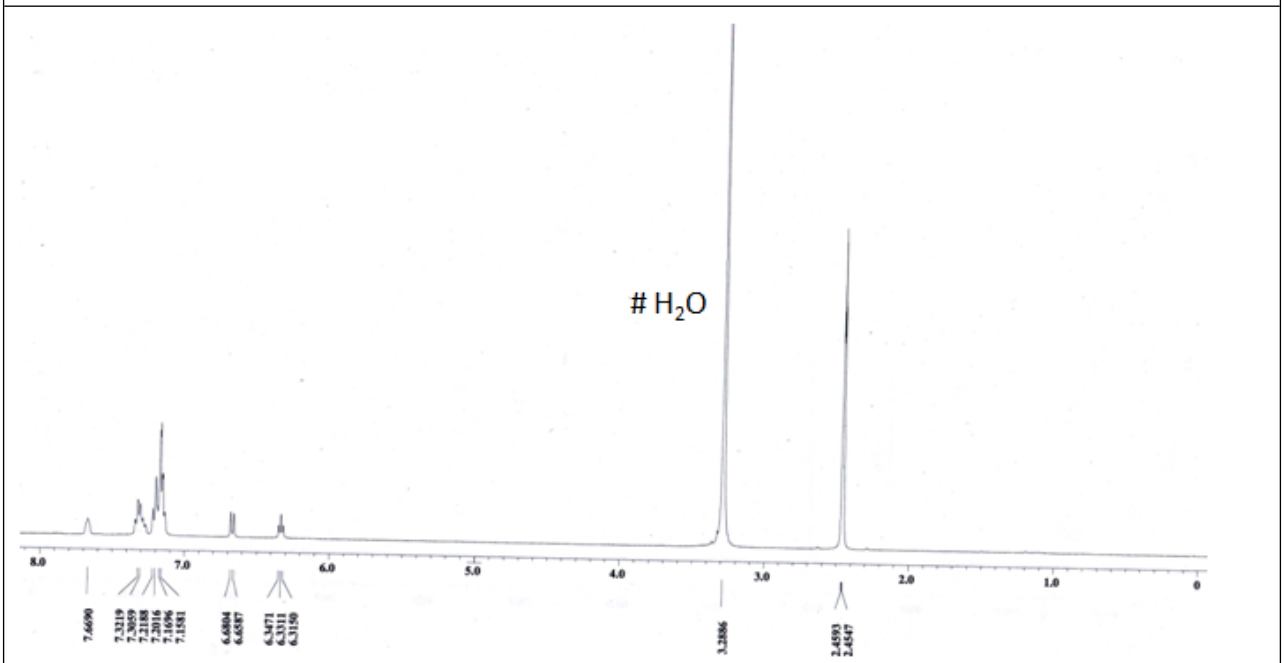


Fig. S5. UV-Vis spectra of **C6**

S1.4 ^{1}H and ^{31}P, and ^{119}Sn NMR spectra of all the complexes: all the spectra were recorded in DMSO-d_{63} at 298 K. solvent residual signals were highlighted in the spectra (DCE represents 1, 2-dichloroethane). [1]

Fig. S6. ^{1}H and ^{31}P NMR of **C1** in DMSO-d_6 at 298K



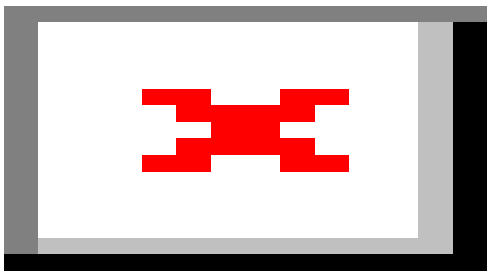


Fig. S7. ^{1}H and ^{31}P NMR of **C2** in DMSO-d_6 at 298K

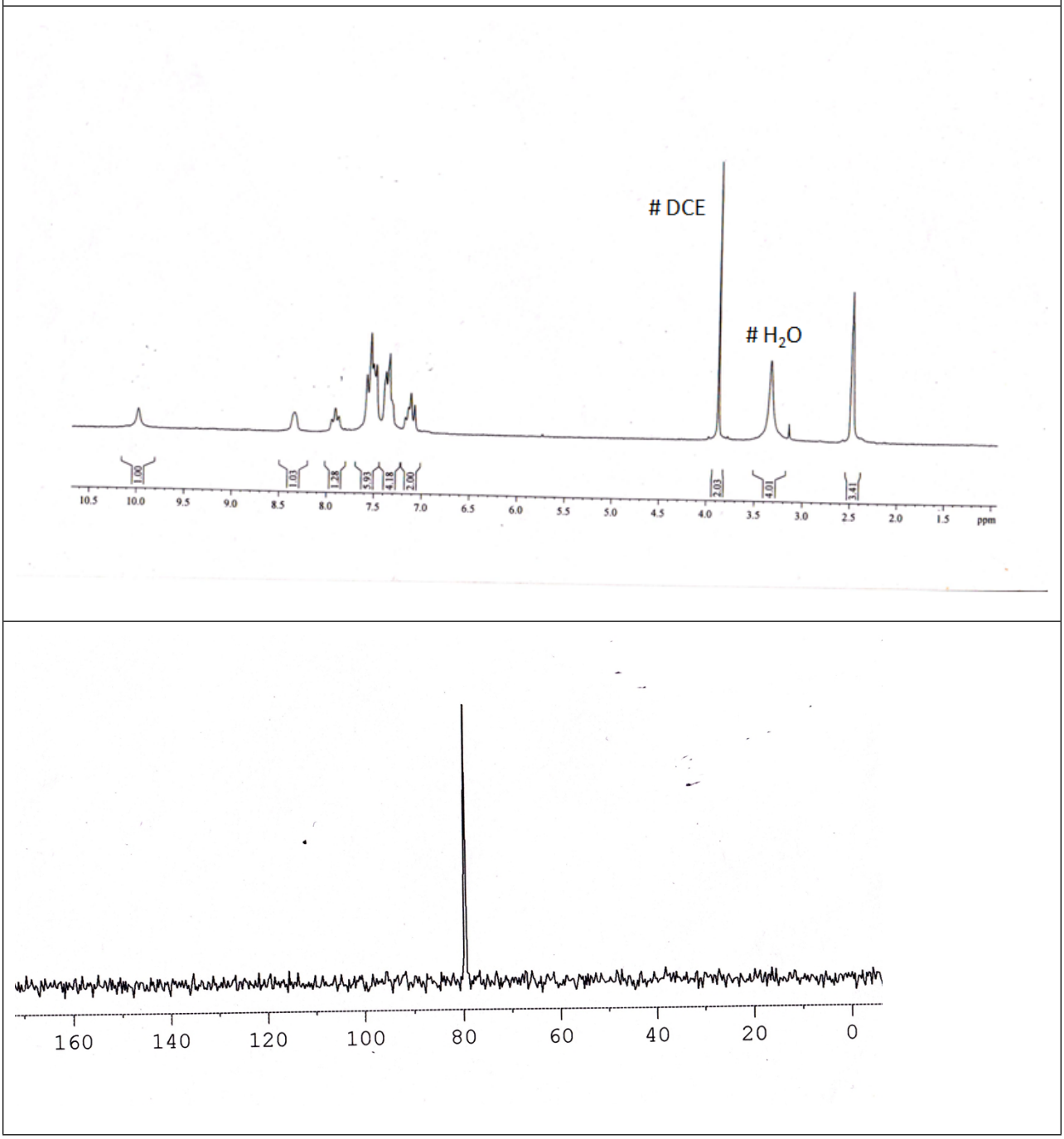
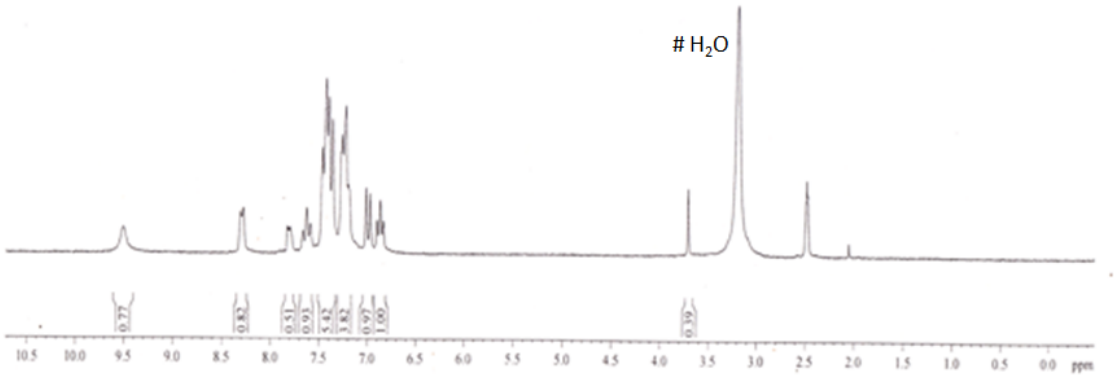
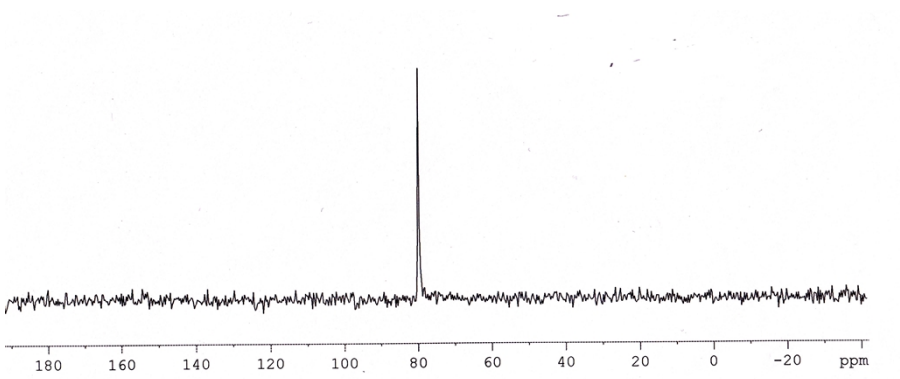


