Electronic Supplementary Information

Mixed-ligand benzaldehyde thiosemicarbazone complexes of palladium containing N,O-donor ancillary ligands: Syntheses, structures and, catalytic application in C-C and C-N coupling reactions

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Table S1 Crystallographic data for [Pd(L-Cl)(q)]

Empirical formula	$C_{17}H_{13}N_4OSClPd$
Formula weight	463.25
Crystal system	Monoclinic
Space group	$P2_1/c$
a /Å	14.643(2)
b /Å	7.9232(11)
c /Å	15.771(2)
α /°	90
β /°	107.518(10)
γ /°	90
V /Å^3	1744.9(4)
Z	4
D_{calcd} /mg m^{-3}	1.763
F(000)	920
λ	0.71073
Crystal size/mm^3	0.23 × 0.24 × 0.25
Temp./K	273
μ /mm^{-1}	1.349
Collected reflections	20164
R_{int}	0.121
Independent reflections	4079
$R1$[a]	0.1257
$wR2$[b]	0.3160
GOF[c]	1.69

[a] $R1 = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$.
[b] $wR2 = [\ \Sigma[\ w(\ F_o^2 - F_c^2)^2] / \Sigma\ [w(\ F_o^2)^2]\ ]^{1/2}$.
[c] $GOF = [\Sigma[w(F_o^2-F_c^2)^2]/(M-N)]^{1/2}$, where M is the number of reflections and N is the number of parameters refined.

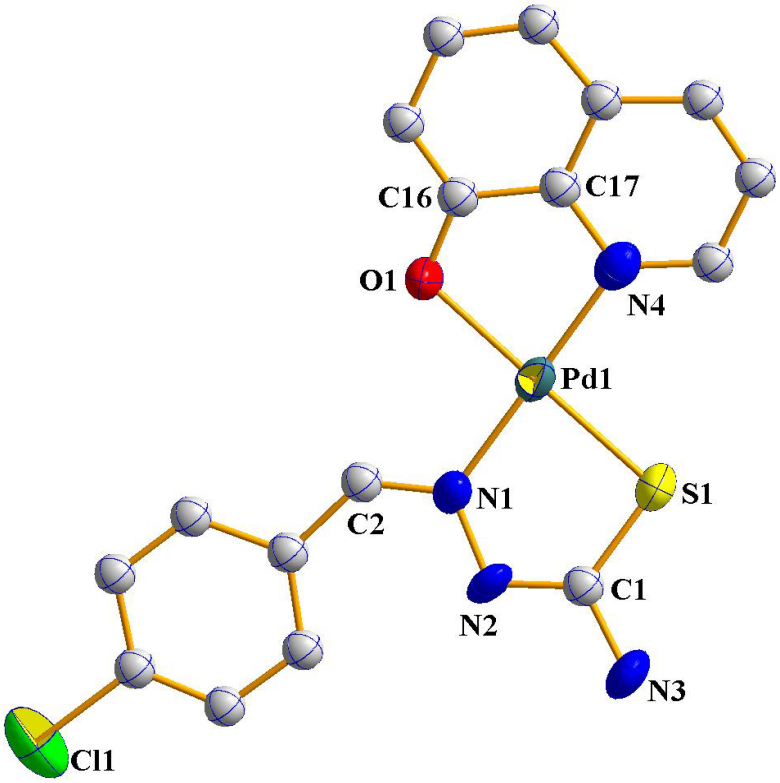

Fig. S1 Structure of [Pd(L-Cl)(q)].

Table S2 Selected bond distances and bond angles for [Pd(L-Cl)(q)]

Bond distances (Å)			
Pd(1)-N(1)	2.015(11)	N(1)-C(2)	1.270(17)
Pd(1)-N(4)	2.029(12)	N(1)-N(2)	1.376(13)
Pd(1)-O(1)	2.075(9)	C(1)-S(1)	1.719(14)
Pd(1)-S(1)	2.237(3)	C(16)-O(1)	1.307(19)
Bond angles (°)			
N(1)-Pd(1)-N(4)	179.2(4)	N(1)-Pd(1)-S(1)	83.3(3)
O(1)-Pd(1)-S(1)	177.6(3)	N(4)-Pd(1)-O(1)	81.9(4)

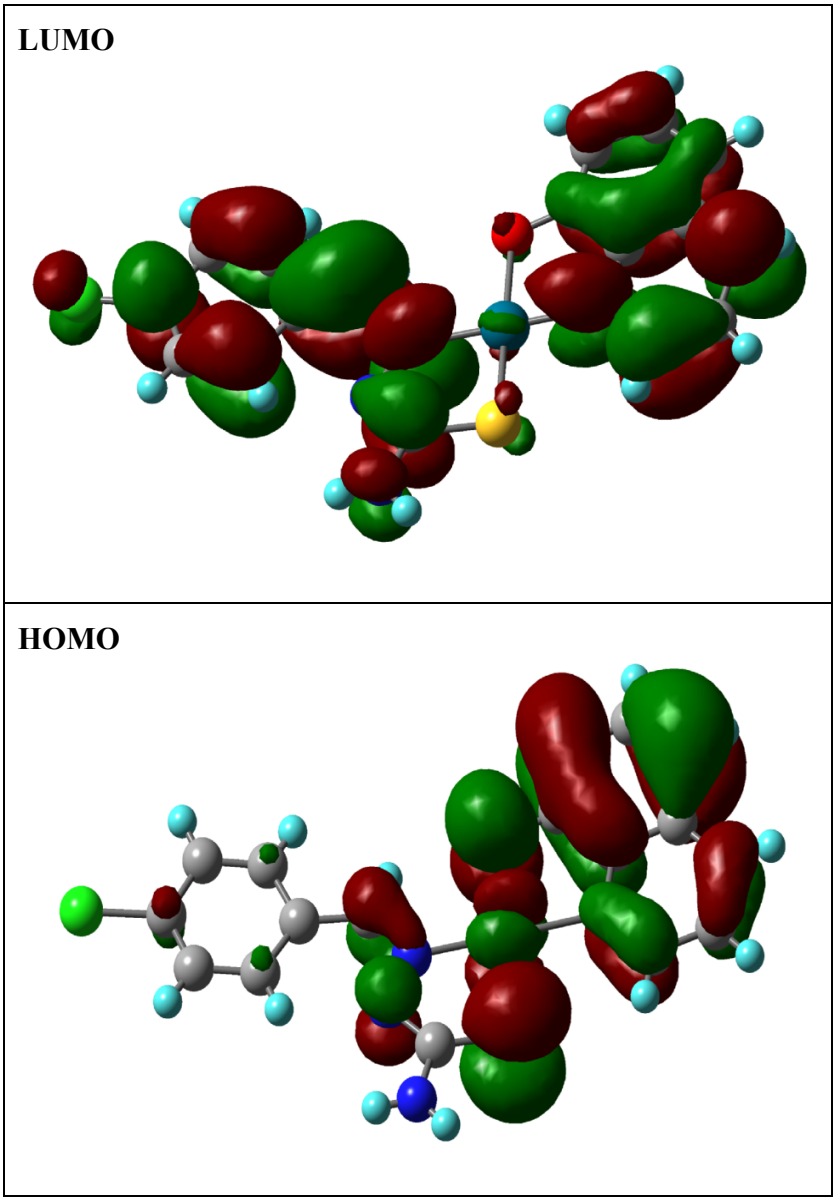

Fig. S2 Contour plots of HOMO and LUMO of [Pd(L-Cl)(q)].