ESI for

Palladium(II) -1-phenylthio-2-arylchalcogenoethane complexes: palladium phosphide nano-peanut and ribbon formation controlled by chalcogen and Suzuki coupling activation

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Table S1. Crystal Data and Structure Refinement Parameters for 1 and 3

Compound	1	3
Empirical formula	$C_{14}H_{14}Cl_2PdS_2$	$C_{15}H_{16}Cl_2OPdSTe$
Formula wt.	423.69	549.25
Colour	Red	Orange
Crystal size, mm^3	0.553 × 0.295 × 0.207	0.517 × 0.301 × 0.225
Crystal system	Monoclinic	Orthorhombic
Space group	$C2/c$	$P2_12_12_1$
Unit Cell dimension	$a = 22.333(3)$ Å $b = 10.6408(15)$ Å $c = 25.506(4)$ Å $\alpha = \gamma = 90.00°$ $\beta = 111.481(2)°$	$a = 8.3567(16)$ Å $b = 14.188(3)$ Å $c = 14.676(3)$ Å $\alpha = \beta = \gamma = 90.00°$
Volume [Å^3]	1621.9(15)	1740.0(6)
Z	4	4
ρ, (calc.) Mg/m^3	1.721	2.097
μ, mm^{-1}	1.714	3.122
$F(000)$	840	1048
θ, range (°)	2.80 to 24.99	2.00 to 25.00
Index ranges	$-22 \leq h \leq 22$ $-9 \leq k \leq 9$ $-14 \leq l \leq 14$	$-9 \leq h \leq 9$ $-16 \leq k \leq 16$ $-17 \leq l \leq 17$
Reflections collected	1400	3057
Independent reflections($R_{int.}$)	1307 [$R(int)$ = 0.0309]	2944 [R_{int} = 0.0420]
Completeness to max. θ, %	99.7	99.9
Max. / min. Transmission	0.558 / 0.711	0.215 / 0.081
Data / restraints / parameters	1400 / 0 / 87	3057 / 0 / 192

Goodness–of–fit on F^2	1.264		1.164
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0354$ $wR_2 = 0.0817$		$R_1 = 0.0398,$ $wR_2 = 0.0745$
R indices (all data)	$R_1 = 0.0386$ $wR_2 = 0.0831$		$R_1 = 0.0419,$ $wR_2 = 0.0754$
Largest diff. peak /hole [e.Å^{-3}]	0.146 / −1.334		0.103 / −0.819
CCDC	1014070		1014071

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) of 1

Bond Length (Å)			
Pd(1)—Cl(1)	2.330(13)	Pd(1)—S(1)	2.285(14)
S(1)—C(7)	1.833(5)	C(2)—C(1)	1.400(6)
C(3)—C(2)	1.381(6)	C(4)—C(5)	1.390(7)
C(6)—C(1)	1.389(6)	C(5)—C(6)	1.383(6)
C(6)—S(1)	1.793(4)	C(7)—C(7)	1.521(9)
Bond Angle (°)			
S(1)—Pd(1)—S(1)	89.11(8)	S(1)—Pd(1)—Cl(1)	177.22(4)
S(1)—Pd(1)—Cl(1)	88.52(6)	Cl(1)—Pd(1)—Cl(1)	93.89(7)
C(6)—S(1)—C(7)	99.4(2)	C(7)—S(1)—Pd(1)	101.99(19)
C(6)—S(1)—Pd(1)	109.28(13)	C(7)—C(7)—S(1)	108.0(4)
C(3)—C(4)—C(5)	120.7(4)	C(2)—C(3)—C(4)	119.6(4)
