List of Supplementary Information

Synthesis and Photocatalytic activity of
Naphthyl-Substituted Photosensitizing BINAP−Palladium Complex

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General. All manipulations were carried out under N_2 atmosphere with use of standard Schlenk techniques. THF, DMSO, DMF, toluene, acetonitrile, CH_2Cl_2, and Et_2O were treated with appropriate drying agents, distilled, and stored under N_2. ^1H, ^{13}C, ^{31}P NMR spectra were recorded on Bruker AVANCE-500 (500 MHz), JEOL JNM-AL400 FT-NMR, and JEOL JNM-270 FT NMR spectrometers. Solvents for NMR measurements ($CDCl_3$, CD_3CN) were dried over molecular sieves, degassed, and stored under N_2. Atmospheric pressure chemical ionization (APCI) and electrospray ionization (ESI) mass spectra were recorded on Bruker MicroTOF II, respectively. [Pd(cod)MeCl] were prepared according to the published procedures [1]. Other chemicals were purchased and used as received.

DFT Study. DFT calculations were performed using the Gaussian-09 Revision D.01 quantum chemistry program package[2] at the B3LYP/LanL2DZ level. We used LanL2DZ pseudo-potential on Pd, 6-31G(d) split-valence basis set on P, N, and C coordinated to Pd, 3-21G on the other C, and H. Geometries of the complexes were optimized without any symmetry constraint. The orbital energies were determined by using minimized singlet geometries to approximate the ground state.

Preparation and spectral data of [(BINAP^{naph})PdMe(MeCN)] (1-Pd).

1 (400 mg, 0.49 mmol) and (COD)PdMeCl (129 mg, 0.49 mmol) were dissolved in CH_2Cl_2 (12 mL) and stirred at room temperature for 1h. The solvent was removed under reduced pressure and resulting solid was washed with ether (3 × 6 mL), and dried in vacuo to give (**1**)PdMeCl (477 mg, 0.49 mmol, >99%) as a pale yellow solid. (**1**)PdMeCl (480 mg, 0.49 mmol) was dissolved in 3 mL CH_2Cl_2 and 7 mL CH_3CN and added $AgBF_4$ solution (95 mg, 0.49 mmol, in 3 mL CH_3CN) and stirred at room temperature for 1h in a Schlenk tube foiled with Al sheet. Resulting mixture was filtered through Celite and the filtrate was concentrated under reduced pressure, precipitated with CH_3CN - Et_2O to give **1-Pd** (467 mg, 0.44 mmol, 88.8%) as a dark yellow solid.

♦ Spectral Data for **1-Pd**.

^1H NMR (500 MHz, CD_3CN, RT, δ/ppm): 8.25 - 6.43 (m, Ar - *H*, 40H), 0.64 (dd, ^2J = 7 Hz, ^2J = 2 Hz, Me - *H*, 3H), CH_3CN proton signal was overlapped with CD_3CN signal.

^{31}P NMR (202 MHz, CD_3CN, RT, δ/ppm): 38.65 (d, $^3J_{P\text{-}P}$ = 42 Hz), 14.97 (d, $^3J_{P\text{-}P}$ = 42 Hz)

^{13}C NMR (125 MHz, CD_3CN, RT, δ/ppm): 140.6 - 122.2 (Ar - C), 13.48 (d, $^3J_{P\text{-}C}$ = 87 Hz, Me - C), CH_3CN carbon signal is overlapped with CD_3CN signal.

ESI-MS : m/z = 984.21466 (M - BF_4), calculated : 984.21403

Anal. Calcd for $C_{63}H_{46}BF_4NP_2Pd$-1.5H_2O: C, 68.84; H, 4.49; N, 1.27. Found: C, 68.98; H, 4.49; N, 1.34.

Preparation and spectral data of [(BINAP)PdMe(MeCN)] (2-Pd).

2 (200 mg, 0.32 mmol) and (COD)PdMeCl (85 mg, 0.32 mmol) were dissolved in 10 mL CH_2Cl_2 and stirred at room temperature for 1h. The solvent was removed from the reaction mixture under reduced pressure. The obtained solid was washed with Et_2O (3 × 3 mL), dried in vacuo to give (**2**)PdMeCl (226 mg, 0.29 mmol, 90%) as a pale yellow solid. (**2**)PdMeCl (215 mg, 0.28 mmol) was dissolved in 2 mL CH_2Cl_2 and 6 mL CH_3CN and added of $AgBF_4$ CH_3CN solution (54 mg, 0.28 mmol) and stirred at room temperature for 1h in a Schlenk tube foiled with Al sheet.. Resulting mixture was filtered through Celite and the filtrate was concentrated under reduced pressure. The resulting solution was precipitated with CH_3CN - Et_2O to give **2-Pd** (230 mg, 0.26 mmol, 96%) as a dark yellow solid.

♦ Spectral Data for **2-Pd**.

^{1}H NMR (500 MHz, CD_3CN, RT, δ/ppm): 7.77 - 6.48 (m, Ar - *H*, 32H), 0.52 (dd, ^2J = 8 Hz, ^2J = 2 Hz, Me - *H*, 3H), CH_3CN proton signal was overlapped with CD_3CN signal.

^{31}P NMR (202 MHz, CD_3CN, RT, δ/ppm): 39.09 (d, $^3J_{P\text{-}P}$ = 43 Hz), 13.80 (d, $^3J_{P\text{-}P}$ = 43 Hz)

^{13}C NMR (125 MHz, CD_3CN, RT, δ/ppm): 140.62 - 122.12 (Ar - C), 13.63 (d, $^3J_{P\text{-}C}$ = 86 Hz, Me - C), CH_3CN carbon signal is overlapped with CD_3CN signal.

ESI-MS : m/z = 784.15151 (M - BF_4), calculated : 784.15143

Anal. Calcd. for $C_{47}H_{38}BF_4NP_2Pd$-$2H_2O$: C, 62.17; H, 4.66; N, 1.54. Found: C, 62.02; H, 4.48; N,1.63.

General procedure for the catalytic polymerization of *p*-methoxystyrene.

Photocatalytic reactions were performed as below. 0.5 mL of a 1 mM CD_3CN solution of catalyst (1 mol%) was added in a 5ϕ quartz NMR tube. 1,1,2,2 - tetrachroloethane (an internalstandard) and a substrate was added in the NMR tube. The system was placed in a water bath, and exposed to 5W LED lamp (λ = 395 nm). The reaction was followed by ^1H NMR after appropriate time intervals.

Figure S1. ^{1}H NMR spectra of **1-Pd** (500MHz, CD_3CN).

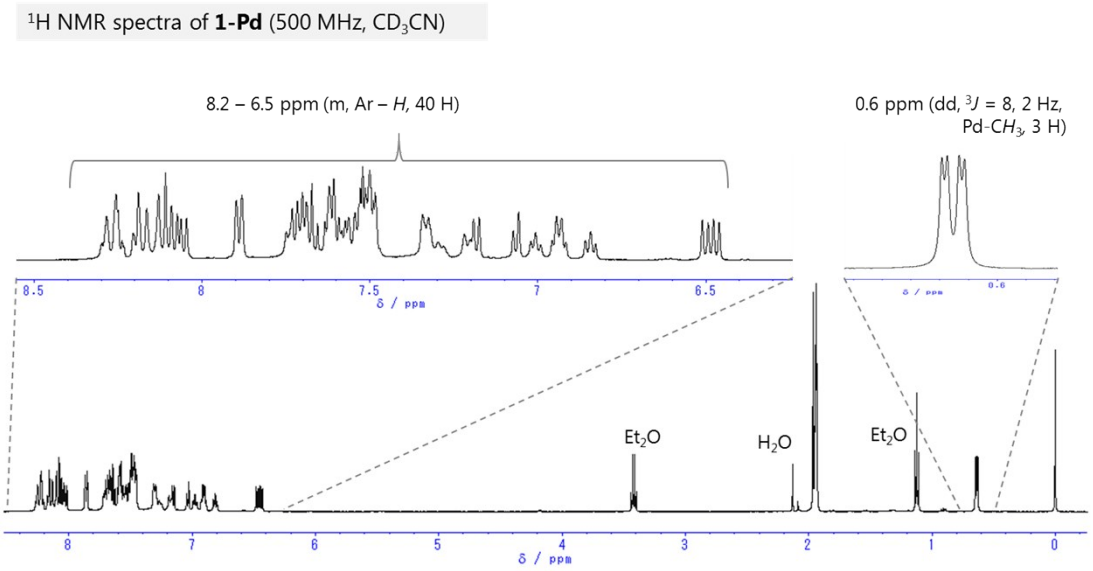


Figure S2. ^{31}P and ^{13}C NMR spectra of **1-Pd**.

