Supplementary Information

Deciphering Anion–π-Acceptor Interactions and Detecting Fluoride Using a Naphthalenediimide-Based Pd(II) Coordination Polymer

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Experimental Section

General Methods and Materials

Starting materials and reagents were purchased from Sigma Aldrich and Cambridge Isotope Laboratory, and used as received. All reactions were performed in dry solvents under N_2 atmosphere unless otherwise specified. The final [Pd(II)(dppe)DPNDI]$_n$ zigzag coordination polymer was characterized by ^{1}H, ^{13}C, ^{19}F NMR and COSY spectroscopy at 298 K in DMSO-d_6 on Bruker Avance 400 MHz and 600 MHz spectrometers. Tetra-*n*-butylammonium (TBA) salts of F^-, Cl^-, Br^-, I^-, AcO^-, $H_2PO_4^-$, NO_2^-, NO_3^- and PF_6^- were purchased from Sigma-Aldrich and were protected from moisture. Freshly prepared solutions of zigzag coordination polymer and anions in dry, HPLC grade solvents were used for all spectroscopic and electrochemical measurements.

DPNDI: DPNDI was prepared as described in the literature.[S1] Briefly, a mixture of 1,4,5,8-naphthalene tetracarboxylic dianhydride (NDA) (0.8 g, 3 mmol) and 4-amino pyridine (0.56 g, 6 mmol) in DMF (20 mL) was heated under reflux for 8 h. A crystalline solid precipitated on cooling and was collected by filtration. The crude product was purified by recrystallization from DMF to obtain compound **1** as an off-white crystalline solid in 81% yield (1.02 g, 2.43 mmol). ^{1}H NMR (400 MHz, DMSO-d_6, 25 °C): δ = 8.81 (dd, J = 1.6 Hz and 3 Hz, 4H$_c$), 8.75 (s, 4H$_a$), and 7.58 (dd, J = 1.6 Hz and 4.5 Hz, 4H$_b$) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25 °C): δ = 162.80, 151.23, 144.0, 131.01, 127.43, 127.21, and 124.96 ppm. MS (HR-ESI, +ve) *m/z*: Observed 421.0942 $[M+H]^+$, $[M+H]^+_{calcd}$ = 421.0937. FT-IR: 3069.97, 1712.27, 1661.71, 1574.39, 1491.67 cm^{-1}.

Pd(II)(dppe)(TfO$^-$)$_2$: The reaction of 1 equiv of Pd(dppe)Cl$_2$ [dppe = 1,2-bis(diphenylphosphino)ethane] with 2 eqiv $AgOSO_2CF_3$ (silver trifluoro methanesulphonate) in DCM resulted in the desired cis bis(triflate) complex (**2**).[S2] ^{1}H NMR (400 MHz, CD_3CN, 25 °C): δ = 7.82–7.76 (m, 12H), 7.68–7.63 (m, 8H), 2.98–2.94 (m, 2H), and 2.88–2.83 (m, 2H) ppm. MS (ESI-MS) *m/z*: 803.14 $[M+H]^+$.

[Pd(II)(dppe)(DPNDI)]$_n$ coordination polymer: A mixture of NPNDI (0.1 g, 0.24 mmol), **2** (0.2 g, 0.24 mmol) in DMF (60 mL) was stirred for 5 h at room temperature. DMF was evaporated under the vacuum and zigzag Pd(II) complex was obtained as an off-white solid in 71% yield (0.84 g, 0.17 mmol). ^{1}H NMR (400 MHz, DMSO-d_6, 25 °C): δ = 8.84 (br, H$_B$ proton, 4H), 8.75 (s, H$_A$ proton, 4H), 7.90–7.85 (m, H$_D$ proton, 8H), 7.78–7.75 (m, H$_F$ proton, 4H), 7.68–7.65 (m, H$_E$ proton, 8 H) and 7.61–7.60 (d, H$_C$ proton, J = 5.4 Hz, 4H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25 °C): δ = 162.23, 162.08, 151.35, 133.37, 133.30, 130.51, 129.67, 129.59, 126.79, 125.64, 125.28, 121.71, 119.58 and 30.71 ppm. ^{19}F NMR (400 MHz, DMSO-d_6, 25 °C): δ = 79.28 ppm. ESIMS (+ve) *m/z*: Observed 462.1 $[\{Pd(dppe)\}_n(DPNDI)_n]^{2n+}$, 1073.0 $[\{Pd(dppe)\}_n(DPNDI)_n(TfO^-)_n]^{n+}$, 548.0 $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)]^{7+}$, 828.9 $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)_3]^{5+}$, 2297.0 $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)_6]^{2+}$. FT-IR: 3058.94, 1720.47, 1679.18, 1664.68, 1644.37, 1608.71, 1582.10, 1497.53 cm^{-1}.

Energy Minimized Structures of DPNDI, TfO$^-$/DPNDI/TfO$^-$ and THF/DPNDI/THF

B3LYP/6-31+G** energy minimization[S3] was conducted using Gaussian 03 Software.[S4] Electrostatic potential (ESP) map has been used to determine the charge distribution of NDI. Electron rich regions are depicted in red and electron deficient regions are in blue.

Electrospray Ionization Mass Spectrometry (ESI-MS)

ESI-MS were recorded on a JEOL AccuTOF JMS-T100LC mass spectrometer using positive ionization mode for the detection of the Pd(II) coordination polymer. ESI-MS shows the presence and isotope distribution patterns of $[\{Pd(dppe)\}_n(DPNDI)_n]^{2n+}$ and $[\{Pd(dppe)\}_n(DPNDI)_n(TfO^-)_n]^{n+}$ [n = 1,2,3,4…] at *m/z* 462.1 and 1073.0 respectively. Moreover, ESI-MS also shows the presence and isotope distribution patterns of $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)]^{7+}$, $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)_3]^{5+}$ and $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)_6]^{2+}$ at *m/z* 548.0, 828.9 and 2297.0 respectively, indicating a preponderance of the

tetranuclear (n=4) complex. ESI-MS data show isotope distribution patterns of DPNDI and TfO^- complexes: [DPNDI·TfO^-] and [TfO^-·DPNDI·TfO^-].