C(6)—C(5)—C(4)	119.3(4)	C(3)—C(2)—C(1)	120.7(4)
C(5)—C(6)—C(1)	121.0(4)	C(5)—C(6)—S(1)	117.8(3)
C(1)—C(6)—S(1)	121.1(3)	C(6)—C(1)—C(2)	118.7(4)

Table S3. Selected Bond Lengths (Å) and Bond Angles (°) of 3

Bond Length (Å)			
Pd(1)—S(1)	2.260(19)	Pd(1)—Cl(1)	2.330(19)
Pd(1)—Cl(2)	2.375(19)	Pd(1)—Te(1)	2.504(8)
C(9)—C(8)	1.525(10)	C(9)—S(1)	1.832(7)
C(5)—C(6)	1.353(10)	C(5)—C(4)	1.358(11)
C(5)—Te(1)	2.128(7)	C(8)—Te(1)	2.117(7)
C(6)—C(7)	1.403(11)	C(7)—C2	1.374(12)
C(2)—O(1)	1.357(10)	C(2)—C(3)	1.364(12)
C(4)—C(3)	1.367(12)	C(10)—C(11)	1.365(13)
C(10)—C(15)	1.367(12)	C(10)—S(1)	1.779(8)
C(11)—C(12)	1.384(13)	C(1)—O(1)	1.417(11)
C(14)—C(13)	1.34(2)	C(14)—C(15)	1.401(17)
C(13)—C(12)	1.34(2)		
Bond Angle (°)			
S(1)—Pd(1)—Cl(1)	175.48(8)	S(1)—Pd(1)—Cl(2)	90.05(7)
Cl(1)—Pd(1)—Cl(2)	93.70(8)	S(1)—Pd(1)—Te(1)	89.97(5)
Cl(1)—Pd(1)—Te(1)	86.19(6)	Cl(2)—Pd(1)—Te(1)	177.90(5)
C(10)—S(1)—C(9)	101.5(4)	C(10)—S(1)—Pd(1)	108.3(3)
C(9)—S(1)—Pd(1)	107.5(2)	C(8)—Te(1)—C(5)	95.3(3)
C(8)—Te(1)—Pd(1)	96.1(2)	C(5)—Te(1)—Pd(1)	98.11(18)
C(8)—C(9)—S(1)	108.7(5)	C(6)—C(5)—C(4)	118.7(7)
C(6)—C(5)—Te(1)	118.1(5)	C(4)—C(5)—Te(1)	123.2(6)
C(9)—C(8)—Te(1)	111.4(5)	C(5)—C(6)—C(7)	120.4(8)
C(2)—C(7)—C(6)	120.2(9)	O(1)—C(2)—C(3)	118.3(8)
O(1)—C(2)—C(7)	123.4(9)	C(3)—C(2)—C(7)	118.3(8)
C(5)—C(4)—C(3)	121.7(9)	C(11)—C(10)—C(15)	121.8(9)
C(11)—C(10)—S(1)	122.0(7)	C(15)—C(10)—S(1)	116.1(8)
C(10)—C(11)—C(12)	117.1(11)	C(2)—C(3)—C(4)	120.7(9)
C(13)—C(14)—C(15)	120.1(15)	C(10)—C(15)—C(14)	118.4(13)
C(12)—C(13)—C(14)	120.1(13)	C(13)—C(12)—C(11)	122.4(14)
C(2)—O(1)—C(1)	118.0(7)		
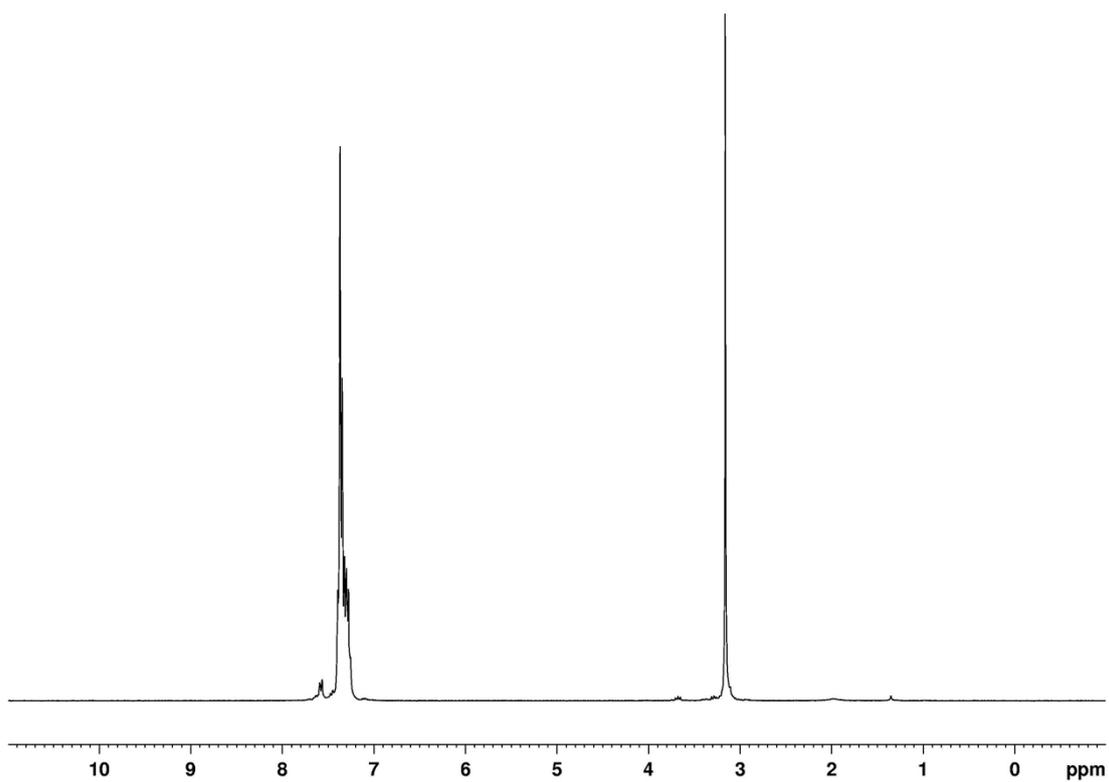
Fig. S1 ^{1}H NMR Spectrum of **L1**
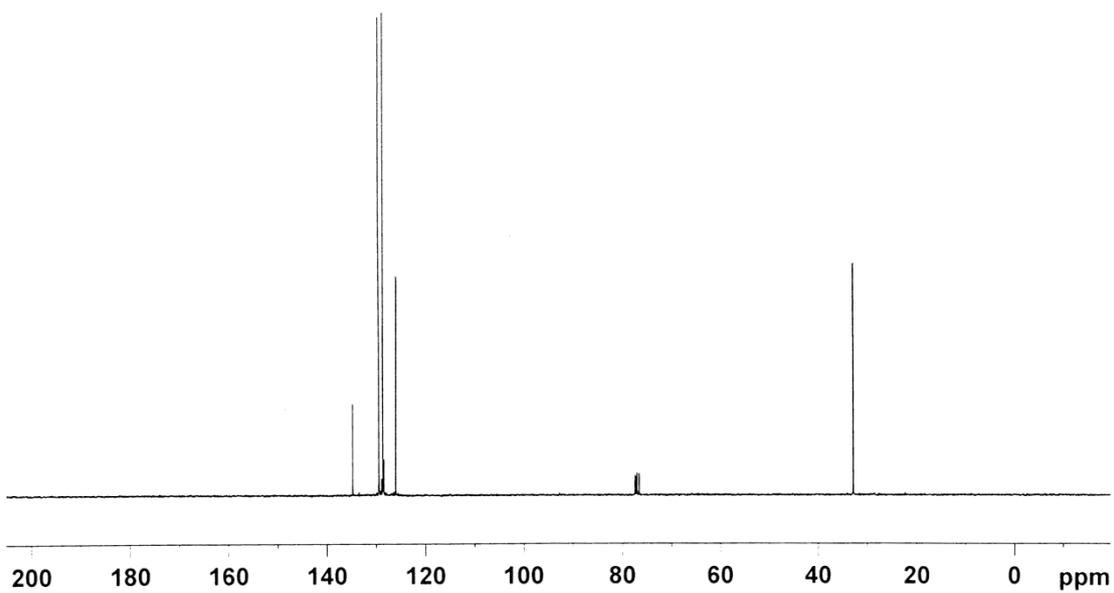
Fig. S2 ^{13}C{^{1}H} NMR Spectrum of **L1**
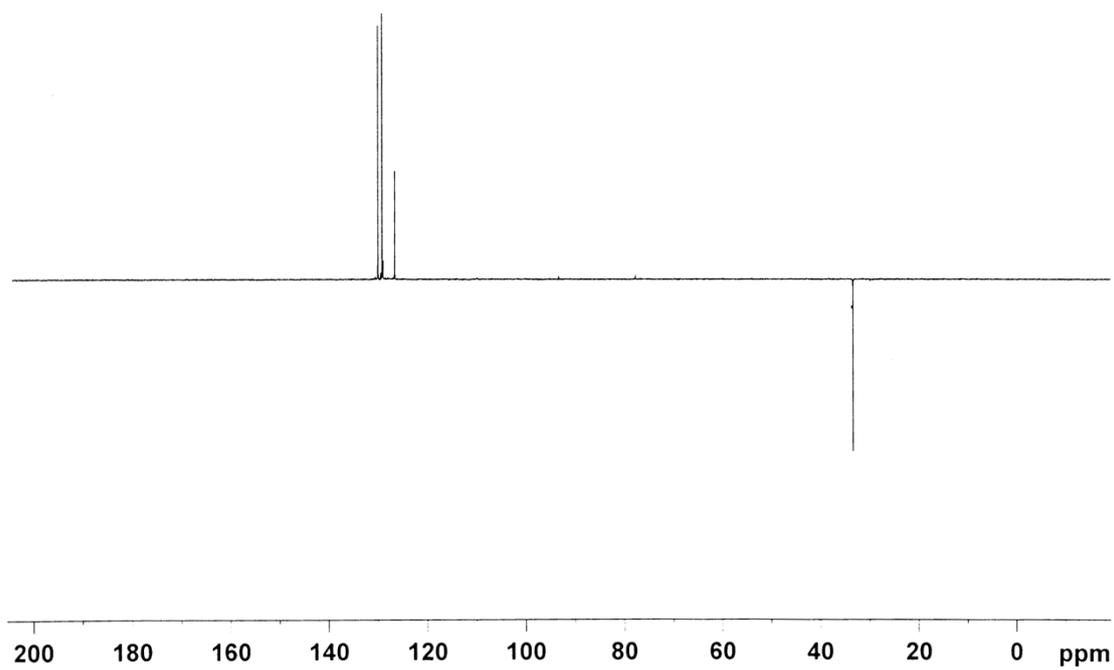
Fig. S3 ^{135}DEPT NMR Spectrum of **L1**
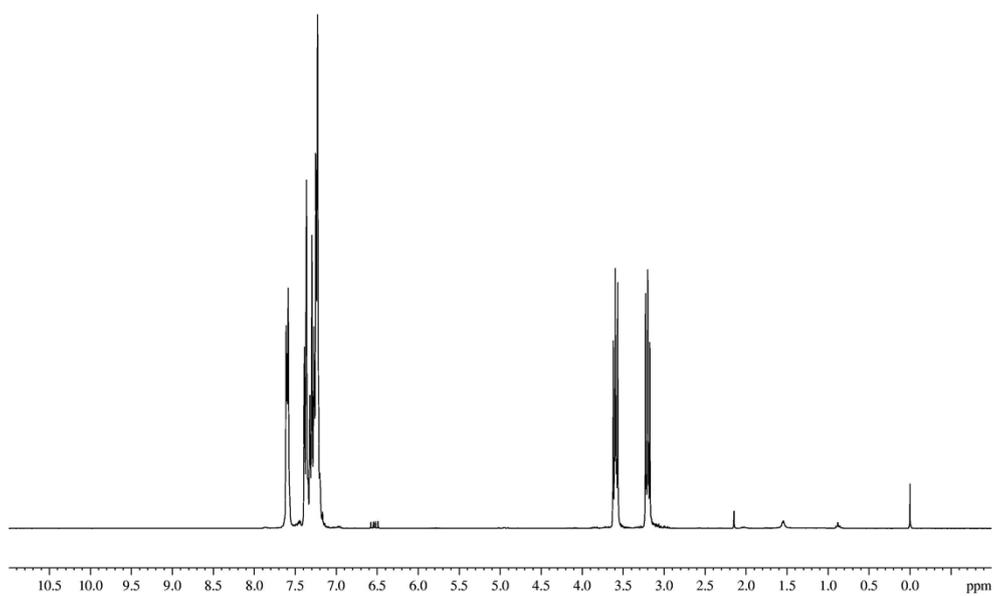
Fig. S4 ^{1}H NMR Spectrum of **L2**
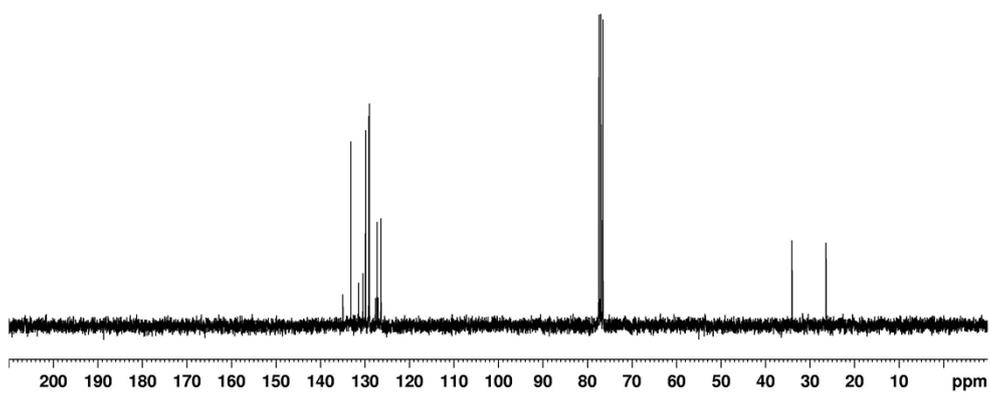
Fig. S5 $^{13}C\{^1H\}$ NMR Spectrum of **L2**
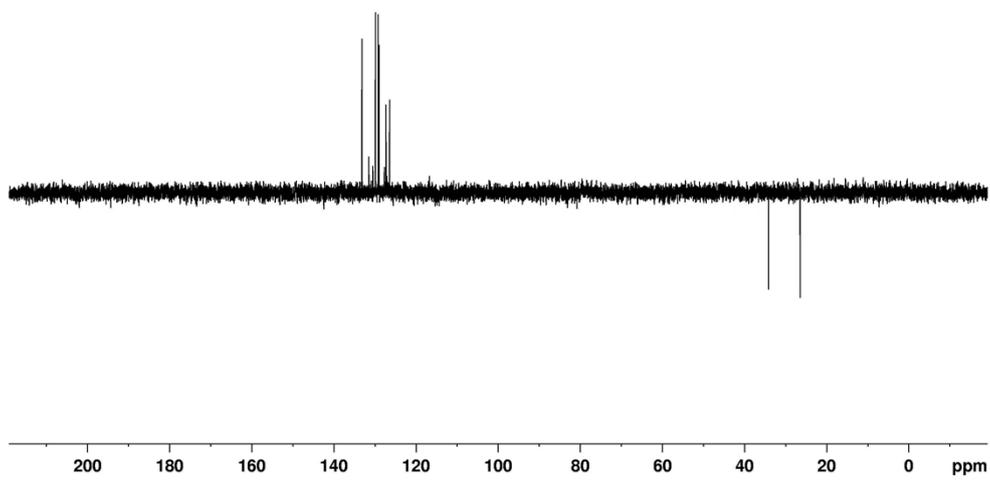
Fig. S6 ^{135}DEPT NMR Spectrum of **L2**
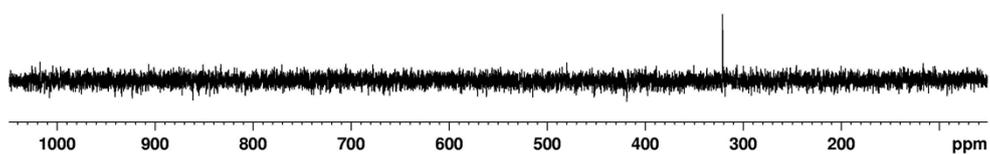
Fig. S7 ^{77}Se$\{^1$H$\}$ NMR Spectrum of **L2**
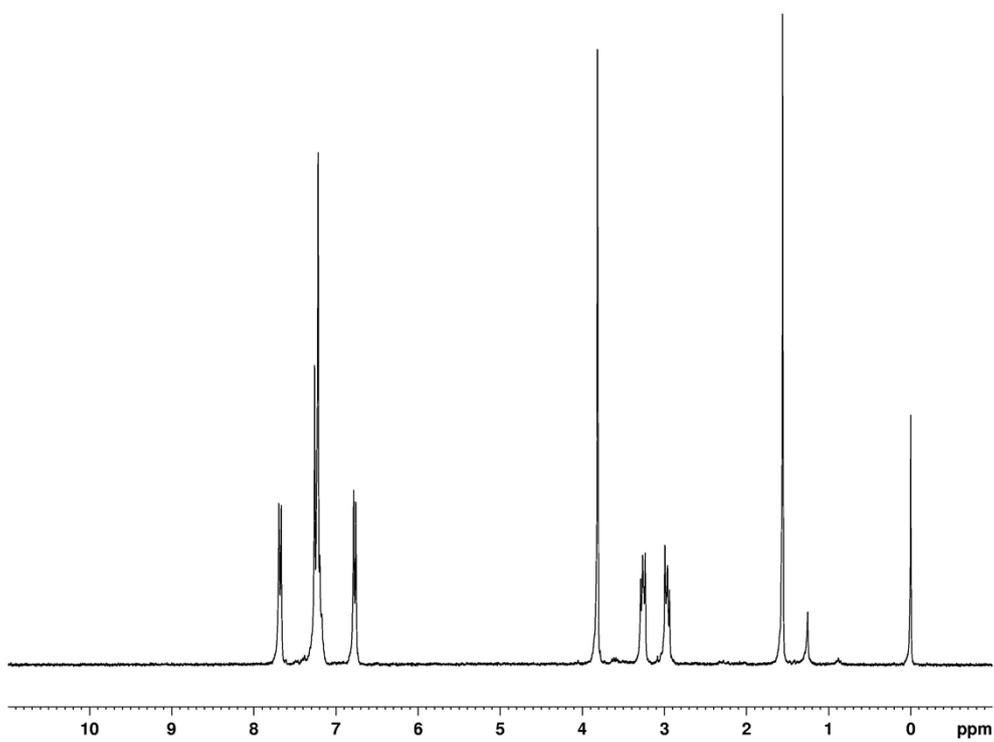

