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SUPPLEMENTARY MATERIAL TO

Catalytic investigation of Pd(II) complexes over Heck–Mizoroki reaction: Tailored synthesis, characterization and density functional theory

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ISOLATED YIELDS AND SPECTROSCOPIC DATA OF SYNTHESIZED COMPOUNDS

2-((E)-(p-tolylimino)methyl)-6-methoxyphenol (L_1)

M.p.: 102 ºC; Yield: 1.115 g (92.60 %). Electronic spectra λ_{max} / nm (ε / mol L^{-1} cm^{-1}) in DMSO: 240 (1220), 360 (385). Selected infrared absorption (KBr, cm^{-1}): ν(O-H), 3217; ν(C-H), 2931; ν(HC=N), 1627; ν(C=C), 1454; ν(C-O), 1265; $\nu(-OCH_3)_{asym}$, 1172; $\nu(-OCH_3)_{sym}$, 1091; $\gamma(C-H)_{in\ plane}$, 1057; $\gamma(C-H)_{out\ plane}$, 740. ^{1}H-NMR spectra (400 MHz, CH_3CN, δ / ppm): (O-H), 13.37 (s, 1H); δ (HC=N), 8.93 (s, 1H), δ $(Ar-H)_{p\text{-}toluidine}$, 7.32 (m, 2H), 7.27 (m, 2H), δ $(Ar-H)_{Vanillin}$, 7.23 (dd, J = 10.6 Hz, 2 Hz, 1H), 7.12 (dd, J = 10.8 Hz, 2.0 Hz, 1H), 6.89 (t, J = 10.4 Hz, 10.4 Hz, 1H); $(-OCH_3)$, 3.42 (s, 3H); $(-CH_3)$, 2.33 (s, 3H). ^{13}C-NMR spectra (400 MHz, CH_3CN, δ / ppm): $(>C=N)_{imine}$, 161.5, (C-OH), 151.7, (Ar-C),150.9 (C_1), 148.1 (C_2), 134.4 (C_3), 128.0 (C_4), 123.7 (C_5), 119.5 (C_6), 119.4 (C_8), 119.2 (C_9), 117.9 (C_{10}), 116.4 (C_{11}), 115.1 (C_{12}); $(O-CH_3)$,55.8; $(-CH_3)$, 20.1. ESI-Mass spectra, (*m/z)*: calculated for $[C_8H_8NO_2+H^+]^+$ = 151.099, $[C_{14}H_{12}NO+H^+]^+$ = 211.026, $[C_{15}H_{14}NO+H^+]^+$ = 225.032, $[C_{14}H_{12}NO_2+H^+]^+$ = 227.014, $[C_{15}H_{15}NO_2+H^+]^+$= 242.116, observed 241.286. Combustion analysis for $C_{15}H_{15}NO_2$: calcd. C 74.67, H 6.27, N 5.81 %. Found C 74.59, H 6.23, N 5.75 %.

2-methoxy-6-((E)-(phenylimino)methyl)phenol (L_2)

M.p.: 95 ºC; Yield: 0.982 g (86.51 %); Electronic spectra λ_{max} / nm (ε / mol L^{-1} cm^{-1}) in DMSO: 250 (1237), 360 (375). Selected infrared absorption

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(KBr, cm^{-1}): *ν*(O-H), 3216; *ν*(C-H), 3034; *ν*(HC=N), 1619; *ν*(C=C), 1464; *ν*(C-O), 1271; $\nu(\text{-OCH}_3)_{asym}$, 1188; $\nu(OCH_3)_{sym}$, 1081. ^{1}H-NMR spectra (400 MHz, CH_3CN, *δ* / ppm): (O-H), 13.34, (s, 1H); (HC=N), 8.92 (s, 1H), (Ar-H), 7.28 (m, $5H)_{aniline}$, 7.20 (dd, J = 9.2 Hz, 2.5 Hz, 1H), 7.13 (dd, *J* = 8.4 Hz, 2.2 Hz, 1H), 6.78 (t, *J* = 8.0 Hz, 8.0 Hz, 1H), (-OCH_3), 3.45 (s, 3H). ^{13}C-NMR spectra (400 MHz, CH_3CN, *δ* / ppm): $(\text{>C=N})_{imine}$,159.2; (C-OH),153.0; (Ar-C),149.5 (C_1), 147.2 (C_2), 135.3 (C_3), 126.5 (C_4), 121.5 (C_5), 118.7 (C_6), 118.1 (C_8), 118.1 (C_9), 115.0 (C_{10}), 114.2 (C_{11}), 113.5 (C_{12}); (O-CH_3), 51.6. ESI-Mass spectra, (*m/z)*: calculated for $[C_8H_8NO_2+H^+]^+$ = = 151.485, $[C_{14}H_{12}NO+H^+]^+$ = 211.152, $[C_{13}H_{10}NO_2+H^+]^+$ = 213.053, $[C_{14}H_{13}NO_2+H^+]^+$ = 228.258, observed 227.351. Combustion analysis for $C_{14}H_{13}NO_2$: calcd. C 73.99, H 5.77, N 6.16 %.Found C 73.92, H 5.69, N 6.08 %.

2-((E)-(4-chlorophenylimino)methyl)-6-methoxy phenol (L_3)

M.p.: 175 ºC; Yield: 1.058 g (81.19 %); Electronic spectra λ_{max}/nm (*ε*/mol L^{-1} cm^{-1}) in DMSO: 245 (1228), 352 (392). Selected infrared absorption (KBr, cm^{-1}): *ν*(O-H), 3249; *ν*(C-H), 3137; *ν*(HC=N), 1613; *ν*(C=C), 1449; *ν*(C-O), 1248; $\nu(\text{-OCH}_3)_{asym}$, 1161; $\nu(\text{-OCH}_3)_{sym}$, 1092. ^{1}H-NMR spectra (400 MHz, CH_3CN, *δ* / ppm): (O-H), 13.32 (s, H); (HC=N), 8.91 (s, 1H), *δ* (Ar-H) 7.45 (m, $4H)_{chloroaniline}$, 7.23 (dd, *J* = 10.5 Hz, 2.4 Hz, 1H), 7.10 (dd, *J* = 9.5 Hz, 3.0 Hz, 1H), 6.95 (t, *J* = 8.4 Hz, 8.4 Hz, 1H); *δ* (-OCH_3), 3.49 (s, 3H); *δ* (-CH_3), 2.33 (s, 3H). ^{13}C-NMR spectra (400 MHz, CH_3CN, *δ* / ppm): $(\text{>C=N})_{imine}$, 157.3; (C-OH),152.3; (Ar-C), 151.7 (C_1), 147. 2 (C_2), 132.0 (C_3), 127.2 (C_4), 124.6 (C_5), 116.8 (C_6), 116.5 (C_8), 116.1 (C_9), 114.9 (C_{10}), 113.2 (C_{11}), 113.0 (C_{12}); (O-CH_3),55.0. ESI-Mass spectra, (*m/z)*: calculated for $[C_8H_8NO_2+H^+]^+$ = 151.359, $[C_{14}H_{12}NO_2+H^+]^+$ = 227.014, $[C_{13}H_9ClNO+H^+]^+$ = 231.026, $[C_{14}H_{12}ClNO_2+H^+]^+$ = 262.706, observed 261.725. Combustion analysis for $C_{14}H_{12}ClNO_2$: calcd. C 64.25, H 4.59, N 5.35 %. Found C 64.17, H 4.52, N 5.24 %.

