Supporting Information

Electronically Regulated Thermally and Light-Gated Electron Transfer from Anions to Naphthalenediimides

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Contents:

Experimental Section

MATERIALS

Chemicals and solvents were purchased from Sigma-Aldrich, Acros Organic, Cambridge Isotope Laboratory, and EMD Chemicals and used as obtained. NDIs **1–7** were synthesized by following the literature procedures[S1] (Scheme S1) and purified by SiO_2 column chromatography. ^1H, ^{13}C, and ^{19}F NMR spectra were recorded at 298 K in deuterated solvents on Bruker Avance 400 MHz and 600 MHz spectrometers. Tetra-*n*-butylammonium (TBA) salts of F^-, AcO^-, $H_2PO_4^-$, Cl^-, Br^-, I^-, and PF_6^- were purchased from Sigma-Aldrich and were protected from moisture. Freshly prepared solutions NDIs and anions in dry, HPLC grade solvents — purchased from Sigma-Aldrich and EMD Chemicals — were used for all spectroscopic and electrochemical measurements.

Synthesis and Characterization of NDI 1–7

All reactions were performed under N_2 atmosphere using dry solvents unless otherwise specified. Analytical thin layer chromatography (TLC) was performed on silica gel 60-F_{254} (Merck) plates and detected under UV lamp and/or by developing with I_2. Column chromatography was performed on silica gel 60 (SorbTech). ^1H and ^{13}C NMR spectra were recorded at 298 K in appropriate deuterated solvents using Bruker Avance 400 MHz and Bruker Avance 600 MHz spectrometers. Electrospray Ionization mass spectra (ESI-MS) were recorded on a JEOL AccuTOF JMS-T100LC ESI mass spectrometer. FT-IR spectra were collected on a PerkinElmer Precisely Spectrum 100 FT-IR Spectrometer.

General Synthesis A (NDIs 2, 4–7): A mixture of 1,4,5,8-naphthalene-tetracarboxylic dianhydride (NDA) (0.8 g, 3 mmol) and an appropriate aromatic amine (6 mmol) in DMF (20 mL) was heated under reflux for 8 h. When the reaction mixture reached room temperature, a crystalline solid precipitated out, which was collected by filtration. The crude product was purified by recrystallization from DMF to obtain compound **2**, **4**-**7** as off-white crystalline solids.

General Synthesis B (NDI 1 and 3): A mixture of NDA (0.8 g, 3 mmol), an appropriate aromatic amine (6 mmol), and imidazole (13.5 g) in pyridine (20 mL) was heated under reflux for 8 h. The solution was allowed to cool to room temperature and then stirred with AcOH (100 mL) for 1 h. H_2O was then added to the solution and stirred for another 1 h. The resulting precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, $CHCl_3$) and crystallized from DMF to obtain pure NDIs **1** and **3** as off-white crystalline solids.

NDI 1: NDI **1** was prepared by following the general synthesis method B using 0.8 g (3 mmol) of NDA and 2.34 g (6 mmol) of 2,6-diiodo-4-nitroaniline. Yield: 67% (2 g, 2 mmol). ^1H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.99 (s, 4H) and 8.8 (s, 4H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 161.07, 148.58, 146.64, 134.09, 132.95, 127.49, 126.55, and 100.73 ppm. HRESIMS (–ve) *m/z*: Observed $[M]^-$ = 1011.6518, $[M]^-_{calcd}$ = 1011.6521. FT-IR: 3072.98 (aromatic CH), 1716.03 (amide C=O stretching), 1677.65 (imide stretching), 1580.14, 1521.01, 1443.86 cm^{-1}.