Fig. S8 ^{1}H NMR Spectrum of **L3**
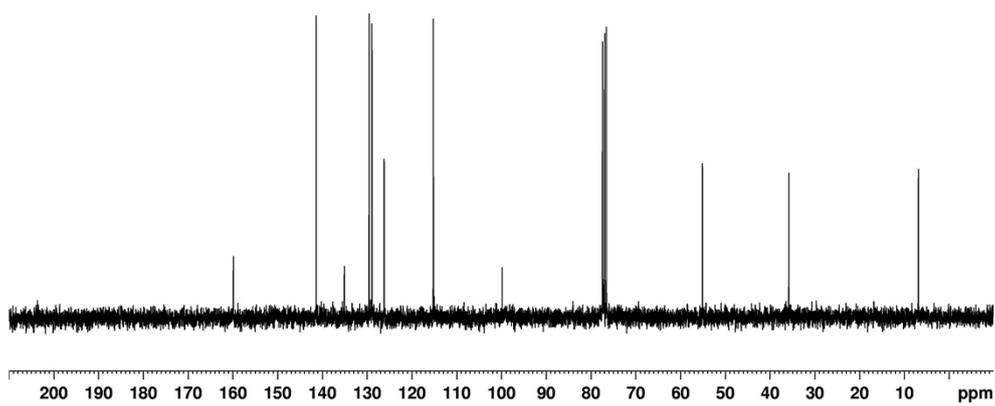
Fig. S9 $^{13}C\{^{1}H\}$ NMR Spectrum of **L3**
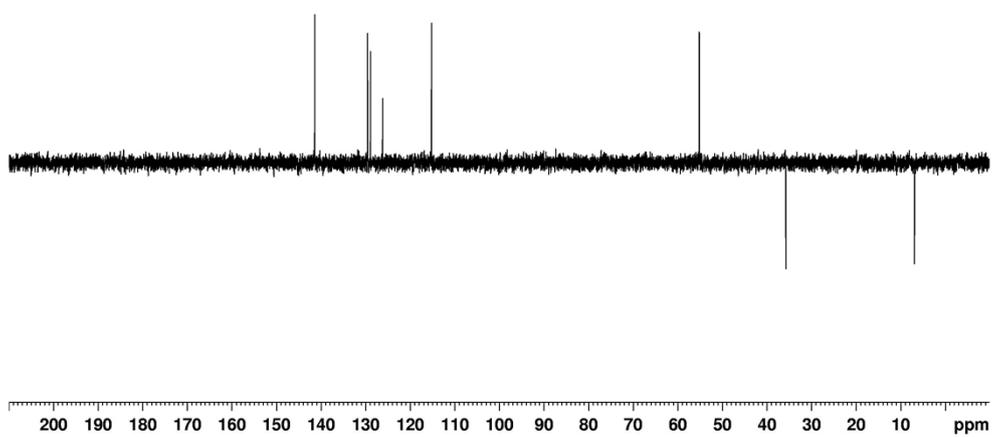
Fig. S10 ^{135}DEPT NMR Spectrum of **L3**
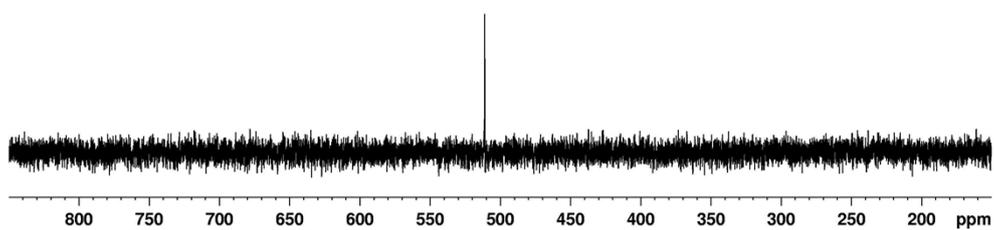
Fig. S11 ^{125}Te{^{1}H} NMR Spectrum of **L3**
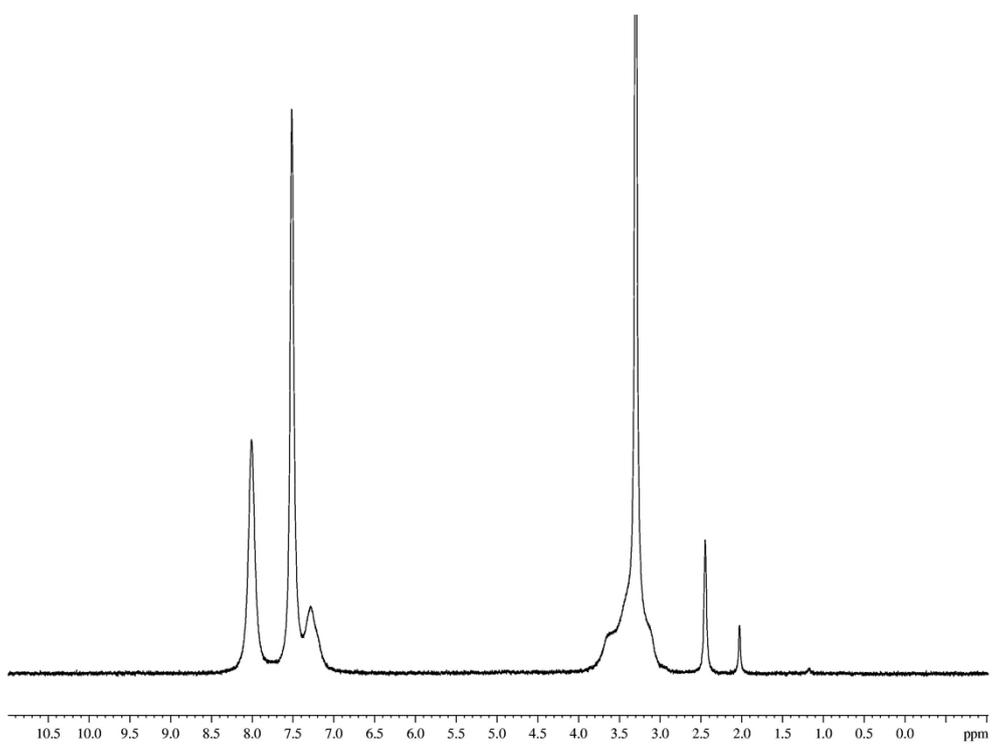
Fig. S12 ^{1}H NMR Spectrum of **1**
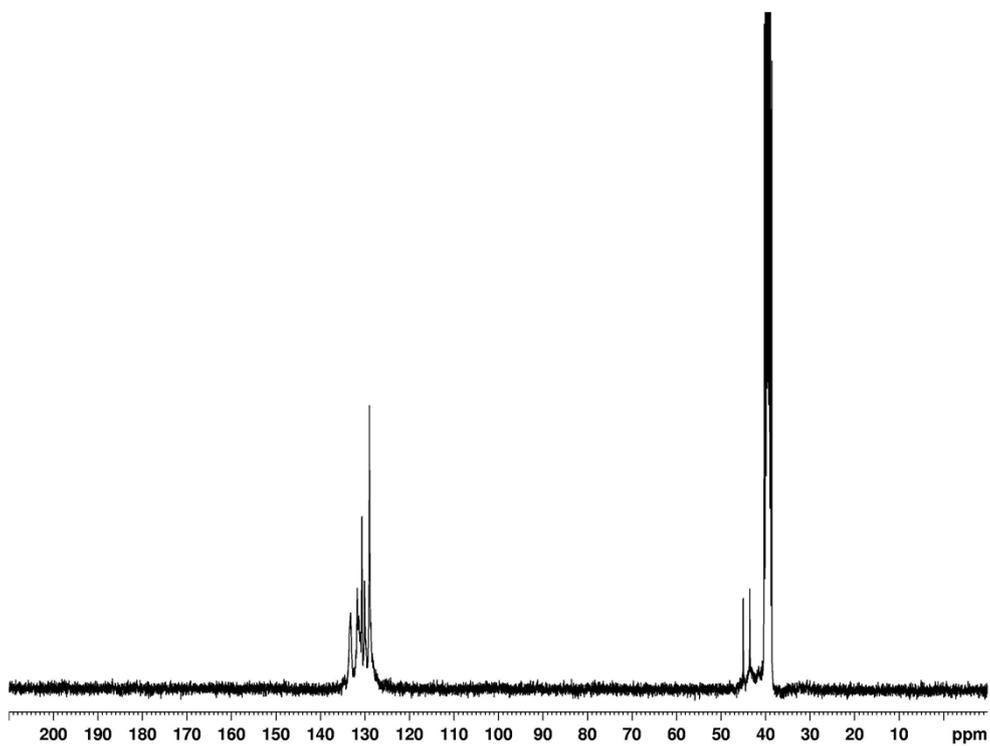
Fig. S13 $^{13}C\{^{1}H\}$ NMR Spectrum of **1**
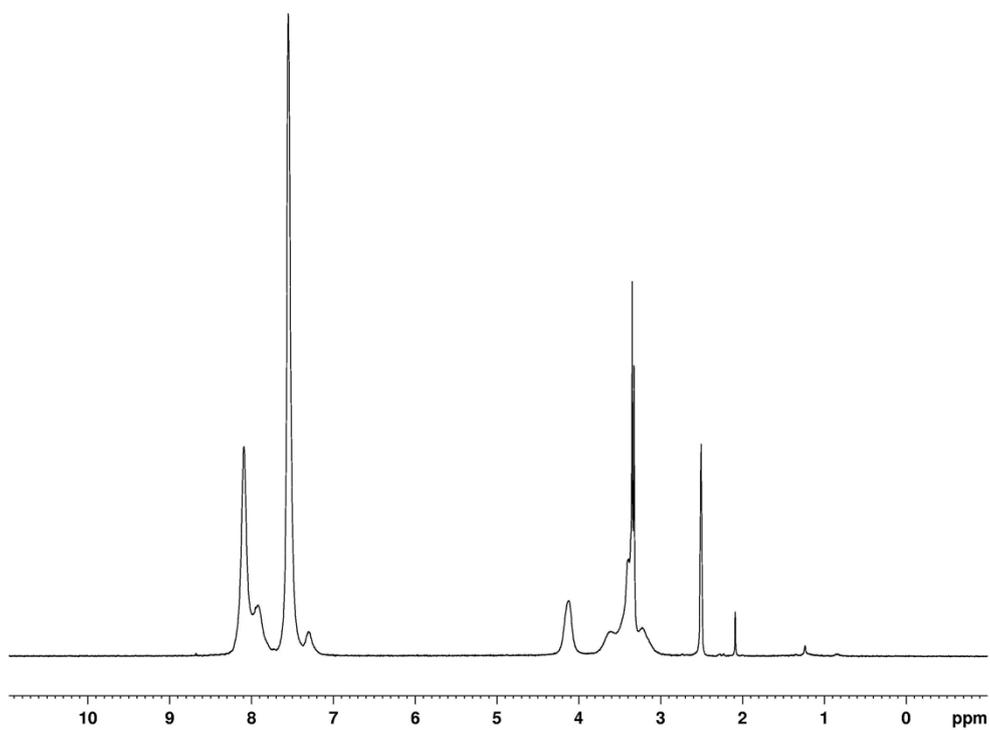
Fig. S14 ^{1}H NMR Spectrum of **2**
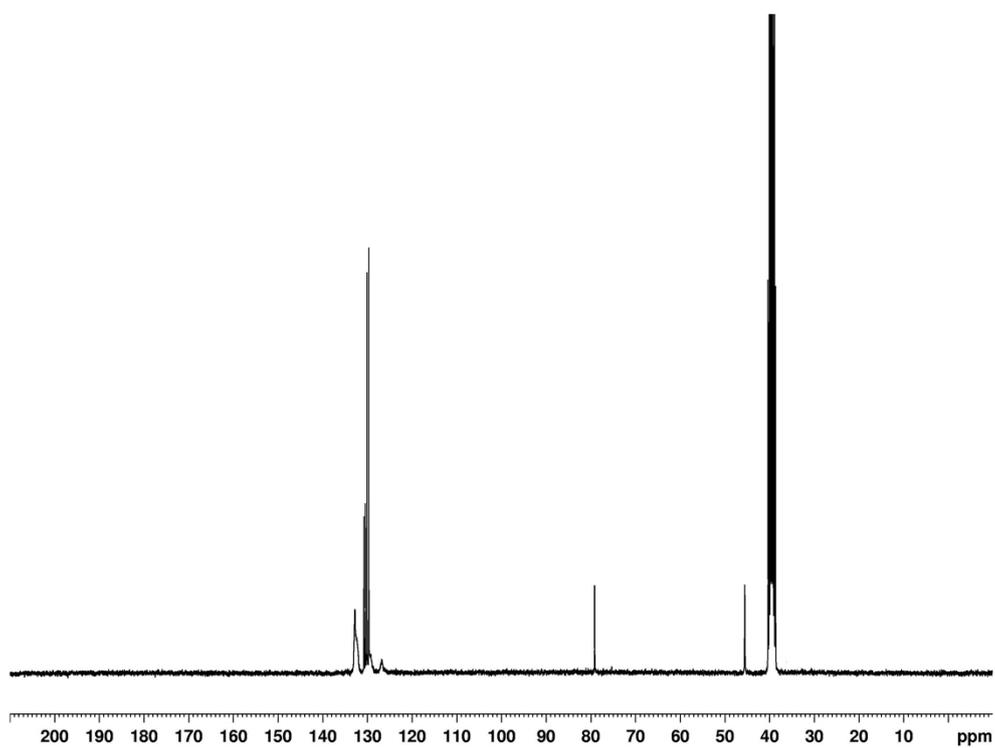
Fig. S15 $^{13}C\{^{1}H\}$ NMR Spectrum of **2**