[Pd(L_1)(imdz)$_2$]Cl (1)

A brown crystalline solid was obtained after recrystallization of impure solid from 1: 1: 2, acetonitrile: acetone: chloroform (v/v) solvent mixture, which was dried in a desiccator over anhydrous calcium chloride under vacuum. M.p.: >300 ºC; Color: brown, Yield: 0.381 g (73.69 %). Electronic spectra λ_{max} / nm (ε / mol L^{-1} cm^{-1}) in DMSO: 703 (29), 600 (98), 440 (286), 400 (421), 370 (759), 260 (1245). Molar conductance Λ_m at 25 ºC (Ω^{-1} cm^2 M^{-1}): 19 in DMSO. Selected infrared absorption (KBr, cm^{-1}): ν(C-H),2843; ν(HC=N), 1602; ν(C=C), 1472; ν(C-O), 1265; $\nu(H_3C\text{-}O)_{asy}$, 1178; $\nu(H_3C\text{-}O)_{sy}$, 1068; $\nu(H_3C)_{in\ plane}$, 1028; $\nu(H_3C)_{out\ of\ plane}$, 752; ν(Pd-O), 534; ν(Pd-N), 453. ^{1}H-NMR spectra (400 MHz, DMSO, *δ* / ppm): 10.94 (s, 2H, $(N\text{-}H)_{imdz}$), 8.99 (s, 1H, -HC=N), 7.34 (d, J = 8.4 Hz, $2H)_{imdz}$, 7.25 (m, $4H)_{imdz}$, (Ar-H), 7.15 (m, $4H)_{p\text{-}toluidene}$, 7.07 (d, *J* = 8.4

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Hz, 1H)$_{vanillin}$, 6.90 (t, J = 8.0 Hz, 8.0 Hz, 1H)$_{vanillin}$, 6.77 (d, J = 7.2 Hz, 1H)$_{vanillin}$, 3.41 (s, 3H, -OCH_3), 2.22 (s, 3H, CH_3). ^{13}C-NMR spectra (400 MHz, dmso, δ / ppm): (>C=N)$_{imine}$, 165.1; (imd-C), 136.5, 136.4, 122.3, 122.1, 122.0, 122.0, (Ar-C), 156.6 (C_1), 150.5 (C_2), 147.8 (C_3), 145.1 (C_4), 131.3 (C_5), 130.0 (C_6), 129.9 (C_7), 116.1 (C_8), 114.5 (C_9), 114.5 (C_{10}), 113.4 (C_{11}), 113.1 (C_{12}); (O-CH_3), 55.8; (-CH_3), 20.5.ESI-Mass spectra, (*m/z)*: calculated for $[C_8H_8O_2N+H^+]^+$ = 151.090, $[C_{15}H_{15}O_2N+H^+]^+$ = 242.172, $[C_8H_7ClO_2$-$NPd+H^+]^+$ = 291.038, $[C_{15}H_{14}O_2NPd+H^+]^+$ =347.697, $[C_{15}H_{14}ClO_2NPd+H^+]^+$= 383.340, $[C_{14}H_{15}N_5O_2Pd+H^+]^+$ = 392.203, $[C_{18}H_{18}N_3O_2Pd+H^+]^+$ = 415.215, $[C_{14}$-$H_{15}ClN_5O_2Pd+H^+]^+$ = 428.210, $[C_{18}H_{18}ClN_3O_2Pd]^+$ = 450.001, $[C_{21}H_{22}N_5O_2Pd]^+$ = 482.857, $[C_{21}H_{22}ClN_5O_2Pd+H^+]^+$ = 519.304, observed 518.258. Combustion analysis for $C_{21}H_{22}ClN_5O_2Pd$: calcd. C 48.63, H 4.28, N 13.51, Pd 20.53 %. Found C 48.54, H 4.23, N 13.44, Pd 20.45 %.

[Pd(L_2)(imdz)$_2$]Cl (2)

The solid obtained was further recrystallized from 1:1:2, acetone: acetonitrile:chloroform (v / v) solvent mixture to yield light brown crystalline solid, which was dried in a desiccator over anhydrous calcium chloride under vacuum. M.p.: >300 ºC; Color: light brown, Yield: 0.345 g (68.59 %); Electronic spectra λ_{max} / nm (ε / mol L^{-1} cm^{-1}) in DMSO: 715 (37), 609 (91), 437 (295), 405 (408), 366 (743), 253 (1264). Molar conductance Λ_m at 25 °C (Ω^{-1} cm^2 M^{-1}): 16 in DMSO. Selected infrared absorption (KBr, cm^{-1}): ν(C-H)$_{arom}$, 2827; ν(HC=N), 1589; ν(C=C), 1438; ν(C-O), 1251; ν(H_3C-O)$_{asym}$, 1172; ν(H_3C-O)$_{sym}$, 1068; ν(Pd-O), 516; ν(Pd-N), 437. ^{1}H-NMR spectra (400 MHz, DMSO, δ / ppm): 10.80 (s, 2H, (N-H)$_{imdz}$), 8.99 (s, 1H, -HC=N), 7.38 (d, J = 8.8 Hz, 2H)$_{imdz}$, 7.27 (m, 4H)$_{imdz}$, (Ar-H), δ 7.22 (m, 5H)$_{aniline}$, 7.18 (dd, J = 9.8 Hz, 2.5 Hz, 1H)$_{vanillin}$, 6.97 (t, J = 8.4 Hz, 8.4 Hz, 1H)$_{vanillin}$, 6.69 (dd, *J = 9.6Hz, 2.2 Hz,* 1H)$_{vanillin}$, 3.48 (s, 3H, -OCH_3).^{13}C-NMR spectra (400 MHz, DMSO, δ / ppm): (>C=N)$_{imine}$, 162.6, (imd-C), 134.6, 134.4, 120.4,120.3, 120.2, 120.1, (Ar-C), 153.1 (C_1), 152.9 (C_2), 144.6 (C_3), 141.8 (C_4), 128.4 (C_5), 126.6 (C_6), 126.2 (C_7), 121.8 (C_8), 117.4 (C_9), 117.1 (C_{10}), 114.8 (C_{11}), 114.6 (C_{12}); (O-CH_3), 52.6. ESI-Mass spectra, (*m/z)*: calculated for $[C_8H_8O_2N+H^+]^+$ = 151.064, $[C_{14}H_{12}O_2N+H]^+$ = 228.258, $[C_8H_7ClO_2NPd+H^+]^+$ = 291.043, $[C_{14}H_{12}O_2NPd+H^+]^+$ = 333.654, $[C_{14}H_{12}ClO_2NPd+H^+]^+$ = 368.283, $[C_{14}H_{15}N_5O_2Pd+H^+]^+$ = 392.218, $[C_{14}H_{11}Cl_2O_2NPd+H^+]^+$ = 401.246, $[C_{14}H_{15}Cl$-$N_5O_2Pd+H^+]^+$ = 428.281, $[C_{20}H_{20}N_5O_2Pd+H^+]^+$ =469.158, $[C_{20}H_{20}ClN_5O_2Pd+H^+]^+$ = 505.035, observed 504.125. Combustion analysis for $C_{20}H_{20}ClN_5O_2Pd$: calcd. C 47.64, H 4.00, N 13.89, Pd 21.12 %. Found C 47.53, H 3.95, N 13.78, Pd 21.01 %.