UV/Vis Spectroscopy

UV/Vis spectra were recorded on a PerkinElmer Lambda-25 UV/Vis spectrophotometer. DPNDI ligand and [Pd(II)(dppe)DPNDI]$_n$ complex concentrations were taken at 10 μM and 2.5 μM, respectively and the TBAX solutions were 30 times more concentrated.

Electrochemistry and Spectroelectrochemistry

Cyclic voltammetry (CV) was conducted on a Princeton Applied Research (PAR) VersaStat-3-200 potentiostat/galvanostat instrument using a standard electrochemical cell, consisting of a glassy carbon working electrode, Pt-wire counter electrode, and Ag/AgCl (3 N aq. NaCl) reference electrode. CV was recorded at 1 mM of DPNDI and Pd(II)(dppe)(DPNDI) containing zigzag coordination polymer in 0.1 M $TBAPF_6$ / DMF supporting electrolyte solution at room temperature at 100 mV/s scan rate.

Spectroelectrochemistry was conducted in an Optically Transparent Thin Layer Electrochemical Cell (OTTLE) fitted with a Pt-gauge working electrode, Pt-wire counter electrode, and Ag/AgCl (3 N aq. NaCl) reference electrode using 0.5 mM of DPNDI and 0.2 mM of [Pd(II)(dppe)DPNDI]$_n$ zigzag coordination polymer in 0.1 M $TBAPF_6$ / DMF supporting electrolyte solution at room temperature. UV/Vis spectra were recorded at 2 min. intervals on a PerkinElmer Lambda-25 UV/Vis spectrophotometer while the applied potential was controlled by the PAR potentiostat, using Virtual Potentiostat software. For the $DPNDI^{\bullet-}$ radical anion formation the applied potential (E_{ap}) was held at –450 mV until the corresponding spectra reached the saturation point and did not show any difference between two consecutive spectra. The same was done for the detection of $DPNDI^{2-}$ by setting E_{ap} at –900 mV.

Crystal Growth and Crystallographic Data

Rectangular shaped single crystals were grown by a slow vapor diffusion of THF into CH_3CN solution of the [Pd(II)(dppe)DPNDI]$_n$ complex. Numerous crystals were analyzed before the most suitable single crystal was mounted on a goniometer head of a Bruker SMART APEX II diffractometer using a nylon loop with a small amount of Paratone oil (Hampton Research). The crystal was cooled to 153 K in a cold stream of N_2 gas. After finding a crystal that indexed to give a satisfactory unit cell, a full low-temperature data set at 153 K was recorded using a sample-to-detector distance of 6 cm. Diffraction data of the compound was measured with Mo Kα (λ = 0.71073 Å) radiation. The size of the crystal required 100 s collection times with omega scans. Even so, reflections were found only at considerably below optimal angles-only about $\theta = 19°$. The Bruker suite of programs on the APEX II was used to integrate the data and SADABS was used for absorption corrections.[S5,S6] The structure was readily solved by direct methods and refined using the SHELXTL.[S7] This crystal has a very open structure containing a lot of disordered THF solvent molecules. The structure shows a zigzag pattern of [Pd(II)(dppe)(DPNDI)]$_n$ chains. We have attempted to resolve solvent molecules, with and without various restraints. Interestingly, all attempts to assign the disordered THF molecules resulted in elevated R-values. THF is known to cause disorder in crystal structures. Since the use of restraints to control the THF molecules yielded problematic results, Platon SQUEEZE program was used. Four tetrahydrofuran molecules were present as the solvent molecule among which two has been removed using SQUEEZE. Thus eight carbon, sixteen hydrogen and two oxygen atoms of tetrahydrofuran molecule were added to the chemical formula to adjust the density, molecular mass and F000 value. In the main residue N2, N4, C21, C27, C28, C32, C33, C37 and C38 were left isotropic since anisotropy for these atoms was not stable." The final R-value was $R1 = 0.0731$ and $wR2 = 0.1950$ for 5085 observed reflections $I > 2\sigma(I)$. In the title compound, [Pd(II)(dppe)DPNDI]$_n$ the complex molecule has crystallographically imposed inversion symmetry. The stereochemistry about each PdN_2P_2 center is square planer. Crystallographic data has been deposited at the Cambridge Crystallographic Data Center with reference number CCDC 841999. These data can be

obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

Formula moiety	$C_{50}H_{36}N_4O_4P_2Pd$, $4(C_4H_8O)$, $2(CF_3O_3S)$
Formula sum	$C_{60}H_{52}F_6N_4O_{12}P_2PdS_2$
Formula weight	1511.58
Crystal system	Monoclinic
Space group	P2(1)/c
a, Å	21.140(4)
b, Å	14.841(3)
c, Å	25.156(5)
β, °	96.51(2)
Z	4
V, Å^3	7842(3)
D_{calcd}, g cm^{-3}	1.411
μ, mm^{-1}	0.395 (Mo Kα)
T, K	153(2)
λ, Å	0.71073 (Mo Kα)
*R*1	0.0731
*wR*2	0.1950
R_{int}	0.0623
No. of reflections measured	23941
No. of independent reflections	6504
Goodness of fit on F^2	1.085
CCDC no	841999

References:

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S4 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03, Revision C.02; Gaussian: Wallingford, CT, **2004**.

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S6 *SADABS*, Bruker AXS Inc., Madison, WI, USA, 2001.

S7 G. M. Sheldrick, *Shelxs97* and *Shelxl97*, Programs for Crystallographic Solution and Refinement. *Acta Crystallogr.*, 2008, **A64**, 112.