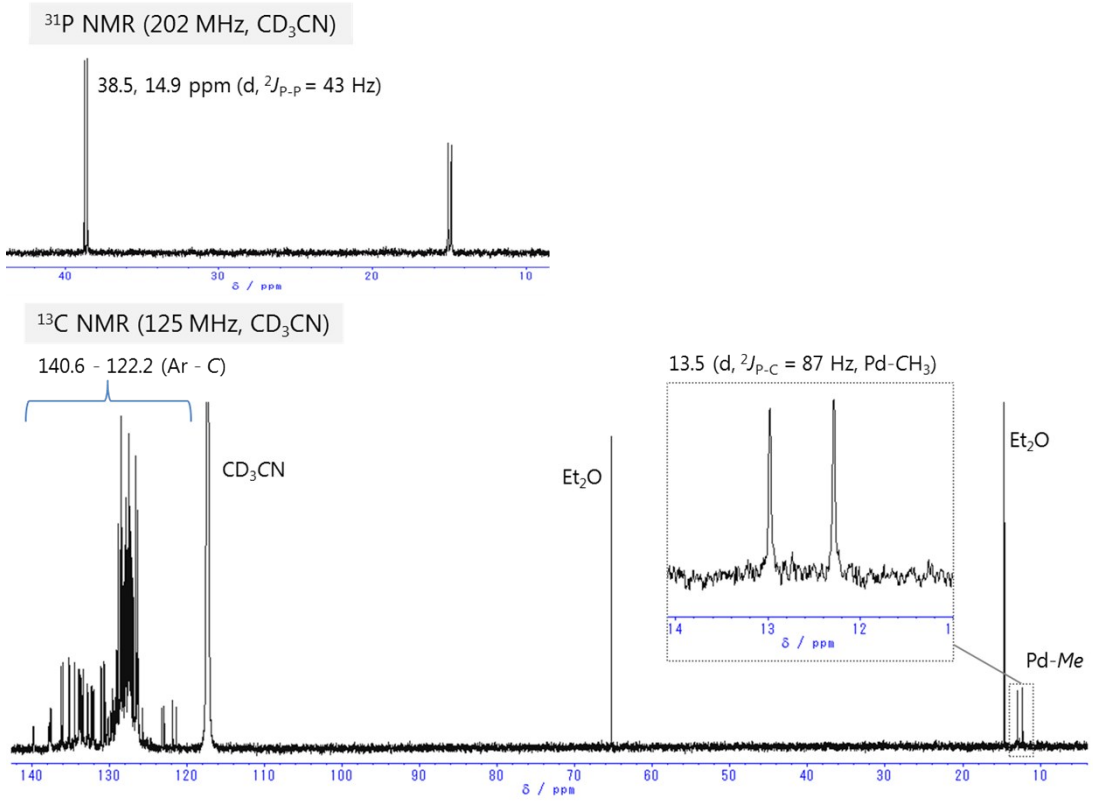


Figure S3. ^{1}H NMR spectra of **2-Pd**.

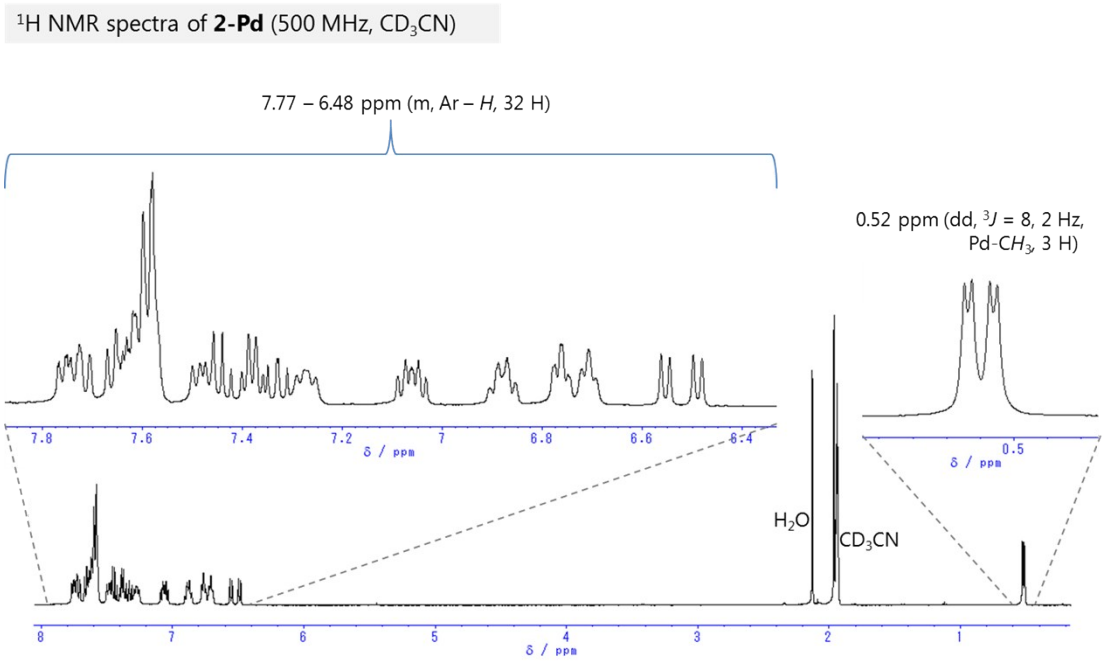


Figure S4. ^{31}P and ^{13}C NMR spectra of **2-Pd**.

