Electronic Supporting Information
For

Shape dependent catalytic activity of nanoflowers and nanospheres of Pd_4S generated via one pot synthesis and grafted on graphene oxide for Suzuki coupling

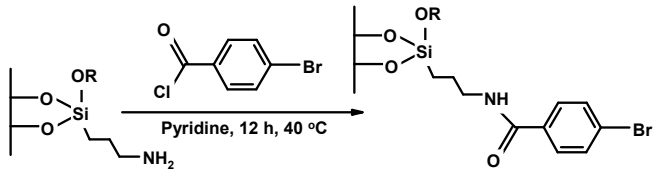
Ved Vati Singh, Umesh Kumar, Sandeep Nath Tripathi, and Ajai Kumar Singh*

Department of Chemistry, Indian Institute of Technology Delhi, New Delhi-110016, India

Email: aksingh@chemistry.iitd.ac.in

S1 Three-phase Test

For immobilization of 4-bromobenzoic acid on silica gel following standard procedure[1-3] was used (Scheme S1).



Scheme S1. Immobilization of 4-bromobenzoic acid on silica

4-Bromobenzoic acid (1.99 g, 10 mmol) was mixed with dry $SOCl_2$ (20 mL) and the mixture refluxed for 3 h. It was cooled and thionyl chloride distilled off to give 4-bromobenzoyl chloride as a white solid. 3-Aminopropyl trimethoxysilane-modified silica (1 g), pyridine (0.4 mL), dry THF (10 mL) and 4-bromobenzoyl chloride (1.150 g, 5.25 mmol) were stirred at 40 °C for 12 h in a round bottom flask under N_2 atmosphere. The suspension was filtered through G-4 crucible and washed with 5% HCl (v/v) (3 × 20 mL) followed by 0.02 M solution of K_2CO_3 in water (2 × 20 mL) and rinsed with distilled water (40 mL) and ethanol (40 mL). The resulting solid was washed with dichloromethane and dried at room temperature in air, resulting in white powder.

Table S1. Selected bond lengths [Å] and bond angles [°]

Compounds	Bond length [Å]		Bond angle [°]	
1	Pd1—S1	2.270(7)	N1—Pd1—S1	97.4(6)
	Pd1—N1	2.047(2)	S1—Pd1—Cl2	83.7(3)
	Pd1—Cl1	2.337(7)	Cl2—Pd1—Cl1	92.7(3)
	Pd1—Cl2	2.304(7)	Cl1—Pd1—N1	86.4(1)
			N1— Pd1— Cl2	176.91(6)
			N1— Pd1— Cl1	86.36(6)
			S1— Pd1— Cl1	175.58(2)
			C6— S1— C7	103.13(13)
			C6— S1— Pd1	105.67(8)
			C6— S1— C7	103.13(13)
			C7— S1— Pd1	111.59(10)

Table S2. Crystallographic data and structure refinement summary for **1**.

	1
Formula	$C_9H_{13}\ Cl_2NPdS$
Formula weight	344.57
T/K	298(2)
λ/Å	0.71073
Cryst system	monoclinic
Space group	*P21/c*
a/Å	10.6716(18)
b/Å	13.846(2)
c/Å	8.2794(14)
α/deg	90.00
β/deg	108.956(3)
γ/deg	90.00
Vol/Å^3	1157.0(3)
Z	4
D_{calcd}/ g.cm^{-3}	1.978
*F(*000)	680
θ range/deg	2.02−25.00
Reflections measured	2040
Reflections used	1958
parameters	127
μ(Mo Kα) (cm^{-1})	2.205
R_1, $wR_2[I > 2\sigma(I)]^a$	0.0198, 0.0207
R_1, wR_2 (all data)^b	0.0486, 0.0490
GOF^c	1.060

$^aR_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $^bwR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $^cS = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)^2]\}^{1/2}$

Table S3. Selected hydrogen bond parameters of **1** (Inter atomic distances in Å and bond angles in deg).

