Electronic Supporting Information

A Phenanthroline-Derived Ligand and Its Complexation with Pd(II): From Ligand Design, Synthesis and Pd(II) Complexes Structures to Its Application

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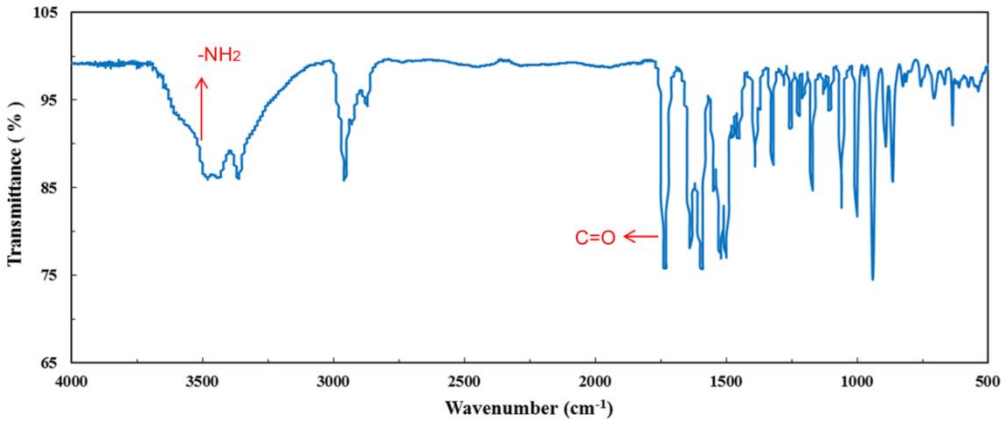

Fig. S1: FT-IR spectrum (KBr) of **3**.

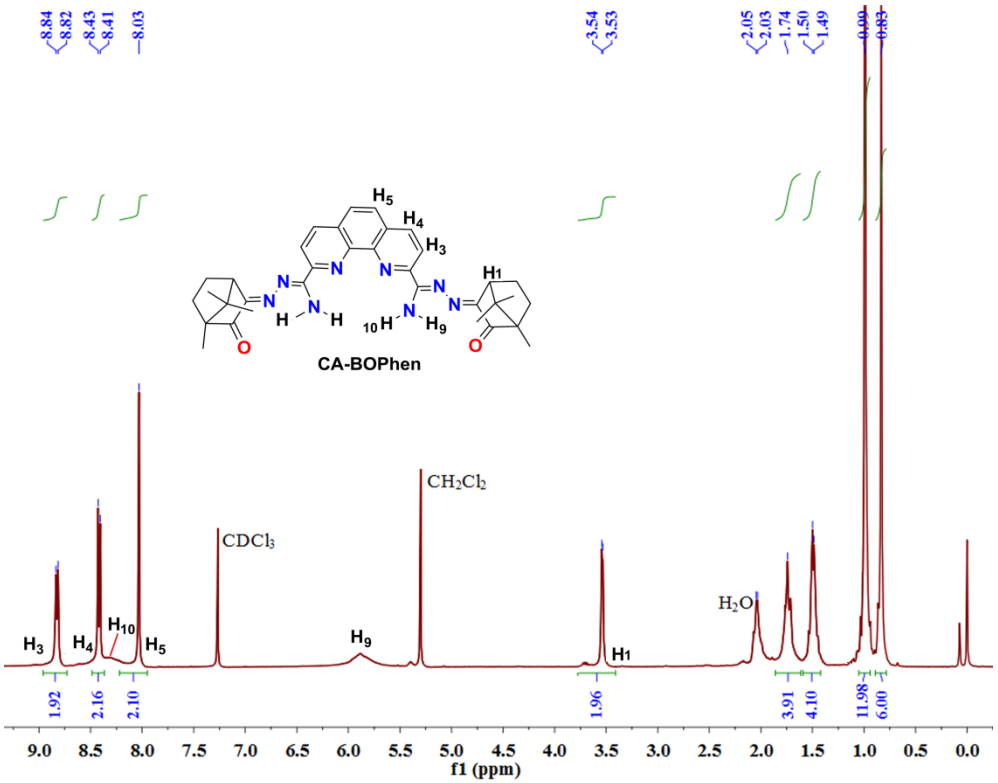

Fig. S2: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of **3**.