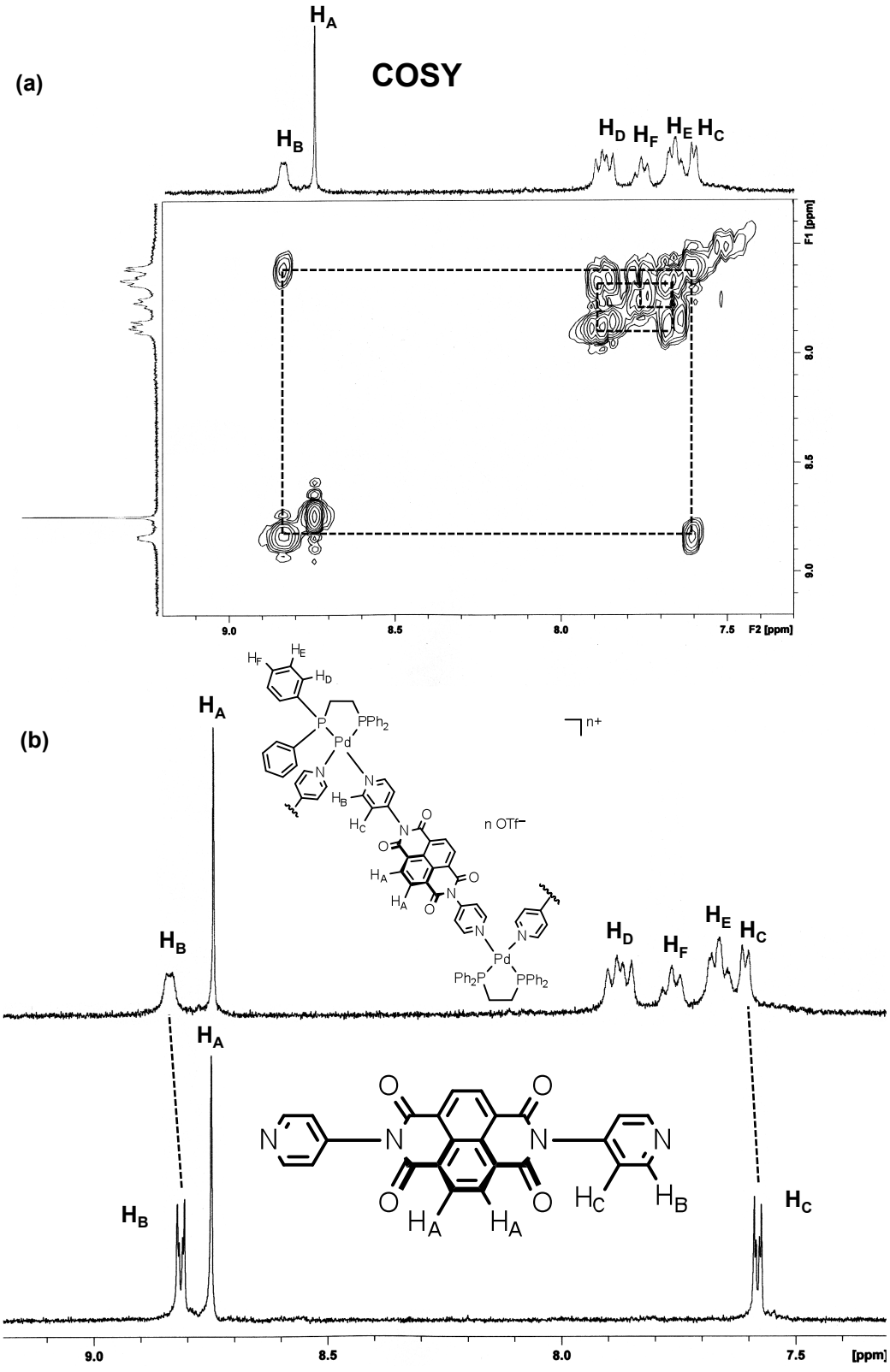

Figure S1. (a) COSY NMR (400 MHz) spectra of the [Pd(II)(dppe)DPNDI]$_n$ coordination polymer in DMSO-d_6 at 298 K. (b)^{1}H NMR spectra (DMSO-d_6, 298 K) of free DPNDI ligand (bottom) and the [Pd(II)(dppe)DPNDI]$_n$ coordination polymer (top) indicating how pyridine protons H_B and H_C of DPNDI ligand shifts to downfield and become broad as a result of the complex formation.