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[Pd(L_3)(imdz)$_2$]Cl (3)

M.p.: >300 ºC; Color: dark brown, Yield: 0.354 g (65.92 %); Electronic spectra λ_{max} / nm (ε / mol L^{-1} cm^{-1}) in DMSO: 711 (32), 605 (104), 445 (282), 403 (419), 375 (751), 248 (1270). Molar conductance Λ_m at 25 ˚C (Ω^{-1} cm^2 M^{-1}): 17 in DMSO. Selected infrared absorption (KBr, cm^{-1}): ν(C-H), 2889; ν(HC=N), 1581; ν(C=C), 1441; ν(C-O), 1247; ν(H_3C-O)$_{asym}$, 1178; ν(H_3C-O)$_{sym}$, 1060; ν(Pd-O), 530; ν(Pd-N), 457. ^{1}H-NMR spectra (400 MHz, DMSO, δ / ppm): 10.78 (s, 2H, (N-H)$_{imdz}$), 8.99 (s, 1H –HC=N), 7.37 (*d, J* = 8.0 Hz, 2H)$_{imdz}$, 7.25 (m, 4H)$_{imdz}$, (Ar-H), 7.20 (m, 4H)$_{chloroaniline}$, 7.15 (dd, *J* = 9.2 Hz, 2.2 Hz, 1H)$_{vanillin}$, 6.90 (t, *J* = 7.2 Hz, 7.2 Hz, 1H)$_{vanillin}$, 6.78 (dd, *J* = 7.4 Hz, 2.4 Hz, 1H)$_{vanillin}$, 3.54 (s, 3H, -OCH_3). ^{13}C-NMR spectra (400 MHz, DMSO, δ / ppm): (>C=N)$_{imine}$, 163.5; (imd-C), 137.6; δ 137.5; 122.3; 122.1; 122.0; 122.0; (Ar-C), 154.2 (C_1), 152.8 (C_2), 148.6 (C_3), 145.2 (C_4), 132.6 (C_5), 130.2 (C_6), 130.0 (C_7), 119.3 (C_8), 115.5 (C_9), 115.2 (C_{10}), 111.8 (C_{11}), 111.5 (C_{12}); (O-CH_3), 58.7. ESI-Mass spectra, (*m/z)*: calculated for $[C_8H_8O_2N+H^+]^+$ = 151.157, $[C_{14}H_{12}ClO_2N+H^+]^+$ = 262.106, $[C_8H_7ClO_2NPd+H^+]^+$ = 291.094, $[C_{14}H_{15}N_5O_2Pd+H^+]^+$ = 392.18, $[C_{17}H_{15}Cl_2N_3O_2Pd+H^+]^+$= 469.134, $[C_{20}H_{19}ClN_5O_2Pd+H^+]^+$ = 505.015, $[C_{20}H_{19}Cl_2N_5O_2Pd+H^+]^+$ = 539.723, observed 538.564. Combustion analysis for $C_{20}H_{19}Cl_2N_5O_2Pd$: calcd. C 44.59, H 3.55, N 13.00, Pd 19.75 %. Found C 44.51, H 3.48, N 12.89, Pd 19.67 %.

Coupling reaction product ((E)-1,2-diphenylethene)

M.p.: 134-135 °C. Color: white crystals. ^{1}H-NMR spectra (400 MHz, DMSO, δ / ppm): 7.614 (t, 2H), 7.239 (t, 2H), 7.293 (t, 2H); 7.287 (d, 2H); 7.267 (d, 2H); δ HC=CH, 4.13 (d, 2H). ^{13}C-NMR spectra (400 MHz, DMSO, δ / ppm): δ 136.99 ($C_{1,9}$); δ 127.27 ($C_{3,11}$); δ 126.12 ($C_{4,12}$); δ 127.62 ($C_{5,13}$); δ 128.67 ($C_{6,14}$); (HC= CH), δ 60.13.

Table S-I. Correlation of experimental FT-IR spectra with theoretical IR spectra for complex **1**

Assignment	Wavelength, cm^{-1}			Deviation, %
	Experimental	Theoretical		
		Unscaled	Scaled	
ν(O-H)	-	-	-	-
ν(C-H)	2843	2835	2840	0.1
ν(-CH=N)	1602	1610	1600	0.1
ν(C=C)	1427	1436	1425	0.1
ν(C-O)	1265	1267	1263	0.1
ν(C-O-C)$_{sym}$	1178	1171	1176	0.1
ν(C-O-C)$_{asym}$	1068	1070	1066	0.1
χ(C-H)$_{in\ plane}$	1028	1013	1026	0.1
χ(C-H)$_{out\ of\ plane}$	752	754	733	0.1
ν(M-O)	534	532	533	0.1
ν(M-N)	453	443	452	0.1

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Table S-II. Selected Mulliken atomic charges of ligands and complexes

