Supplementary materials

Synthesis, spectral characterization, and theoretical investigation of Pd(II) complex incorporating unsymmetrical tetradentate Schiff base ligand and its application in Suzuki–Miyaura cross-coupling reaction

Hadi Kargar [a,*], Mehdi Fallah-Mehrjardi [b], Reza Behjatmanesh-Ardakani [b], Khurram Shahzad Munawar [c,d], Mehrnaz Bahadori [e], Majid Moghadam [e]

[a] Department of Chemical Engineering, Faculty of Engineering, Ardakan University, P.O. Box 184, Ardakan, Iran

[b] Department of Chemistry, Payame Noor University (PNU), 19395-4697, Tehran, Iran

[c] Department of Chemistry, University of Sargodha, Punjab, Pakistan

[d] Department of Chemistry, University of Mianwali, Mianwali, Pakistan

[e] Catalysis Division, Department of Chemistry, University of Isfahan, 81746-73441, Isfahan, Iran

[*] Corresponding author's e-mail: h.kargar@ardakan.ac.ir; hadi_kargar@yahoo.com

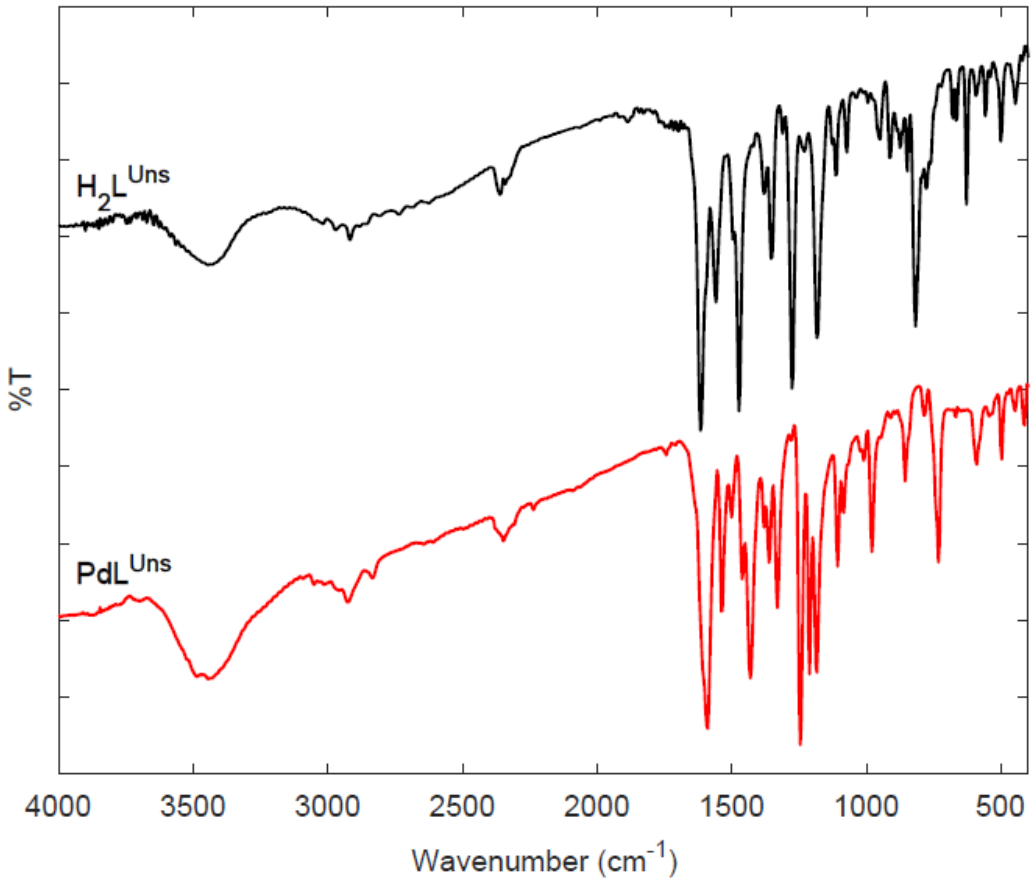

Figure S1. The experimental FT-IR stacked spectrum of **H_2L^{Uns}** and **PdL^{Uns}**.