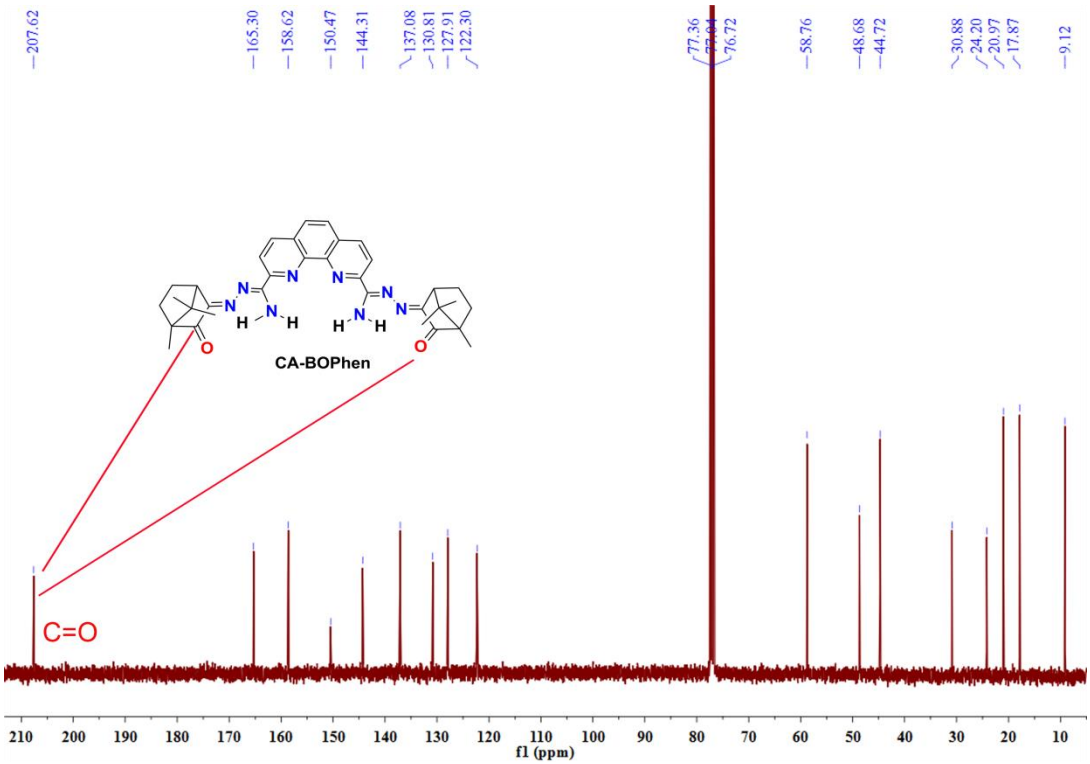

Fig. S3: ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of **3**.

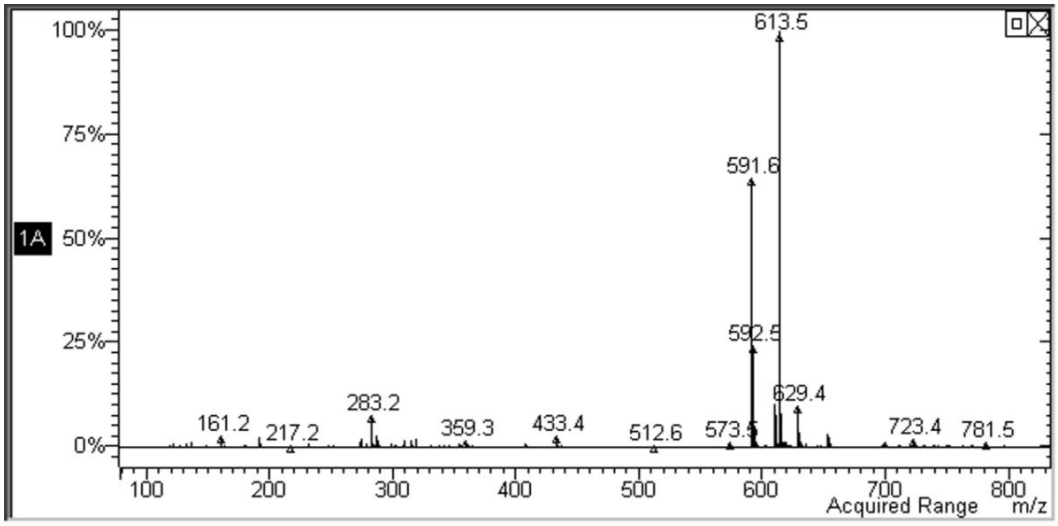

Fig. S4: ESI-MS of **3**, main peaks: 591.60 $[M+H]^+$, 613.5 $[M+Na]^+$ (100%).