Atoms	Mulliken atomic charge					
	Ligand			Complex		
	L_1	L_2	L_3	1	2	3
C (connected to O)	(C2) 0.355	(C2) 0.396	(C2) 0.396	(C2) 0.396	(C2) 0.394	(C2) 0.384
C′ OCH_3 (connected to O)	(C1) 0.086	(C1) 0.075	(C1) 0.075	(C1) 0.076	(C1) 0.072	(C1) 0.052
C (connected to imine N)	(C20) 0.356	(C21) 0.354	(C20) 0.354	(C20) 0.343	(C20) 0.359	(C20) 0.350
H (connected to O)	(H33) 0.356	(H27) 0.356	(H27) 0.355	-	-	-
O	(O22) -0.687	(O23) -0.679	(O23) -0.679	(O22) -0.678	(O27) -0.656	(O21) -0.669
N (imine)	(N25) -0.671	(N25) -0.615	(N22) -0.615	(N23) -0.582	(N22) -0.582	(N24) -0.578
N (Imdz)	-	-	-	(N33) -0.655	(N29) -0.611	(N31) -0.674
N′ (Imdz)	-	-	-	(N43) - 0.640	(N39) -0.653	(N33) -0.654
Pd	-	-	-	1.324	1.331	1.340

Table S-III. The calculated quantum chemical parameters of ligands and complexes

Quantum parameter	Ligand			Complex		
	L_1	L_2	L_3	1	2	3
E_{HOMO} / eV	-5.937	-5.980	-6.271	-4.508	-3.986	-5.490
E_{LUMO} / eV	-2.029	-0.595	-2.236	-3.137	-3.197	-3.771
ΔE / eV	3.907	5.384	4.035	1.371	0.789	1.719
χ / eV	3.983	3.288	4.254	3.822	3.591	4.631
η / eV	1.953	2.692	2.017	0.685	0.394	0.859
Σ / eV^{-1}	0.511	0.371	0.495	1.458	2.534	1.163
μ / eV or Pi	-3.983	-3.288	-4.254	-3.822	-3.591	-4.319
2n	3.907	5.384	4.035	1.371	0.789	1.791
S / eV^{-1}	0.255	0.185	0.247	0.729	1.267	0.581
Ω / eV	4.061	2.007	4.485	10.657	13.347	12.472
ΔN_{max} / eV	2.038	1.221	2.108	5.575	6.103	5.386
E, TD- F / TD-KS	-785.615	-746.303	-856.915	-1378.681	-1339.642	-1354.039
Dipole moment, D	4.959	4.445	4.044	12.793	12.533	12.318

Table S-IV. Geometrically optimized bond lengths of ligands and complexes

Bonds	Bond length, Å					
	Ligand			Complex		
	L_1	L_2	L_3	1	2	3
C-O	(C2-O22) 1.431	(C2-O23) 1.430	(C2-O23) 1.435	(C2-O22) 1.431	(C2-O21) 1.435	(C2-O21) 1.437
H-O	(H33-O22)	(H27-H23)	(H27-O23)	-	-	-

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	0.968	0.961	0.960			
C=N (imine)	(C20=N25) 1.298	(C21=N25) 1.293	(C20=N22) 1.297	(C20=N23) 1.299	(C20=N22) 1.298	(C20= N24) 1.299
C-O (O-CH_3)	(C21-O23) 1.430	(C22-O24) 1.430	(C21-O24) 1.430	(C24-O31) 1.430	(C23-O27) 1.434	(C23-O22) 1.431
C-Cl			(C12-Cl25) 1.761	-	-	(C12-Cl25) 1.760
Pd-O	-	-	-	(Pd32-O22) 1.942	(Pd28-O21) 1.942	(Pd30 -O21) 1.941
Pd -N	-	-	-	Pd32-N23 (phen) 1.981	Pd28-N22 (phen) 1.980	Pd30-N24 (phen) 1.980
Pd –N (Imdz)	-	-	-	Pd32 N33 1.978	Pd28-N29 1.977	Pd30-N31 1.976
Pd -N′ (Imdz)				Pd32 N43 1.979	Pd32-N39 1.976	Pd32-N33 1.974

Table S-V. Geometrically optimized bond angles of ligands and complexes

Angles	Bond angle, °					
	Ligand			Ligand		
	L_1	L_2	L_3	1	2	3
∠C-C-O	(∠C3-C2-O22) 119.999	(∠C3-C2-O23) 119.997	(∠C3-C2-O23) 119.994	(∠C3-C2-O22) 122.849	(∠C3-C2-O21) 122.842	(∠C3-C2-O21) 122.616
∠C-O-H	(∠C2-O22-H33) 109.471	(∠C2-O23-H27) 109.471	(∠C2-O23-H27) 109.471	-	-	-
∠C=N-C	(∠C3-C20-N25) 120.004	(∠C3-C21-N25) 120.007	(∠C3-C21-N22) 120.005	(∠C3-C22-N23) 123.139	(∠C3-C22-N22) 123.137	(∠C3-C20-N24) 123.142
∠H-C=N (imine)	(∠H26-C20-N25) 119.999	(∠H26-C21-N25) 119.998	(∠H26-C20-N22) 119.997	(∠H38-C20-N23) 118.400	(∠H34-C20-N22) 118.400	(∠H26-C20-N24) 118.925
∠C-O-C O-CH_3	(∠C1-O23-C21) 109.471	(∠C1-O24-C22) 109.472	(∠C1-O24-C21) 109.471	(∠C1-O31-C24) 109.492	(∠C1-O27-C23) 109.490	(∠C1-O22-C23) 109.471
∠N(imine)-Pd-O	-	-	-	(∠N23-Pd32-O22) 92.855	(∠N22-Pd28-O21) 92.848	(∠N24-Pd30-O21) 92.841
∠N-Pd-O (Imdz)	-	-	-	(∠N23-Pd32-O22) 92.855	(∠N22-Pd28-O21) 92.860	(∠N24-Pd30-O21) 92.853
∠N-Pd-N	-	-	-	(∠N43-Pd32-N33) 87.534	(∠N39-Pd28-N29) 87.534	(∠N39-Pd30-O31) 87.748
∠N(imdz-Pd-O	-	-	-	(∠N43-Pd32-O22) 125.874	(∠N39-Pd28-O21) 125.874	(∠N33-Pd30-O21) 125.425
∠N(imine)-Pd-N	-	-	-	(∠N23-Pd32-N33) 90.697	(∠N22-Pd28-N29) 90.695	(∠N24-Pd30-N31) 90.629

Table S-VI. Catalysis of Heck-Mizoroki reaction in different condition by complexes