Fig. S8. ^{1}H, ^{31}P, and ^{119}Sn NMR of **C3** in DMSO-d_6 at 298K





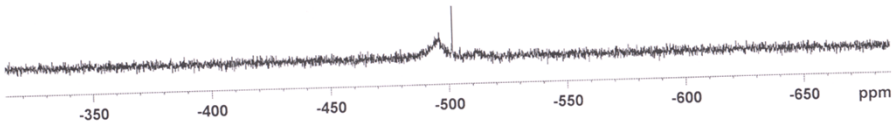
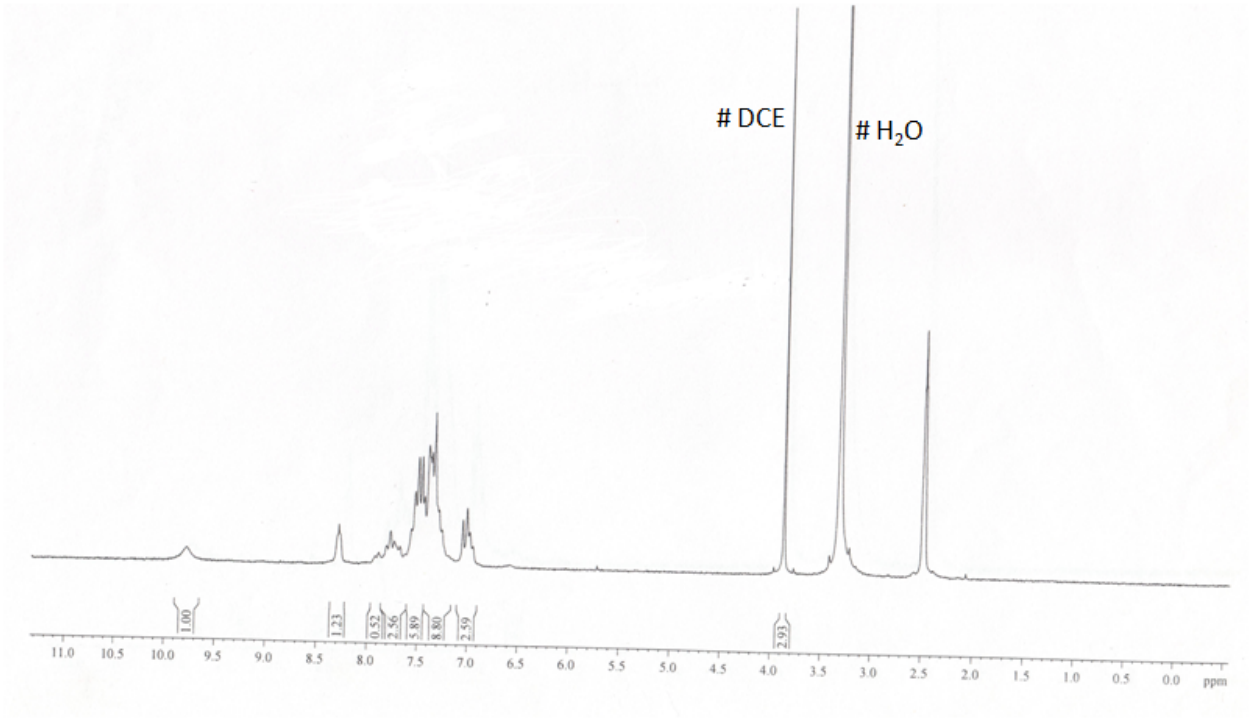
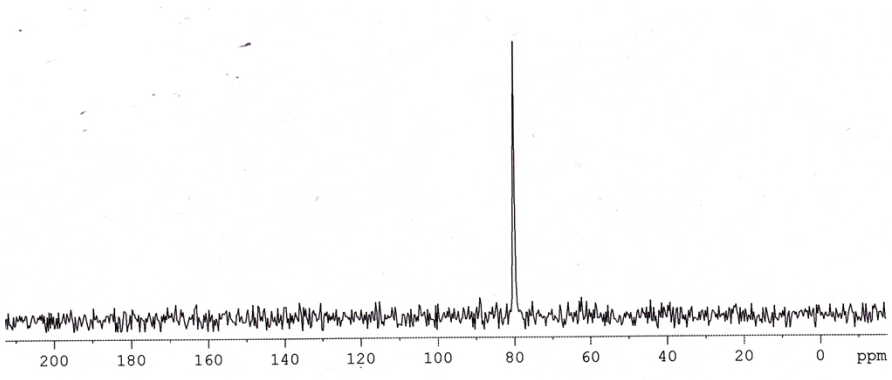


Fig. S9. ^{1}H, ^{31}P, and ^{119}Sn NMR of **C4** in DMSO-d_6 at 298K





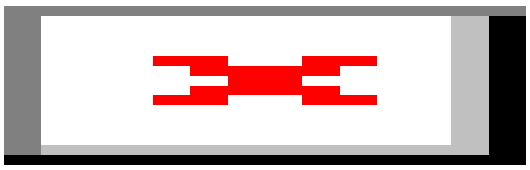
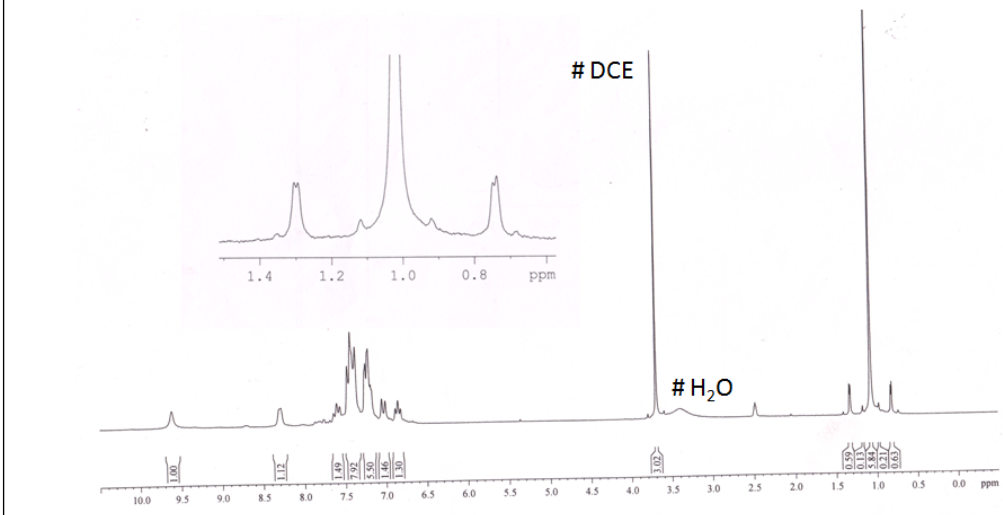
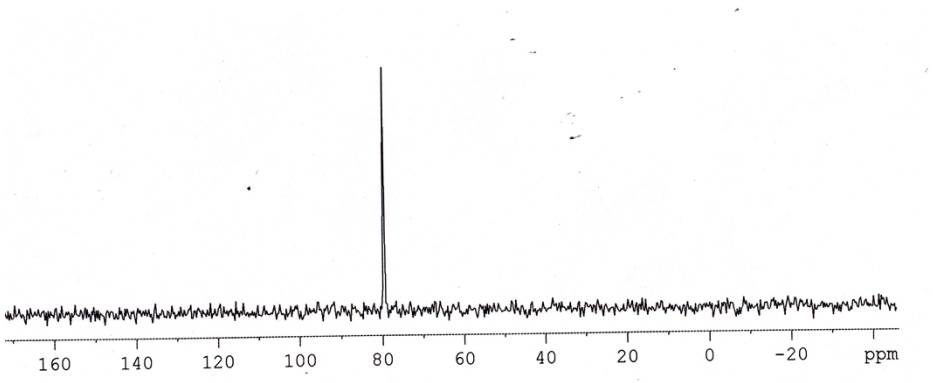