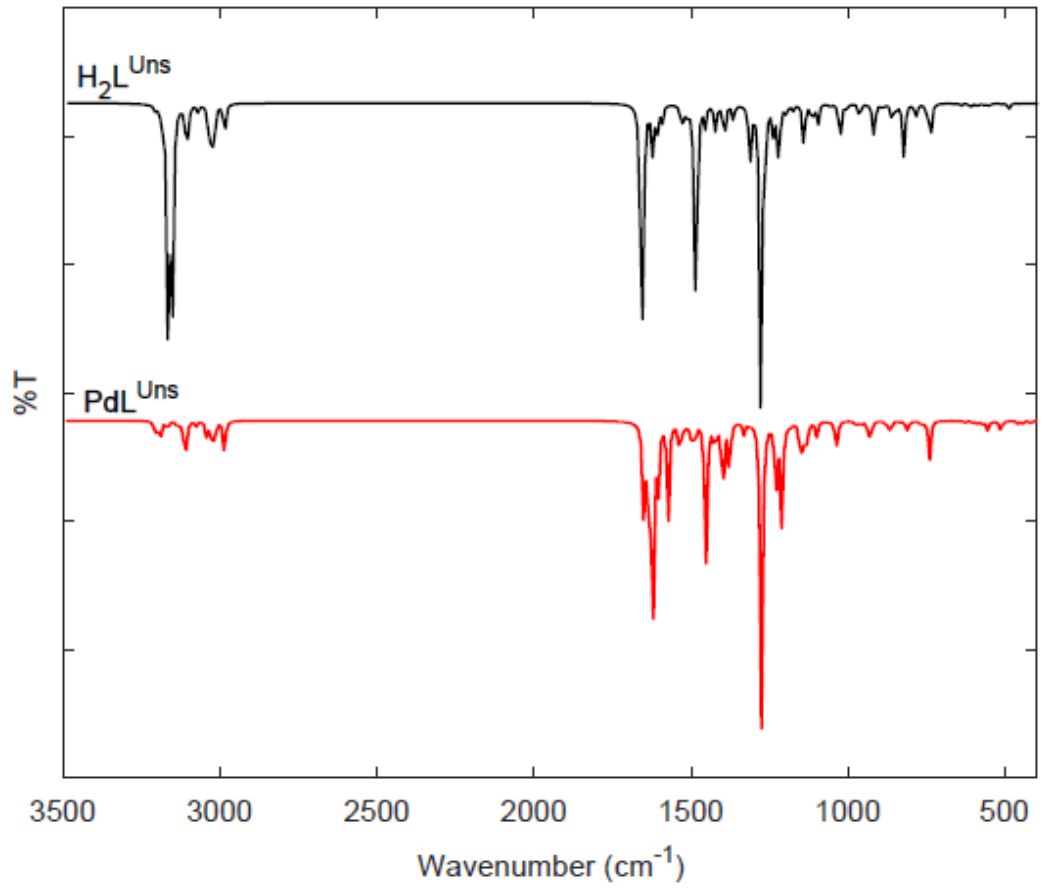

Figure S2. The theoretical stacked FT-IR spectrum of **H_2L^{Uns}** and **PdL^{Uns}**.