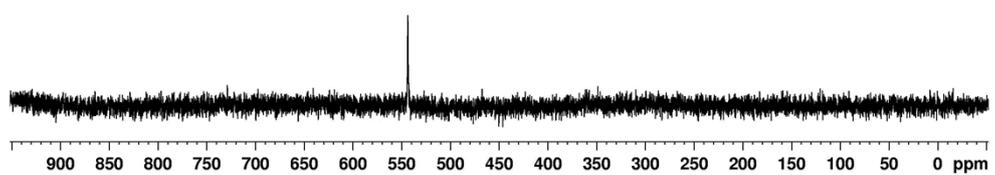
Fig. S16 $^{77}Se\{^{1}H\}$ NMR Spectrum of **2**
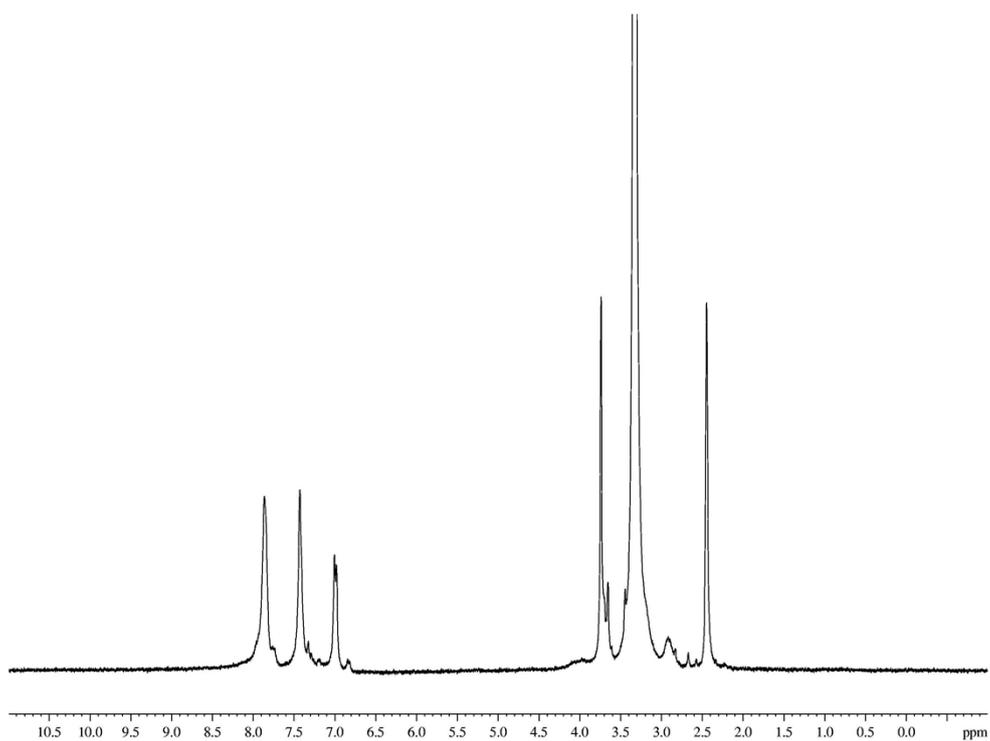
Fig. S17 ^{1}H NMR Spectrum of **3**
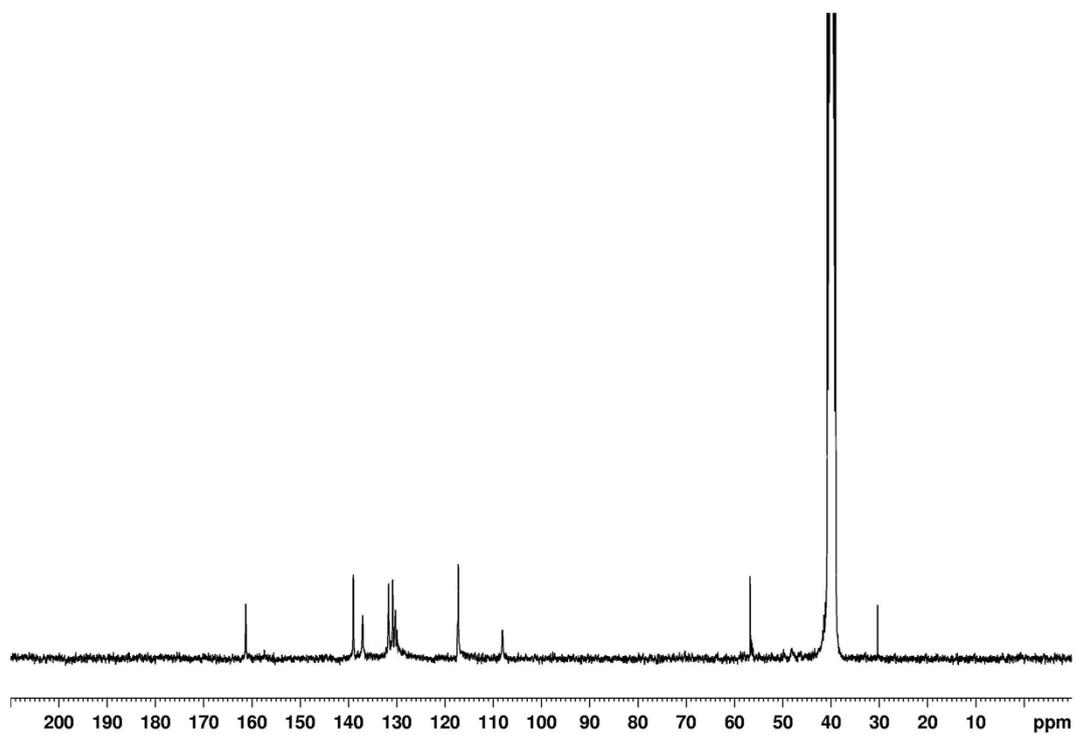
Fig. S18 ^{13}C{^{1}H} NMR Spectrum of **3**
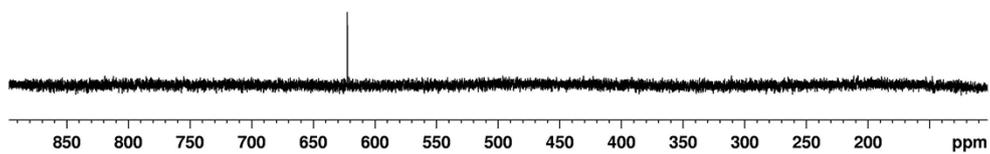
Fig. S19 ^{125}Te{^{1}H} NMR Spectrum of **3**
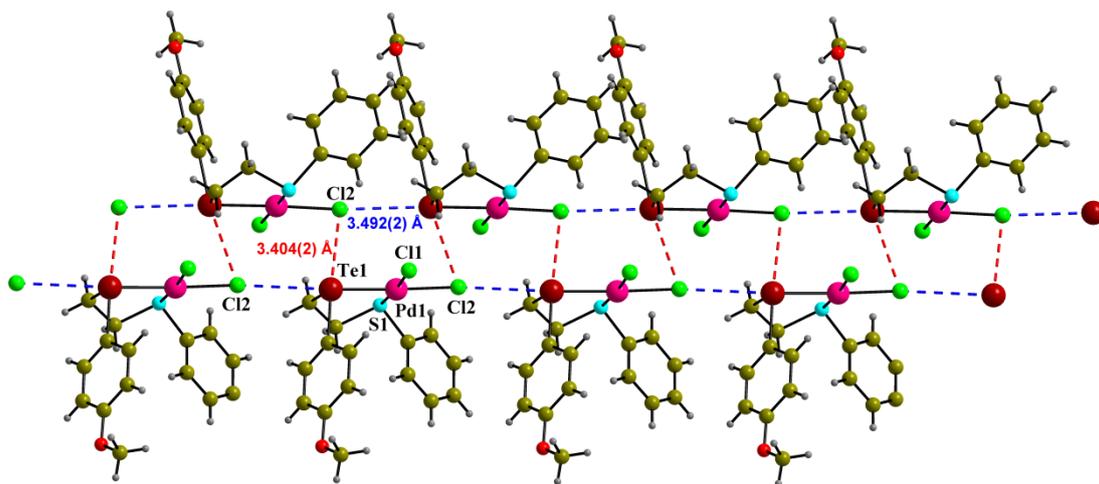
Fig. S20 Molecular Packing of **3** showing Cl⋯Te Interaction
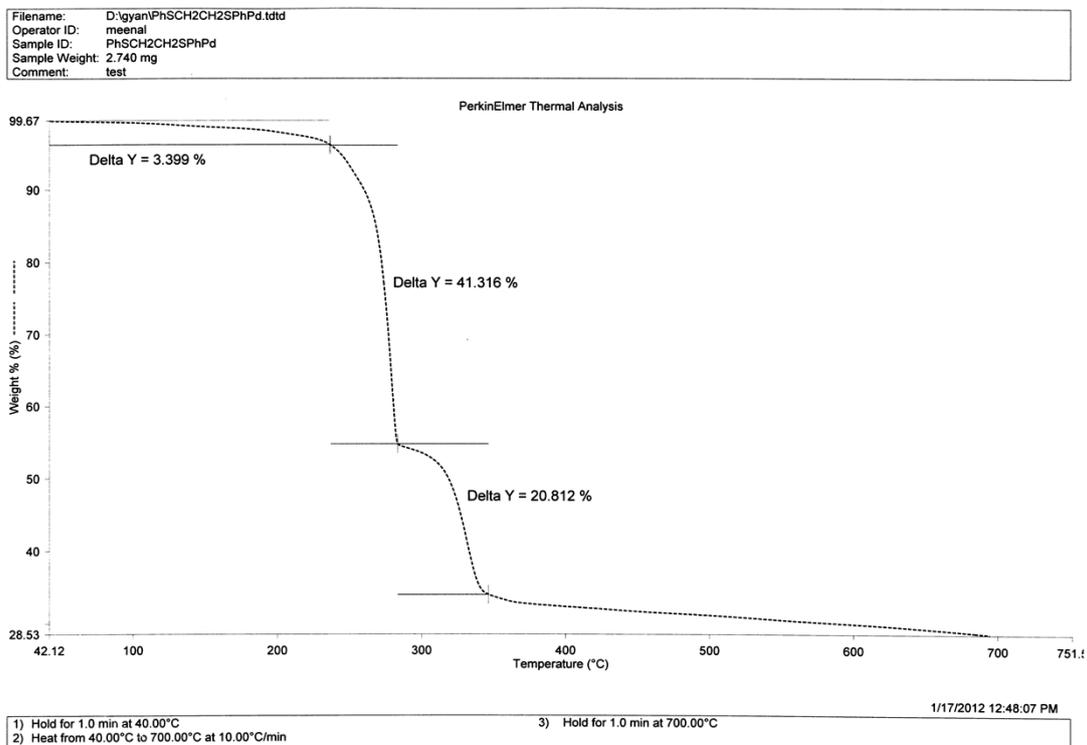
Filename: D:\gyan\PhSCH2CH2SPhPd.tdtd
Operator ID: meenal
Sample ID: PhSCH2CH2SPhPd
Sample Weight: 2.740 mg
Comment: test