Fig. S10 ^{1}H, ^{31}P, and ^{119}Sn NMR of **C5** in DMSO-d_6 at 298K





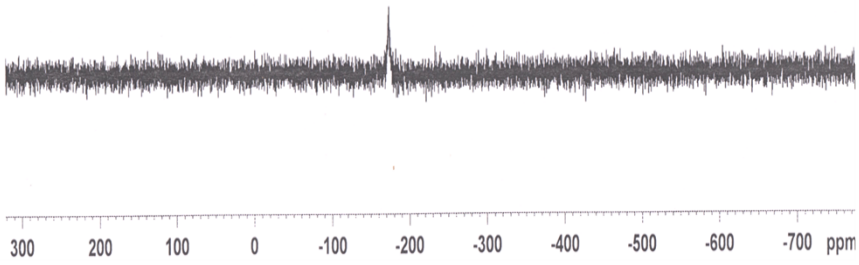
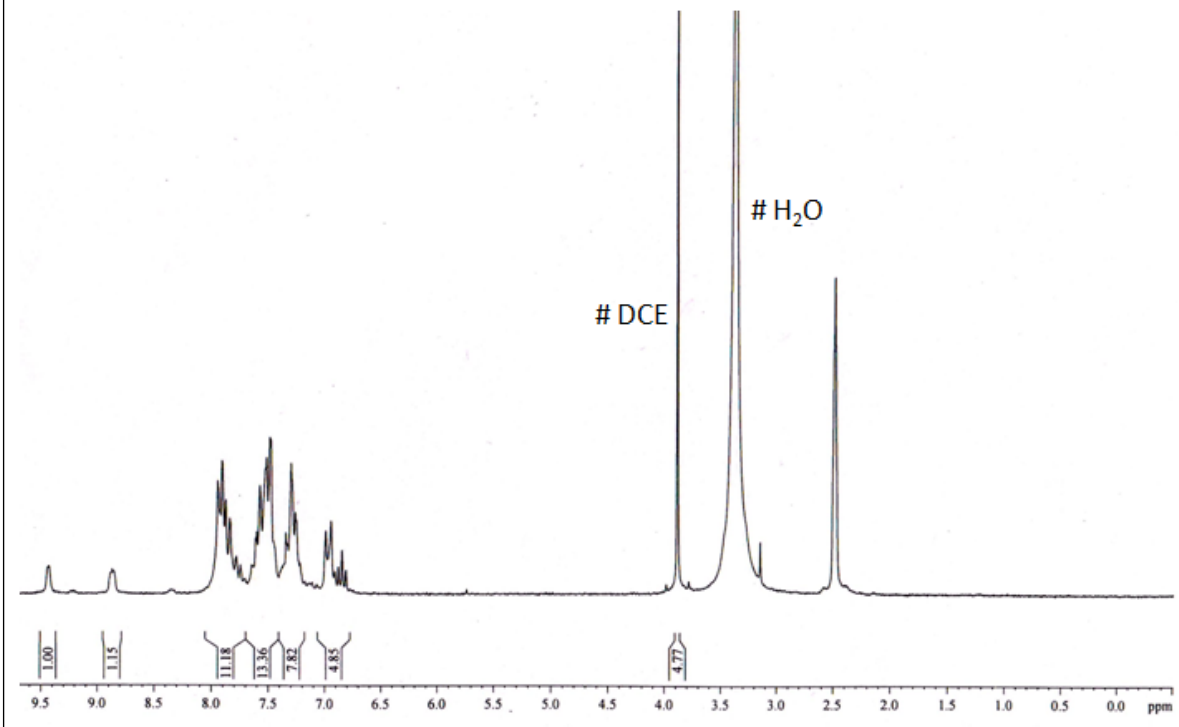


Fig. S11 ^{1}H and ^{31}P NMR of **C6** in DMSO-d_6 at 298K



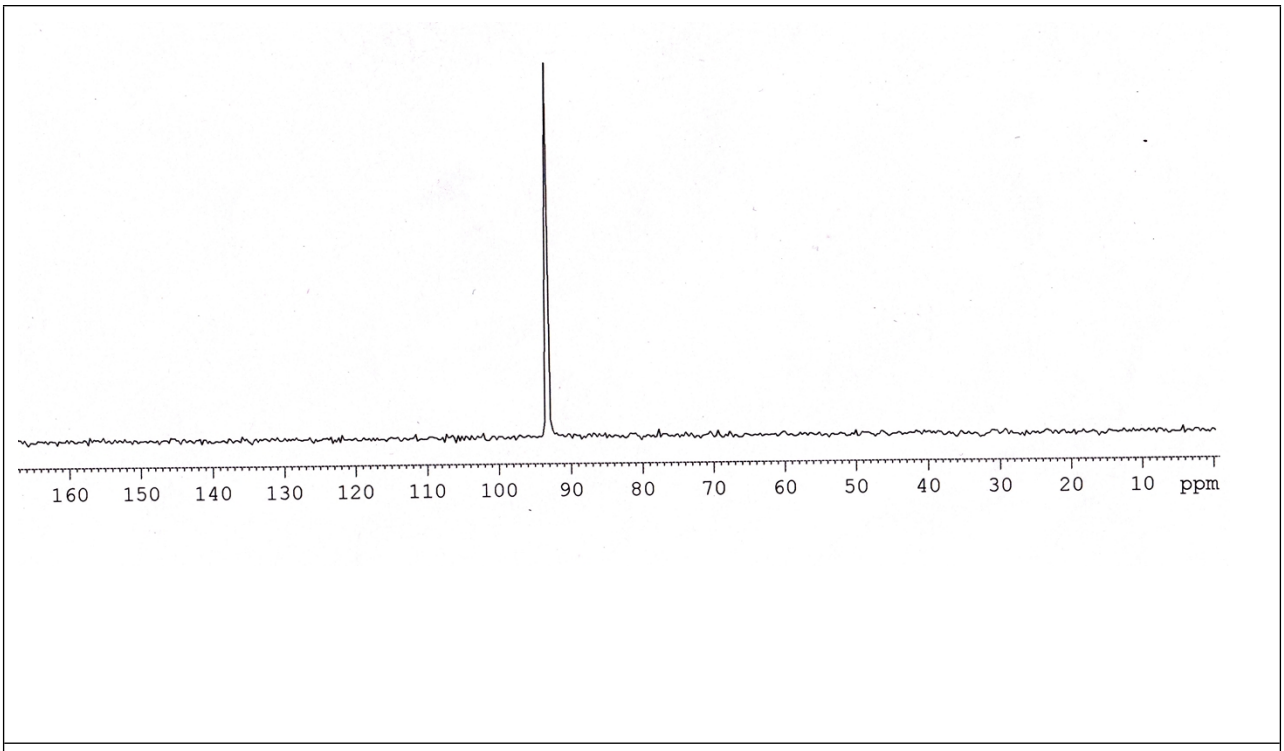
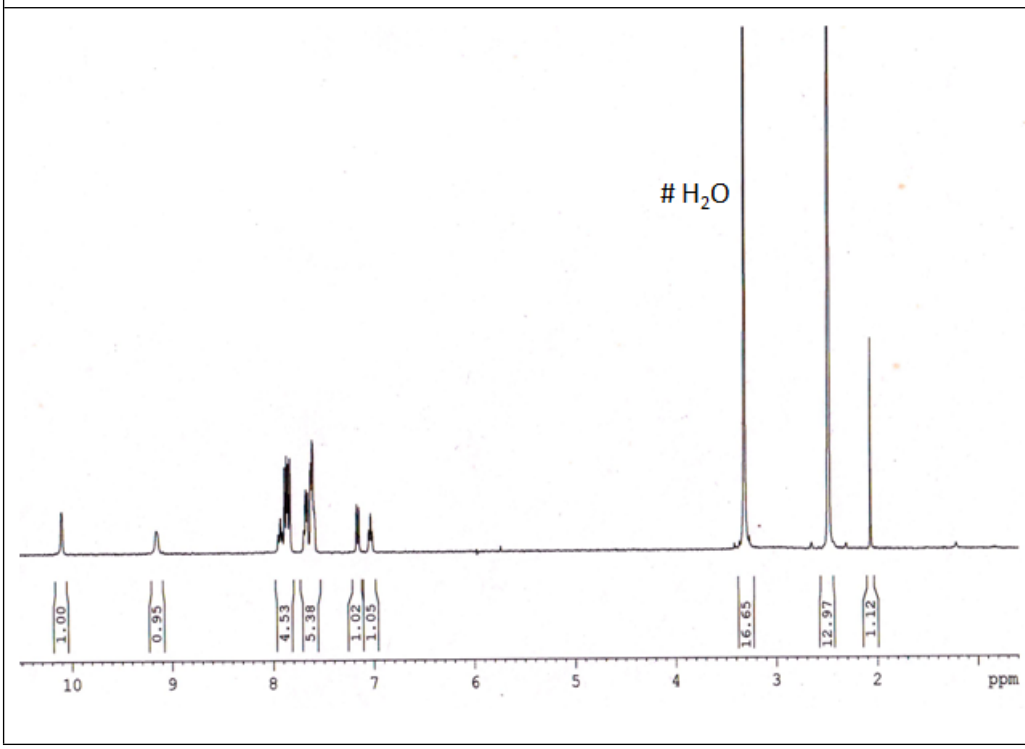
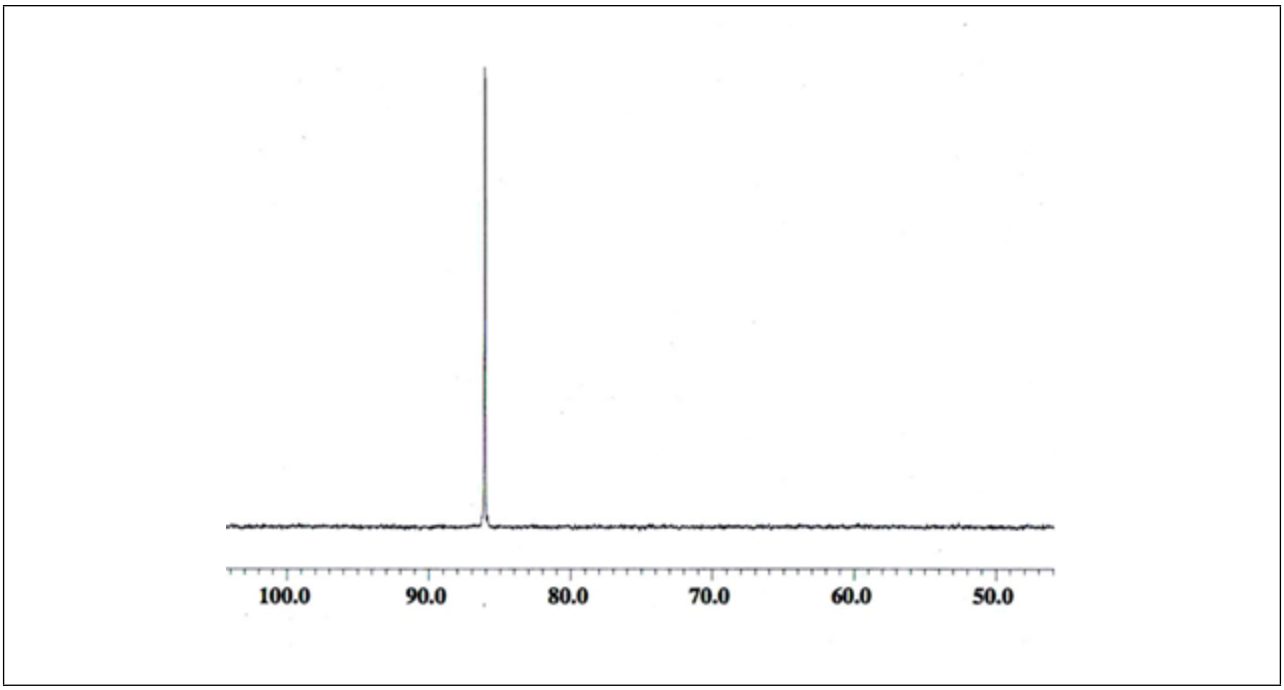