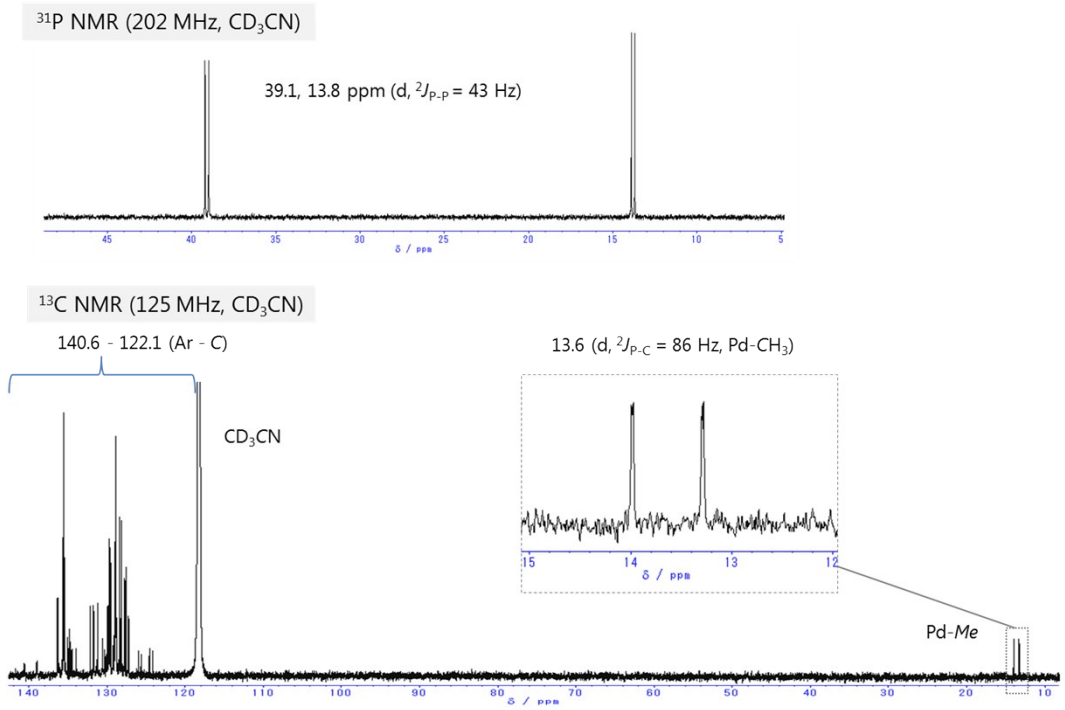
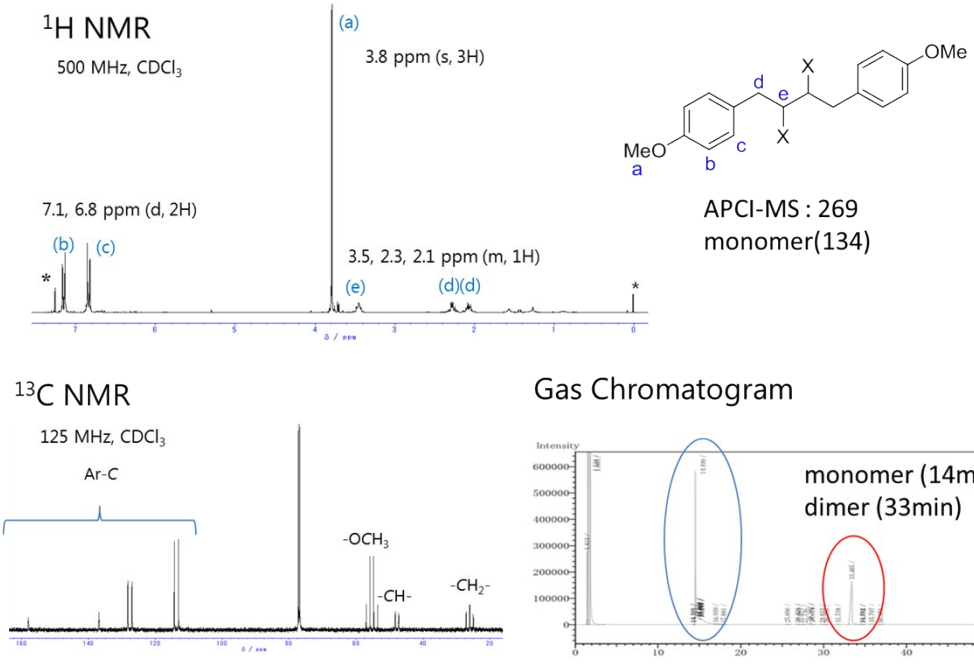


Figure S5. NMR and GC spectral data of dimer.



^{1}H NMR (500MHz, $CDCl_3$, RT, δ/ppm): 7.13 (d, J = 5 Hz, 2H, Ar-H), 6.82 (d, J = 5 Hz, 2H, Ar-H), 3.77 (s, 3H, OMe-H), 3.44 (t, J = 15 Hz, 1H), 2.27 (m, 1H), 2.06 (m, 1H).
^{13}C NMR (125MHz, $CDCl_3$, RT, δ/ppm): 158.0 (s), 136.9 (s), 127.6 (d), 113.7 (d), 55.29(q), 47.8 (d), 26.0 (t).
APCI-MS : 269.1852

Figure S6. Reaction of **1-Pd** toward 4-methoxystyrene under irradiated and dark conditions. (1 mol% CD_3CN solution in 5f quartz NMR tube, λ_{irr} = 395 nm. Plot of polymer yield vs. time).

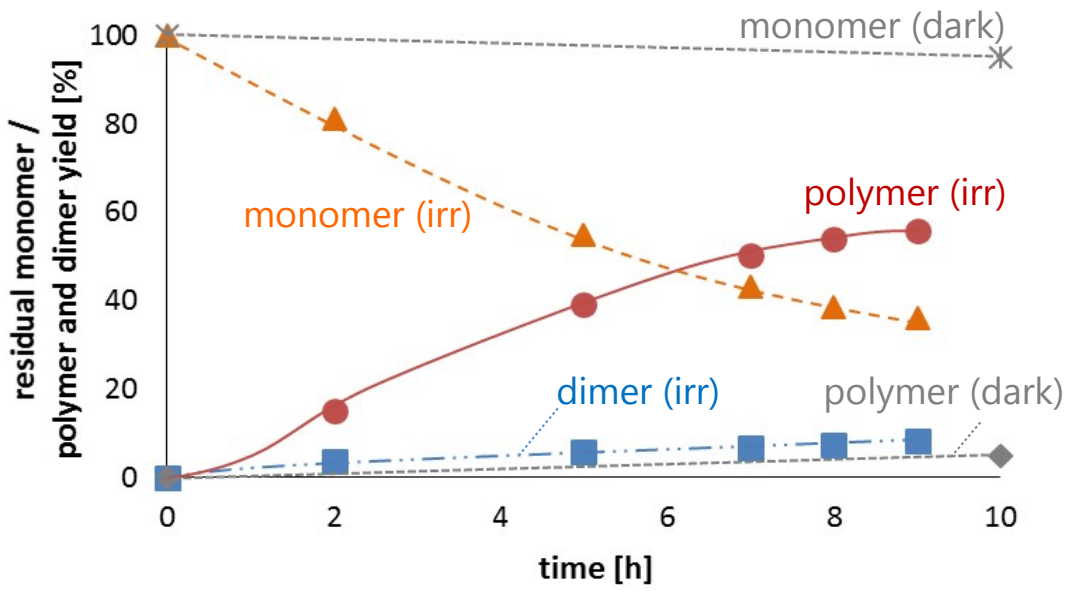
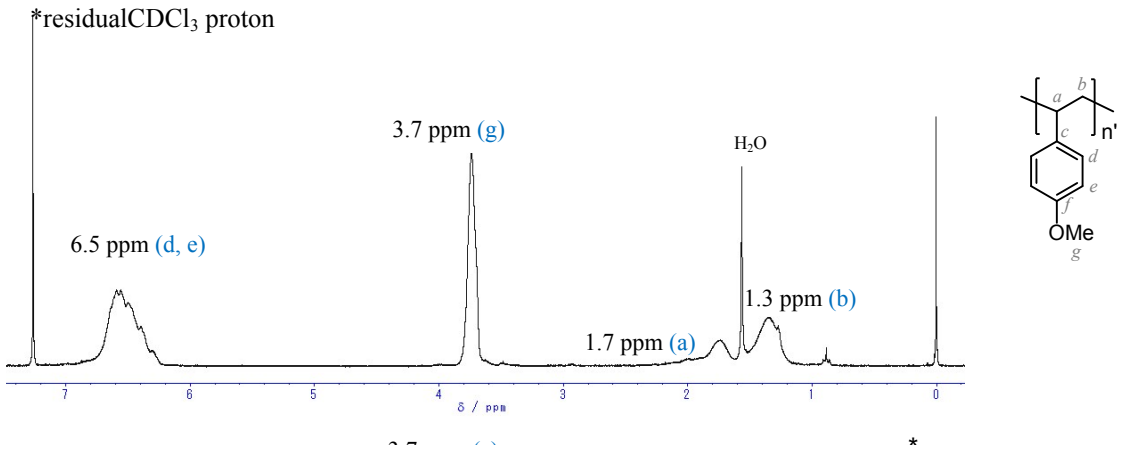