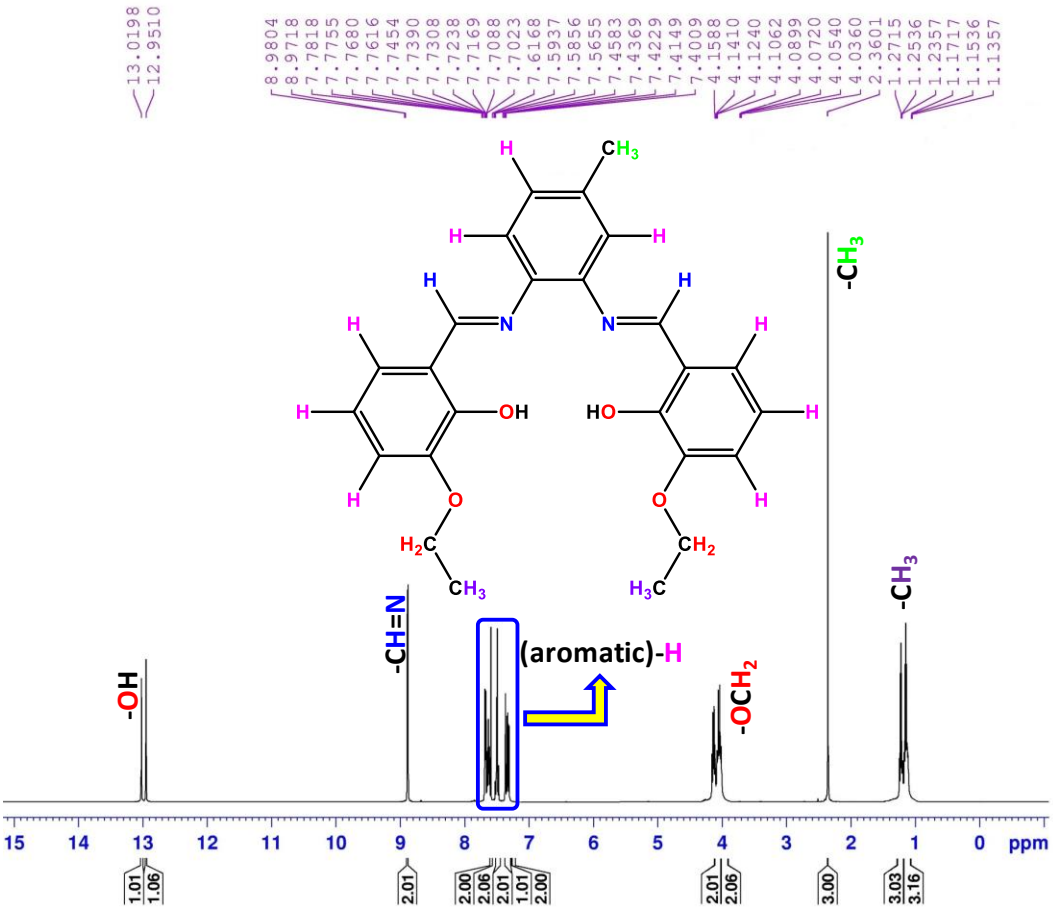

Figure S3. ^{1}H NMR spectrum of the $\mathbf{H_2L^{Uns}}$ in $CDCl_3$.