Fig. S12 ^{1}H and ^{31}P NMR of **C7** in DMSO-d_6 at 298K





^{1}H and ^{13}C NMR spectra of all the coupling products: all the spectra were recorded in $CDCl_3$ at 298 K. solvent residual signals were highlighted in the spectra.

Fig. S13. ^{1}H and ^{13}C NMR of **1a** in $CDCl_3$ at 298K

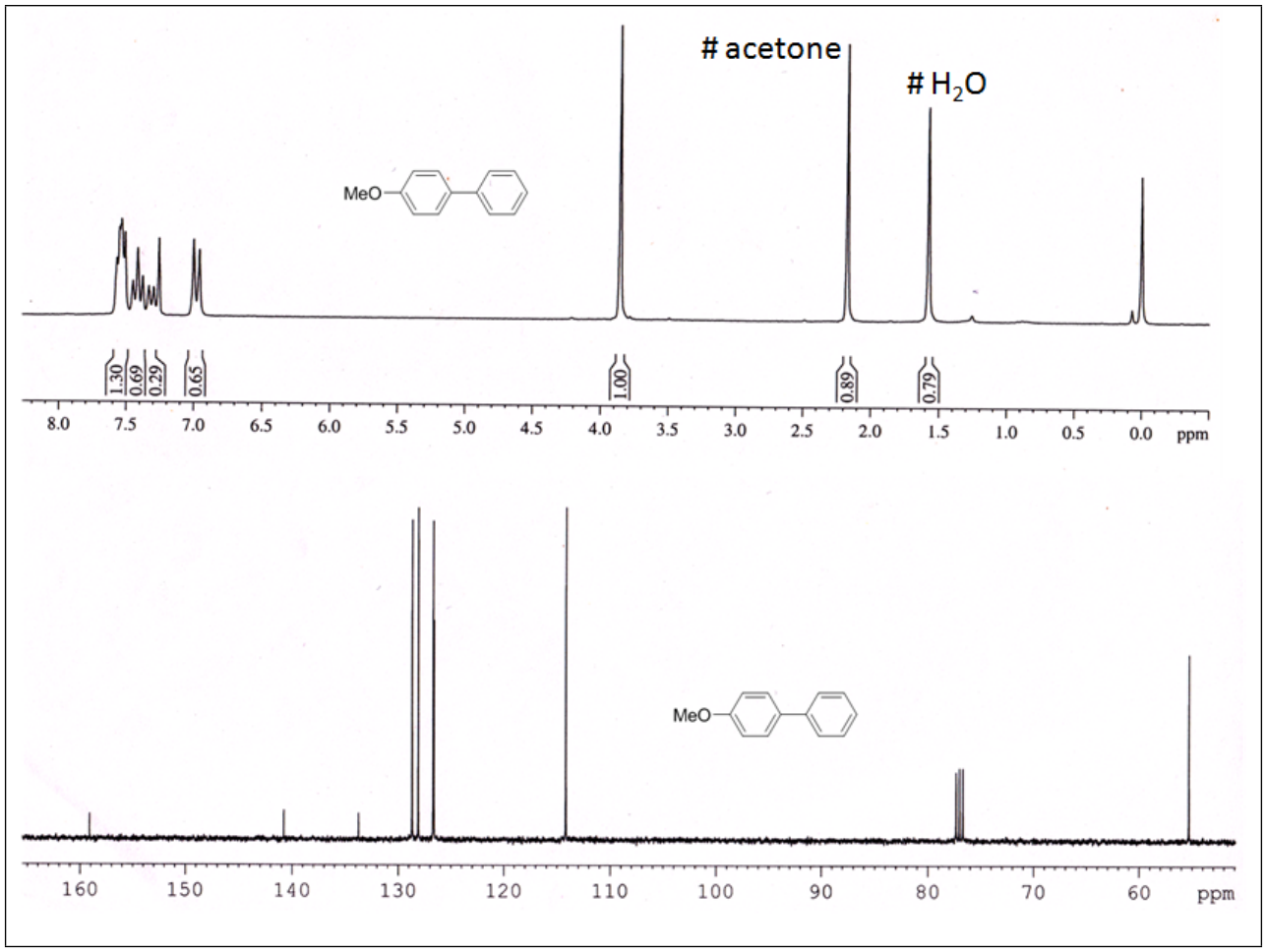


Fig. S14. ^{1}H and ^{13}C NMR of **1b** in $CDCl_3$ at 298K

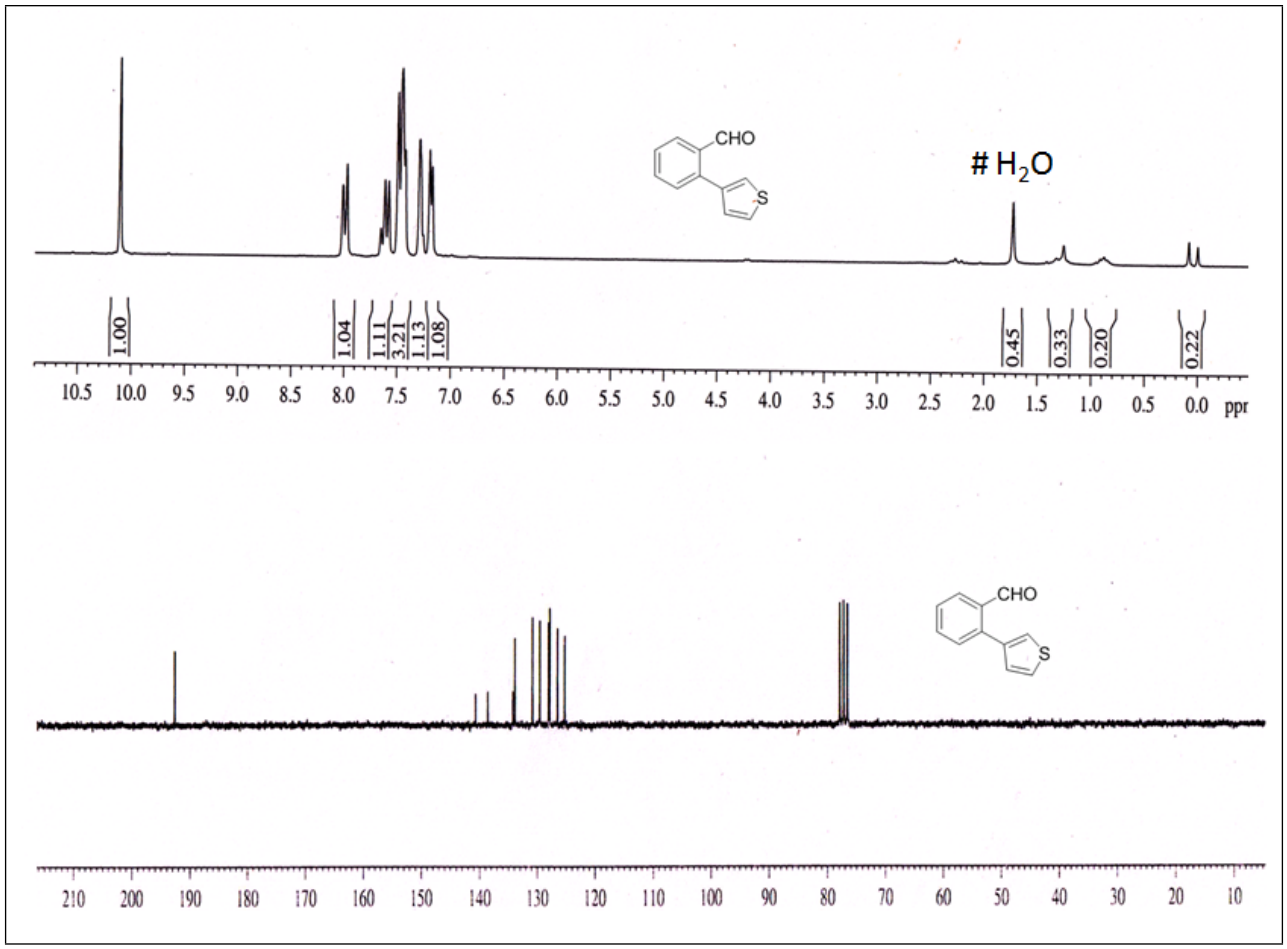

CHO
S
H_2O
1.00
1.04
1.11
3.21
1.13
1.08
0.45
0.33
0.20
0.22
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
CHO
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