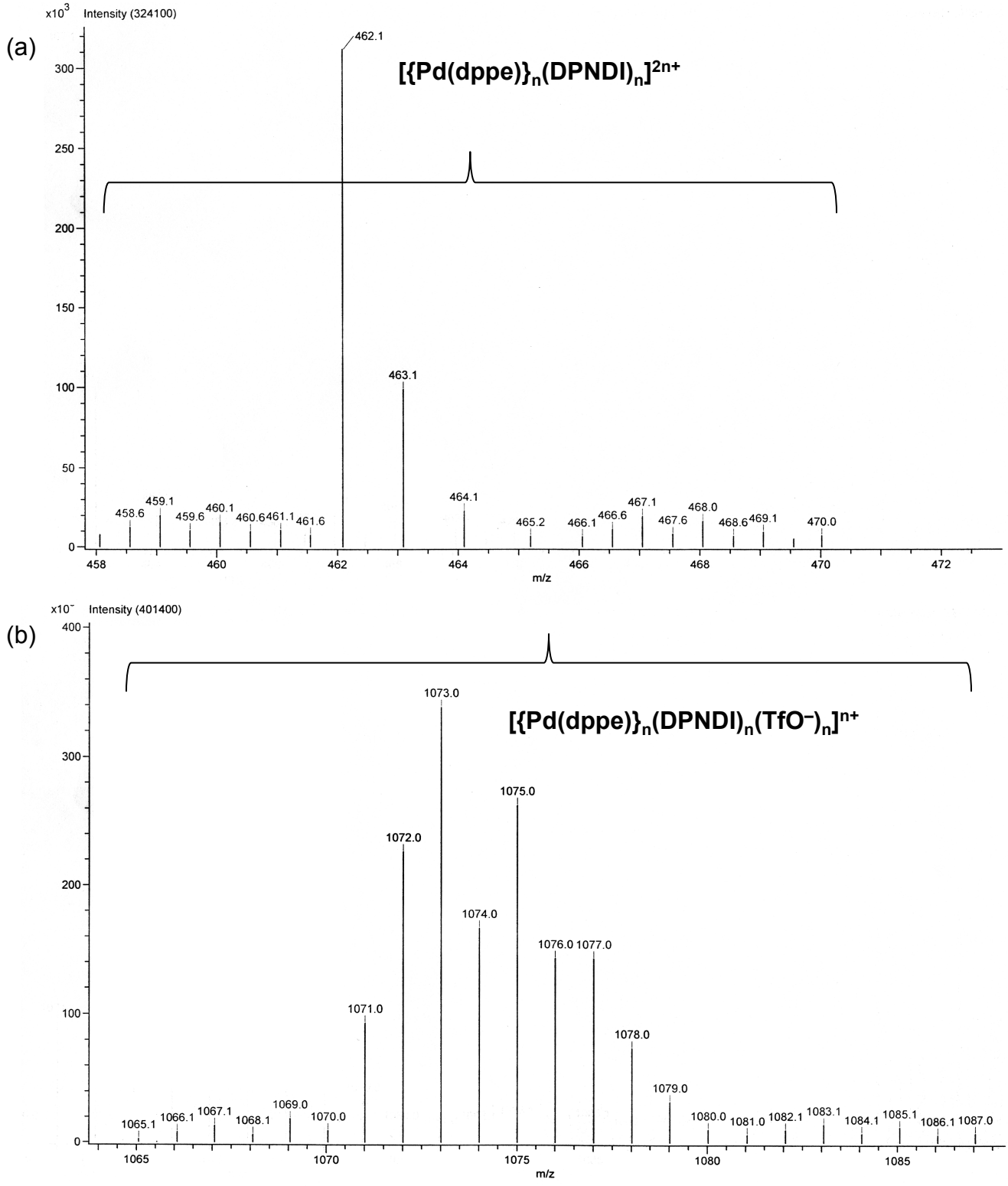

Figure S2(a and b). ESI-MS shows the presence and isotope distribution patterns of $[\{Pd(dppe)\}_n(DPNDI)_n]^{2n+}$ (a) and $[\{Pd(dppe)\}_n(DPNDI)_n(TfO^-)_n]^{n+}$ where n=1,2,3,4…….

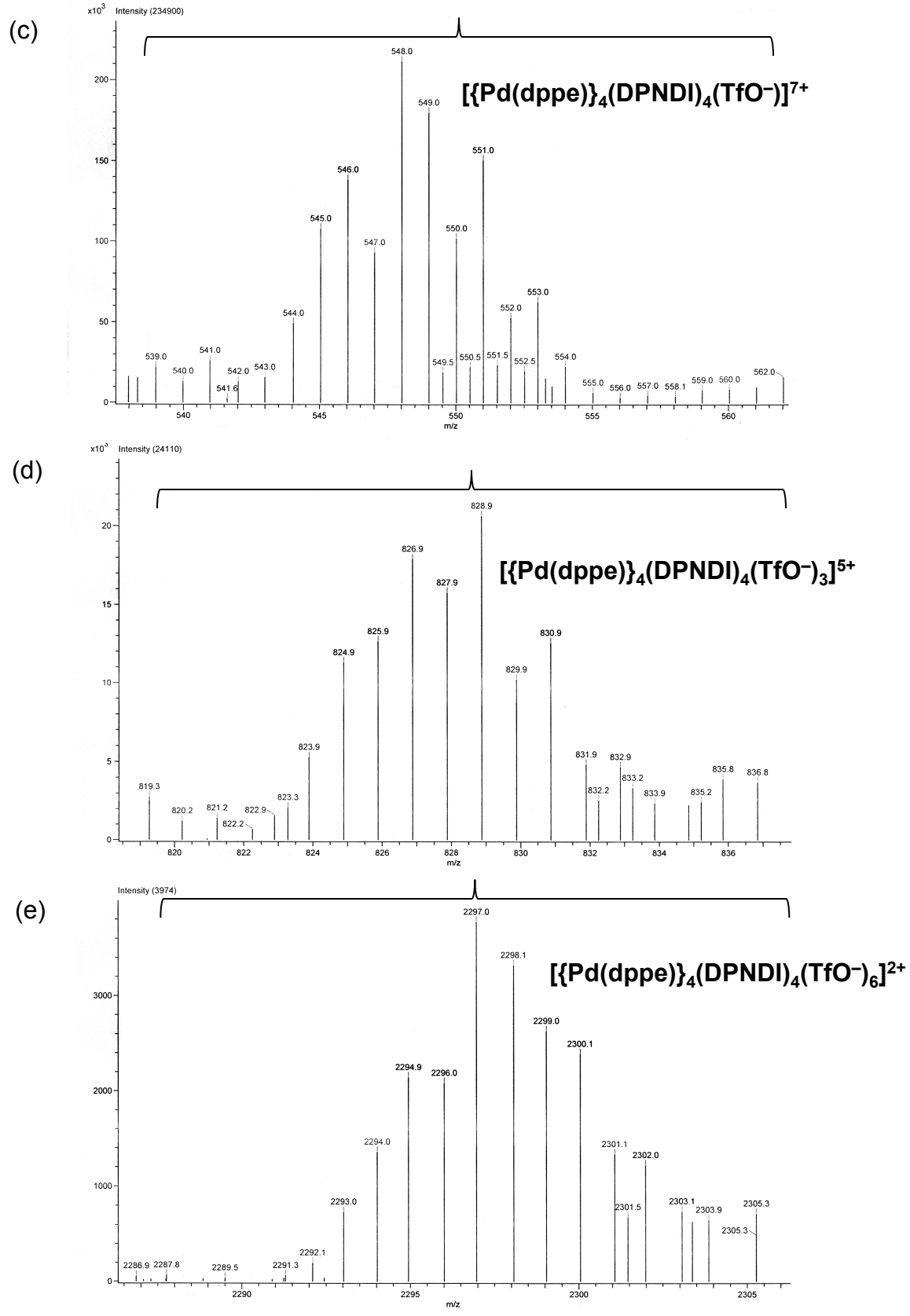

Figure S2(c-e). ESI-MS shows the presence and isotope distribution patterns of (c) $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)]^{7+}$, (d) $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)_3]^{5+}$ and (e) $[\{Pd(dppe)\}_4(DPNDI)_4(TfO^-)_6]^{2+}$.