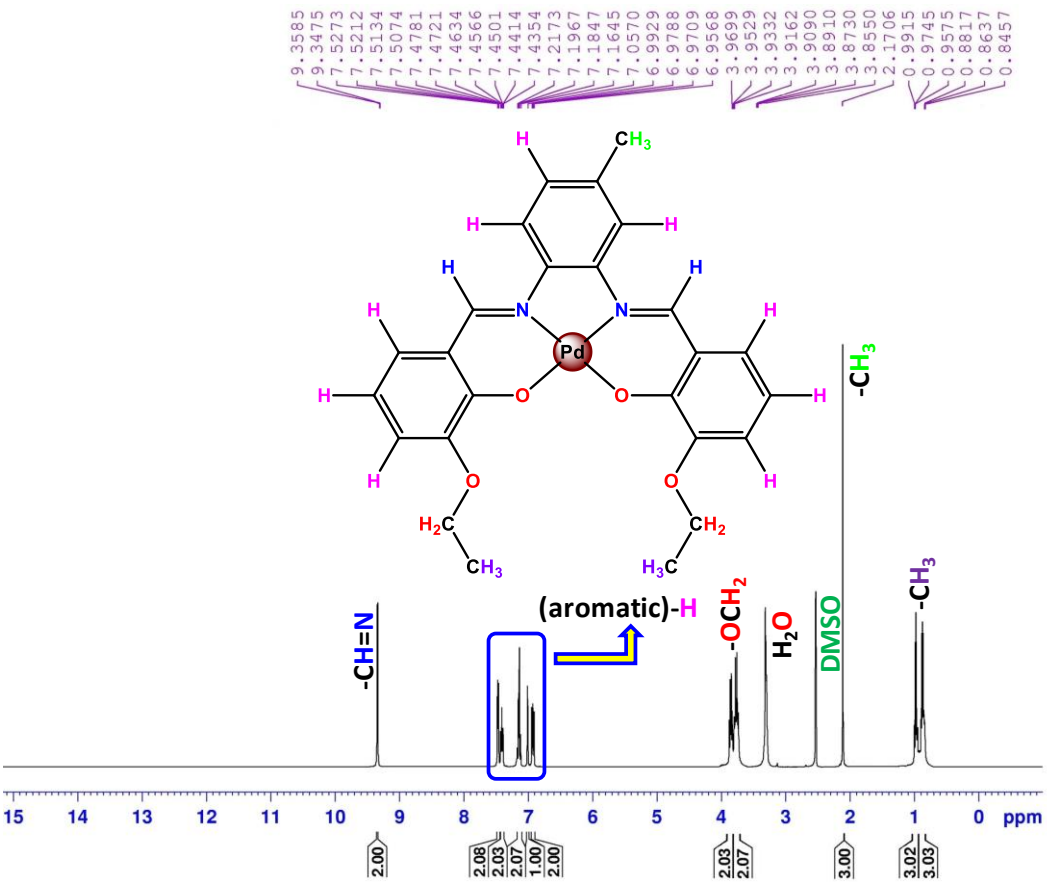

Figure S4. ^{1}H NMR spectrum of the $\mathbf{PdL^{Uns}}$ in DMSO-d_6.

Table S1. The experimentally obtained and theoretically calculated IR vibrational data (cm^{-1}) as well as relative errors (%) for the synthesized compounds[a]

Compound		υ(HC=N)	υ(C–O)	υ(M–O)	υ(M–N)
H_2L^{Uns}	Experimental	1616	1277	-	-
	Calculated	1607	1273	-	-
	Relative error (%)	-0.56	-0.31	-	-
PdL^{Uns}	Experimental	1589	1330	590	497
	Calculated	1594	1329	592	495
	Relative error (%)	0.31	-0.08	0.34	-0.40

[a]Relative error (%) = $(X^{Calc} - X^{Exp})*100/X^{Exp}$

Table S2. Experimental and theoretically derived chemical shifts (ppm) for ^{1}H NMR spectra of the synthesized compounds[a]

Compound		**–CH_3**	**–CH_3**	**–CH_2–O**	**H (aromatic)**	**–CH=N**	**OH**
H_2L^{Uns}	Experimental	1.15 & 1.25	2.36	4.06 & 4.13	7.40-7.78	8.97 & 8.98	12.95 & 13.02
	Calculated	1.45	2.50	4.02 & 4.03	7.14-7.44	8.97 & 8.98	13.64 & 13.66
PdL^{Uns}	Experimental	0.86 & 0.97	2.17	3.88 & 3.94	6.96-7.53	9.35 & 9.36	-
	Calculated	1.57 & 1.58	2.57	4.08	6.96-8.23	9.47 & 9.53	-

[a]The average values acquired from the B3LYP/Def2-TZVP level of theory are used to determine the chemical shifts.