D–H····A	D–H	H····A	D····A	D–H····A
N1–H1A····Cl2	0.90	2.70	3.14	136
C8–H8B····Cl2	0.97	2.95	3.69	134.
N1–H1A····Cl2	0.90	2.56	3.34	146

S2. Powder XRD of Pd_4S, GO and GO-Pd_4S nanocomposites (nanoflowers and nanospheres)

The powder X-ray diffraction pattern of Pd_4S nanoparticles (Fig. S1) was indexed[4] on the basis of a primitive tetragonal unit cell (JCPDS #73−1387) with the refined lattice parameter = 10.87 Å and d values (*hkl*): 3.77 (101), 3.61 (110), 2.79 (002), 2.55 (200), 2.45 (102), 2.32 (201), 2.28 (210), 2.21 (112), 2.11 (211), 1.88 (202), 1.77 (212), 1.75 (103), 1.63 (301), 1.61 (310), 1.55 (311), 1.51 (222), 1.50 (203), 1.45 (302), 1.44 (213), 1.41 (320), 1.39 (312), 1.37 (321). PXRD pattern of graphene oxide[5] was recorded and shown in Fig S2. The powder X-ray diffraction pattern of GO-Pd_4S nanocomposites are also shown in Fig. S3 and Fig. S4 respectively.

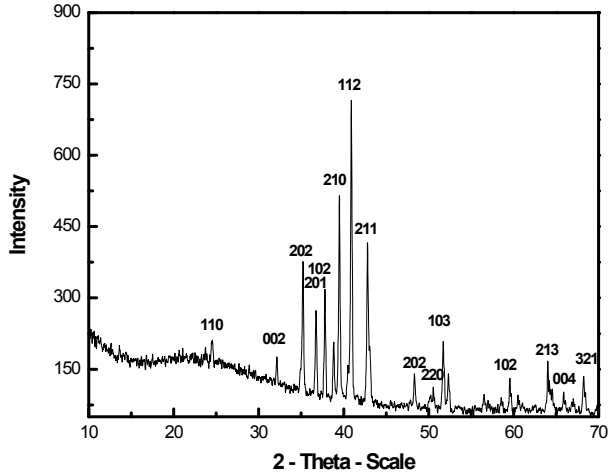


Fig. S1. PXRD pattern of Pd_4S NPs

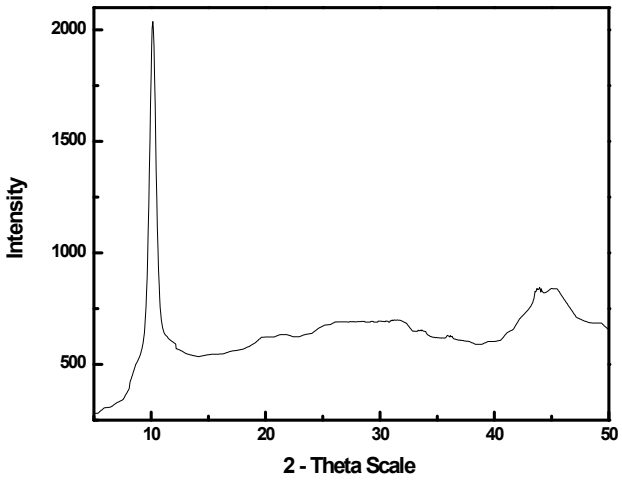


Fig. S2. PXRD pattern of Graphene oxide (GO)

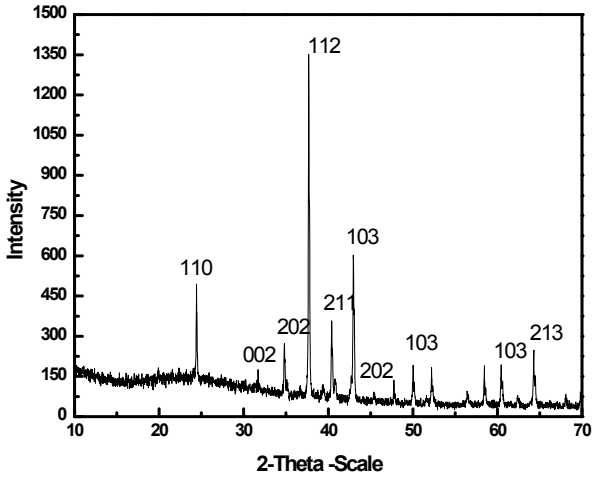


Fig. S3 PXRD pattern of nanoflowers GO-Pd_4S.