Ent.	Catal load, μmol	Solv.	*T* / ° C	Base	*t* / h	Yield*, % 1	TOF, h^{-1}	Yield*, % 2	TOF, h^{-1}	Yield*, % 3	TOF, h^{-1}
1	0.1	DMF+ Water	80	K_2CO_3	8	44.656	302.5	42.285	287.5	39.476	267.5
2	0.2	DMF+ Water	80	K_2CO_3	8	57.633	195.62	54.637	185.62	51.524	175
3	0.3	DMF+ Water	80	K_2CO_3	8	68.326	158.25	62.392	166.25	58.518	136.62
4	0.4	DMF+	80	K_2CO_3	8	89.694	152.5	76.240	129.68	74.823	127.62

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		Water									
5	0.5	DMF+ Water	80	K_2CO_3	8	89.308	121.5	76.005	103.25	74.661	127.18
6	0.6	DMF+ Water	80	K_2CO_3	8	89.246	101.03	76.404	86.45	74.856	87.16
7	0.4	DMF	80	K_2CO_3	8	72.519	123.12	69.725	118.43	68.214	112.8
8	0.4	Toluene	80	K_2CO_3	8	46.259	78.43	41.034	69.68	40.473	68.81
9	0.4	Aceto-nitrile	80	K_2CO_3	8	38.549	65.31	35.559	60.31	35.415	60.06
10	0.4	Water	80	K_2CO_3	8	29.746	50.31	28.854	48.81	27.964	47.56
11	0.4	DMF+ Water	25	K_2CO_3	8	24.572	44.06	22.554	38.18	19.863	46.06
12	0.4	DMF+ Water	40	K_2CO_3	8	35.877	60.56	34.168	57.81	21.468	36.31
13	0.4	DMF+ Water	50	K_2CO_3	8	65.568	111.31	62.359	105.93	59.216	100.62
14	0.4	DMF+ Water	60	K_2CO_3	8	69.847	118.8	68.526	116.31	62.163	105.68
15	0.4	DMF+ Water	70	K_2CO_3	8	78.442	133.1	73.056	124.06	71.225	120.93
16	0.4	DMF+ Water	90	K_2CO_3	8	89.524	152.31	76.164	129.37	74.001	125.68
17	0.4	DMF+ Water	100	K_2CO_3	8	89.512	152.18	76.408	129.62	74.614	126.93
18	0.4	DMF+ Water	80	Na_2CO_3	8	69.465	117.81	64.556	109.68	60.509	113.18
19	0.4	DMF+ Water	80	CH_3COONa	8	44.656	75.68	42.465	72.18	42.148	71.56
20	0.4	DMF+ Water	80	NaOH	8	39.694	67.56	35.469	60.6	31.968	54.06
21	0.4	DMF+ Water	80	KOH	8	28.989	49.06	26.989	45.68	24.382	41.31
22	0.4	DMF+ Water	80	K_2CO_3	2	31.297	212.75	30.857	208.75	28.957	196.25
23	0.4	DMF+ Water	80	K_2CO_3	4	61.846	210.12	60.761	189.37	55.872	189.37
24	0.4	DMF+ Water	80	K_2CO_3	6	65.648	148.75	61.299	139.2	58.469	132.08
25[#]	0.4	DMF+ Water	80	K_2CO_3	8	41.984	71.31	39.914	67.81	36.710	62.18
26[##]	0.4	DMF+ Water	80	K_2CO_3	8	-	-	-	-	-	

Reaction condition: Bromobenzene (0.5 mmol); Styrene (0.6 mmol); Potassium carbonate (0.75 mmol).
[*]Yield after column chromatography. [#]Only $PdCl_2$ used as catalyst. [##]Schiff base ligands as catalyst.

Table S-VII. Heck-Mizoroki reactions with different substituents catalyzed by complex **1** under optimized reaction conditions

Entry	X	Y	Catalyst loading, μmol	Solvents	*T* / ºC	Base	*t* / h	*Yield, %	TOF, h^{-1} Complex **1**
1	Cl	H	0.4	DMF+ Water	80	K_2CO_3	8	43.710	74.06
2	Br	H	0.4	DMF+ Water	80	K_2CO_3	8	89.694	152.5
3	I	H	0.4	DMF+	80	K_2CO_3	8	89.899	152.7

(CC) 2021 SCS.

				Water					
4	Br	CHO	0.4	DMF+ Water	80	K_2CO_3	8	67.872	115.2
5	Br	OCH_3	0.4	DMF+ Water	80	K_2CO_3	8	59.660	101.25

Substituted aryl halides (0.5 mmol) (XC_6H_4Y; where X = Cl/ Br/ I and Y = H/ CHO/OCH_3). In each case styrene (0.6 mmol) and as base potassium carbonate (0.75 mmol) was used. *Yield after column chromatography

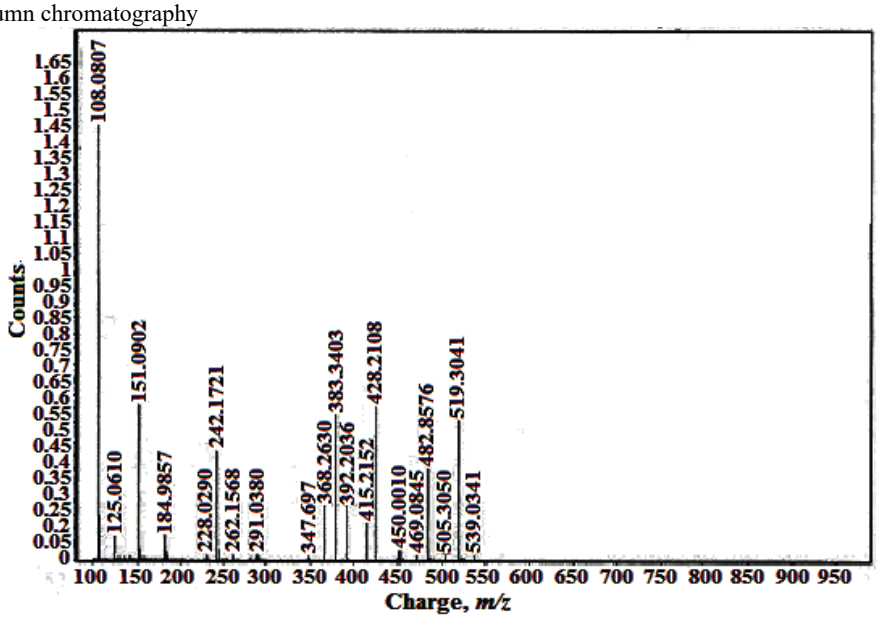

Fig. S-1. ESI-Mass spectrum of complex **1**.

(CC) 2021 SCS.