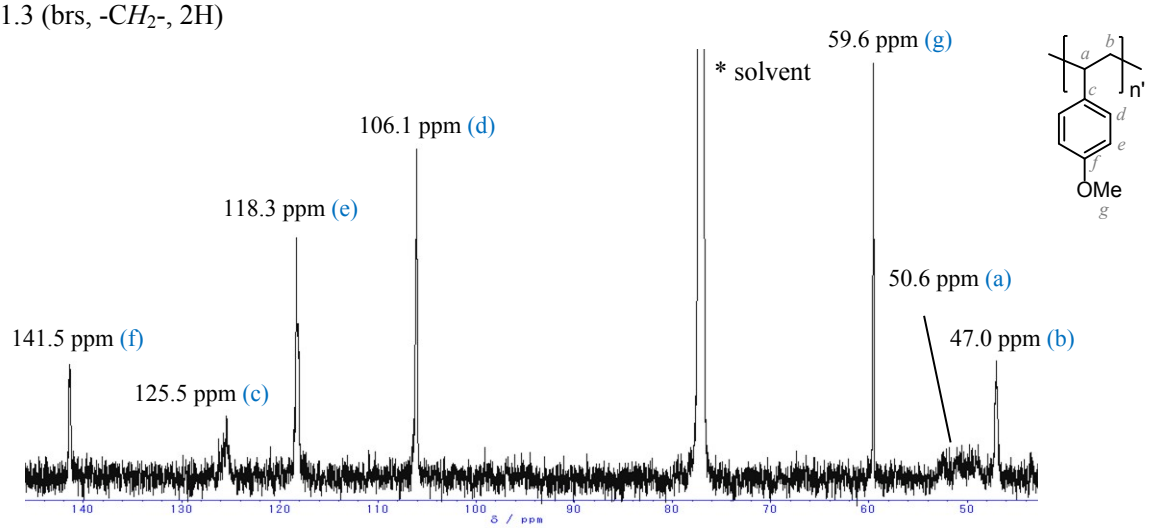
Figure S7. NMR spectra of poly(*p*-methoxystyrene) (a) ^{1}H NMR spectra (270 MHz, $CDCl_3$, r.t). (b) ^{13}C NMR spectra (100 MHz, $CDCl_3$, r.t.).

(a)



^{1}H NMR (500MHz, $CDCl_3$, RT, δ/ppm): 6.5 (brs, Ar-*H*, 4H), 3.7 (brs, -OC*H*$_3$, 3H), 1.7 (brs, -C*H*-, 1H), 1.3 (brs, -C*H*$_2$-, 2H)

(b)



^{13}C NMR (125MHz, $CDCl_3$, RT, δ/ppm): 141.5 (s), 125.5 (brs), 118.3 (s), 106.1 (s), 59.6 (s), 50.6 (m), 47.0 (s)

Figure S8. Plot of polymer yield vs. time for the samples with various catalyst concentrations (λ_{irr} = 395 nm in CD_3CN solution).

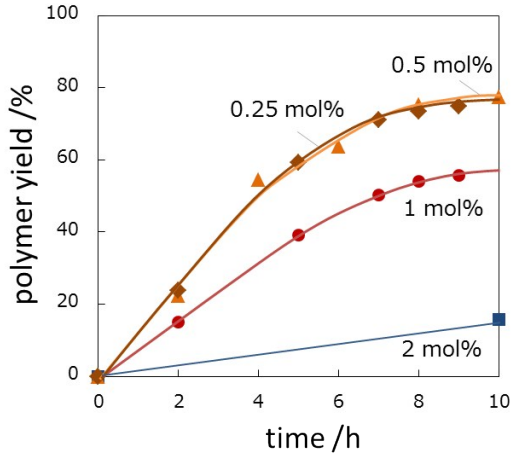


Figure S9. Comparison of catalyst activity between **1-Pd** and **2-Pd** (1 mol% CD_3CN solution, λ_{irr} = 395 nm. Plot of polymer yield vs. time).

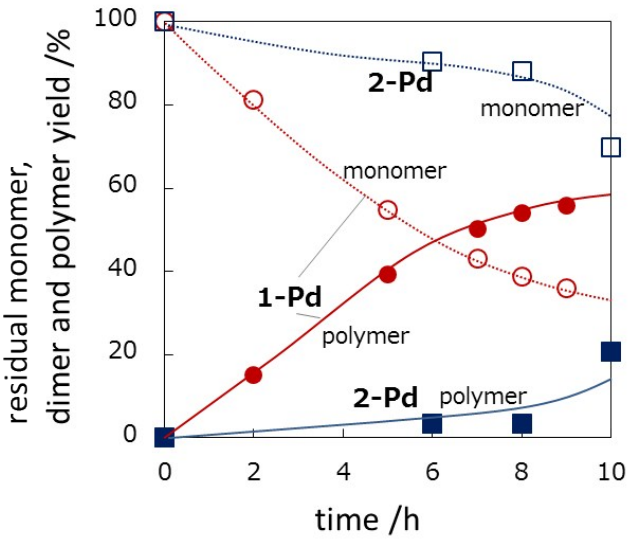


Figure S10. ESI spectra of the reaction mixture (CD_3CN).