PerkinElmer Thermal Analysis

Delta Y = 3.399 %

Delta Y = 41.316 %

Delta Y = 20.812 %

1/17/2012 12:48:07 PM

1) Hold for 1.0 min at 40.00°C
2) Heat from 40.00°C to 700.00°C at 10.00°C/min

3) Hold for 1.0 min at 700.00°C

Fig. S21 TGA Spectrum of **1**

PerkinElmer Thermal Analysis

Delta Y = 5.014 %

Delta Y = 37.741 %

Delta Y = 24.918 %

Weight % (%)

Temperature (°C)

12/26/2011 3:16:39 PM

1) Heat from 50.00°C to 700.00°C at 7.00°C/min   2) Hold for 1.0 min at 700.00°C

Fig. S22 TGA Spectrum of **2**

PerkinElmer Thermal Analysis

Delta Y = 2.985 %

Delta Y = 30.459 %

Delta Y = 26.026 %

Weight % (%)

Temperature (°C)

12/26/2011 4:37:51 PM

1) Heat from 50.00°C to 700.00°C at 8.00°C/min   2) Hold for 1.0 min at 700.00°C
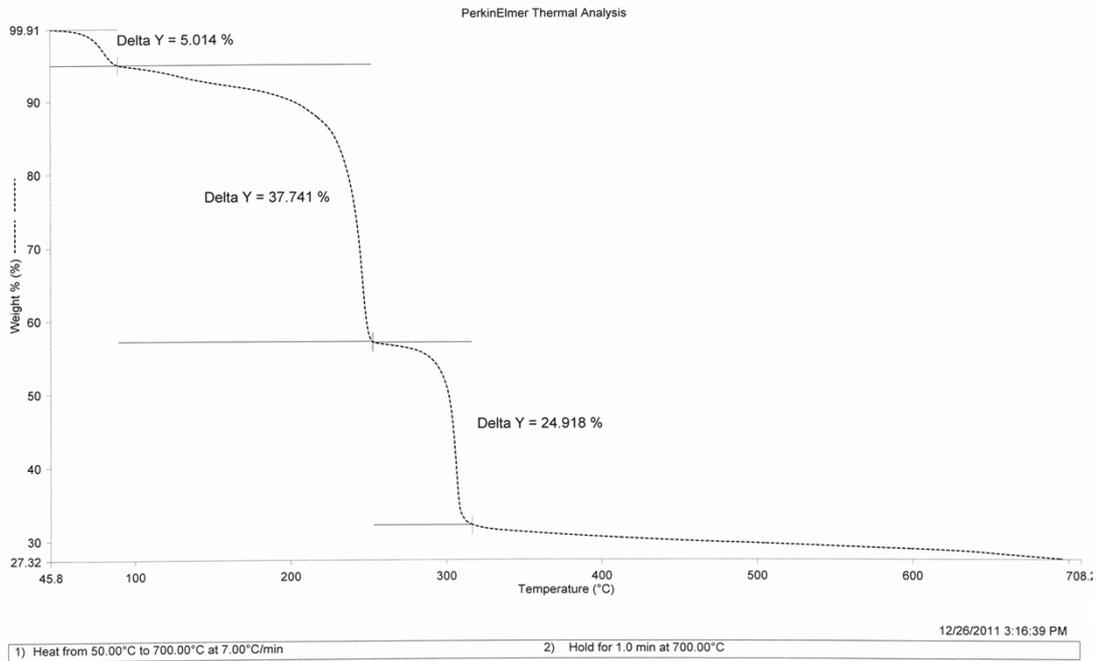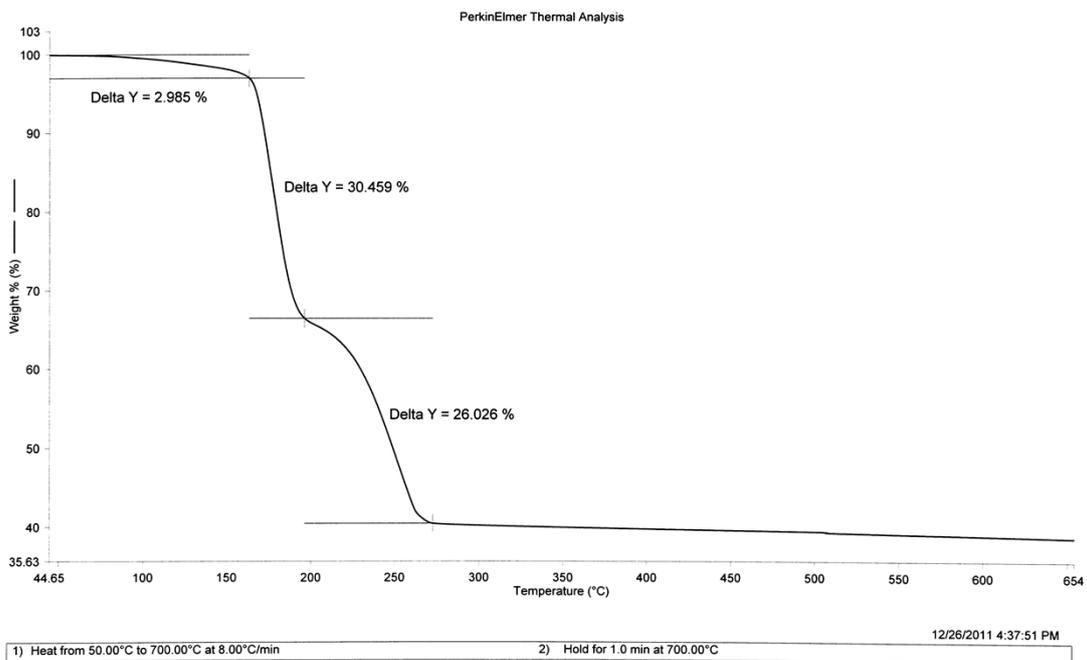
Fig. S23 TGA Spectrum of **3**
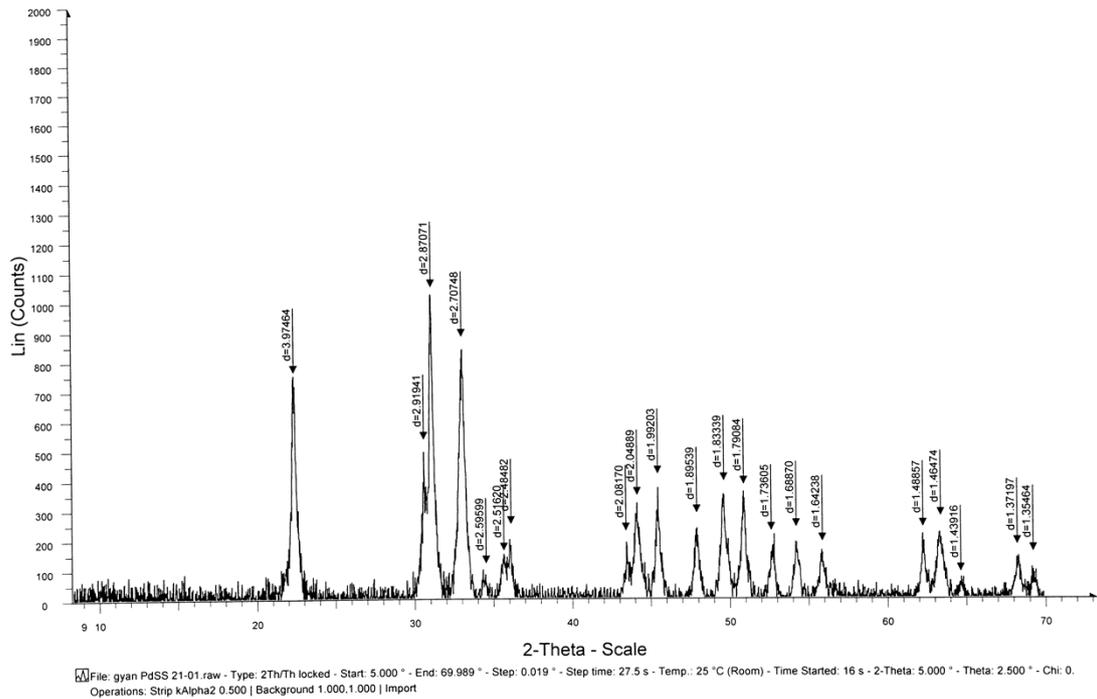
Fig. S24 PXRD of PdP$_2$ Nanoparticles Obtained from **1**
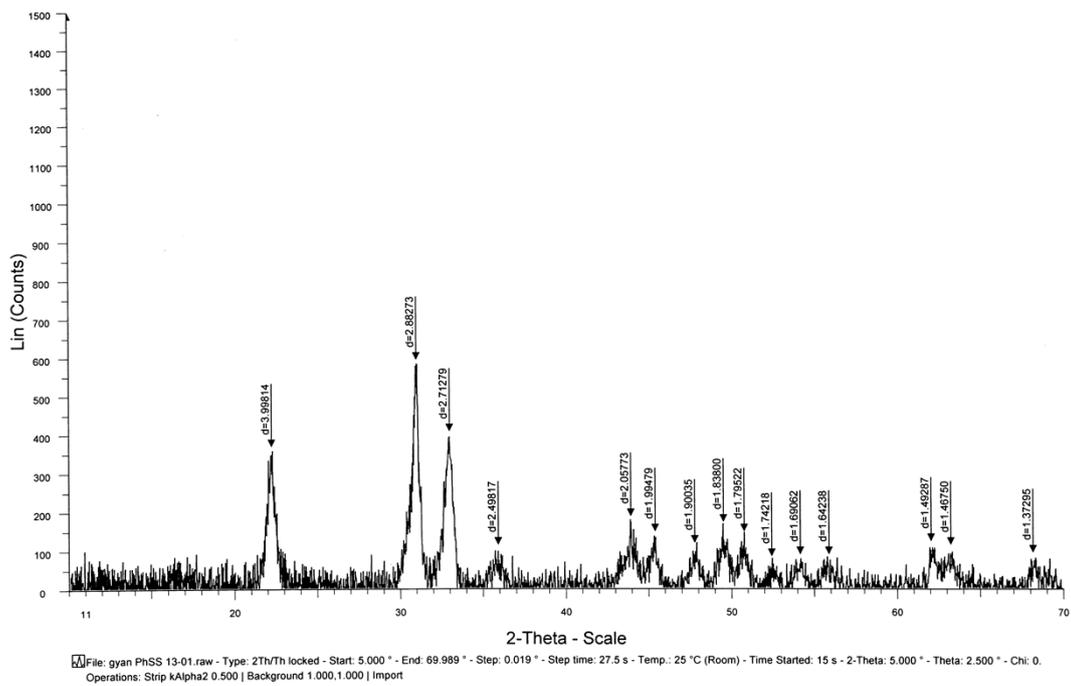
Fig. S25 PXRD of PdP$_2$ Nanoparticles Obtained from **2**
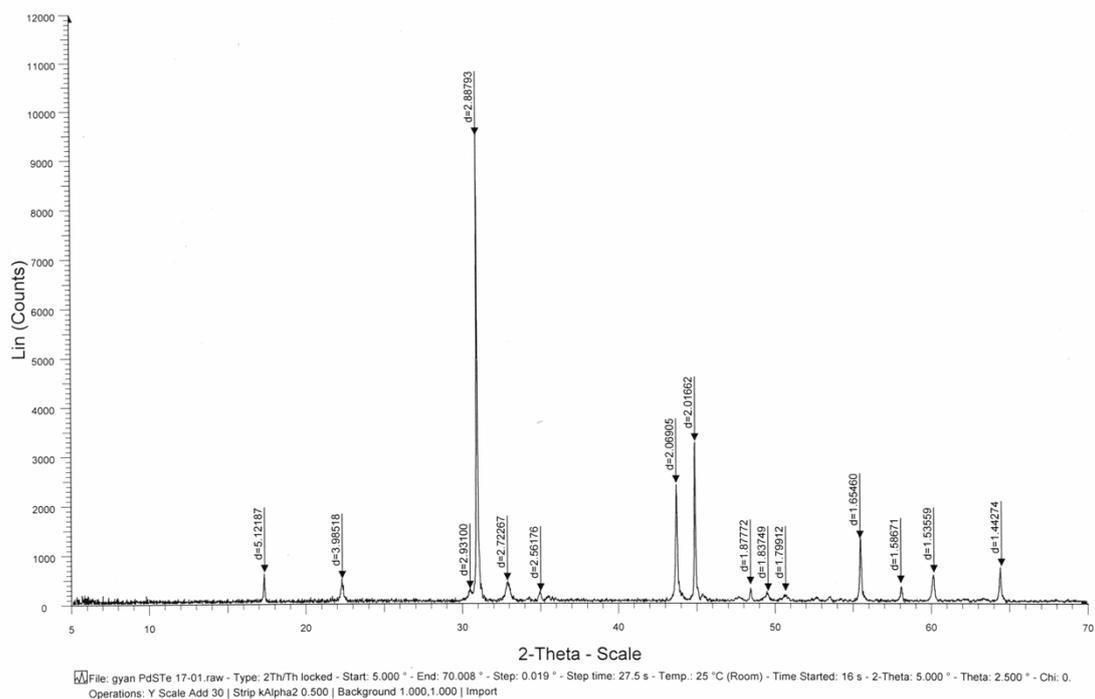
Fig. S26 PXRD of PdP$_2$ Nanoparticles Obtained from **3**
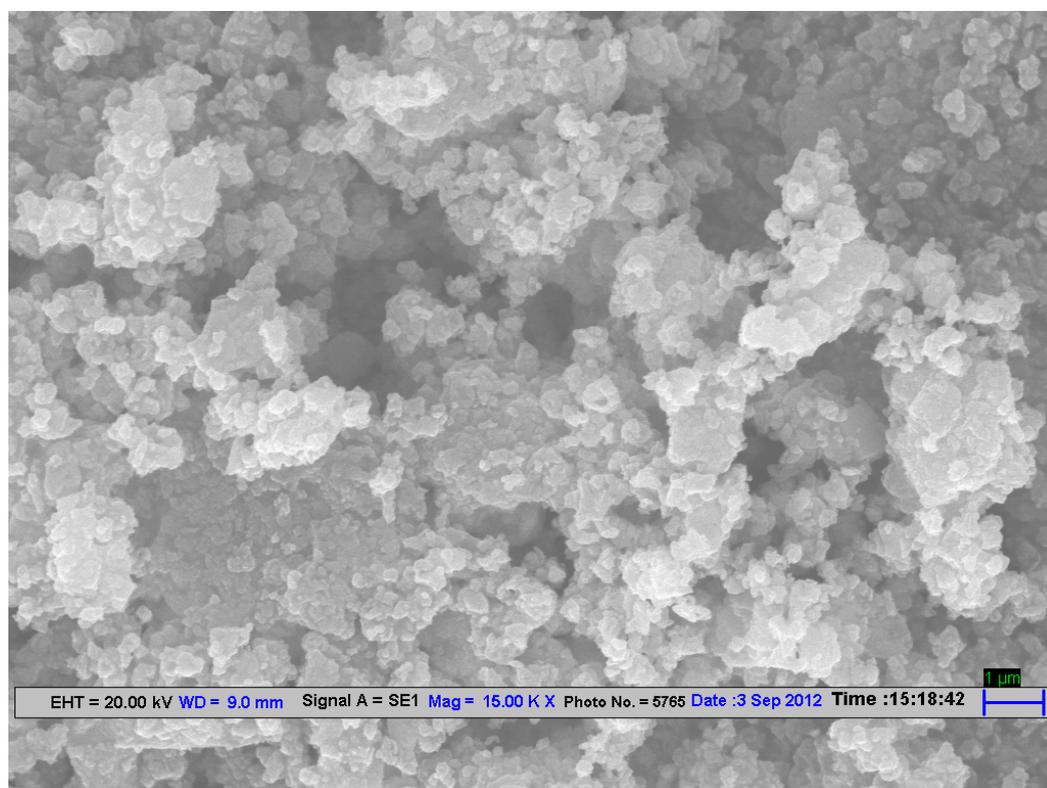
Fig. S27 SEM Image of Decomposition Product (Pd Nanoparticles Protected by Ligand) of **1** Obtained after Suzuki Coupling Reaction
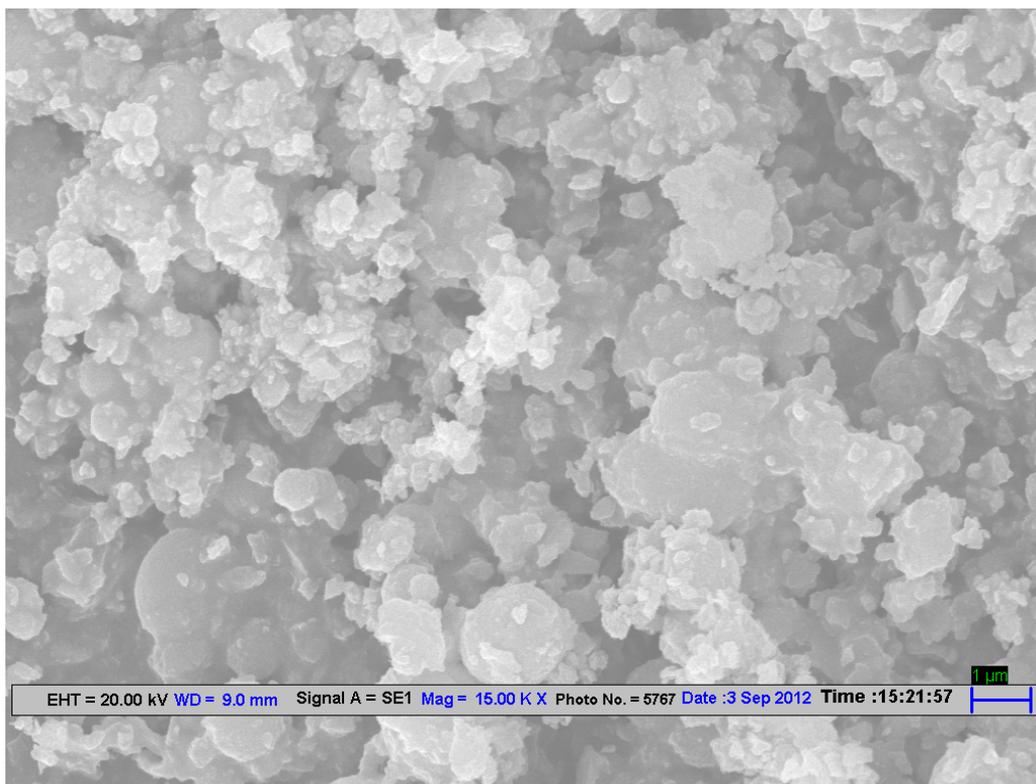
Fig. S28 SEM Image of Decomposition Product (Pd Nanoparticles Protected by Ligand) of **2** Obtained after Suzuki Coupling Reaction
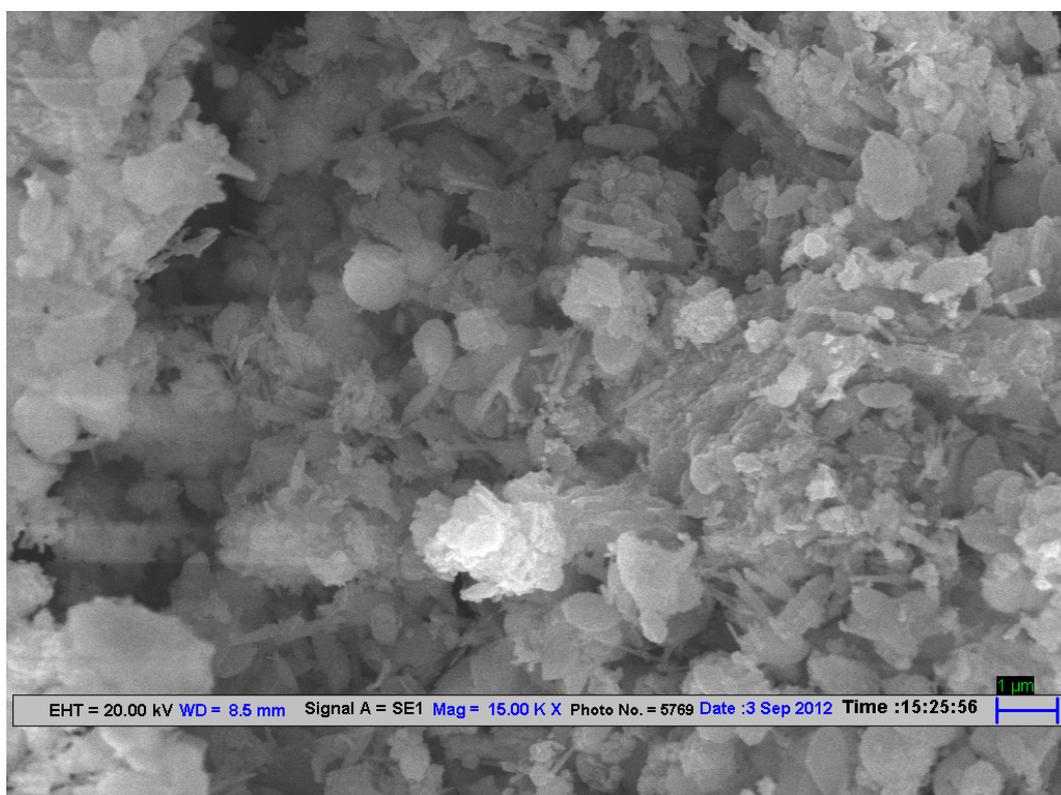