Fig. S15. ^{1}H and ^{13}C NMR of **1c** in $CDCl_3$ at 298K

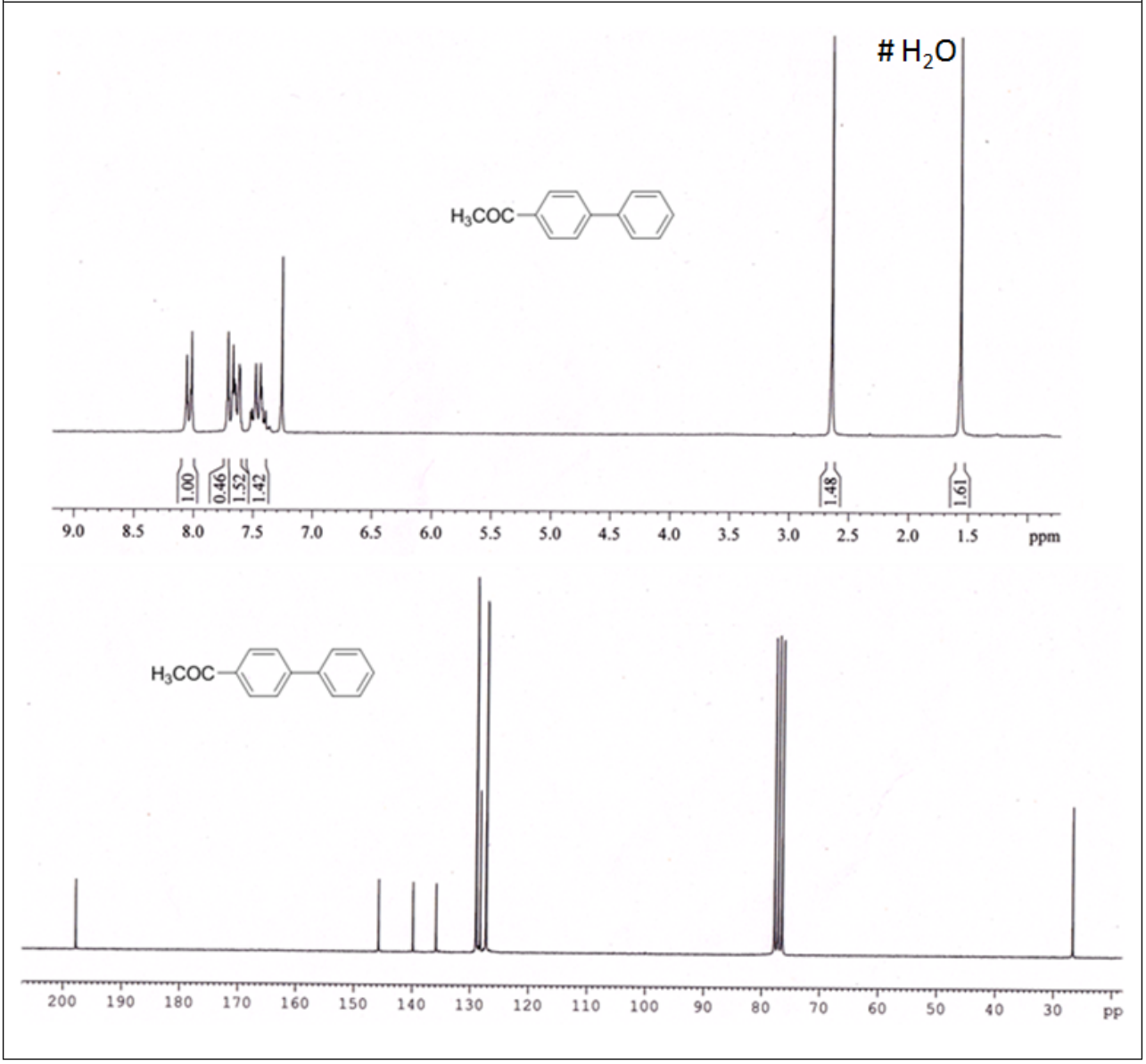


Fig. S16. ^{1}H and ^{13}C NMR of **1d** in $CDCl_3$ at 298K