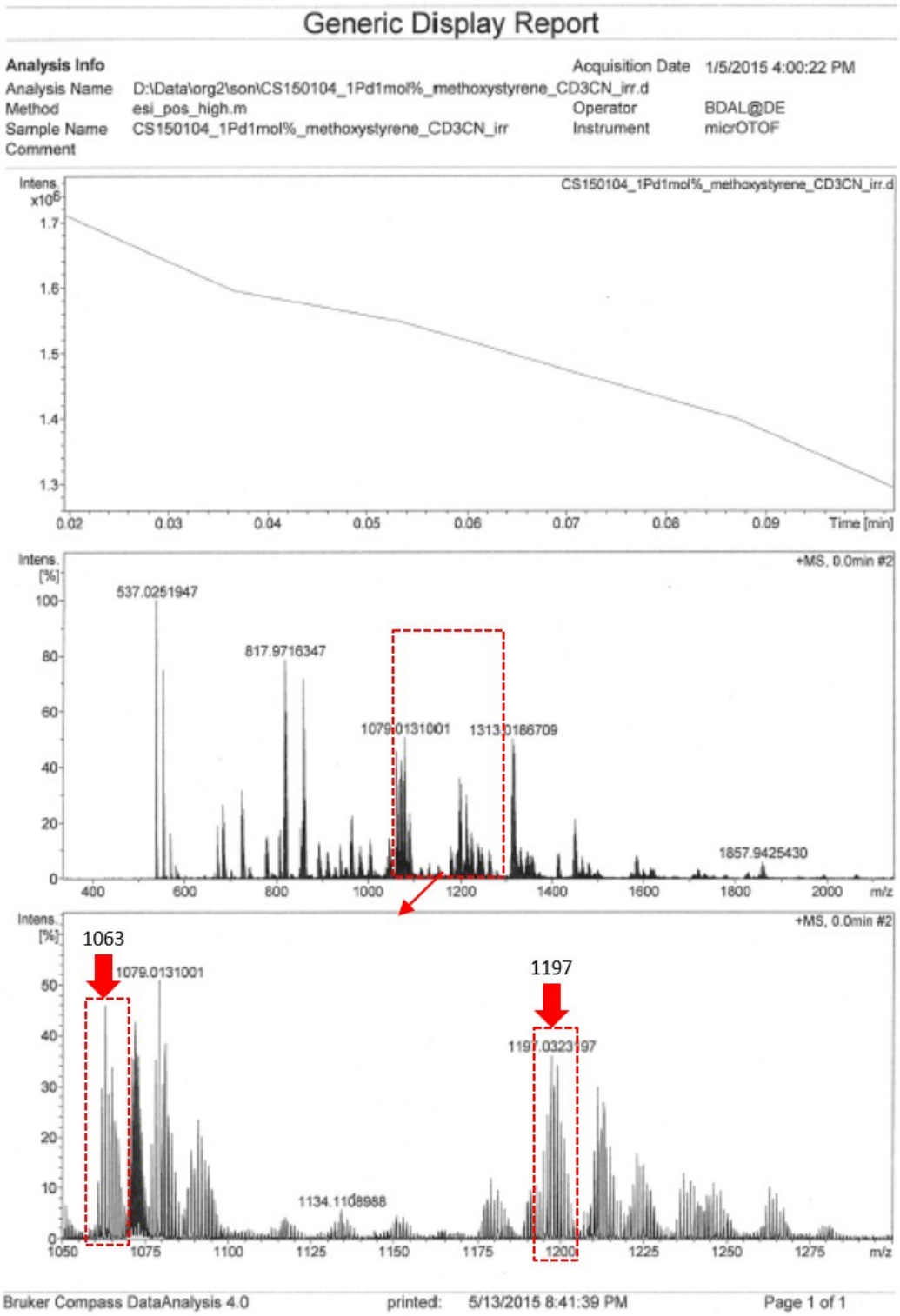


Table S1. Crystal data and structure refinement for **1.**

Empirical formula	C60 H40 P2	
Formula weight	822.86	
Temperature	93(2) K	
Wavelength	0.71075 Å	
Crystal system	monoclinic	
Space group	C2	
Unit cell dimensions	a = 19.756(11) Å	α= 90°.
	b = 10.922(6) Å	β= 92.043(7)°.
	c = 10.065(5) Å	γ = 90°.
Volume	2170(2) $Å^3$	
Z	2	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	0.141 mm^{-1}	
F(000)	860	
Crystal size	0.50 x 0.40 x 0.20 mm^3	
Theta range for data collection	3.61 to 27.50°.	
Index ranges	-25<=h<=25, -14<=k<=14, -12<=l<=13	
Reflections collected	11446	
Independent reflections	4954 [R(int) = 0.0199]	
Completeness to theta = 27.50°	99.4 %	
Max. and min. transmission	0.9723 and 0.9326	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4954 / 1 / 360	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.0968	
R indices (all data)	R1 = 0.0386, wR2 = 0.0979	
Absolute structure parameter	0.00(7)	
Largest diff. peak and hole	1.418 and -0.209 $e.Å^{-3}$	

Figure S11. ORTEP diagram of **1**.