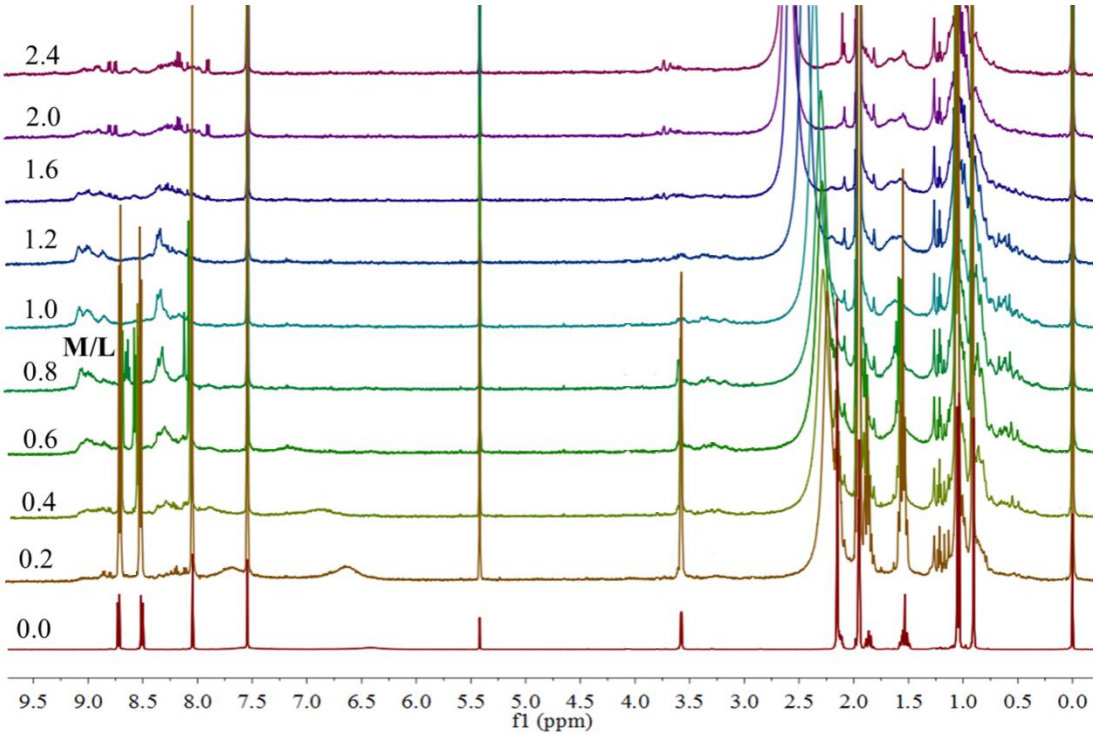

Fig. S5: Stacked ^{1}H NMR spectra (500 MHz, 295 K) of **3** (5.3mM) titrated with $Pd(NO_3)_2$ in CD_3CN/CCl_3D (7/3, v/v); M/L = Pd equivalents.