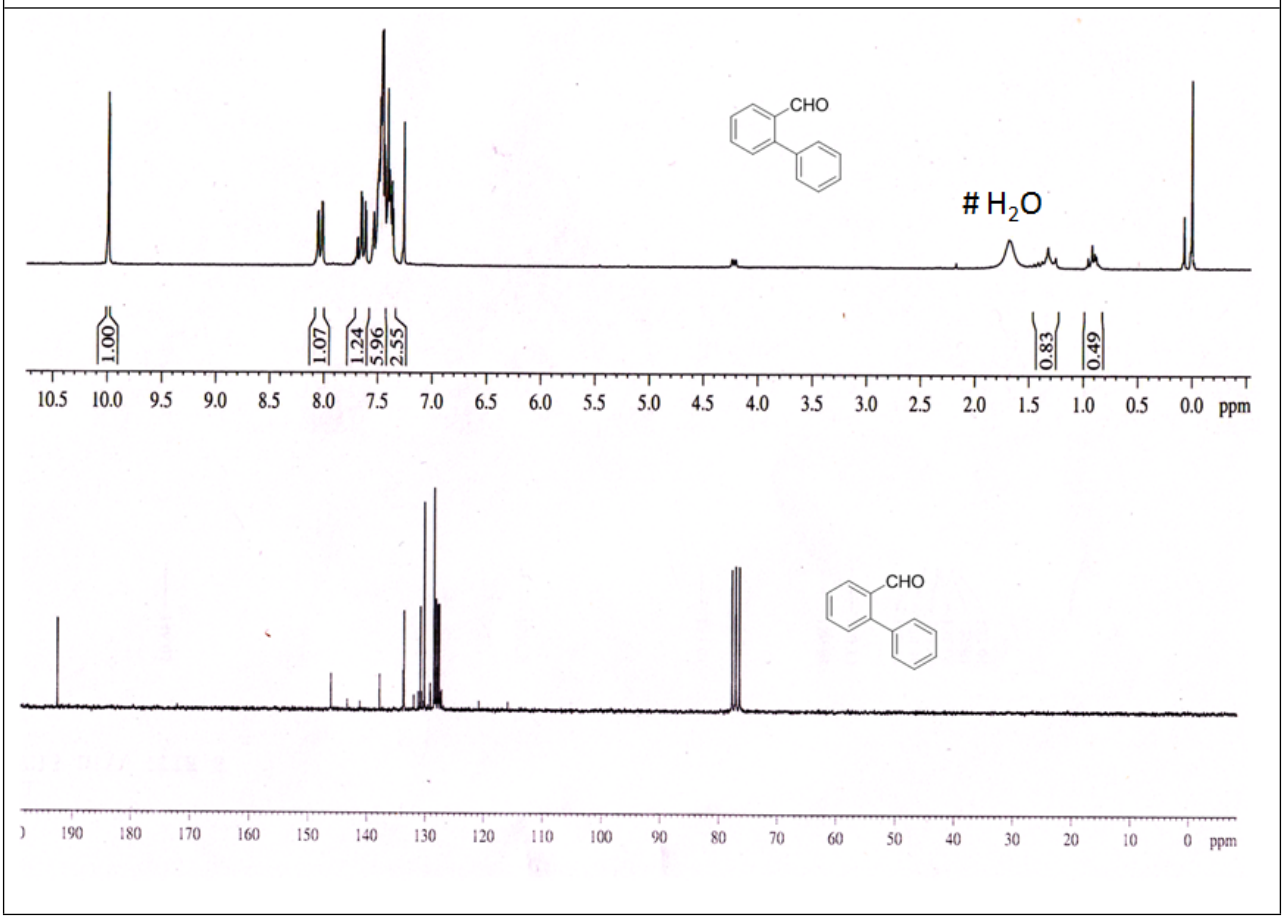


Fig. S17. ^{1}H and ^{13}C NMR of **1e** in $CDCl_3$ at 298K

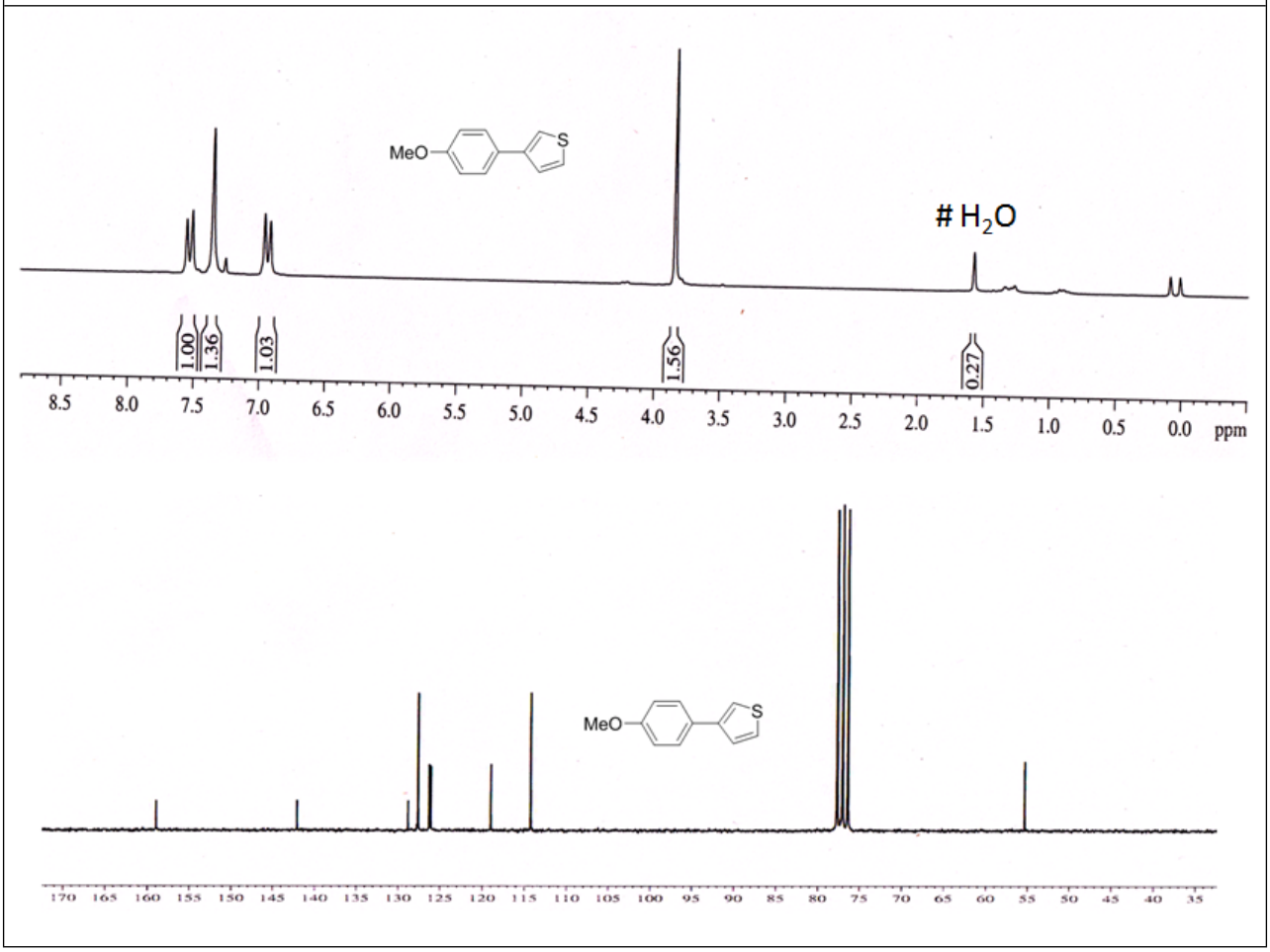
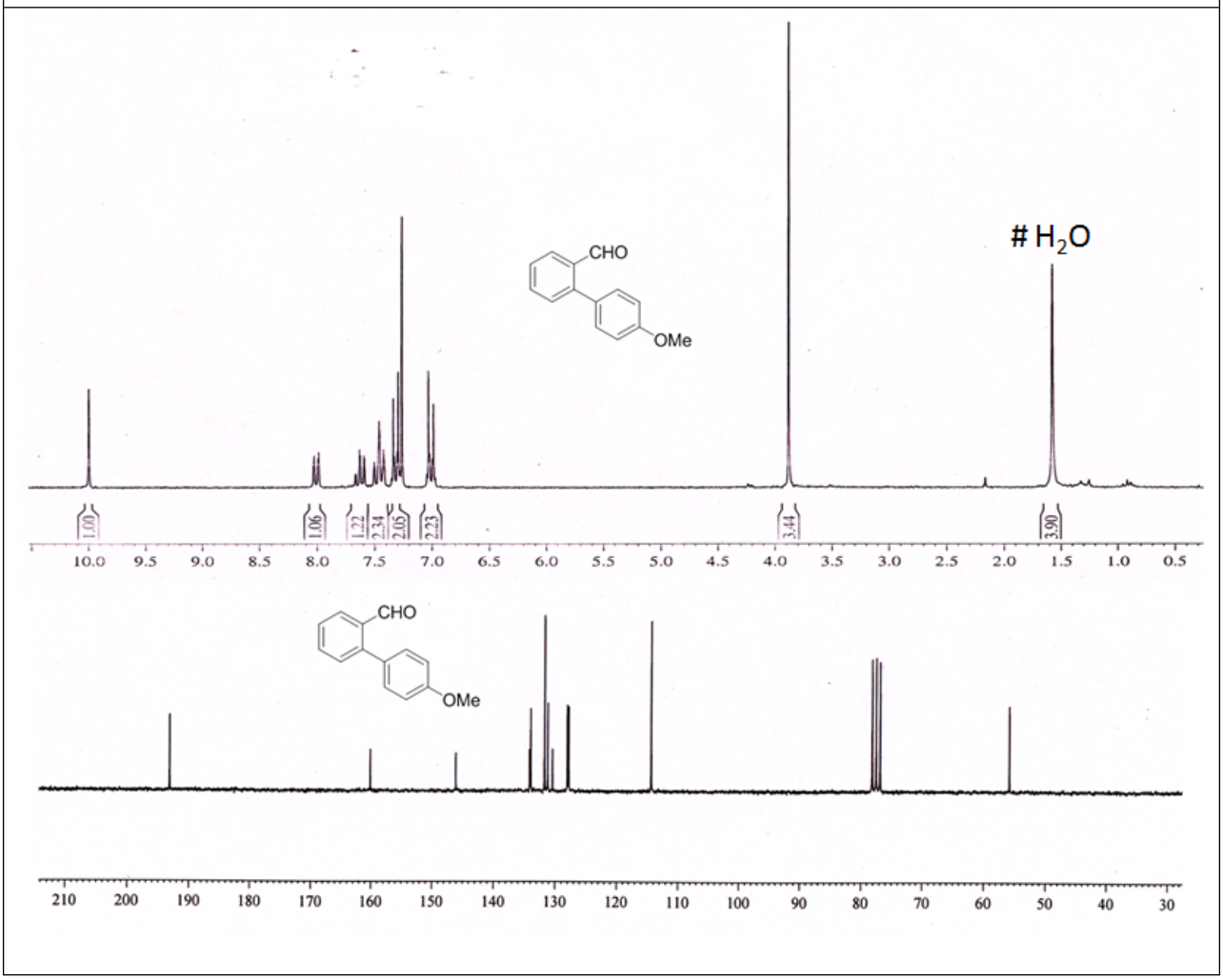