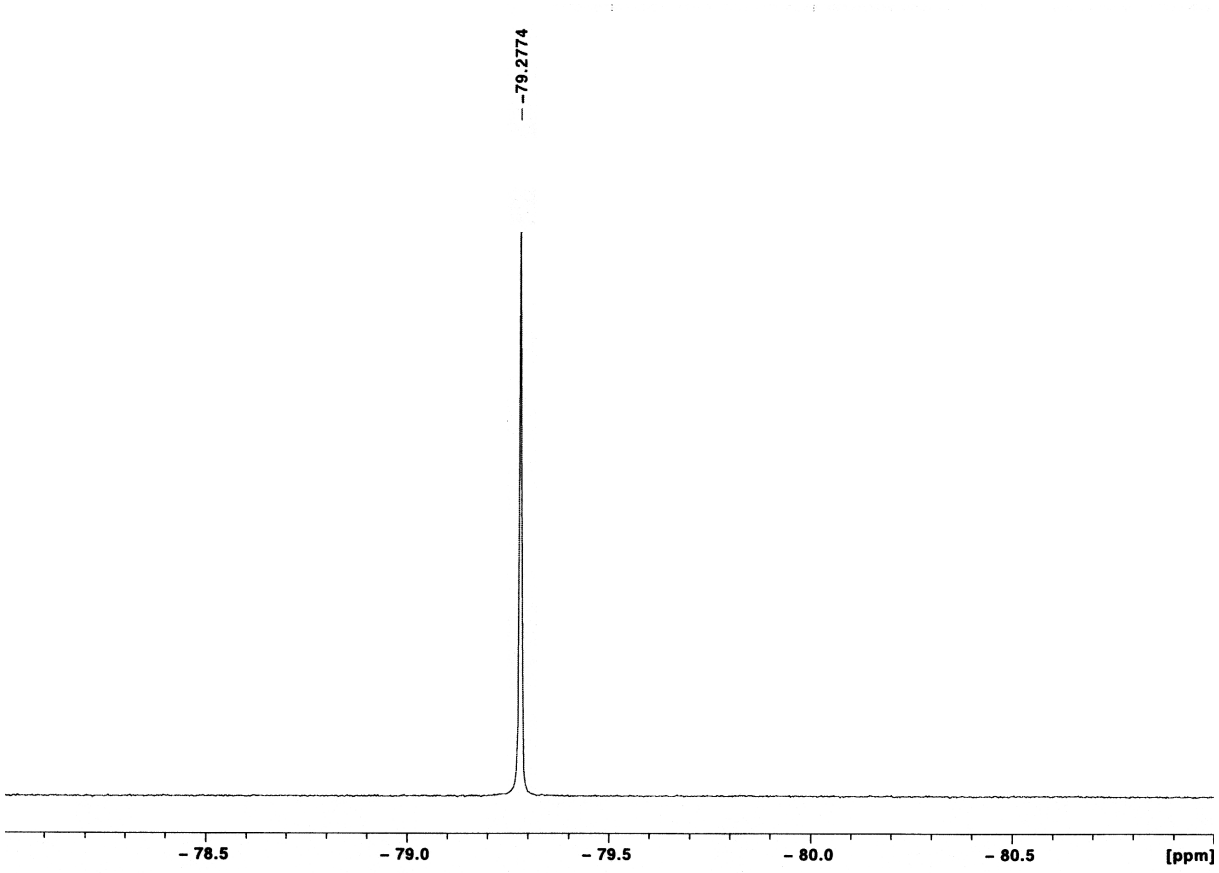

Figure S3. ^{19}F NMR spectrum of TfO^- in $[Pd(II)(dppe)DPNDI]_n$ coordination polymer (DMSO-d_6, 298 K).

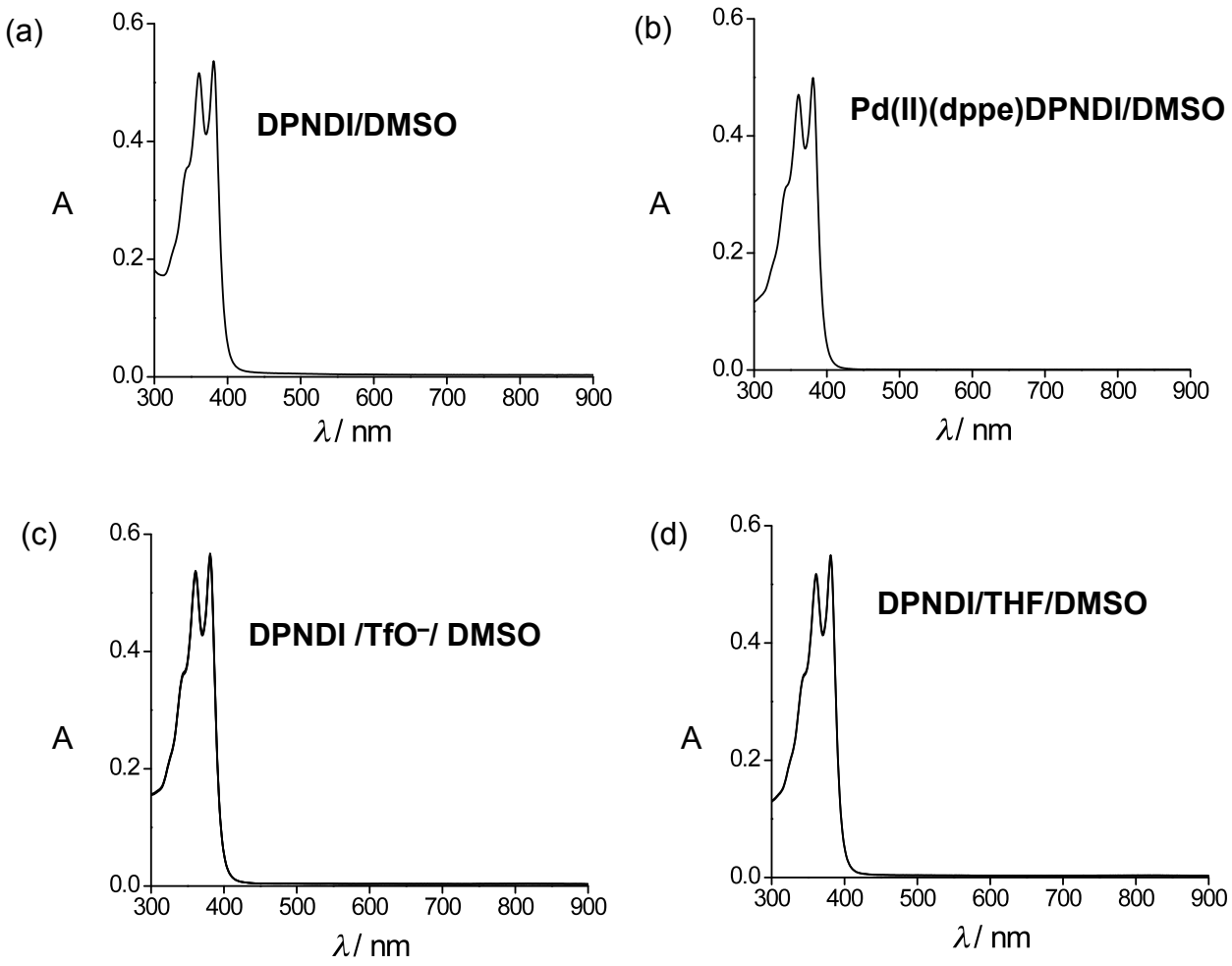

Figure S4. UV/Vis spectra of (a) free DPNDI ligand (10 μM/DMSO) and (b) $[Pd(II)(dppe)DPNDI]_n$ coordination polymer (2.5 μM/DMSO). UV/Vis spectra of free DPNDI ligand in DMSO with (c) TfO^- and (d) THF.