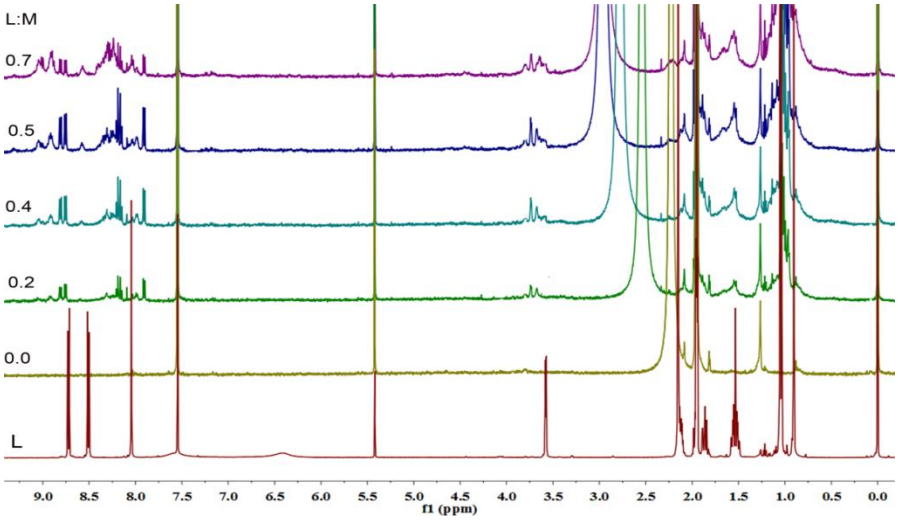

Fig. S6: Stacked ^{1}H NMR spectra (500 MHz, 295 K,) of $Pd(NO_3)_2$ (4.5 mM) titrated with various equivalents (0~0.7) of **3** in CD_3CN/CCl_3D (7/3, *v*/*v*), L:M=**3** equivalents.