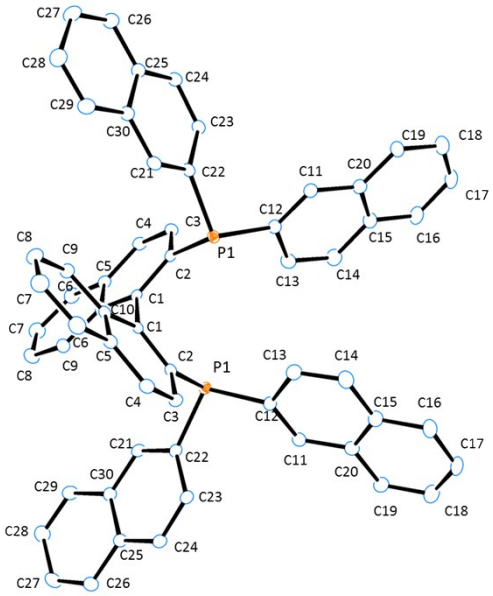


Figure S12. ^{1}H NMR chart of **1-Pd**

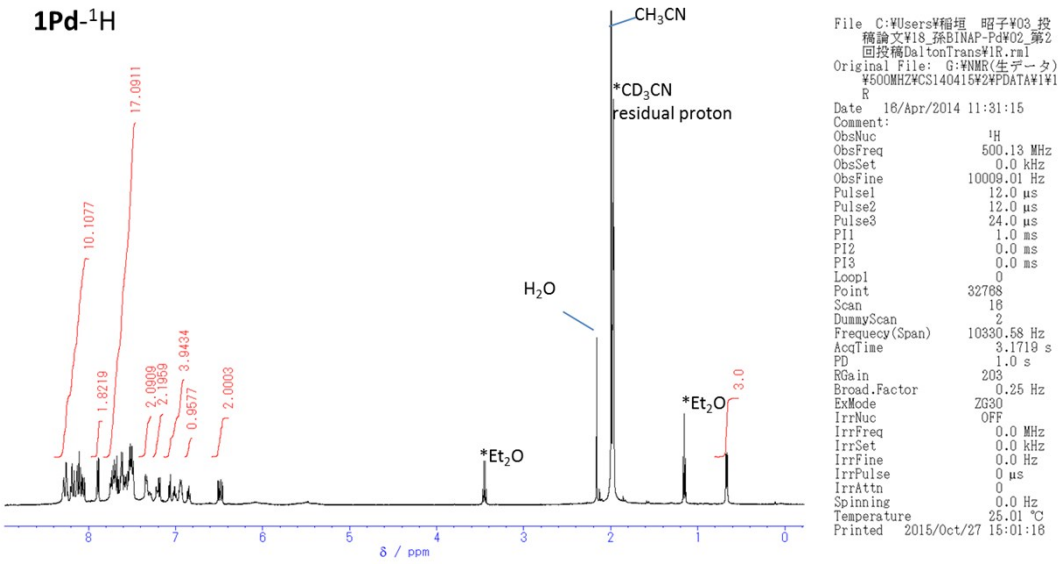


Figure S13. ^{13}C NMR chart of **1-Pd**

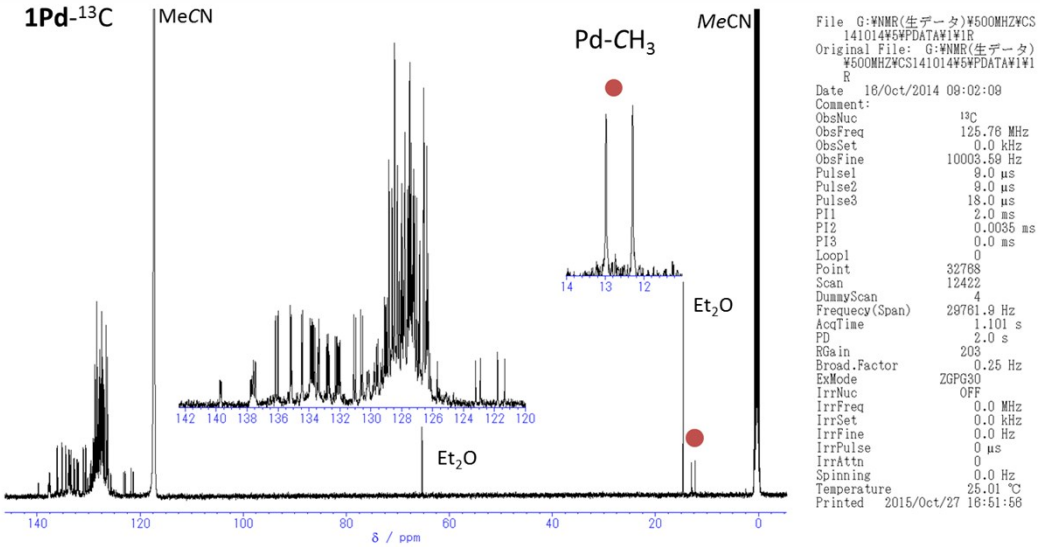


Figure S14. ^{1}H NMR chart of **2-Pd**

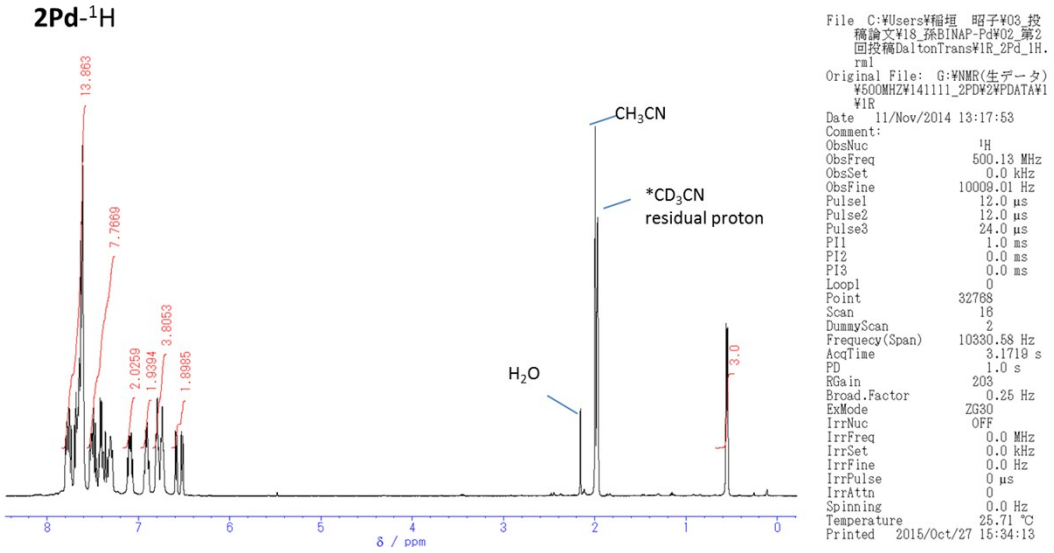


Figure S15. ^{13}C NMR chart of **2-Pd**

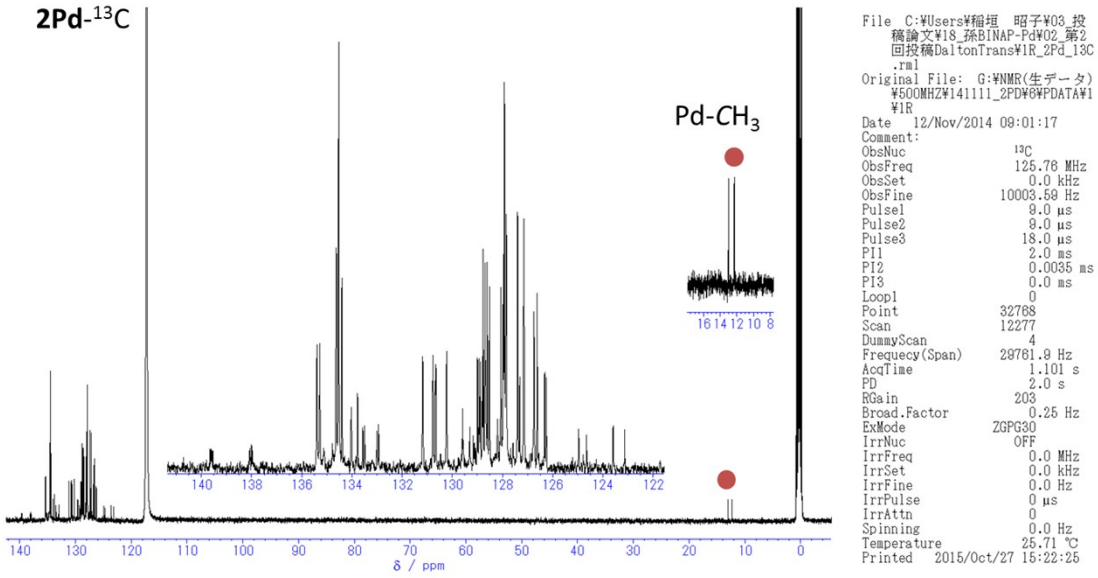


Table S2.Optimized geometry of **1-Pd**

atom	x	y	z
Pd	0.1115300000	-0.1774610000	1.8486590000
P	-1.7543680000	-0.1704250000	0.5041120000
P	1.7071620000	0.1594070000	-0.0082000000
C	-1.1215210000	-0.7691270000	3.4302120000
N	1.6759760000	-0.0495350000	3.3105080000
C	2.5690600000	-0.0180450000	4.0411540000
C	3.7232510000	0.0027110000	4.9348120000
C	-1.5591580000	0.9496010000	-0.9567280000
C	-2.2593130000	2.1948260000	-0.9257380000
C	-2.0923850000	3.1336920000	-1.9118400000
C	-1.2161630000	2.8997520000	-3.0003330000
C	-1.0403650000	3.8592830000	-4.0351170000
C	-0.1982810000	3.6051840000	-5.0917470000
C	0.5083720000	2.3784880000	-5.1556590000
C	0.3626410000	1.4315920000	-4.1681770000
C	-0.5040840000	1.6572010000	-3.0584920000
C	-0.6850460000	0.6800990000	-2.0154340000
C	0.0610820000	-0.6180570000	-2.1709120000
C	1.2225010000	-0.8969050000	-1.4461260000
C	1.9523990000	-2.0916220000	-1.7167470000
C	1.5283910000	-2.9815700000	-2.6725480000
C	0.3539010000	-2.7364140000	-3.4283240000
C	-1.2082210000	-3.3642880000	-5.1827820000
C	-1.9356550000	-2.1688810000	-4.9571220000
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C	-6.6231400000	2.1460340000	3.3482180000
C	-6.4642560000	3.2437230000	4.1625910000
C	-5.1817360000	3.8224050000	4.3497960000
C	-4.0804070000	3.2933160000	3.7183570000
C	-4.2099750000	2.1599930000	2.8663490000
C	-3.0956870000	1.5868860000	2.2008770000
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C	-1.7636590000	-2.9448640000	0.5444360000
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C	2.7021710000	4.4623460000	-1.4647690000
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C	4.5614560000	0.2605800000	0.2847930000
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C	5.9421000000	-3.9120750000	2.8199690000
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C	4.6548870000	-2.2049010000	1.6598640000
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C	-0.0887870000	-3.6402960000	-4.4336750000