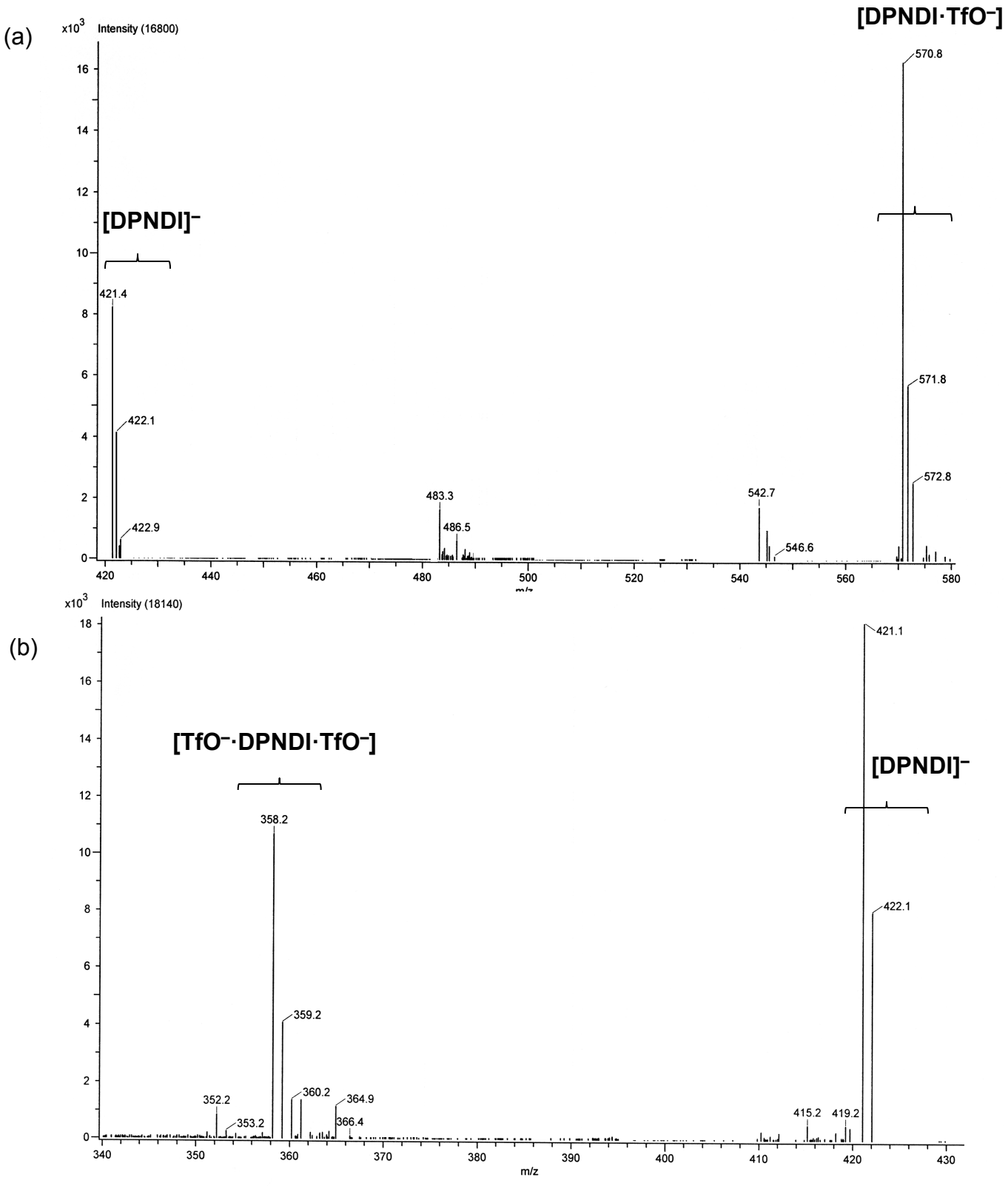

Figure S5(a and b). ESI-MS shows the presence and isotope distribution patterns of (a) $[DPNDI]^-$ and $[DPNDI{\cdot}TfO^-]$ in the presence of 1 equiv of TfO^- ion and (b) $[DPNDI]^-$ and $[TfO^-{\cdot}DPNDI{\cdot}TfO^-]$ in the presence of excess TfO^- ion.

(a)

(b)