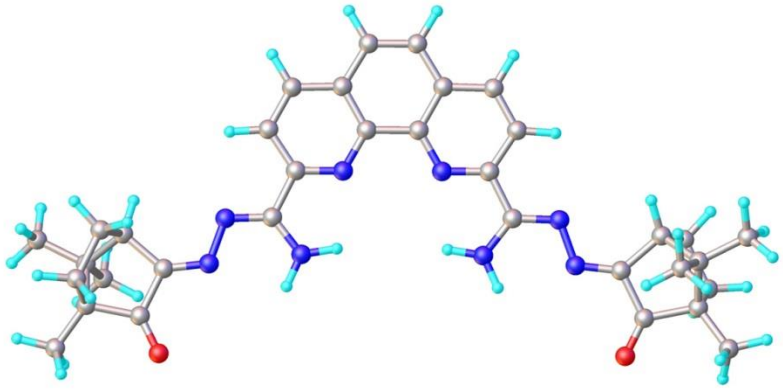

Fig. S7a: Optimized structure of the ligand **3**

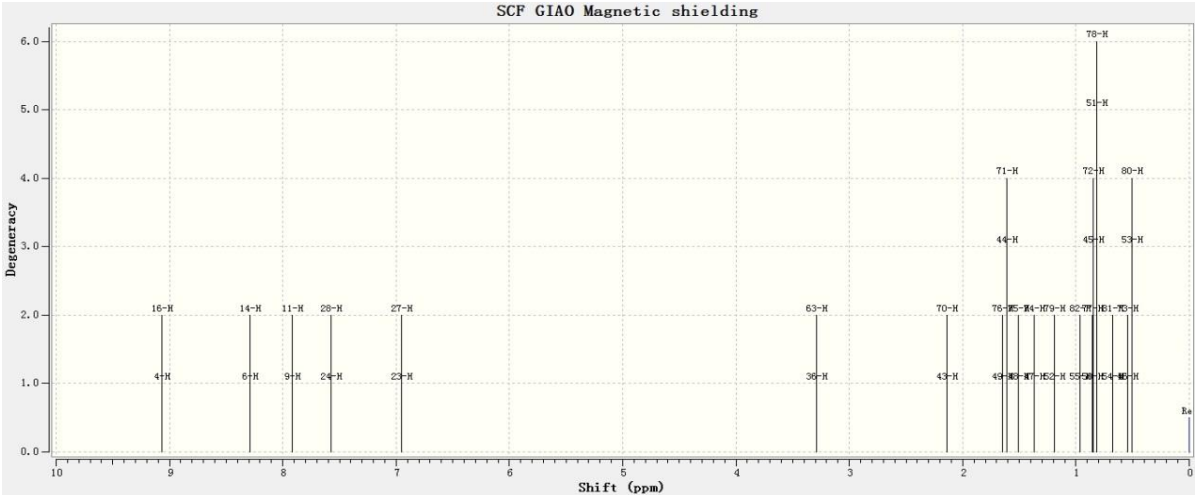

Fig. S7b: Calculated ^{1}H NMR spectrum of the ligand **3**

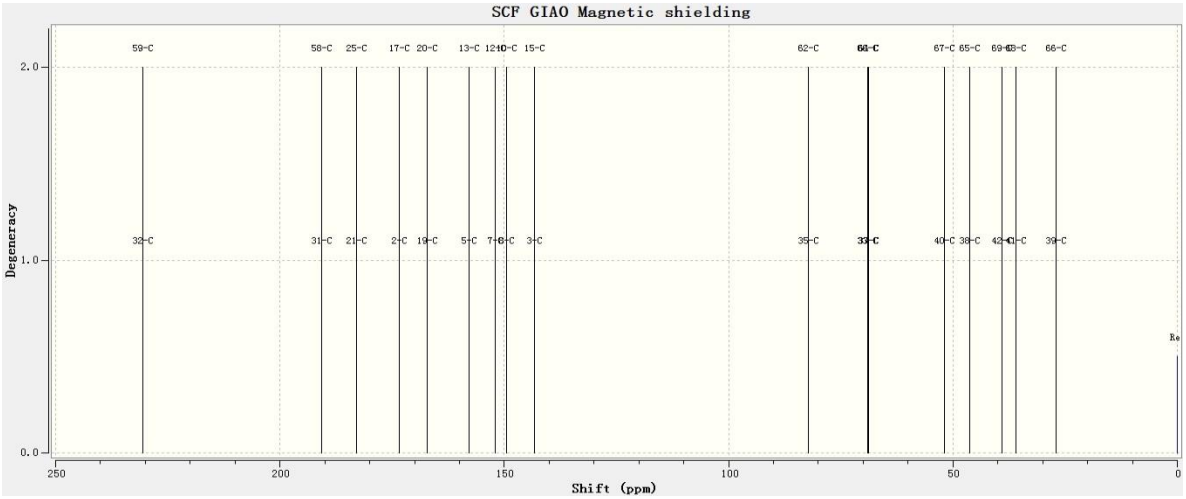

Fig. S7c: Calculated ^{13}C NMR spectrum of the ligand **3**

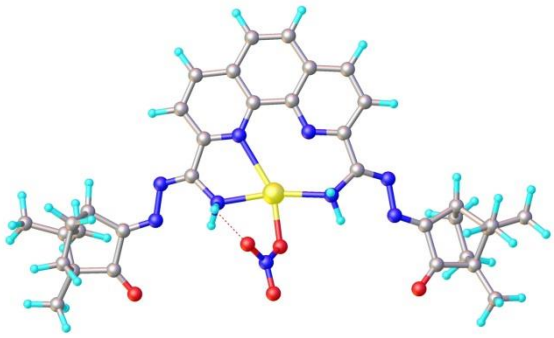

Fig. S8a: Optimized structure of the 1:1 complex $[Pd(NO_3)(\mathbf{3})]^+$

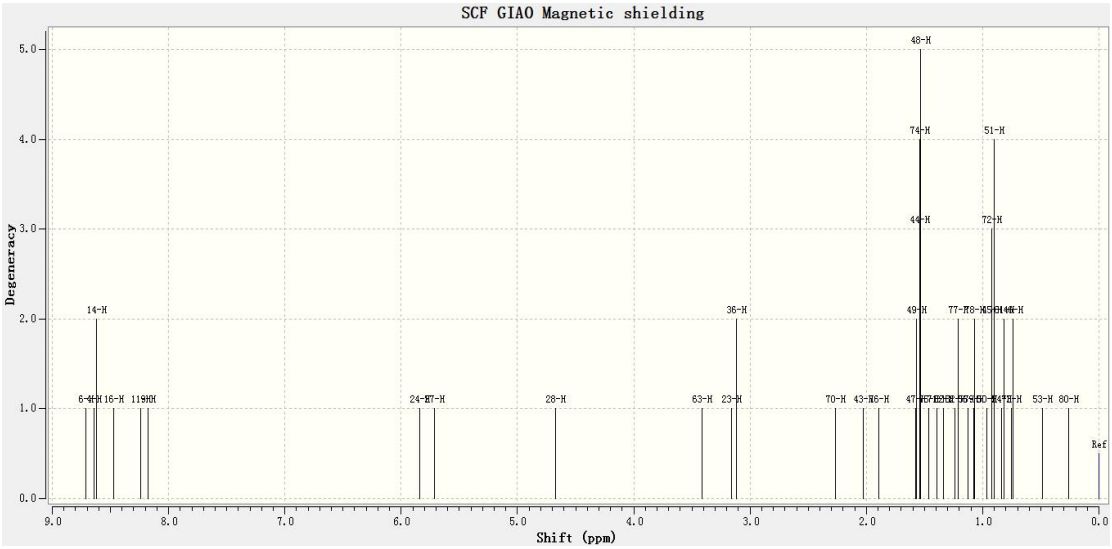

Fig. S8b: Calculated ^{1}H NMR spectrum of the 1:1 complex $[Pd(NO_3)(\mathbf{3})]^+$