Fig. S29 SEM Image of Decomposition Product (Pd Nanoparticles Protected by Ligand) of **3** Obtained after Suzuki Coupling Reaction
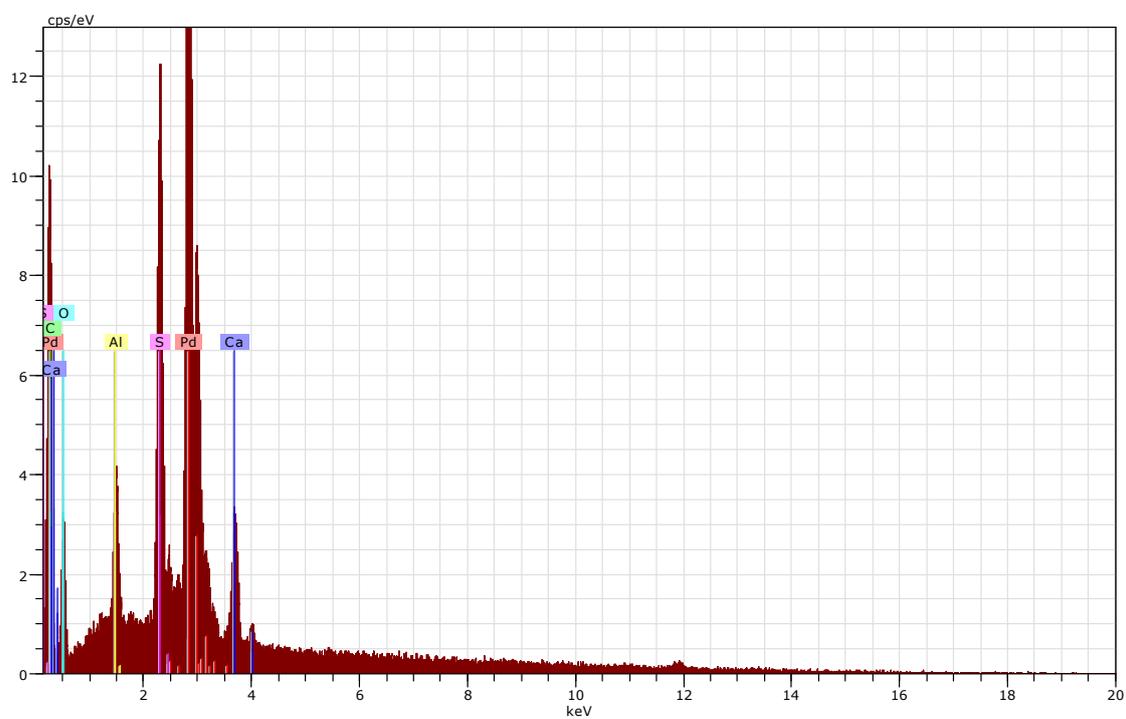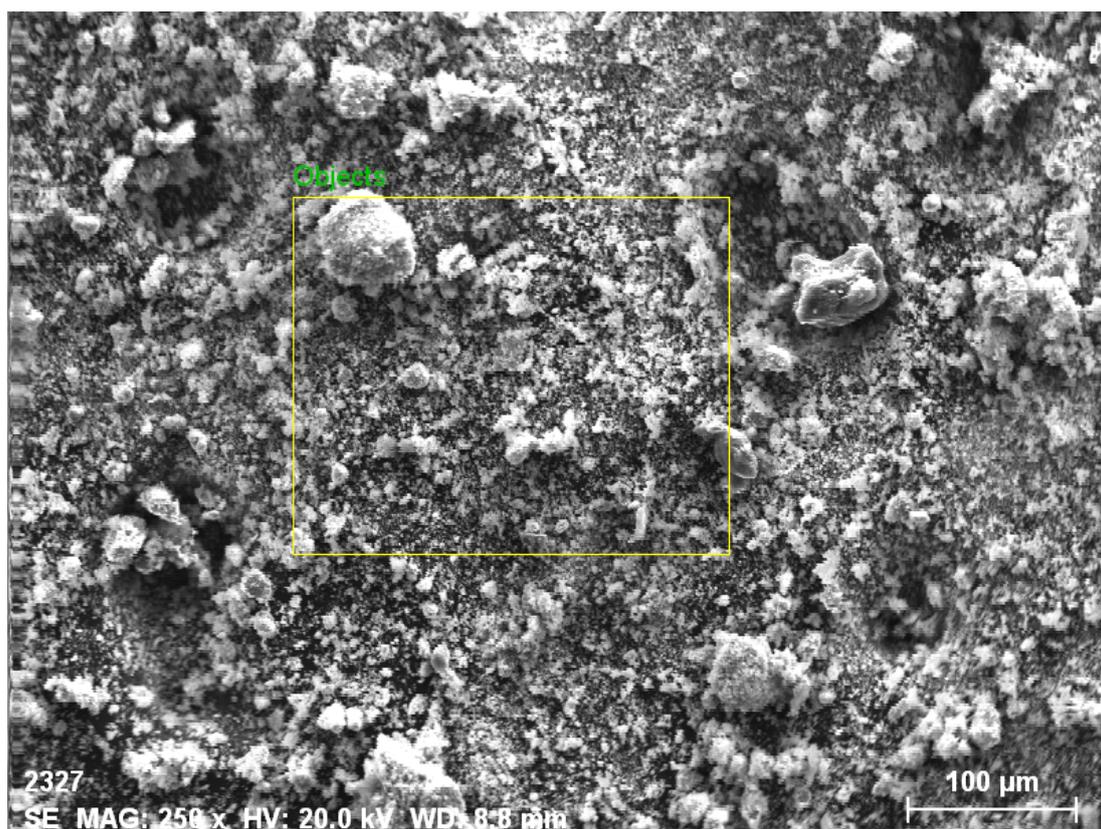
Fig. S30 SEM−EDX of Decomposition Product (Pd nanoparticles protected by Ligand) of **1** Obtained after Suzuki Coupling Reaction
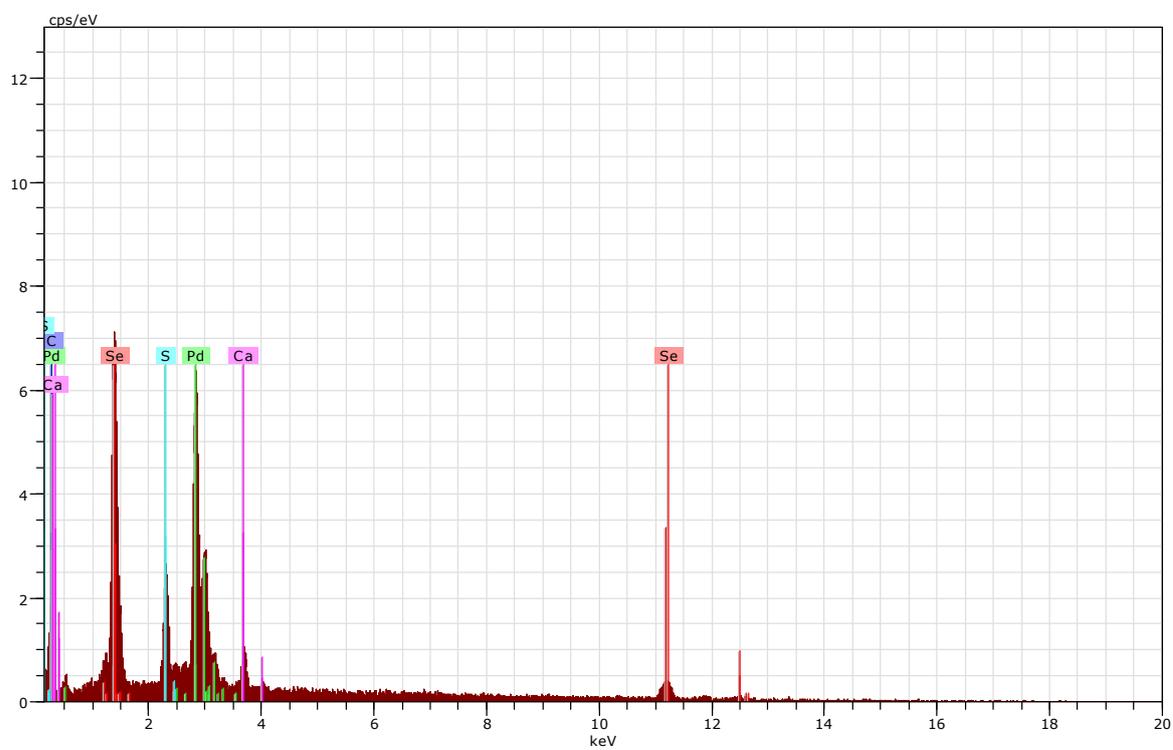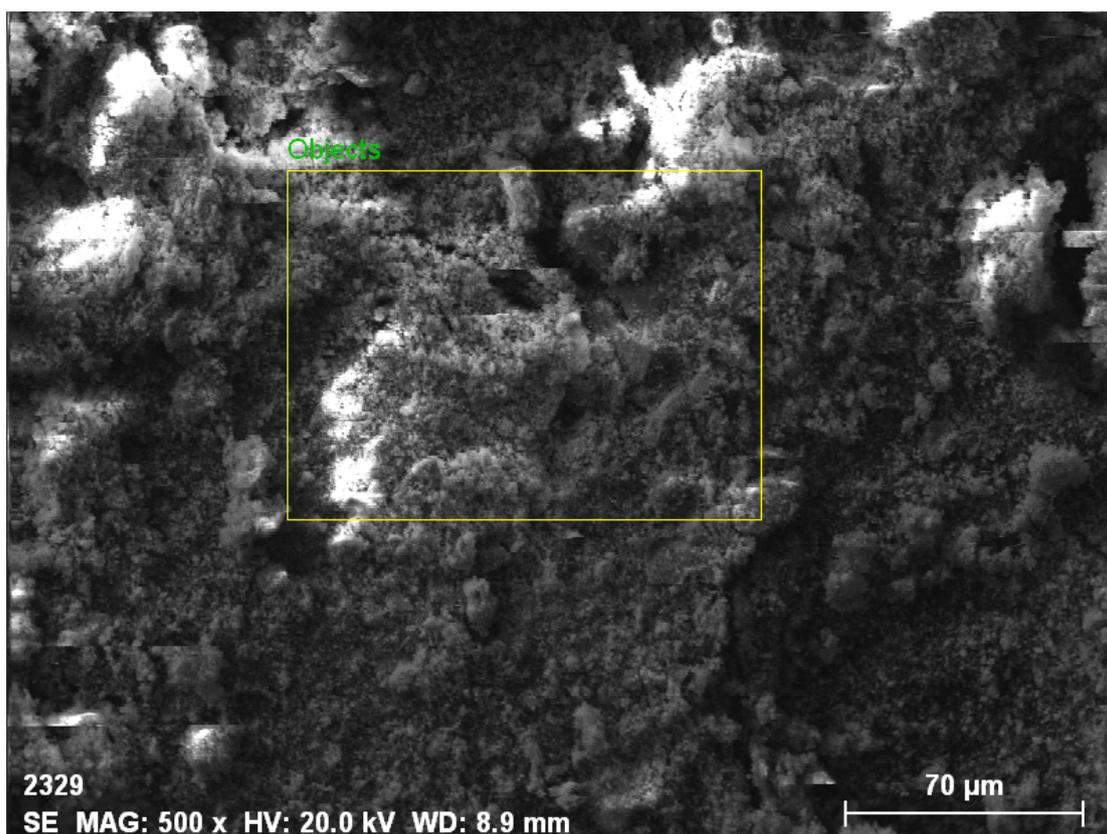
Fig. S31 SEM−EDX of Decomposition Product (Pd nanoparticles protected by Ligand) of **2** Obtained after Suzuki Coupling Reaction
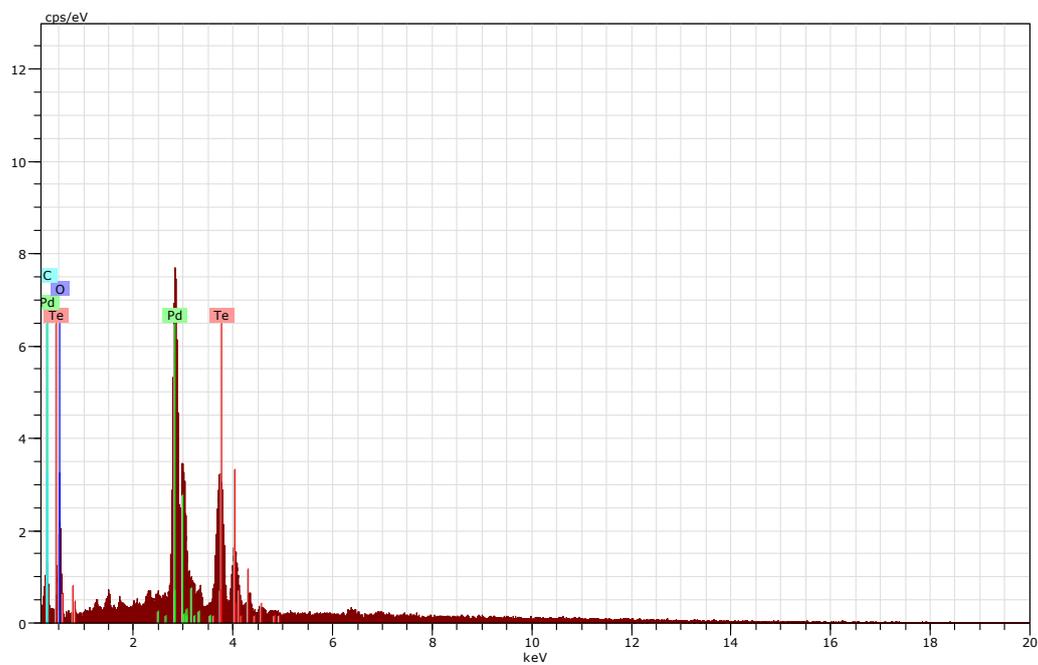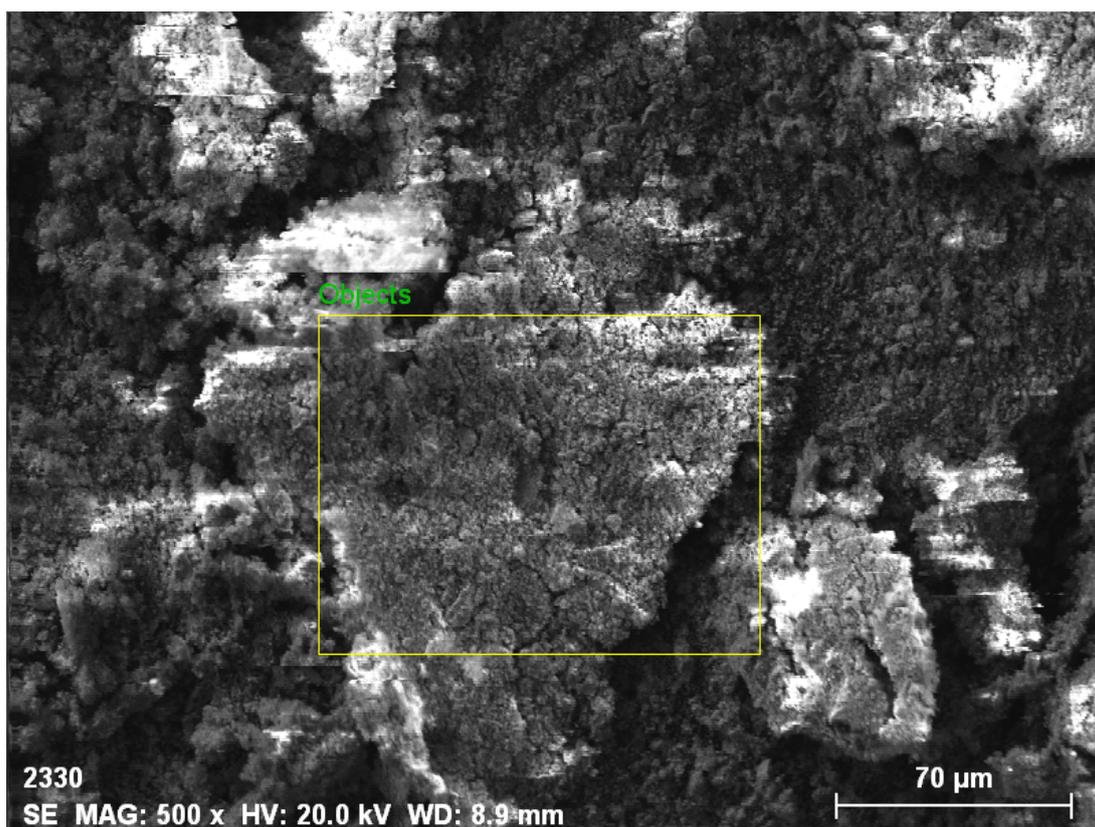