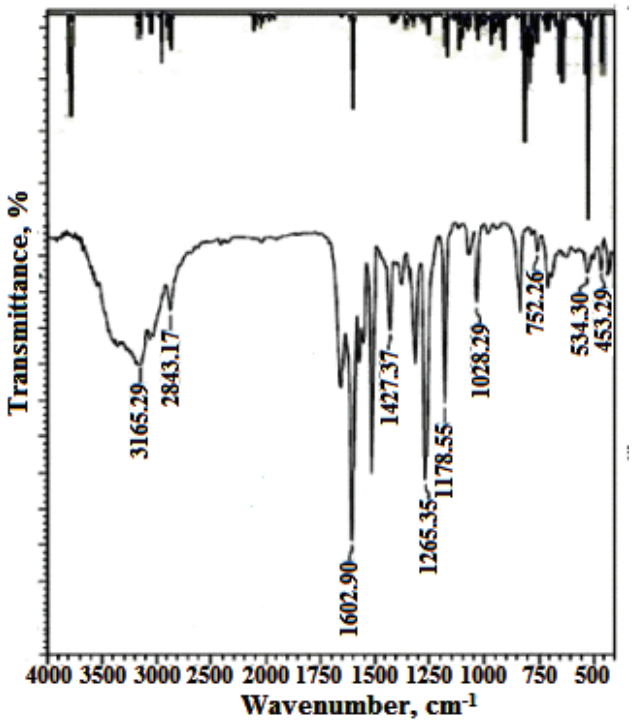

Fig. S-2. Experimental and theoretical FT-IR spectrum of complex **1**.

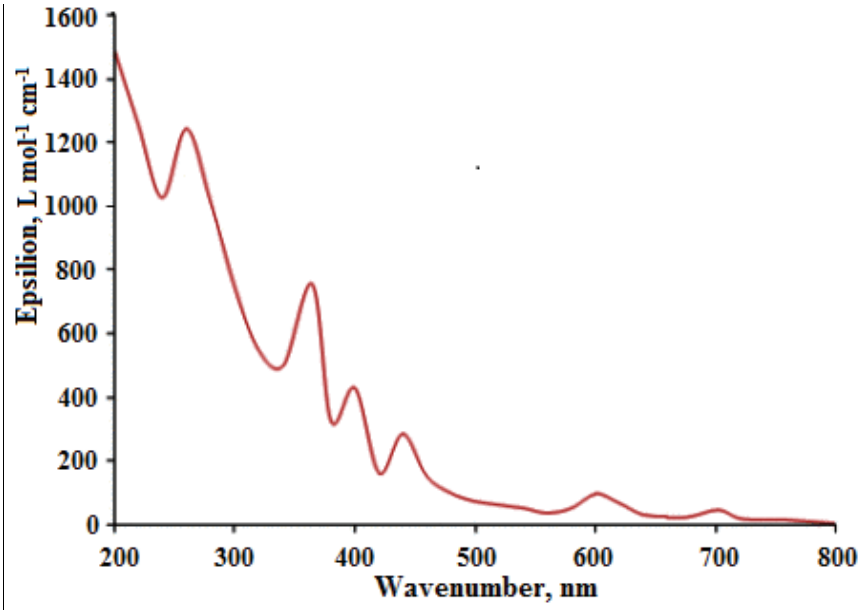

Fig. S-3. UV-Vis spectra spectrum of complex **1**.

(CC) 2021 SCS.

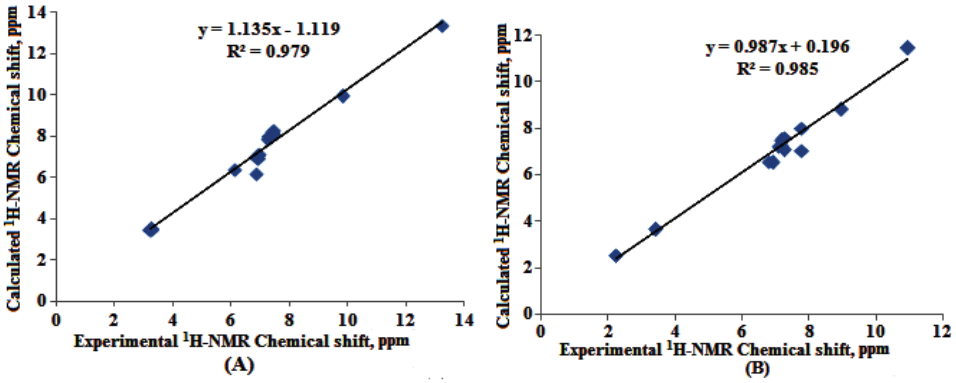

Fig. S-4. ^{1}H-NMR correlation diagram for (A) L_1 and (B) complex **1**.

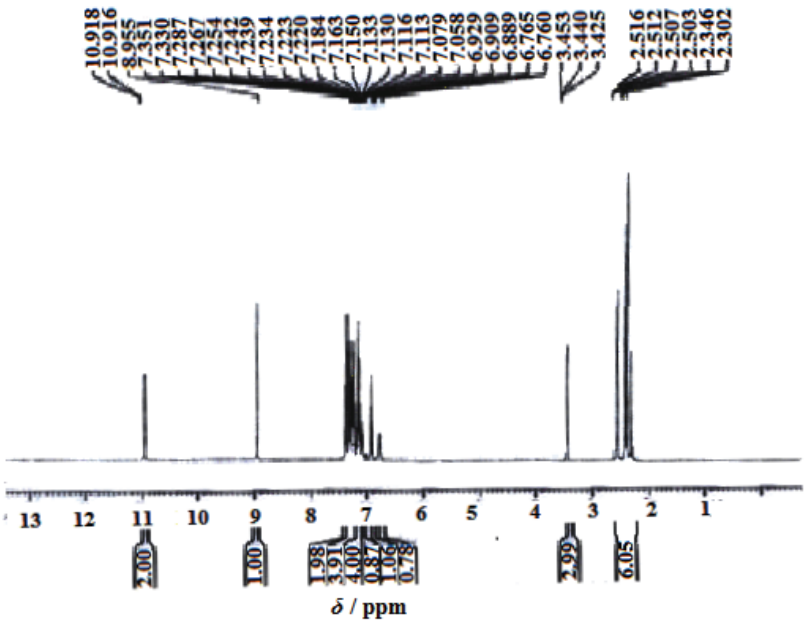

Fig. S-5. ^{1}H-NMR spectrum of complex **1**.

(CC) 2021 SCS.