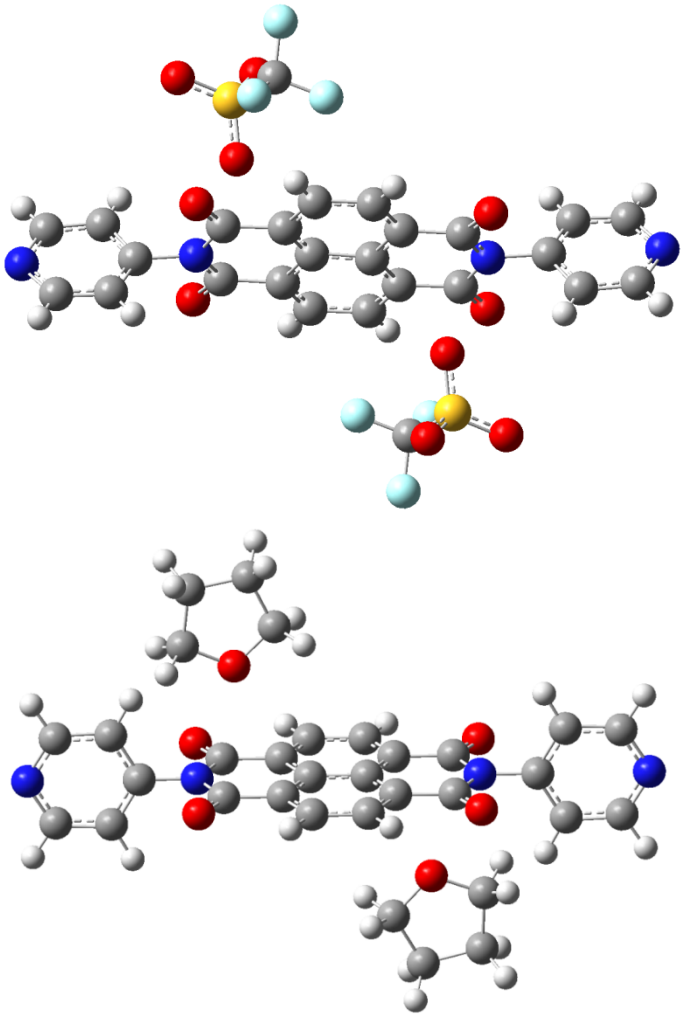

Figure S6 (a and b). B3LYP/6-31+G** energy minimized structure of (a) [TfO^{-}·DPNDI·TfO^{-}] complex and (b) [THF·DPNDI·THF] complex.

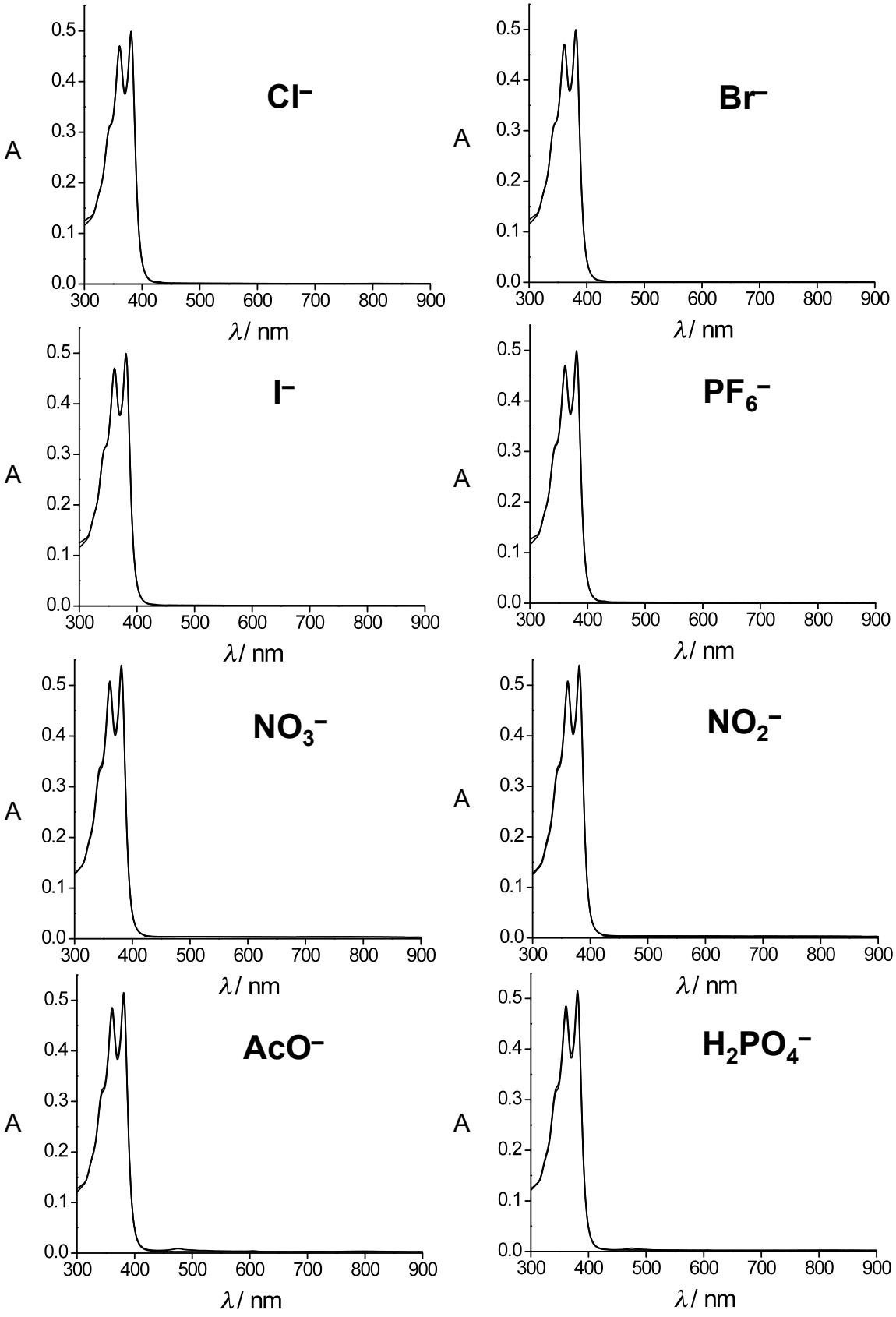

Figure S7. UV/Vis spectra of $[Pd(II)(dppe)DPNDI]_n$ coordination polymer (2.5 μM/DMSO) with excess amounts (50 equiv.) TBAX (X^- = Cl^-, Br^-, I^-, PF_6^-, NO_3^-, NO_2^-, AcO^-, and $H_2PO_4^-$)

Cartesian coordinates and total energies (Hartrees) of B3LYP/6-31+G energy minimized structures of NDI/anion complexes**