NDI 2: NDI **2** was prepared by following the general synthesis method A using 0.8 g (3 mmol) of NDA and 0.77 g (6 mmol) of 2,6-difluoro-aniline. Yield: 90% (1.3 g, 2.7 mmol). ^1H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.84 (s, 4H), 7.76–7.68 (m, 2H), and 7.44 (t, J = 8.4 Hz, 4H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 162.77, 157.86, 132.62, 132.11, 127.70, 126.71, 113.03, and 111.77 ppm. HRESIMS (+ve) *m/z*: Observed $[M+H]^+$ = 491.0661, $[M]^+_{calcd}$ = 490.0577. FT-IR: 3074.77 (aromatic CH), 1718.04 (amide C=O stretching), 1677.68 (imide stretching), 1597.10, 1580.10, 1497.17, 1473.67 cm^{-1}.

NDI 3: NDI **3** was prepared by following the general synthesis method B using 0.8 g (3 mmol) of NDA and 2.15 g (6 mmol) of 2,6-diiodo-4-toludine. Yield: 73% (2.1 g, 2.2 mmol). ^1H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.94 (s, 4H), 7.92 (s, 4H), and 2.36 (s, 6H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 161.49, 143.21, 140.78, 139.42, 137.13, 131.95, 127.32, 97.69, and 20.46 ppm. HRESIMS

(+ve) *m/z*: Observed $[M+H]^+$ = 950.7216, $[M]^+_{calcd}$ = 949.7132. FT-IR: 3069.97 (aromatic CH), 1717.21 (amide C=O stretching), 1681.69 (imide stretching), 1579.40, 1530.20, 1447.96 cm^{-1}.

NDI 4: NDI **4** was prepared by following the general synthesis method A using 0.8 g (3 mmol) of NDA and 0.83 g (6 mmol) of 4-nitroaniline. Yield: 77% (1.2 g, 2.3 mmol). ^{1}H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.76 (s, 4H), 8.45 (d, J = 8.9 Hz, 4H), and 7.82 (d, J = 8.9 Hz, 4H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 162.69, 147.41, 141.61, 130.80, 130.43, 126.99, 126.73, and 124.22 ppm. ESI-MS (–ve) *m/z*: Observed 508.7 $[M]^-$, $[M]^-_{calcd}$ = 508.1. FT-IR: 3082.37 (aromatic CH), 1707.02 (amide C=O stretching), 1663.56 (imide stretching), 1577.00, 1522.18, 1497.12 cm^{-1}.

NDI 5: NDI **5** was prepared by following the general synthesis method A using 0.8 g (3 mmol) of NDA and 0.56 g (6 mmol) of aniline. Yield: 83% (1 g, 2.5 mmol). ^{1}H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.73 (s, 4H), 7.59–7.46 (m, 10H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 162.89, 135.56, 130.39, 128.97, 128.90, 128.43, 126.96, and 126.67 ppm. HRESIMS (+ve) *m/z*: Observed $[M+H]^+$ = 419.1030, $[M]^+_{calcd}$ = 418.0954. FT-IR: 3071.97 (aromatic CH), 1710.71 (amide C=O stretching), 1665.65 (imide stretching), 1583.41, 1478.51, 1455.15 cm^{-1}.

NDI 6: NDI **6** was prepared by following the general synthesis method A using 0.8 g (3 mmol) of NDA and 0.74 g (6 mmol) of *p*-anisidine. Yield: 87% (1.2 g, 2.6 mmol). ^{1}H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.71 (s, 4H), 7.36 (d, J = 8.8 Hz, 4H), and 7.09 (d, J = 8.9 Hz, 4H), 3.85 (s, 6H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 163.10, 159.09, 138.5, 130.41, 129.97, 127.98, 127.00, 114.19, and 55.37 ppm. HRESIMS (–ve) *m/z*: Observed $[M+H]^+$ = 479.1246, $[M]^+_{calcd}$ = 478.1165. FT-IR: 3061.62 (aromatic CH), 1706.70 (amide C=O stretching), 1667.17 (imide stretching), 1608.43, 1580.10, 1510.85, 1455.15 cm^{-1}.