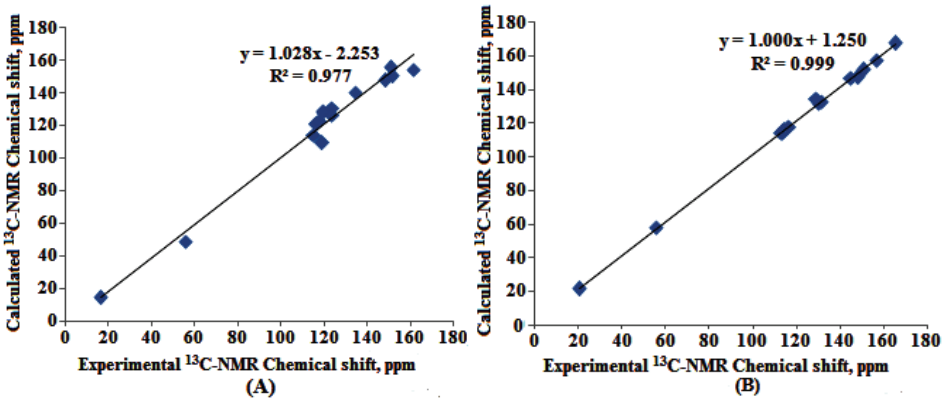

Fig. S-6. ^{13}C-NMR correlation diagram for (A) L_1 and (B) complex **1**.

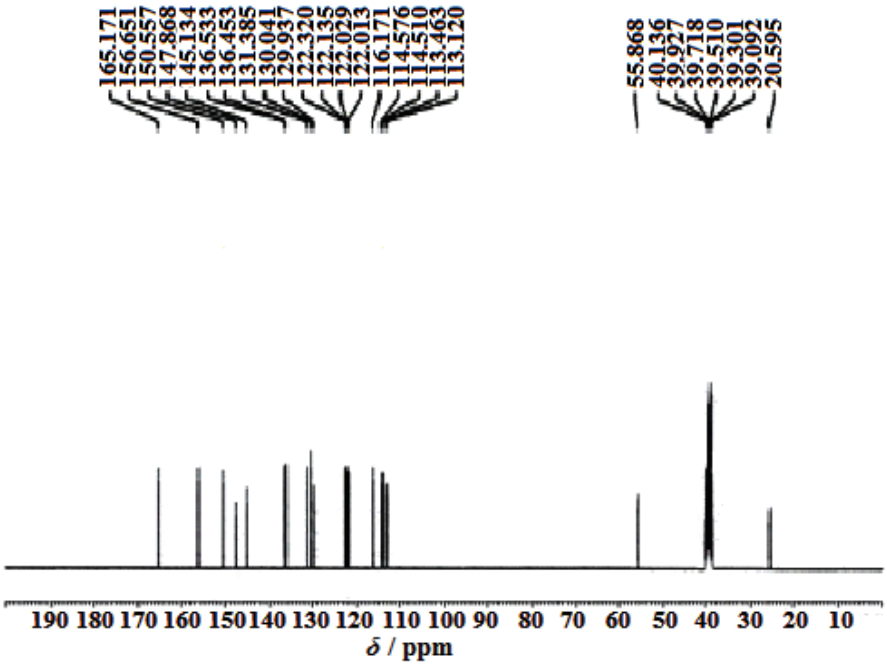

Fig. S-7. ^{13}C-NMR spectrum of complex **1**.

(CC) 2021 SCS.

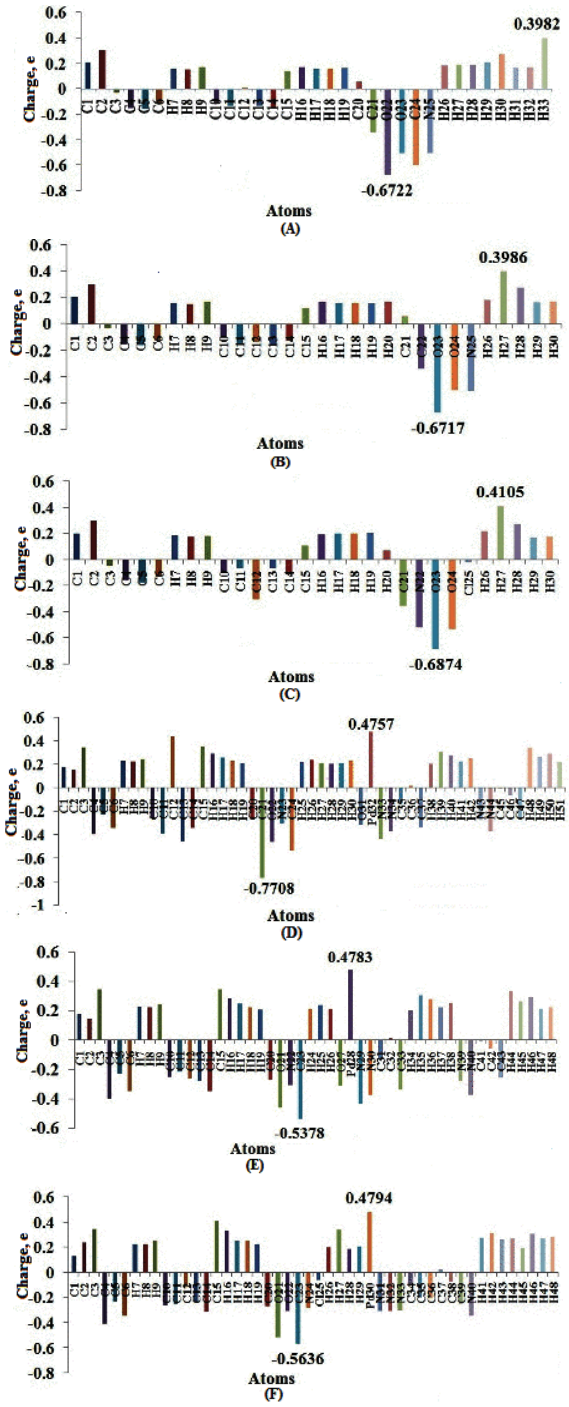

Fig. S-8. Mulliken atomic charge plot of $\mathbf{L}_1$, $\mathbf{L}_2$, $\mathbf{L}_3$, complexes **1**, **2** and **3**.

(CC) 2021 SCS.