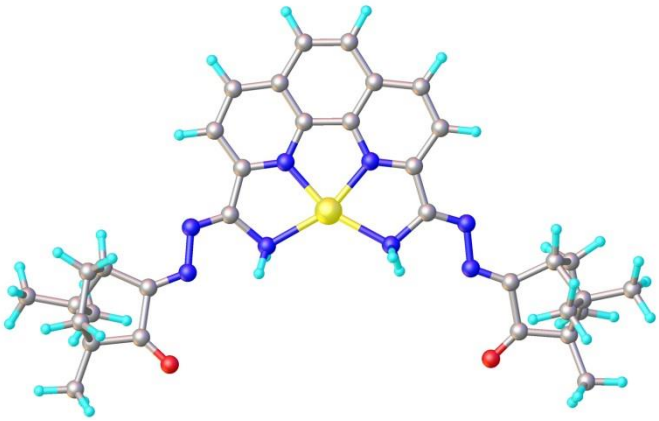

Fig. S9a: Optimized structure of the 1:1 complex [(**3**)Pd]$^{2+}$

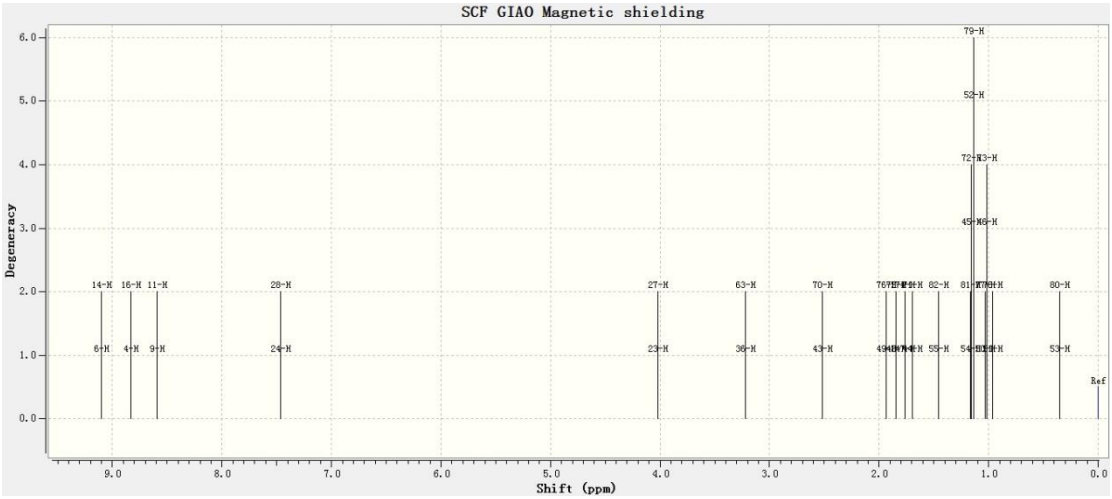

Fig. S9b: Calculated ^{1}H NMR spectrum of the 1:1 complex [(**3**)Pd]$^{2+}$

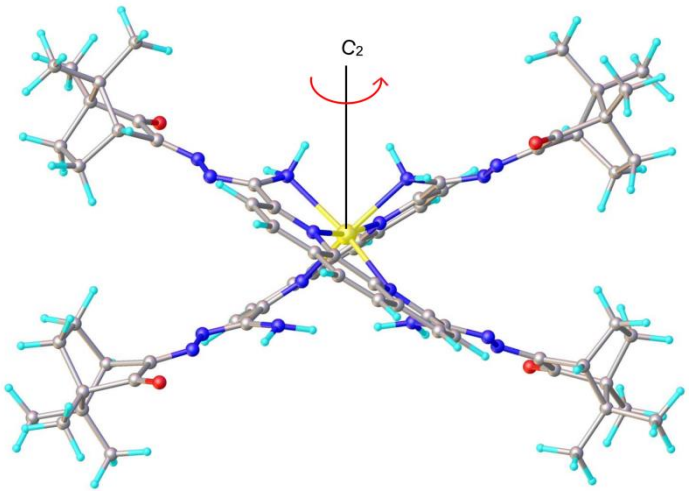

Fig. S10a: Optimized structure of the 2:1 complex $[(\mathbf{3})_2Pd]^{2+}$ with C_2 symmetry.