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H	3.4548560000	-0.4134930000	5.9112770000
H	4.5288980000	-0.5964080000	4.4955580000
H	4.0750580000	1.0310900000	5.0692180000
H	2.8585780000	-2.2922840000	-1.1627310000
H	2.0998230000	-3.8822790000	-2.8690760000
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H	-1.5353530000	-4.0536610000	-5.9518040000
H	-2.8094620000	-1.9549280000	-5.5613340000
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H	1.1663840000	2.1856140000	-5.9947280000
H	-0.0730870000	4.3377750000	-5.8799800000
H	-1.5870630000	4.7936960000	-3.9743210000
H	-2.6413960000	4.0680650000	-1.8704730000
H	-2.9422350000	2.3955750000	-0.1135780000
H	-2.1150230000	2.0229720000	2.3679760000
H	-4.6432380000	-0.9650650000	0.5622820000
H	-6.6006380000	-0.0156010000	1.7031610000
H	-3.0985130000	3.7326830000	3.8598020000
H	-7.6017650000	1.7012610000	3.2058910000
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H	-7.3200730000	3.6739650000	4.6686400000
H	-1.0411390000	-2.8476540000	1.3484030000
H	-3.5473350000	-1.0703330000	-1.6737300000
H	-4.3370380000	-3.3012120000	-2.3527750000
H	-1.0053800000	-5.3103130000	1.6269450000
H	-4.3226640000	-5.7729290000	-2.0609950000
H	-1.8106600000	-7.5471970000	0.9430790000
H	-3.4629970000	-7.7756620000	-0.8948300000
H	4.5186060000	1.2052800000	-0.2403180000
H	6.6756750000	0.3543420000	0.5764420000
H	3.8229810000	-4.0123390000	2.5204350000
H	7.9986690000	-1.4011230000	1.7559350000
H	5.9953220000	-4.8566620000	3.3479050000
H	8.0752010000	-3.5562080000	2.9650110000
H	1.0757520000	2.7611250000	1.0420920000
H	3.0775590000	1.2066180000	-2.4432040000
H	3.6474940000	3.4971040000	-3.1558310000
H	0.9872630000	5.2106660000	1.4227560000
H	3.5847470000	5.9517480000	-2.7625880000
H	1.5681590000	7.5046700000	0.7020310000
H	2.8641300000	7.8720780000	-1.3828680000

SCF energy : -3279.43079059 Hartree

Table S3. Optimized geometry of **2-Pd**

atom	x	y	z
Pd	1.1640380000	1.8972590000	-0.0581060000
P	-1.1060330000	1.5886210000	-0.2488410000
P	1.6829210000	-0.5057340000	0.1341770000
C	0.8010900000	3.9510890000	0.1019060000
N	3.2443180000	2.4137560000	-0.0822100000
C	4.3642170000	2.6923560000	-0.0940990000
C	5.7888430000	3.0096460000	-0.0831800000
C	-1.5112400000	0.0306920000	-1.1615340000
C	-1.9476820000	0.1645800000	-2.5155700000
C	-2.1574280000	-0.9336810000	-3.3099360000
C	-1.9520920000	-2.2440190000	-2.8113000000
C	-2.1749050000	-3.3920460000	-3.6202870000
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C	-1.5708020000	-4.8244790000	-1.7683480000
C	-1.3423280000	-3.7336570000	-0.9612970000
C	-1.5242110000	-2.4075000000	-1.4526110000
C	-1.2986860000	-1.2461920000	-0.6304460000
C	-0.8818920000	-1.4953740000	0.7947190000
C	-1.8683610000	-2.0109640000	1.7045500000
C	-3.2235740000	-2.2282710000	1.3188550000
C	-4.1430830000	-2.7231710000	2.2150320000
C	-3.7635560000	-3.0291150000	3.5461340000
C	-2.4636160000	-2.8392640000	3.9514120000
C	-1.4867250000	-2.3352930000	3.0487250000
C	-0.1333770000	-2.1671940000	3.4367300000
C	0.8015210000	-1.6905990000	2.5515490000
C	0.4412170000	-1.3404750000	1.2167580000
C	-1.9889710000	1.5795690000	1.3431710000
C	-3.3079010000	1.0989190000	1.4388850000
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C	-3.3767200000	1.7412860000	3.7711180000
C	-2.0645820000	2.2117310000	3.6853130000
C	-1.3704750000	2.1317840000	2.4773320000
C	-1.9234310000	2.9026770000	-1.2418360000
C	-1.2712460000	3.3855940000	-2.3936480000
C	-1.8696480000	4.3637920000	-3.1858810000
C	-3.1172490000	4.8861910000	-2.8309680000
C	-3.7612910000	4.4267950000	-1.6821400000
C	-3.1714000000	3.4387230000	-0.8886450000
C	1.8950860000	-1.5247740000	-1.3635650000
C	2.0698850000	-0.8773220000	-2.5977290000
C	2.3044740000	-1.6228120000	-3.7546450000
C	2.3631020000	-3.0164690000	-3.6880610000
C	2.1813610000	-3.6681730000	-2.4646800000
C	1.9462410000	-2.9291320000	-1.3054610000
C	3.2776130000	-0.6982910000	1.0381050000
C	4.2881440000	-1.5758300000	0.6138680000
C	5.5014370000	-1.6441830000	1.3054930000
C	5.7206140000	-0.8440080000	2.4274810000
C	4.7224520000	0.0370310000	2.8576160000
C	3.5148740000	0.1170600000	2.1642500000
H	-0.2194430000	4.2173210000	0.3850530000
H	1.5113070000	4.2895060000	0.8659760000
H	1.0449510000	4.3878460000	-0.8730550000
H	6.3098170000	2.3070750000	0.5769170000
H	6.2012180000	2.9236670000	-1.0942210000
H	5.9459160000	4.0308800000	0.2798450000
H	1.8297550000	-1.5835790000	2.8673980000
H	0.1593040000	-2.4341440000	4.4464430000
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H	-3.5181690000	-2.0095580000	0.3015920000
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H	-2.1684200000	-5.5264840000	-3.7309440000
H	-2.4997220000	-3.2493130000	-4.6449670000
H	-2.4957880000	-0.8077600000	-4.3326520000
H	-2.1266150000	1.1507530000	-2.9179920000

H	2.7523690000	0.8142110000	2.4965130000
H	4.8837850000	0.6575020000	3.7317950000
H	6.6582730000	-0.9077350000	2.9669030000
H	6.2708070000	-2.3284740000	0.9676100000
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H	-1.3604500000	4.7258730000	-4.0712340000
H	-3.5777990000	5.6527950000	-3.4423990000
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H	-3.7858320000	0.6508010000	0.5758820000
H	-5.0070510000	0.8029650000	2.7197190000
H	-3.9141060000	1.8032610000	4.7097880000
H	-1.5822150000	2.6392560000	4.5561880000
H	-0.3517990000	2.4964730000	2.4083870000

SCF energy : -2668.24628571 Hartree

Figure S16, Molecular orbital diagram of **1-Pd** (left) and **2-Pd** (right).