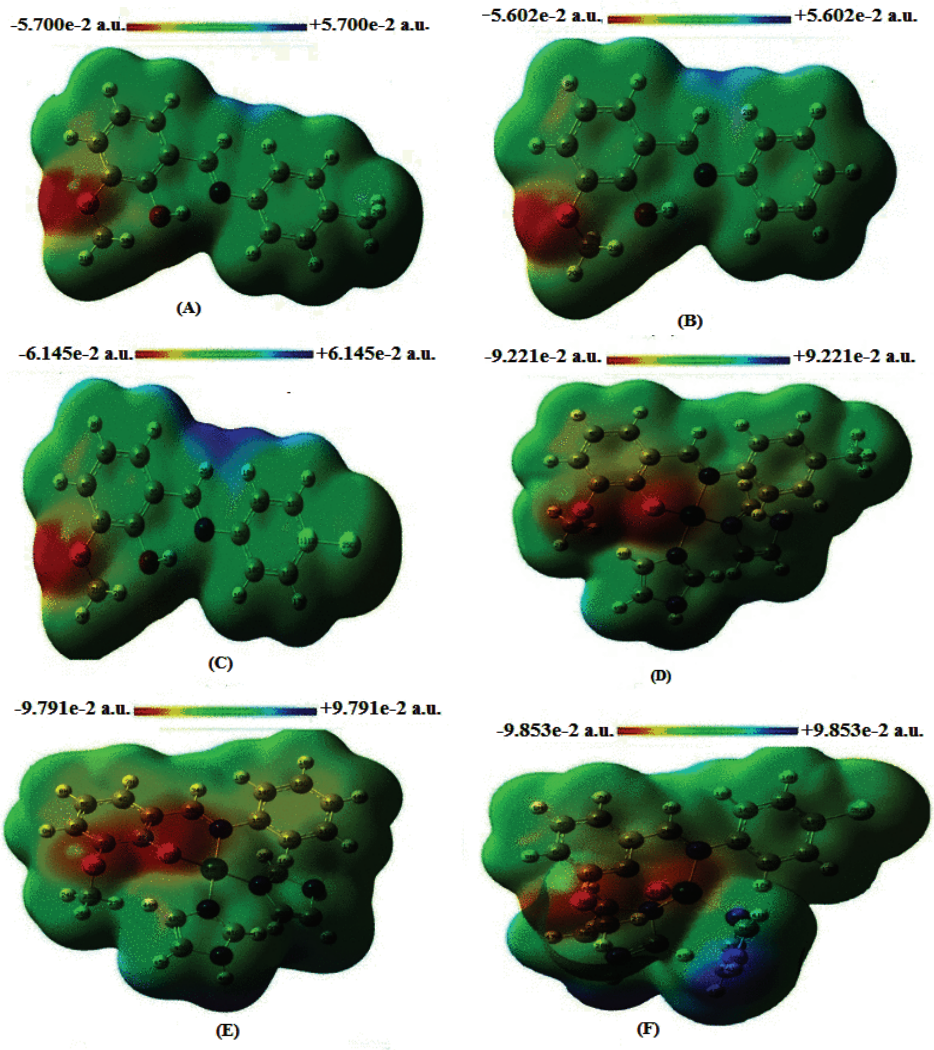

Fig. S-9. Molecular Electrostatic Potential of $\mathbf{L}_1$, $\mathbf{L}_2$, $\mathbf{L}_3$, complexes **1**, **2** and **3**.

(CC) 2021 SCS.

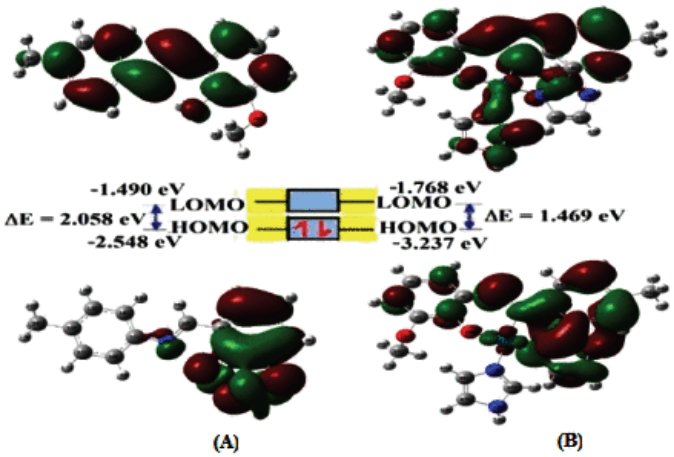

Fig. S-10. HOMO-LUMO structure with energy level diagram of (A) $\mathbf{L}_1$ (B) complex **1**.

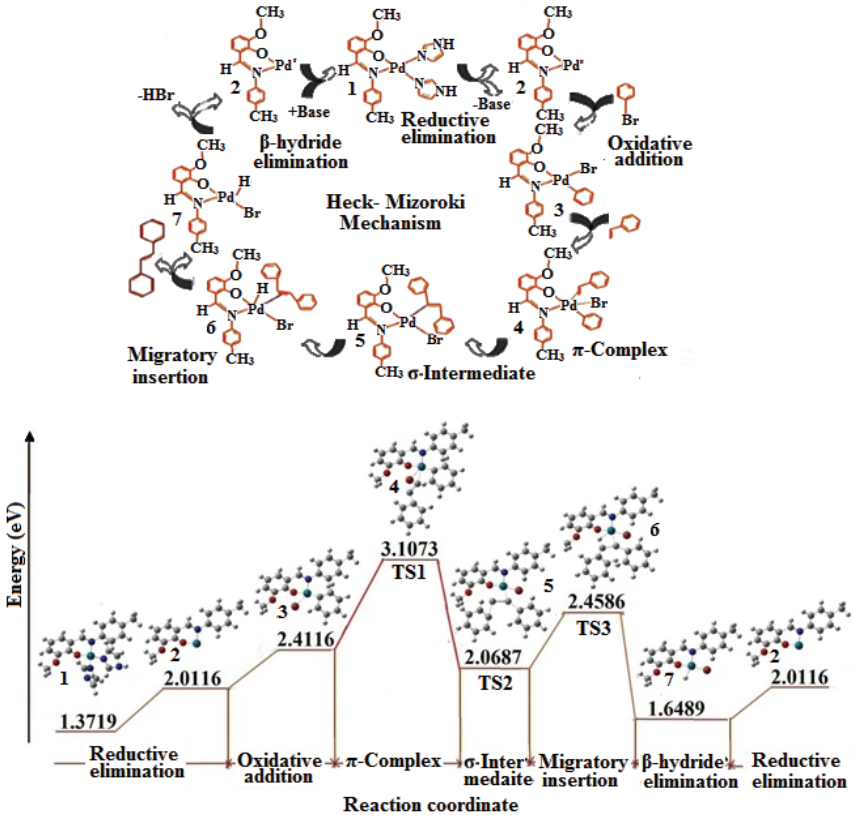

Fig. S-11. Proposed mechanism and energy profiles of *the* full catalytic species using complex **1**.

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