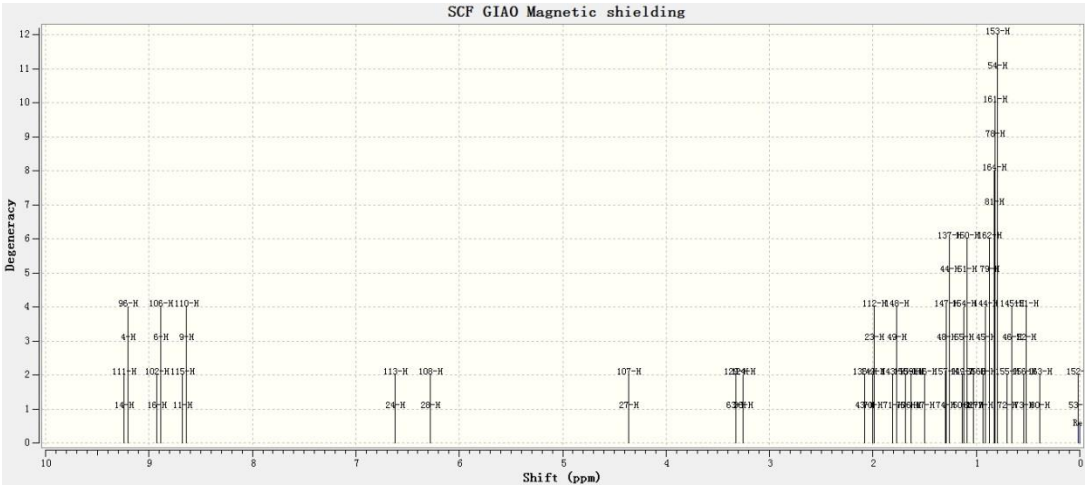

Fig. S10b: Calculated ^{1}H NMR spectrum of the 2:1 complex $[(\mathbf{3})_2Pd]^{2+}$.

Table S1. Separation factor (SF) of Pd(II) over other tested metals in different HNO_3 concentrations.

$[HNO_3]$ (M)	$SF_{Pd/Li}$	$SF_{Pd/Na}$	$SF_{Pd/K}$	$SF_{Pd/Rb}$	$SF_{Pd/Cs}$	$SF_{Pd/Mg}$	$SF_{Pd/Ca}$	$SF_{Pd/Sr}$	$SF_{Pd/Ba}$
0.4	195	79.7	96.7	20.1	179	357	185	101	406
1.0	77.2	41.6	43.4	39.7	73.2	127	135	66.0	84.6
2.0	88.9	41.9	82.2	36.6	56.3	301	175	66.1	103
3.0	113	96.7	59.6	20.5	63.8	357	74.1	72.8	127
4.0	109	71.5	72.0	21.0	77.1	505	58.2	112	272
5.0	48.2	99.2	112	23.0	73.7	336	1081	166	1908
6.0	77.2	98.7	281	18.1	94.1	384	675	392	1350

Table S2. Separation factor (SF) of Pd(II) over other tested metals in different HNO_3 concentrations.

$[HNO_3]$ (M)	$SF_{Pd/Fe}$	$SF_{Pd/Co}$	$SF_{Pd/Ni}$	$SF_{Pd/Zr}$	$SF_{Pd/Ru}$	$SF_{Pd/La}$	$SF_{Pd/Nd}$	$SF_{Pd/Yb}$	$SF_{Pd/Y}$
0.4	140	1480	815	20.0	929	929	195	1609	268
1.0	228	92.9	62.6	41.9	59.2	60.7	53.0	85.7	77.3
2.0	237	300	104	56.6	38.7	38.7	102	112	261
3.0	206	130	111	30.2	20.3	39.0	110	190	112
4.0	272	209	261	27.2	20.2	26.4	1418	72.5	89.3
5.0	161	253	287	23.0	25.9	612	927	154	477
6.0	318	325	397	24.5	23.2	1298	1607	1125	1298