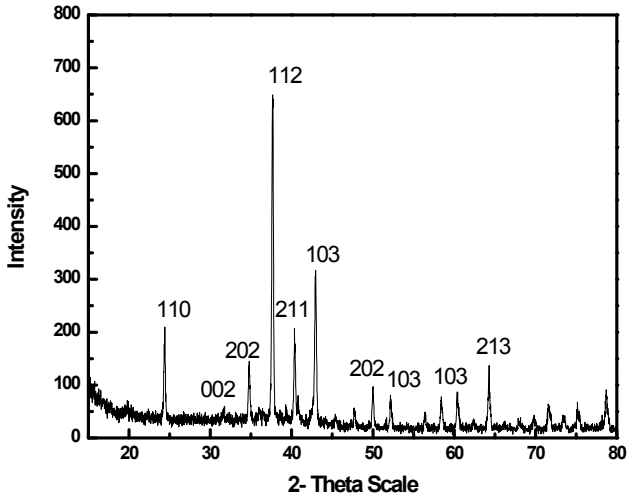


Fig. S4 PXRD pattern of nanospheres GO-Pd_4S.

S3. TEM−EDX of Pd_4S nanocomposites

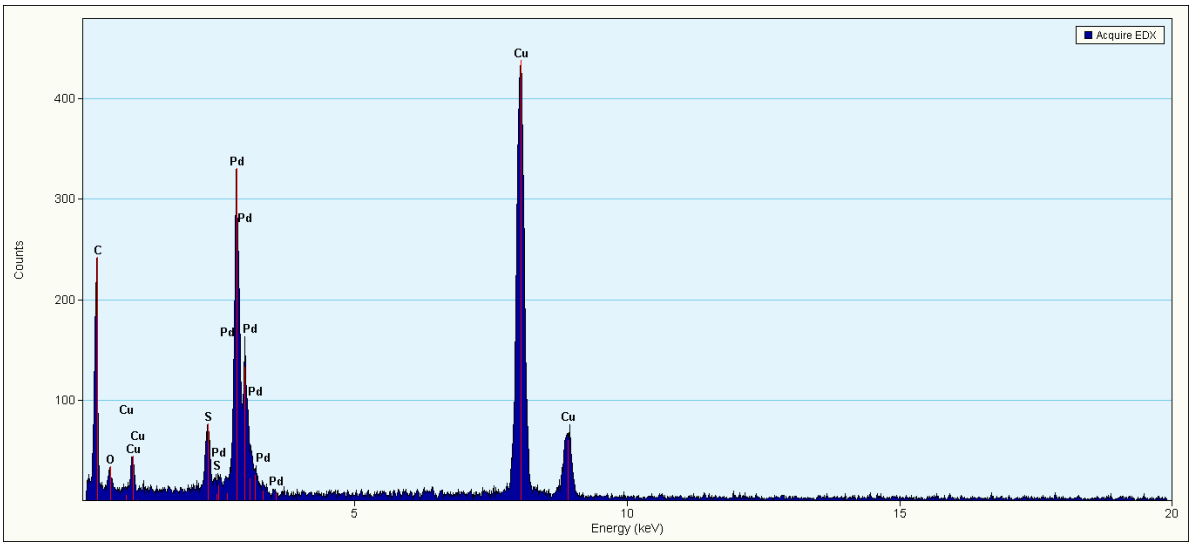


Fig. S5 TEM−EDX of nanoflowers GO-Pd_4S

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