DPNDI•2TfO$^-$

C	1.39764300	6.55972200	2.40691700
H	1.37337500	7.41307900	1.98951800
C	1.81145400	5.25074600	4.24647100
H	2.07129300	5.17505700	5.15625100
C	1.03328800	5.47039300	1.67209500
H	0.72762900	5.54905000	0.77481200
C	1.50237100	4.14954400	3.60162800
H	1.53675700	3.30805900	4.04152100
C	1.13788400	4.22968500	2.31194000
N	0.76861200	3.02608000	1.56462100
C	-0.47045900	2.45321700	1.88204400
C	1.64786400	2.59123900	0.60235400
C	-1.94697400	0.50311000	1.51963200
H	-2.57194500	0.88749200	2.12448500
C	-0.77291500	1.15611400	1.23470100
C	0.11600300	0.63667900	0.31742300
C	1.37540700	1.27929400	-0.02999300
C	2.22439600	0.73611400	-0.91227900
H	3.02532100	1.19470000	-1.13222600
N	1.78806800	6.48848500	3.69160600
O	2.65760100	3.23682200	0.31242400
O	-1.19068200	2.96968400	2.69184800
C	-1.39764300	-6.55972200	-2.40691700
H	-1.37337500	-7.41307900	-1.98951800
C	-1.81145400	-5.25074600	-4.24647100
H	-2.07129300	-5.17505700	-5.15625100
C	-1.03328800	-5.47039300	-1.67209500
H	-0.72762900	-5.54905000	-0.77481200
C	-1.50237100	-4.14954400	-3.60162800
H	-1.53675700	-3.30805900	-4.04152100
C	-1.13788400	-4.22968500	-2.31194000
N	-0.76861200	-3.02608000	-1.56462100
C	0.47045900	-2.45321700	-1.88204400
C	-1.64786400	-2.59123900	-0.60235400
C	1.94697400	-0.50311000	-1.51963200
H	2.57194500	-0.88749200	-2.12448500
C	0.77291500	-1.15611400	-1.23470100
C	-0.11600300	-0.63667900	-0.31742300
C	-1.37540700	-1.27929400	0.02999300
C	-2.22439600	-0.73611400	0.91227900
H	-3.02532100	-1.19470000	1.13222600
N	-1.78806800	-6.48848500	-3.69160600
O	-2.65760100	-3.23682200	-0.31242400
O	1.19068200	-2.96968400	-2.69184800
O	-0.58451400	3.59597400	-1.04724600
F	-3.20000800	3.12996700	0.30992500
O	0.58451400	-3.59597400	1.04724600
F	3.20000800	-3.12996700	-0.30992500
S	1.72918600	-4.29053300	1.52038200
O	2.05329600	-5.51640000	0.84729500
O	1.83822400	-4.34841300	2.93678900
C	3.11262100	-3.21604500	1.01225500

F	4.29794800	-3.61378300	1.49963700
F	2.94812400	-1.97533700	1.47214300
S	-1.72918600	4.29053300	-1.52038200
O	-2.05329600	5.51640000	-0.84729500
O	-1.83822400	4.34841300	-2.93678900
C	-3.11262100	3.21604500	-1.01225500
F	-4.29794800	3.61378300	-1.49963700
F	-2.94812400	1.97533700	-1.47214300

Total energy = −3364.6552446

DPNDI•2THF

N	3.47643200	0.79940000	0.00458300
C	2.84472400	0.66406700	1.25963800
C	1.39955700	0.31171700	1.23817200
C	0.72990800	0.13034000	0.00199000
C	1.41015300	0.27779900	-1.23291700
C	2.85549600	0.62958000	-1.25165400
C	0.71211100	0.16191400	2.43316200
C	-0.65317600	-0.20658100	0.00068400
C	-1.33341300	-0.35406700	1.23559200
C	-0.65622100	-0.17143600	2.43187000
C	-2.77875100	-0.70587400	1.25433000
N	-3.39970200	-0.87563800	-0.00190800
C	-2.76800400	-0.74025600	-1.25696400
C	-1.32283100	-0.38793100	-1.23549800
C	-0.63538300	-0.23813500	-2.43048800
C	0.73296000	0.09517300	-2.42919600
H	1.27640300	0.21378000	-3.36034300
H	-1.17083500	-0.38232900	-3.36265500
H	1.24755800	0.30612600	3.36532800
H	-1.19966200	-0.29006200	3.36301800
O	3.48798100	0.76836700	-2.28548600
O	3.46833300	0.83127400	2.29465500
O	-3.39162300	-0.90741500	-2.29198200
O	-3.41122600	-0.84469700	2.28816200
C	4.88387400	1.14225600	0.00591200
C	5.84959900	0.14104700	0.02422000
C	7.19169700	0.52727500	0.02465600
N	7.59750000	1.80330400	0.00847400
C	6.65032800	2.74974500	-0.00898600
C	5.28096300	2.47545100	-0.01110800
H	5.56999400	-0.90694600	0.03775300
H	7.97569600	-0.22612400	0.03868800
H	7.00001600	3.77931300	-0.02194600
H	4.55072300	3.27744400	-0.02559600
C	-4.80714500	-1.21849100	-0.00323700
C	-5.77285900	-0.21730100	-0.02314500
C	-7.11495800	-0.60352500	-0.02351700
N	-7.52077300	-1.87953100	-0.00579800
C	-6.57360900	-2.82595100	0.01319700
C	-5.20424400	-2.55166000	0.01538400
H	-5.49324500	0.83067100	-0.03798000
H	-7.89894900	0.14985800	-0.03879300
H	-6.92330500	-3.85550000	0.02740300

H	-4.47401300	-3.35363500	0.03117200
C	-4.59186500	2.61344100	0.13071000
O	-3.19822700	2.31783300	0.00284300
C	-2.44153800	3.52207900	-0.14940200
C	-3.39405500	4.71265200	-0.12199700
C	-4.78655500	4.12423900	0.05939700
H	-5.11442700	2.07942700	-0.70401300
H	-4.92432600	2.18969100	1.11300900
H	-1.70450300	3.55059100	0.69378800
H	-1.89465200	3.44029900	-1.12368600
H	-3.13810200	5.40423800	0.71773200
H	-3.32545300	5.29556600	-1.07302400
H	-5.26467600	4.50563600	0.99475000
H	-5.45203000	4.39696500	-0.79600600
C	4.33126300	-2.34533300	-0.04501400
O	2.91837400	-2.14643300	0.05571000
C	2.23615200	-3.40298000	0.09599700
C	3.26333600	-4.52730900	0.01672300
C	4.62007900	-3.84240100	-0.07459200
H	4.66495500	-1.83123700	-0.98275500
H	4.79352300	-1.84250600	0.84295300
H	1.65643900	-3.42651300	1.05432000
H	1.52783900	-3.41524100	-0.77184300
H	3.20396600	-5.18127200	0.92102000
H	3.07725500	-5.17016500	-0.87829700
H	5.27593300	-4.13530700	0.78156700
H	5.14922400	-4.12420000	-1.01775000

Total energy = −1906.7059077