Fig. S32 SEM−EDX of Decomposition Product (Pd nanoparticles protected by Ligand) of **3** Obtained after Suzuki Coupling Reaction
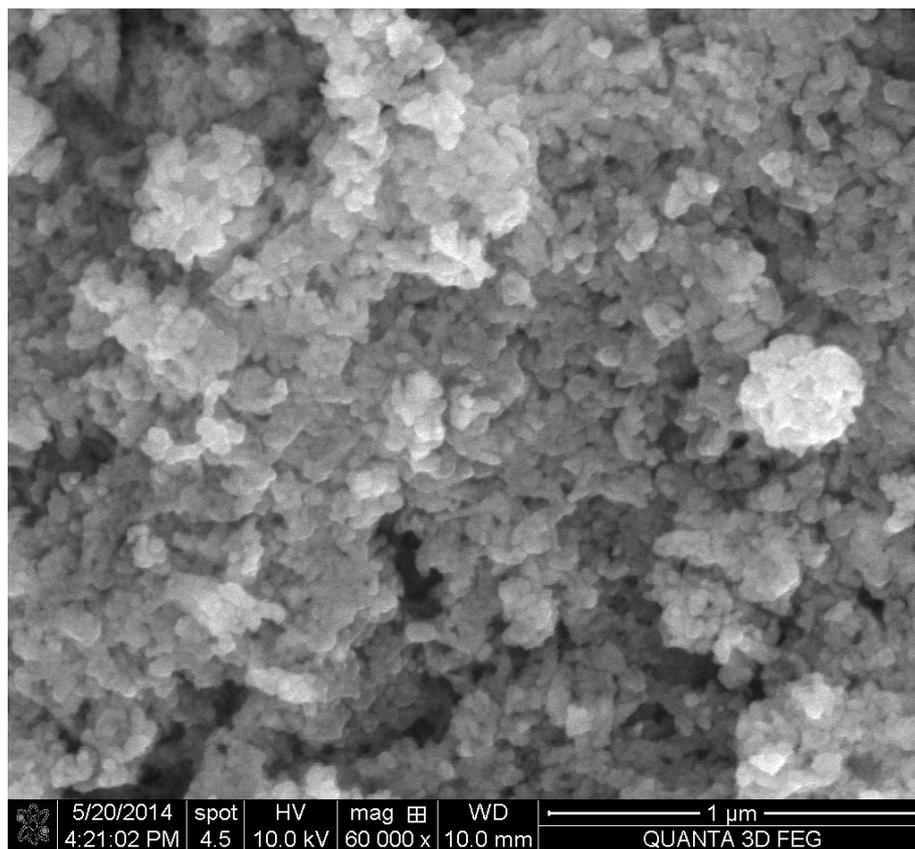
Fig. S33 FE-SEM image of PdP$_2$ NPs obtained from complex **1**
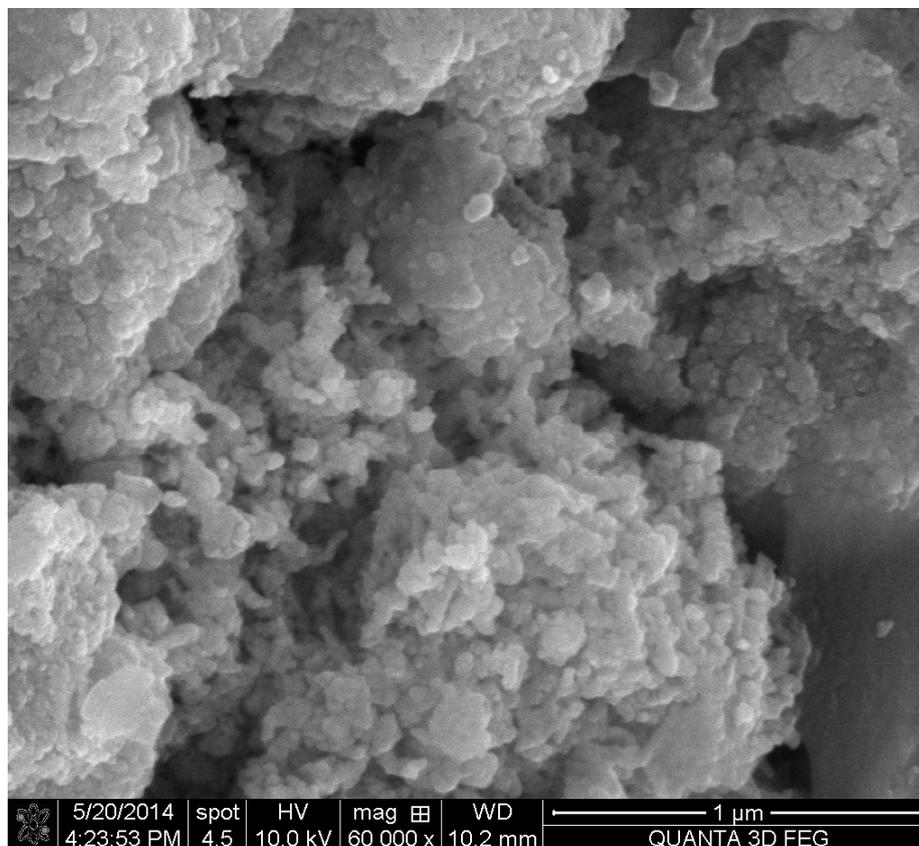
Fig. S34 FE-SEM image of PdP$_2$ NPs obtained from complex **2**
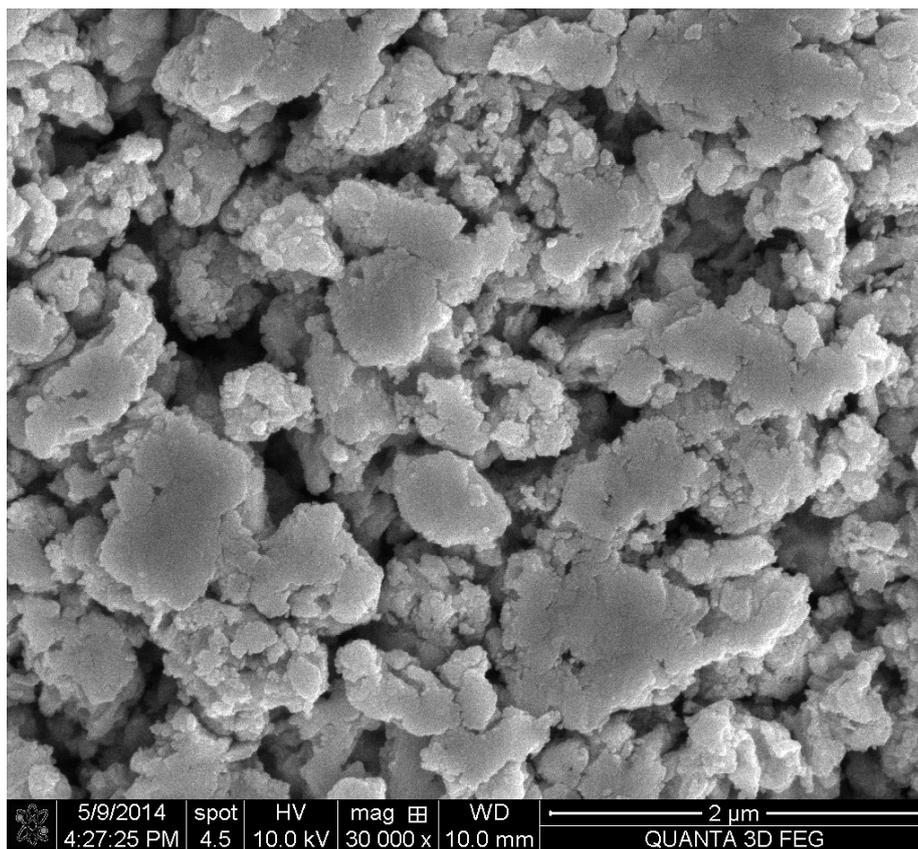
Fig. S35 FE-SEM image of PdP$_2$ NPs obtained from complex **3**
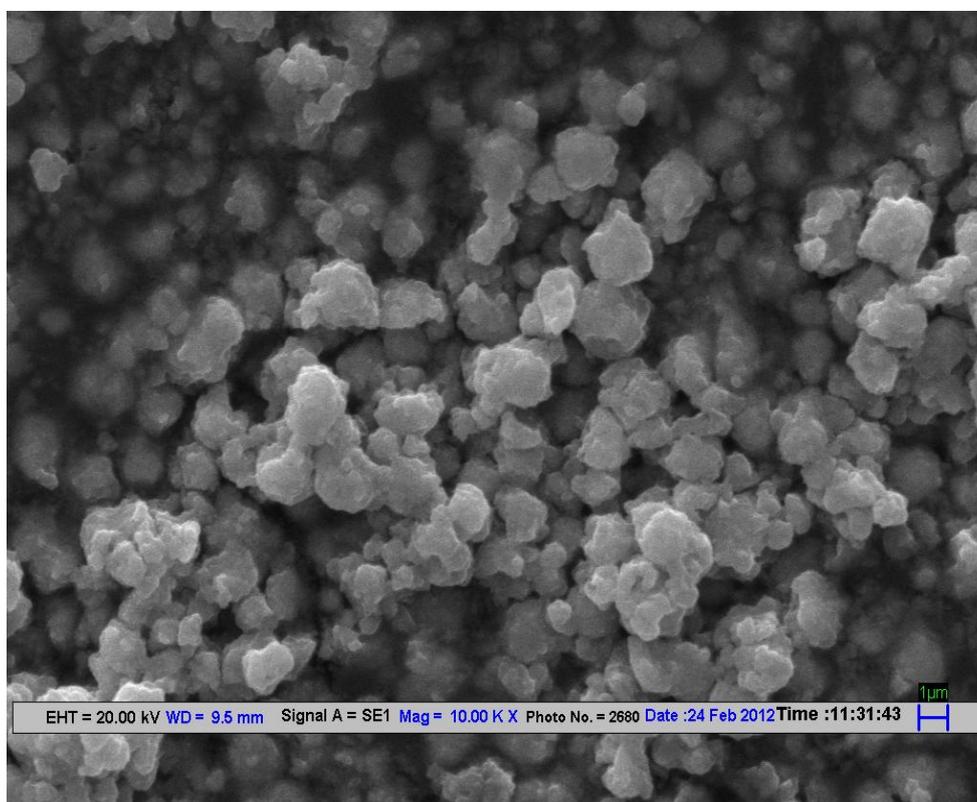
Fig. S36 SEM Image of PdP$_2$ Nanoparticles obtained from **1**
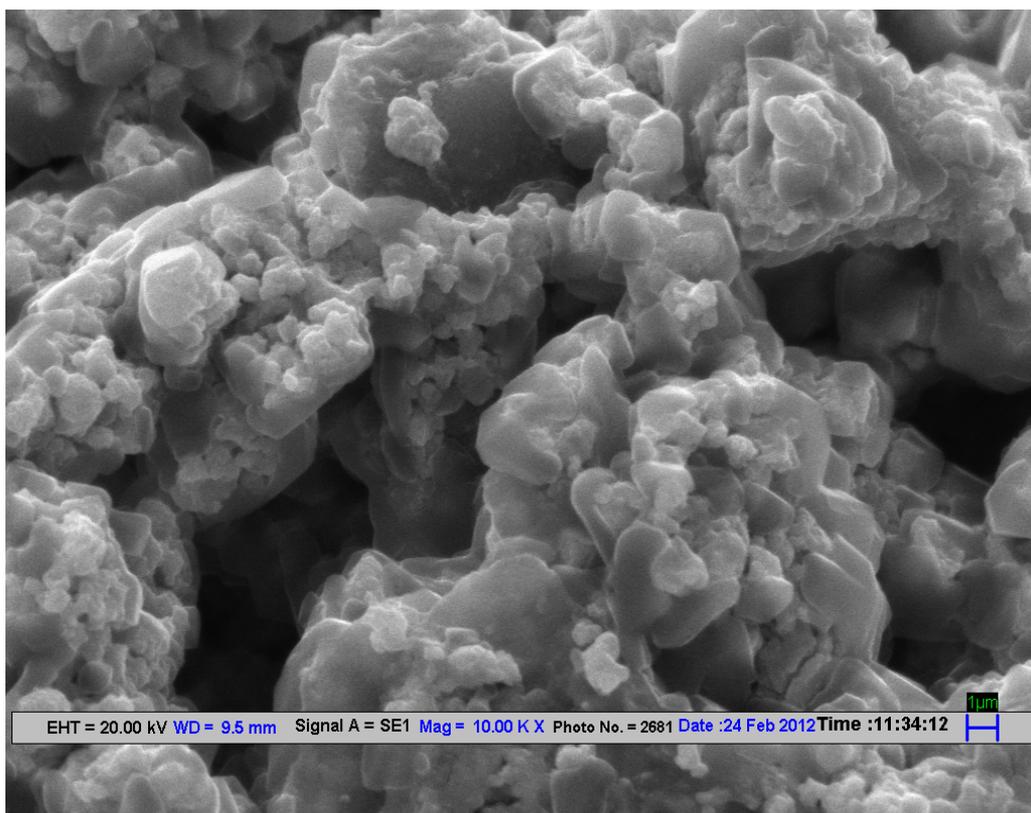