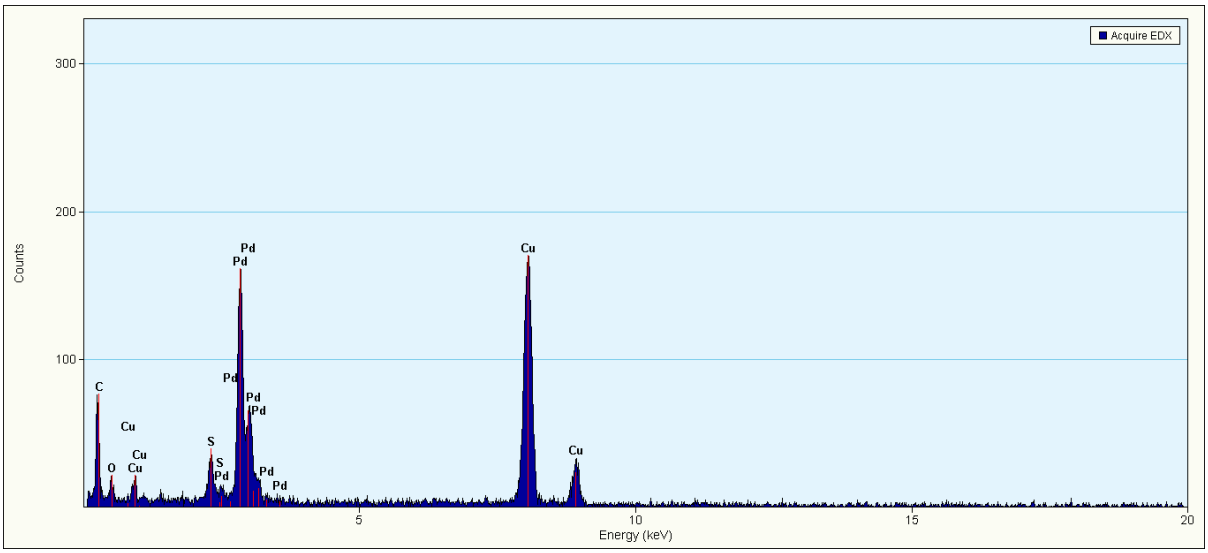


Fig. S6 TEM−EDX of nanospheres GO-Pd_4S

S4. Size distribution of GO-Pd_4S nanocomposites

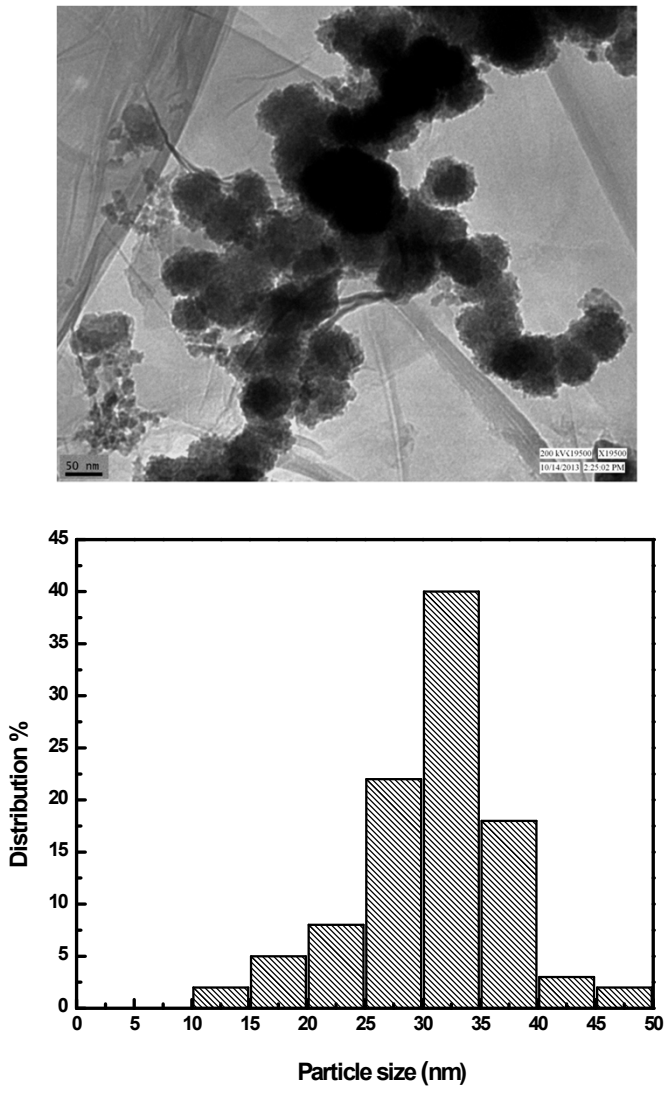


Fig. S7 TEM image and size distribution of GO-Pd_4S nanoflowers.