Fig. S18. ^{1}H and ^{13}C NMR of **1f** in $CDCl_3$ at 298K



Optimized Geometry:

C-1

Cartesian Coordinates (Angstroms):

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3	7	0	2.524374	1.546198	0.473435
4	6	0	-1.567509	1.159438	1.881669
5	6	0	-0.772961	2.382358	-1.851051
6	1	0	-0.285942	1.630519	-2.100731
7	6	0	-0.997761	2.650551	-0.508258
8	6	0	-1.294496	0.935536	3.209145
9	1	0	-0.443099	1.113793	3.538194
10	6	0	2.039851	2.542102	1.275907
11	6	0	4.221422	3.605437	1.157649
12	1	0	4.823506	4.258787	1.432702
13	6	0	3.752968	1.663877	-0.075944
14	1	0	4.028682	1.022473	-0.690246
15	6	0	2.949226	3.576206	1.686516
16	1	0	2.681912	4.219343	2.302846
17	7	0	0.773052	2.570881	1.676275
18	6	0	-2.264779	0.450041	4.061951
19	1	0	-2.059870	0.288983	4.954632
20	6	0	-2.858505	0.911652	1.408010
21	1	0	-3.058113	1.044452	0.509472
22	6	0	-1.727589	3.770175	-0.156116
23	1	0	-1.885089	3.956366	0.741358
24	6	0	-2.219216	4.605436	-1.120541
25	1	0	-2.720735	5.350384	-0.878697
26	6	0	-3.845188	0.465617	2.282301
27	1	0	-4.715887	0.344166	1.978865
28	6	0	-1.268788	3.225557	-2.806368
29	1	0	-1.127888	3.039448	-3.706642
30	6	0	-1.973516	4.345340	-2.442166
31	1	0	-2.285335	4.929495	-3.095301
32	6	0	-3.531175	0.204780	3.595136
33	1	0	-4.178462	-0.138558	4.167734
34	6	0	4.600642	2.675556	0.229128
35	1	0	5.429838	2.736981	-0.187583
36	15	0	-0.207248	-1.613817	-0.770858
37	7	0	2.524451	-1.546057	-0.473484
38	6	0	-1.567466	-1.159516	-1.881676
39	6	0	-0.772814	-2.382452	1.851116
40	1	0	-0.285833	-1.630587	2.100791
41	6	0	-0.997614	-2.650598	0.508245
42	6	0	-1.294479	-0.935598	-3.209155
43	1	0	-0.443076	-1.113810	-3.538212
44	6	0	2.039974	-2.541987	-1.275950
45	6	0	4.221603	-3.605205	-1.157715
46	1	0	4.823719	-4.258443	-1.432714
47	6	0	3.753057	-1.663670	0.075883
48	1	0	4.028743	-1.022172	0.690241

49	6	0	2.949399	-3.576102	-1.686488
50	1	0	2.682113	-4.219193	-2.302896
51	7	0	0.773173	-2.570833	-1.676306
52	6	0	-2.264796	-0.450156	-4.061951
53	1	0	-2.059905	-0.289086	-4.954633
54	6	0	-2.858470	-0.911718	-1.407944
55	1	0	-3.058062	-1.044609	-0.509464
56	6	0	-1.727386	-3.770261	0.156111
57	1	0	-1.884886	-3.956519	-0.741281
58	6	0	-2.218959	-4.605548	1.120541
59	1	0	-2.720440	-5.350523	0.878702
60	6	0	-3.845187	-0.465816	-2.282284
61	1	0	-4.715888	-0.344412	-1.978840
62	6	0	-1.268587	-3.225619	2.806358
63	1	0	-1.127687	-3.039502	3.706631
64	6	0	-1.973259	-4.345439	2.442164
65	1	0	-2.285040	-4.929611	3.095301
66	6	0	-3.531200	-0.204962	-3.595122
67	1	0	-4.178513	0.138341	-4.167714
68	6	0	4.600783	-2.675223	-0.229138
69	1	0	5.429987	-2.736685	0.187504

C-2

Cartesian Coordinates (Angstroms):

1	7	0	0.548081	-2.737707	1.331459
2	1	0	0.210789	-3.287791	1.899948
3	6	0	-0.624739	2.410273	1.806518
4	1	0	-0.040248	1.731099	2.055458
5	7	0	1.030032	2.429191	-1.573669
6	1	0	0.800902	2.919031	-2.242339
7	6	0	-2.667445	-2.912260	-0.068941
8	1	0	-2.910301	-2.918599	0.828754
9	6	0	4.405790	-3.127499	0.105820
10	1	0	5.294929	-3.172288	-0.163170
11	6	0	-0.824898	-0.880957	3.352151
12	1	0	0.045561	-1.194442	3.447195
13	6	0	-1.530781	-2.249836	-0.466025
14	6	0	-3.479842	-3.593525	-1.033516
15	1	0	-4.225589	-4.075791	-0.757416
16	6	0	-2.035197	-2.869353	-2.766610
17	1	0	-1.829793	-2.817478	-3.672112
18	6	0	-1.206123	-2.274260	-1.817079
19	1	0	-0.410874	-1.881214	-2.096545
20	6	0	-0.907868	2.625718	0.479906
21	6	0	1.853932	-2.877368	0.947837
22	6	0	-2.713922	0.134538	4.275980
23	1	0	-3.144031	0.549742	4.988413
24	6	0	-2.234835	4.477607	1.019353

25	1	0	-2.767934	5.190292	0.749710
26	6	0	-3.160073	-3.533476	-2.343638
27	1	0	-3.709608	-3.948017	-2.968851
28	6	0	-1.227191	3.227212	2.792229
29	1	0	-1.068661	3.079558	3.696679
30	6	0	3.810743	-4.183896	0.695658
31	1	0	4.283785	-4.979218	0.789172
32	6	0	-2.054904	4.247425	2.376818
33	1	0	-2.490926	4.779394	3.002662
34	6	0	-1.472927	-0.397942	4.486508
35	1	0	-1.086555	-0.435295	5.331735
36	6	0	-1.641949	3.674412	0.050260
37	1	0	-1.747027	3.852583	-0.856433
38	6	0	-0.980715	0.842535	-3.294671
39	1	0	-0.090371	0.921893	-3.551143
40	6	0	-2.718882	1.001690	-1.627921
41	1	0	-3.023697	1.171459	-0.765858
42	6	0	-1.944002	0.427161	-4.209562
43	1	0	-1.688791	0.241928	-5.084408
44	6	0	-3.560573	0.605427	-2.612763
45	1	0	-4.458280	0.558899	-2.374296
46	6	0	-3.294232	0.280951	-3.843051
47	1	0	-3.944652	-0.023703	-4.433971
48	6	0	-1.375340	1.142767	-1.967363
49	46	0	1.199309	-0.118078	-0.005827
50	15	0	-0.404182	-1.502881	0.704434
51	15	0	-0.123002	1.528786	-0.748839
52	7	0	2.680235	1.350299	-0.383234
53	7	0	2.423840	-1.819111	0.355471
54	6	0	3.923980	1.357721	0.072858
55	1	0	4.167575	0.686977	0.669111
56	6	0	-2.622520	-0.385470	1.969948
57	1	0	-3.006809	-0.326290	1.125158
58	6	0	2.504277	-4.109581	1.167236
59	1	0	2.088917	-4.822062	1.596873
60	6	0	4.876520	2.278236	-0.267931
61	1	0	5.735843	2.231813	0.084734
62	6	0	3.653668	-1.957731	-0.093589
63	1	0	4.039998	-1.252978	-0.561526
64	6	0	-1.386073	-0.922727	2.114204
65	6	0	-3.333310	0.087909	3.106837
66	1	0	-4.219233	0.360359	3.030338
67	6	0	2.337368	2.376379	-1.172381
68	6	0	3.278585	3.352824	-1.619156
69	1	0	3.024664	4.017308	-2.218180
70	6	0	4.517964	3.292895	-1.164023
71	1	0	5.147737	3.920310	-1.437181