Fig. S37 SEM Image of PdP$_2$ Nanoparticles obtained from **2**
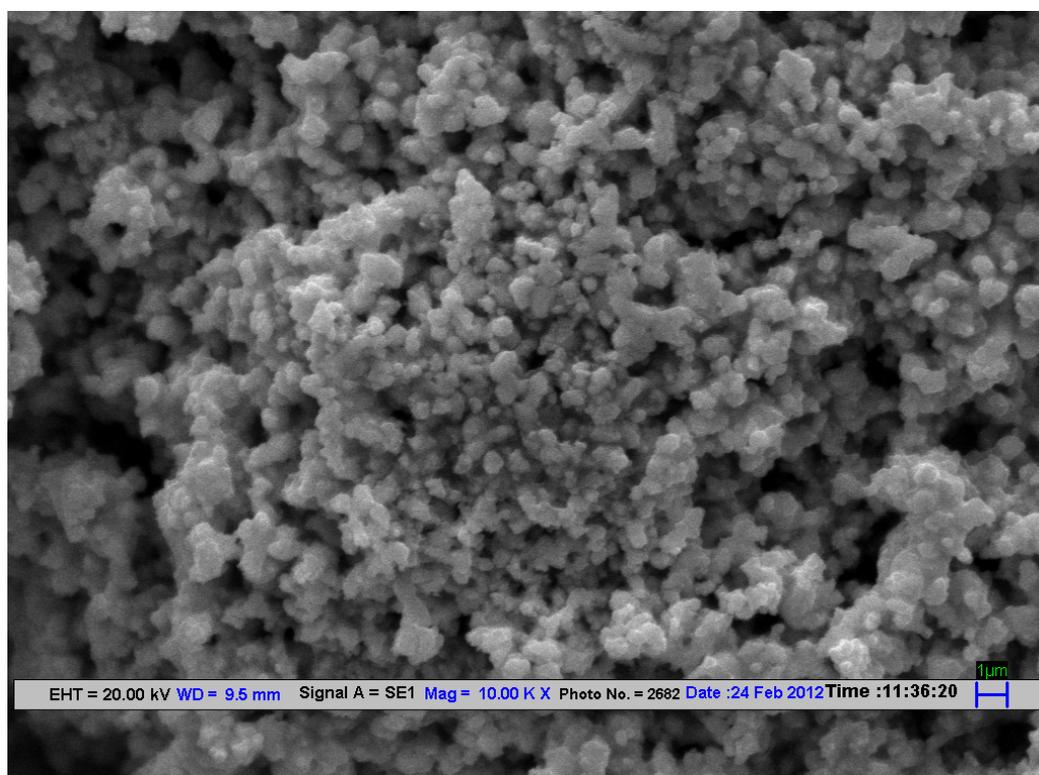
**Fig. S38** SEM Image of PdP$_2$ Nanoparticles obtained from **3**
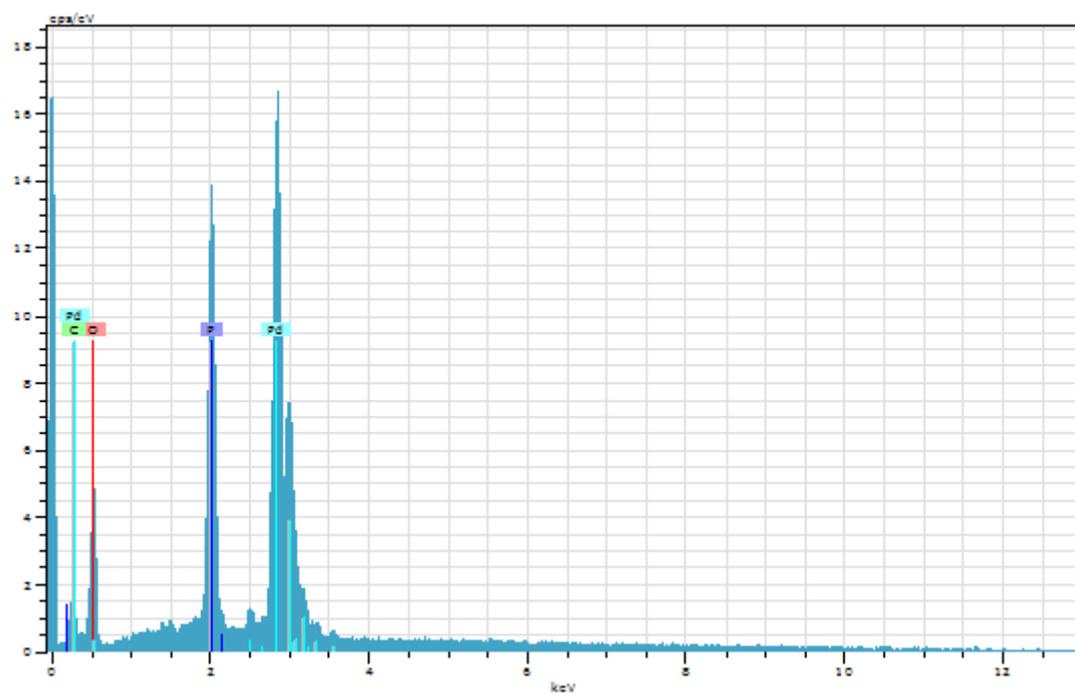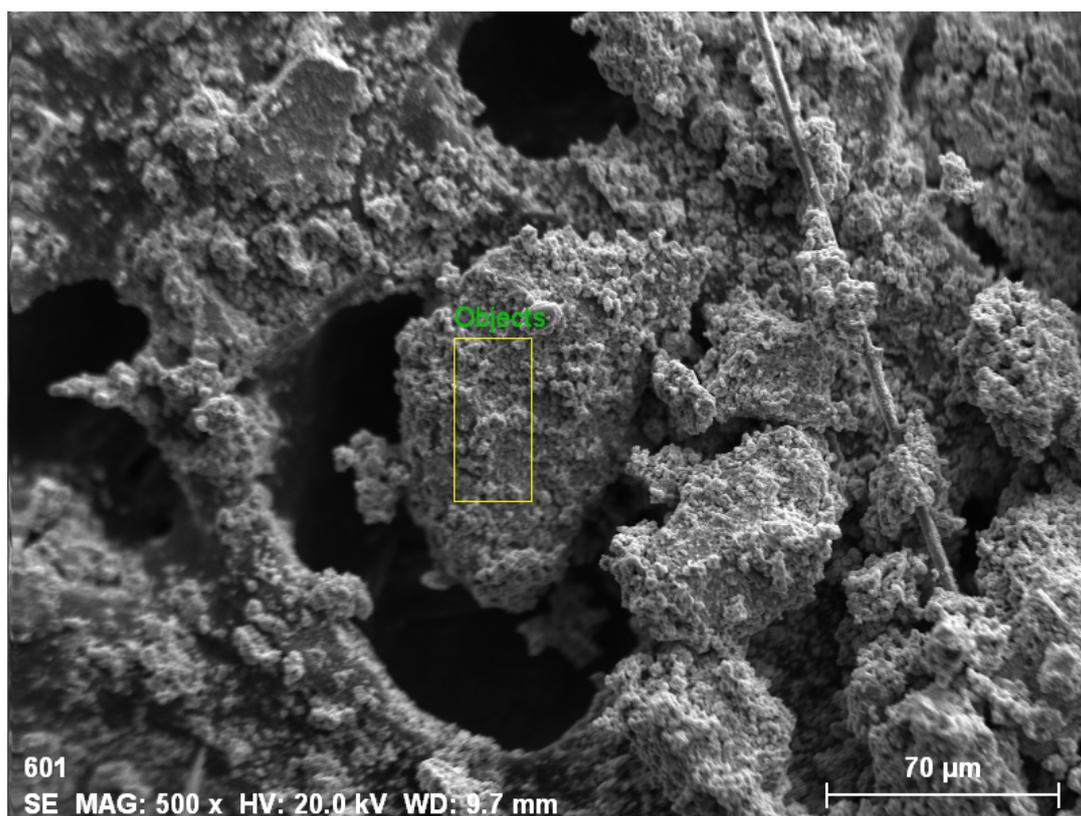
Fig. S39 SEM EDX of PdP$_2$ Nanoparticles obtained from **1**
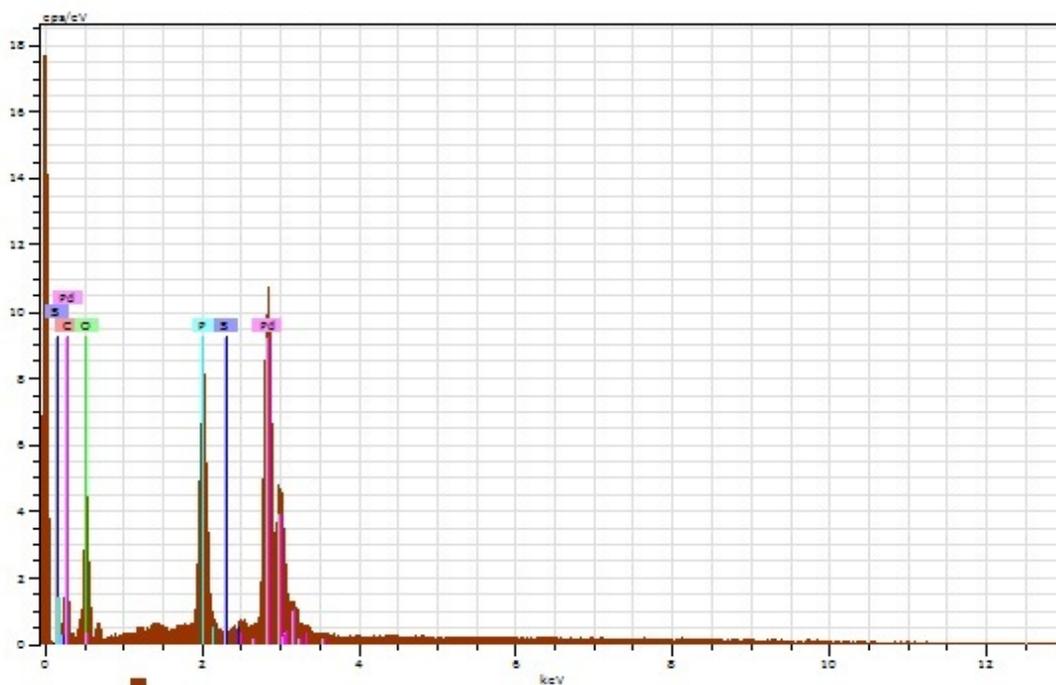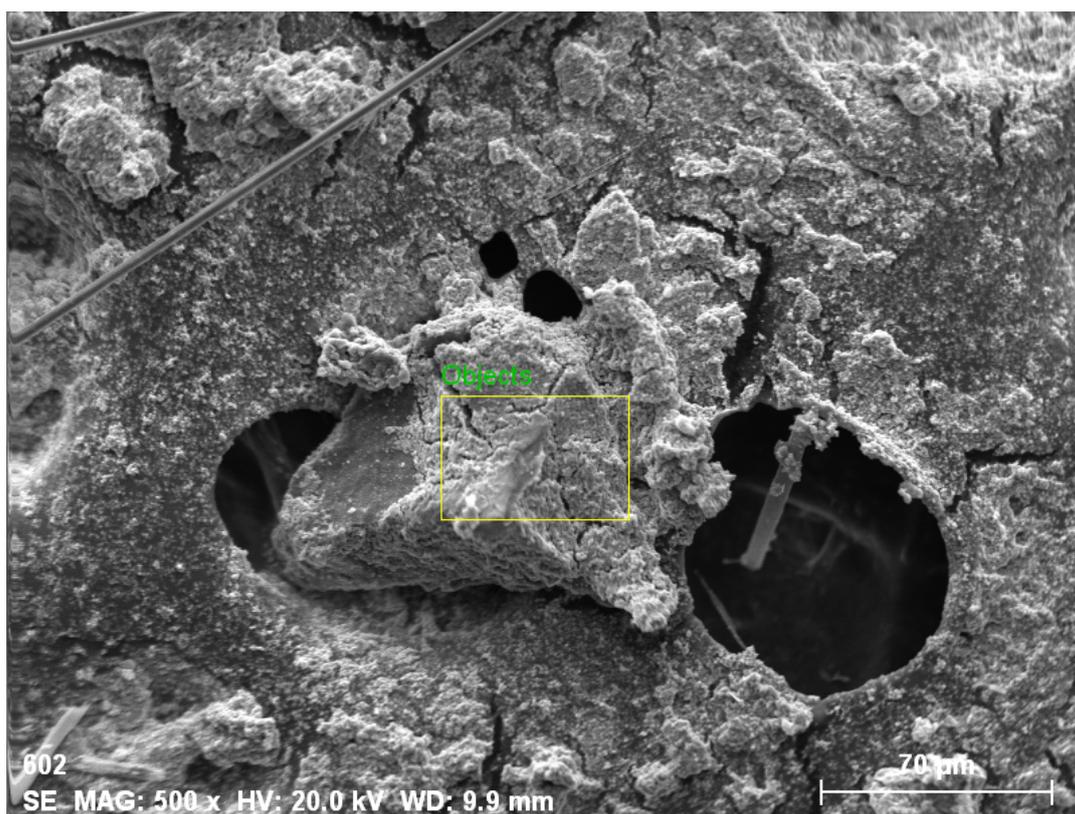
**Fig. S40** SEM EDX of PdP$_2$ Nanoparticles obtained from **2**
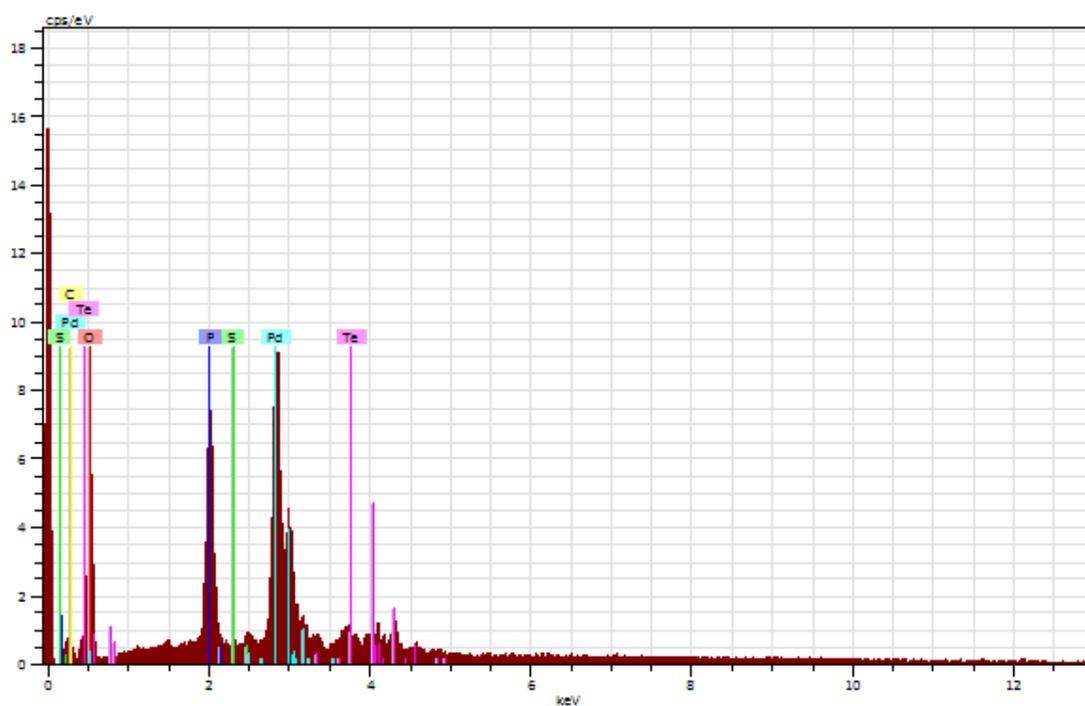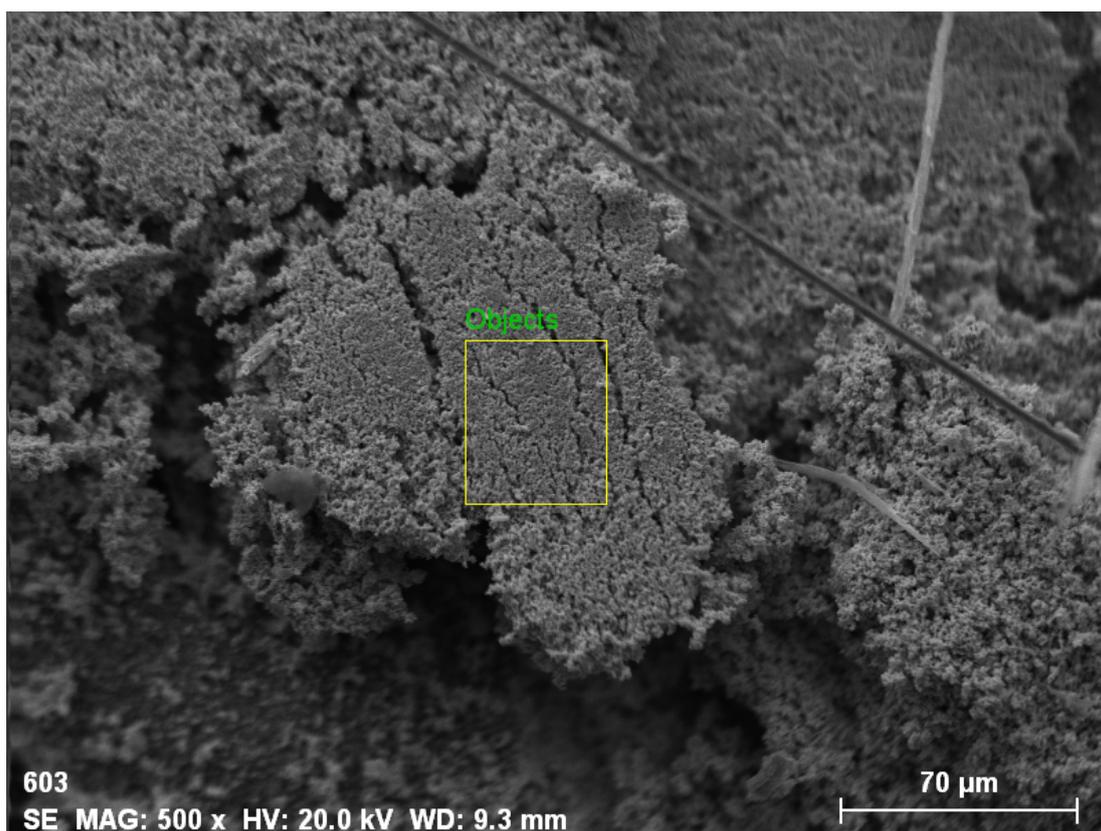
Fig. S41 SEM EDX of PdP_2 Nanoparticles obtained from **3**