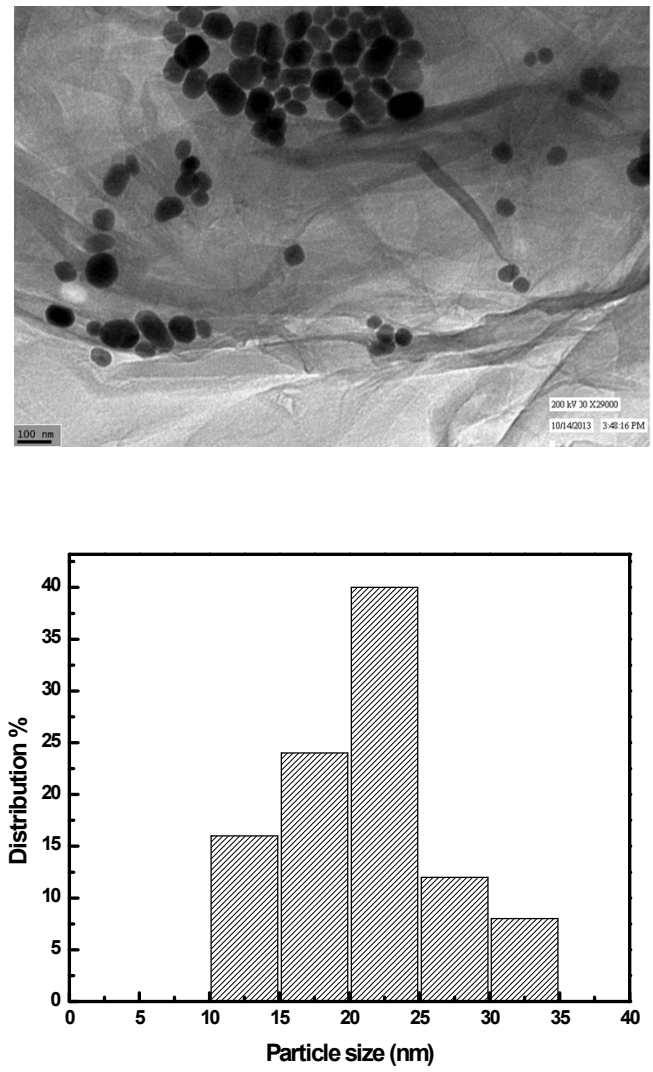
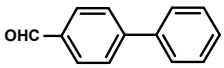


Fig. S8 TEM image and size distribution of nanospheres GO-Pd_4S.

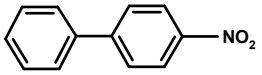
S5. Spectroscopic data of coupled products

4−Phenylbenzaldehyde (light yellow solid)



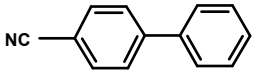
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.537−7.447 (m, 3H), 7.678−7.616 (m, 2H), 7.822 (d, J = 9.0 Hz, 2H), 7.994 (d, J = 5.4 Hz, 2H), 10.081 (s, 1H).

4-Nitrobiphenyl (Pale yellow solid)



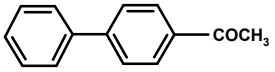
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.462−7.571 (m, 3H), 7.663 (d, J = 8.5 Hz, 2H), 8.050 (d, J = 8.7 Hz, 2H), 8.225 (d, J = 8.7 Hz, 2H).

4-Phenylbenzonitrile (pale yellow solid)



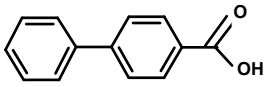
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.367−7.338 (m, 3H, aromatic), 7.492−7.413 (m, 2H, aromatic), 7.563−7.499 (m, 4H, aromatic).

4−Acetylbiphenyl (white solid)



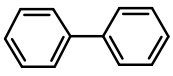
^{1}H NMR (300 MHz, $CDCl_3$): δ 2.595 (s, 3H), 7.554−7.507 (m, 3H), 7.630−7.601 (m, 4H), 7.844 (d, J = 6.6 Hz, 2H).

Biphenyl-4-carboxylic acid (White solid)



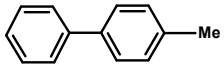
^{1}H NMR (300 MHz, DMSO): δ 7.324−7.423 (m, 3H), 7.769 (d, J = 7.0 Hz, 2H), 7.791 (d, J = 8.3 Hz, 2H), 8.034 (d, J = 8.2 Hz, 2H)

Biphenyl (white solid)



^{1}H NMR (300 MHz, $CDCl_3$): δ 7.526 (t, J = 6.9 Hz, 2H), 7.596 (t, J = 7.2 Hz, 4H), 7.775 (d, J = 7.2 Hz, 4H).