C-6

Cartesian Coordinates (Angstroms):

1	46	0	1.048153	-0.473358	-0.088404
2	15	0	-0.947634	0.546859	0.065242
3	35	0	3.239011	-1.487798	-0.254087
4	7	0	-0.420448	2.185887	0.247597
5	7	0	1.812043	1.491240	0.123934
6	6	0	0.925969	2.504325	0.286902
7	6	0	-2.010040	0.219483	1.512207
8	6	0	-2.069601	0.585794	-1.372347
9	6	0	3.134566	1.768029	0.133351
10	1	0	3.774783	0.902760	-0.004174
11	6	0	1.355796	3.828173	0.478051
12	1	0	0.623124	4.618357	0.608939
13	6	0	-2.888146	-0.529469	-1.620774
14	1	0	-2.866432	-1.380578	-0.947686
15	6	0	-3.305519	0.755985	1.601039
16	1	0	-3.724827	1.317189	0.770182
17	6	0	-3.708739	-0.551403	-2.747155
18	1	0	-4.335255	-1.418195	-2.936618
19	6	0	-2.072004	1.662547	-2.270914
20	1	0	-1.425209	2.517279	-2.097638
21	6	0	3.626392	3.051260	0.312165
22	1	0	4.697061	3.220795	0.313658
23	6	0	2.715719	4.097155	0.490689
24	1	0	3.062723	5.116011	0.637186
25	6	0	-1.495003	-0.536789	2.576337
26	1	0	-0.507391	-0.980033	2.492835
27	6	0	-3.719558	0.529944	-3.632118
28	1	0	-4.360002	0.507676	-4.509474
29	6	0	-3.547508	-0.194903	3.811037
30	1	0	-4.146414	-0.358944	4.702717
31	6	0	-4.067654	0.552393	2.750856
32	1	0	-5.069393	0.968116	2.815249
33	6	0	-2.265549	-0.740793	3.721654
34	1	0	-1.866324	-1.335490	4.538115
35	6	0	-2.900269	1.634600	-3.393923
36	1	0	-2.899908	2.473929	-4.083779
37	1	0	-1.070622	2.931184	0.467090
38	35	0	-0.092745	-2.600383	-0.263104

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Cartesian Coordinates (Angstroms):

1	46	0	0.859716	-0.085497	-0.032529
2	15	0	-1.243331	0.701747	0.038592
3	53	0	3.336314	-0.904547	-0.120373

4	7	0	-0.913125	2.399001	0.127405
5	7	0	1.386695	1.963950	0.069074
6	6	0	0.386363	2.874347	0.161496
7	6	0	-2.285551	0.337811	1.491492
8	6	0	-2.337094	0.525009	-1.410350
9	6	0	2.667806	2.393462	0.075591
10	1	0	3.406385	1.602373	-0.002899
11	6	0	0.656299	4.248263	0.277050
12	1	0	-0.165271	4.953717	0.352473
13	6	0	-3.016270	-0.690893	-1.599687
14	1	0	-2.907646	-1.492723	-0.876380
15	6	0	-3.635876	0.723529	1.534347
16	1	0	-4.102970	1.182237	0.666878
17	6	0	-3.809085	-0.874526	-2.731196
18	1	0	-4.327411	-1.818195	-2.874640
19	6	0	-2.448804	1.539592	-2.372101
20	1	0	-1.908658	2.472725	-2.243876
21	6	0	3.004238	3.733631	0.181926
22	1	0	4.047817	4.026914	0.184368
23	6	0	1.975400	4.674593	0.287643
24	1	0	2.199249	5.733840	0.376131
25	6	0	-1.704807	-0.289437	2.604542
26	1	0	-0.671137	-0.618361	2.558182
27	6	0	-3.929922	0.144426	-3.679733
28	1	0	-4.548118	-0.003897	-4.560784
29	6	0	-3.804255	-0.117991	3.794952
30	1	0	-4.395480	-0.298366	4.688601
31	6	0	-4.389098	0.499992	2.686331
32	1	0	-5.433274	0.798861	2.715128
33	6	0	-2.466257	-0.514628	3.751971
34	1	0	-2.014972	-1.009731	4.606878
35	6	0	-3.248599	1.349298	-3.499962
36	1	0	-3.333643	2.141048	-4.239066
37	1	0	-1.649098	3.074785	0.294831
38	53	0	-0.092816	-2.514662	-0.095280

$SnCl_4$

Cartesian Coordinates (Angstroms):

1	50	0	0.000036	0.000015	0.000000
2	17	0	1.878696	1.328852	0.000000
3	17	0	0.000036	-1.328664	1.878577
4	17	0	0.000036	-1.328664	-1.878577
5	17	0	-1.878873	1.328432	0.000000

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.004720 (Hartree/Particle)

Thermal correction to Energy= 0.012428

Thermal correction to Enthalpy= 0.013372
Thermal correction to Gibbs Free Energy= -0.030752
Sum of electronic and zero-point Energies= -1843.648219
Sum of electronic and thermal Energies= -1843.640511
Sum of electronic and thermal Enthalpies= -1843.639567
Sum of electronic and thermal Free Energies= -1843.683691

$PhSnCl_3$

Cartesian Coordinates (Angstroms):

1	50	0	-0.714801	0.000029	-0.006692
2	17	0	-1.696303	-0.011224	2.132505
3	17	0	-1.554789	-1.908573	-1.096856
4	17	0	-1.551700	1.921444	-1.076570
5	6	0	1.411744	-0.000538	-0.002728
6	6	0	2.104946	-1.214361	0.012406
7	6	0	2.105243	1.213107	0.011737
8	6	0	3.498759	-1.209183	0.037492
9	1	0	1.573752	-2.163196	-0.008531
10	6	0	3.499073	1.207592	0.036826
11	1	0	1.574191	2.162011	-0.009726
12	6	0	4.193386	-0.000872	0.052294
13	1	0	4.040031	-2.151556	0.044811
14	1	0	4.040572	2.149838	0.043620
15	1	0	5.280068	-0.001013	0.071907

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.094542 (Hartree/Particle)
Thermal correction to Energy= 0.106151
Thermal correction to Enthalpy= 0.107095
Thermal correction to Gibbs Free Energy= 0.052289
Sum of electronic and zero-point Energies= -1614.870275
Sum of electronic and thermal Energies= -1614.858666
Sum of electronic and thermal Enthalpies= -1614.857722
Sum of electronic and thermal Free Energies= -1614.912528

Me_2SnCl_2

Cartesian Coordinates (Angstroms):

1	50	0	0.000000	0.274904	0.000000
2	17	0	1.883342	-1.132193	0.000000
3	17	0	-1.883344	-1.132191	0.000000
4	6	0	0.000001	1.316077	-1.846997
5	1	0	0.000000	0.591654	-2.665959
6	1	0	-0.892787	1.943277	-1.926238
7	1	0	0.892792	1.943274	-1.926238
8	6	0	0.000001	1.316077	1.846997
9	1	0	0.892792	1.943275	1.926238
10	1	0	-0.892788	1.943276	1.926239
11	1	0	0.000001	0.591654	2.665959

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.075575 (Hartree/Particle)
Thermal correction to Energy= 0.084881
Thermal correction to Enthalpy= 0.085825
Thermal correction to Gibbs Free Energy= 0.039083
Sum of electronic and zero-point Energies= -1003.179926
Sum of electronic and thermal Energies= -1003.170619
Sum of electronic and thermal Enthalpies= -1003.169675
Sum of electronic and thermal Free Energies= -1003.216417

References:

[1] G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics* 2010, **29**, 2176