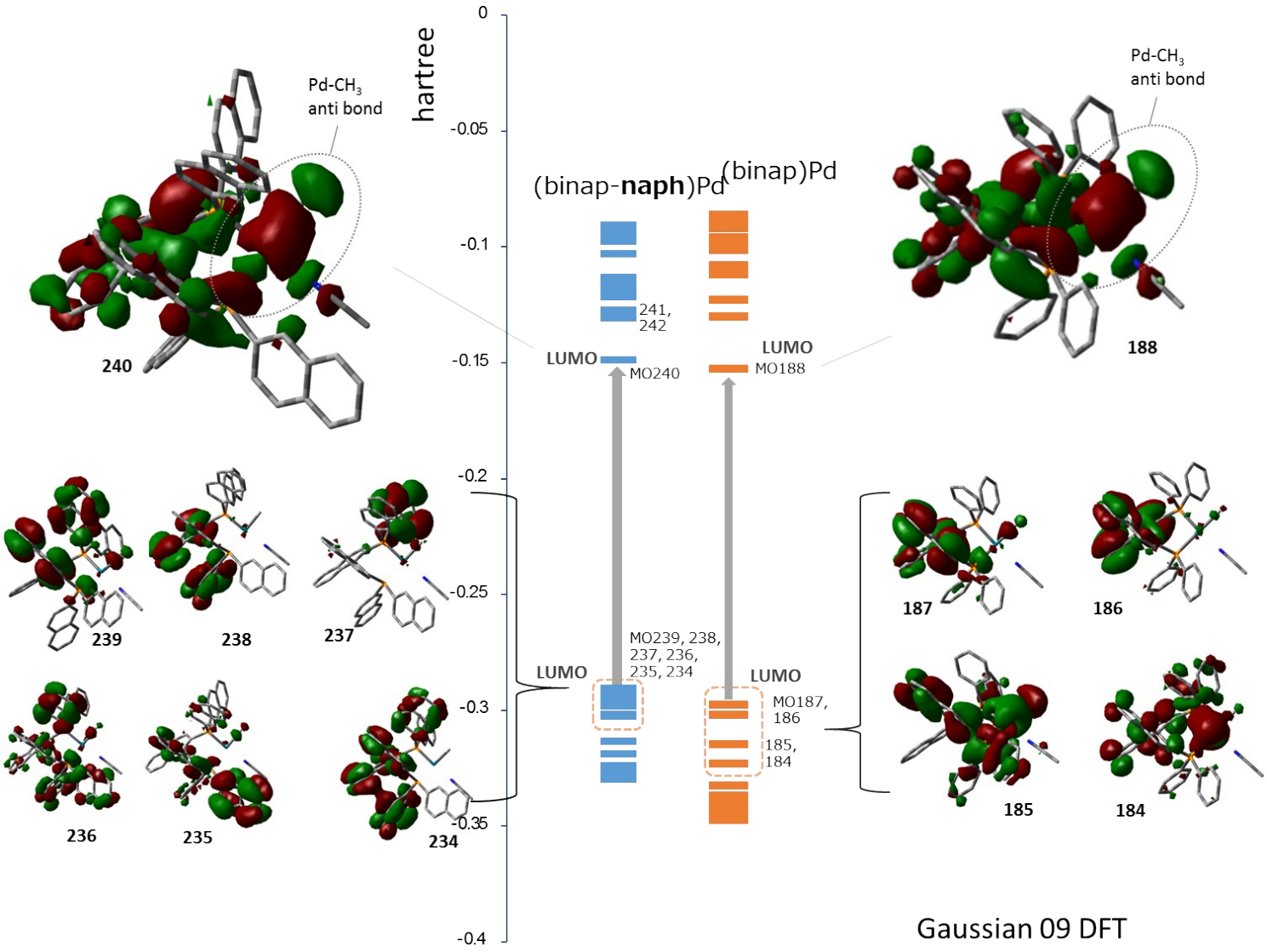


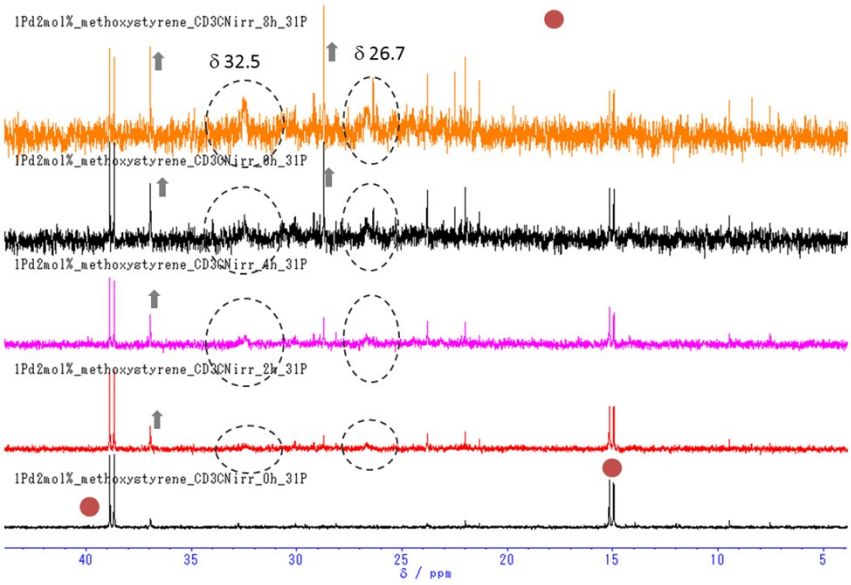
Table S4. TDDFT calculation result (**1-Pd**)

state	Energy /eV (wavelength /nm)	f	Excitation with oscillator strength
1	3.4800 eV (356.28 nm)	f=0.0037	236 ->**240**: 0.16379 238 ->**240**: -0.24985 **239** ->**240**: 0.62427
2	3.5868 eV (345.67 nm)	f=0.0170	236 ->**240**: -0.15368 238 ->**240**: 0.59532 **239** ->**240**: 0.29695
3	3.7157 eV (333.67 nm)	f=0.0053	232 ->**240** : 0.11540 236 ->**240**: -0.25578 237 ->**240**: 0.58927 238 ->**240**: -0.17260
4	3.7583 eV (329.90 nm)	f=0.0153	236 ->**240**: 0.57257 237 ->**240**: 0.33770 238 ->**240**: 0.18364
5	3.8934 eV (318.45 nm)	f=0.0007	233 ->**240**: 0.11554 234 ->**240**: 0.63546 235 ->**240**: -0.13199 **239** ->241: -0.11331
6	3.9457 eV (314.22 nm)	f=0.0400	233 ->**240**: 0.24050 235 ->**240**: 0.61640

Table S5. TDDFT calculation result (**2-Pd**)

state	Energy /eV (wavelength /nm)	f	Excitation with oscillator strength
1	3.5466 eV (349.59 nm)	f=0.0067	**187** ->**188**: 0.68289
2	3.7476 eV (330.84 nm)	f=0.0301	186 ->**188**: 0.66739 **187** ->189: 0.11408
3	3.9228 eV (316.06 nm)	f=0.0522	176 ->**188**: -0.10815 182 ->**188**: -0.10172 184 ->**188**: -0.41679 185 ->**188**: 0.41714 186 ->**188**: -0.13182
4	4.0612 eV (305.29 nm)	f=0.0500	174 ->**188**: 0.10233 184 ->**188**: 0.38823 185 ->**188**: 0.50791 186 ->189: 0.11721 **187** ->189: -0.11015
5	4.2070 eV (294.71 nm)	f=0.0050	186 ->**188**: -0.10449 **187** ->189: 0.66084
6	4.2972 eV (288.52 nm)	f=0.0349	186 ->189: 0.66705

Figure S17, ^{31}P NMR time course in the catalytic reaction of **1-Pd** with *p*-methoxystyrene



File G:¥NMR(生データ)¥500MHZ¥CS150104_2¥2¥PDATA¥1¥1R
Original File: G:¥NMR(生データ)¥500MHZ¥CS150104_2¥10¥PDATA¥1¥1r
Date 04/Jan/2015 10:18:14
Comment: 1Pd2mol%_methoxystyrene_CD3CNirr_0h_31P

ObsNuc	^{31}P
ObsFreq	202.46 MHz
ObsSet	0.0 kHz
ObsFine	9993.888 Hz
Pulse1	11.7 µs
Pulse2	11.7 µs
Pulse3	23.4 µs
PI1	2.0 ms
PI2	0.0 ms
PI3	0.0 ms
Loop1	0
Point	131072
Scan	64
DummyScan	4
Frequecy(Span)	81521.74 Hz
AcqTime	1.6078 s
PD	2.0 s
RGain	203
Broad.Factor	0.25 Hz
ExMode	ZGPG30
IrrNuc	OFF
IrrFreq	0.0 MHz
IrrSet	0.0 kHz
IrrFine	0.0 Hz
IrrPulse	0 µs
IrrAttn	0
Spinning	0.0 Hz
Temperature	25.01 ℃
Printed	2015/Oct/27 20:13:44

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