4-Methylbiphenyl (colorless solid)



^{1}H NMR (300 MHz, $CDCl_3$): δ 2.377 (s, 3H), 7.213 (d, J = 8.4 Hz, 2H), 7.284−7.213 (m, 1H), 7.406−7.390 (m, 2H), 7.414 (d, J = 8.7 Hz, 2H), 7.538−7.443 (m, 2H).

S6. References

1. J. Rebek, F. Gavina, *J. Am. Chem. Soc*. 1974, **96**, 7112.
2. J. Rebek, D. Brown, S. Zimmerman, *J. Am. Chem. Soc.* 1975, **97**, 454.
3. I. W. Davies, L. Matty, D.L. Hughes, P.J. Reider, *J. Am. Chem. Soc*., 2001, **123,** 10139.
4. Powder Diffraction Files Nos. 73-1424, JCPDS-ICDD, International Centre for Diffraction Data, Swarthmore, PA, 1990.
5. S. Park, J. An, I. Jung, R.D. Piner, S.J. An, X.Li, A. Velamakanni, R.S. Ruoff, *Nano Lett*, 2009, **9**, 1593.

S 7. NMR Spectra

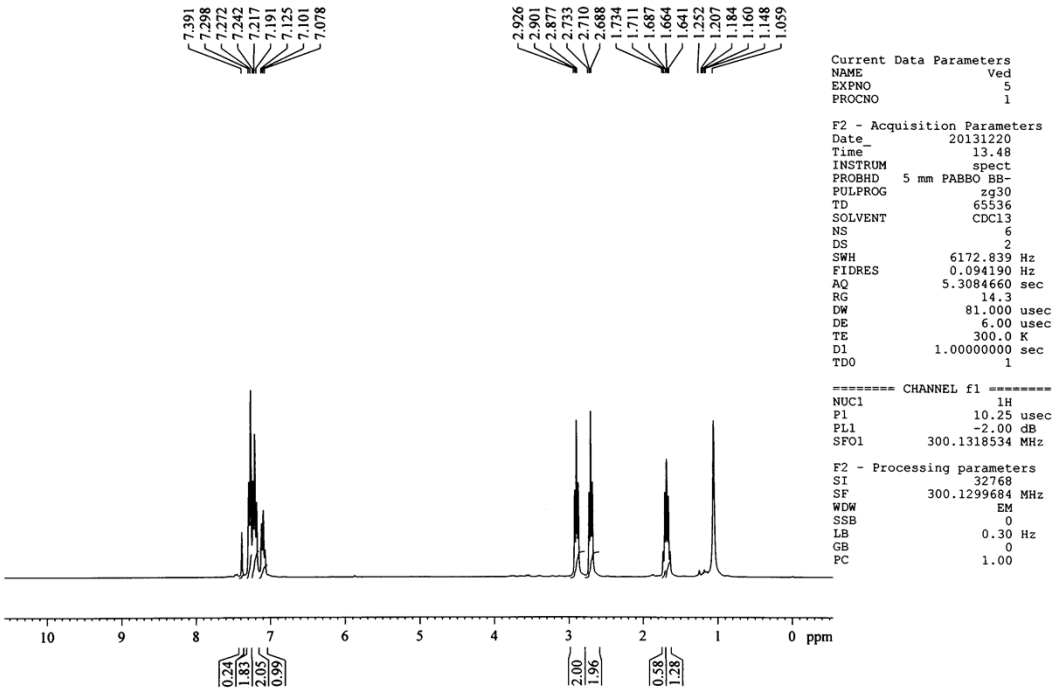


Fig. S9 ^{1}H NMR of Ligand (**L)**

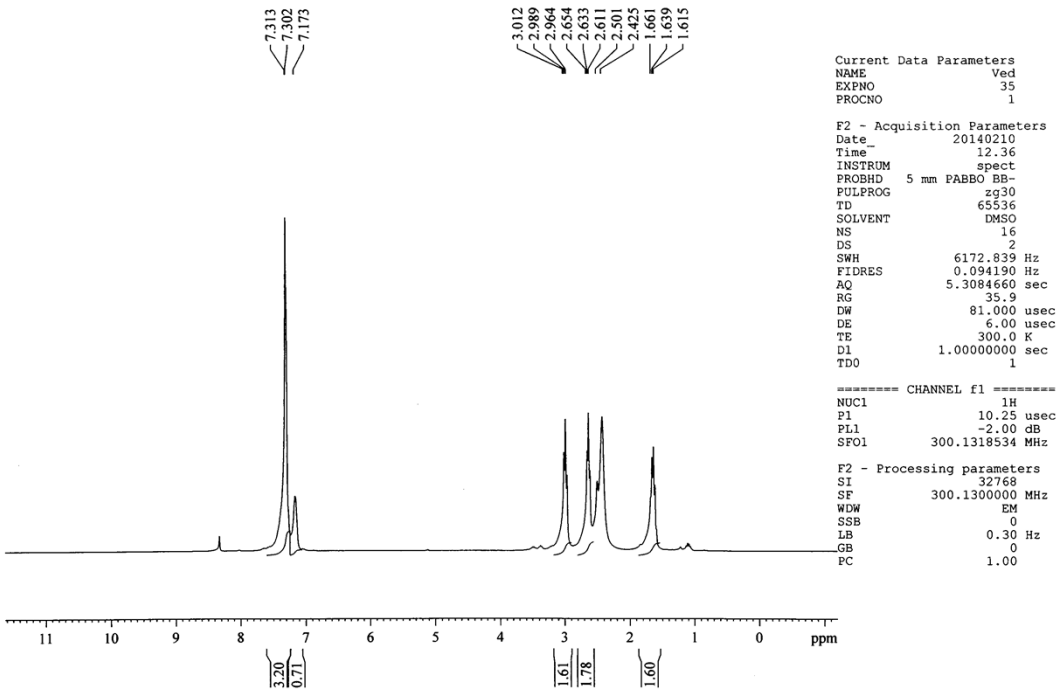


Figure S10 ^{1}H NMR of Complex (**1)**

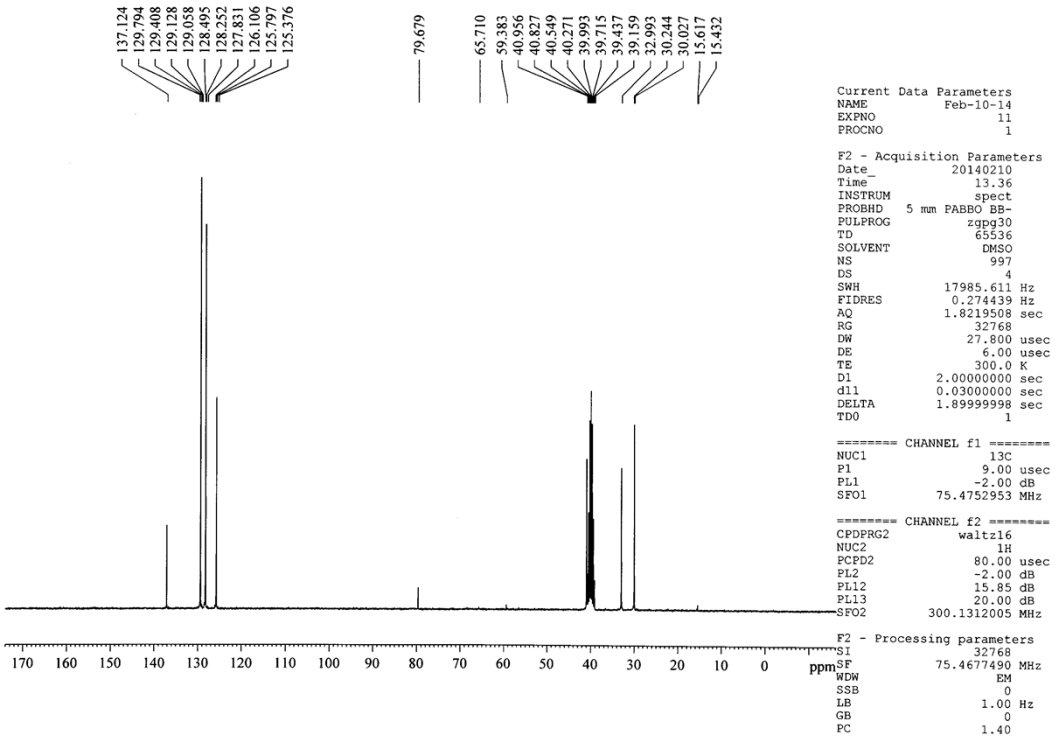


Fig. S11 $^{13}C\{^{1}H\}$ NMR of Complex **1**