NDI 7: NDI **7** was prepared by following the general synthesis method A using 0.8 g (3 mmol) of NDA and 0.64 g (6 mmol) of *p*-toludine. Yield: 87% (1.2 g, 2.6 mmol). ^{1}H NMR (400 MHz, DMSO-d_6, 25°C): δ = 8.71 (s, 4H), 7.37–7.31 (m, 8H), and 2.41 (s, 6H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6, 25°C): δ = 162.94, 138.4, 135.3, 130.38, 129.41, 128.65, and 126.95, 120.4, and 20.74 ppm. ESI-MS (–ve) *m/z*: Observed 446.1 $[M]^-$, $[M]^-_{calcd}$ = 446.1. FT-IR: 3038.70 (aromatic CH), 1710.02 (amide C=O stretching), 1671.32 (imide stretching), 1580.93, 1514.03, 1447.13 cm^{-1}.

METHODS

UV/Vis Spectroscopy

UV/Vis spectra were recorded on a PerkinElmer Lambda-25 UV/Vis spectrophotometer. UV/Vis studies of NDIs (30 μM) were conducted in ODCB or MeCN. For the association constant (K_a) determination, UV/Vis studies were done using 0.5 mM NDI solutions that were titrated with 25 mM (50-times more concentrated) stock solutions of the anions from 4:1 to 1:50 NDI:anion ratio. To allow equilibriums to reach, these solution mixtures were kept in the dark at room temperature for 2 h. Anion-induced absorption changes of NDIs at 475 (λ_{max} of $NDI^{\bullet-}$) nm were used for the determination of the K_as using Benesi-Hildebrand method (Figure S6).[S2] Excellent linear fits of [NDI]/Abs (y-axis) vs 1/[anion] (x-axis) plots (Origin Software) show good agreement for 1:1 NDI•anion complex formation, K_as (y-intercept/slope) of which vary depending on the NDI's π-acidity and anion's Lewis basicity. The least square fits provide the correlation coefficient greater than 0.99 in all cases. Each NDI/anion titration was repeated at least twice and the K_a of a given NDI/anion interaction obtained from each set of UV/Vis data is highly reproducible and reliable. To avoid PET from anions to ^{1}*NDIs, UV/Vis experiments were conducted in dark and the samples were carefully protected from the ambient light.

To investigate the anion-mediated PET phenomena, the NDIs solutions (ODCB or MeCN) in the presence of anions were irradiated with a Scientific Instrument, Inc. DynaLume SunLite Hi-Intensity Illuminator fitted with a 15W 12V W-Ar bulb (40,000 Lux) and UV/Vis spectra were recorded at 2 min.

intervals. In the events of PET, the anion-generated $NDI^{\bullet-}$ signals displayed instantaneous amplification and became saturated within 10 min.

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 for 0.5 mM NDI solutions in the presence of 0.1 M $TBAPF_6$ in ODCB or MeCN at room temperature with 100 mV/s scan rate (Figure S3).

Spectroelectrochemistry (Figure S5) 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 solutions of NDI in 0.1 M $TBAPF_6$ in ODCB or MeCN at room temperature. UV/Vis spectra were recorded at 2 min. intervals on a PerkinElmer Lambda-25 UV/Vis spectrophotometer while the applied potential (E_{ap}) was controlled by the PAR potentiostat, using Virtual Potentiostat software. For the $NDI^{\bullet-}$ radical anion formation the E_{ap} was set at certain potentials until the corresponding spectra reached the saturation point and displayed two consecutive identical spectra.

NMR Experiments

^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded at 298 K in appropriate deuterated solvents using Bruker Avance 400 MHz and Bruker Avance 600 MHz spectrometers. For ^{1}H NMR titrations of NDIs with anions, samples were prepared and handled in the dark unless mentioned otherwise to avoid PET from the anions to NDIs. Addition of 1 equiv of X^- ($X^- = F^-$, AcO^-, and $H_2PO_4^-$) to NDI **1** (CD_3CN, 298 K) made the ^{1}H NMR signal of NDI core protons (H_A, 8.93 ppm) disappear, as NDI **1** was reduced to the $NDI^{\bullet-}$ radical anion. The Cl^- ion did not form $NDI^{\bullet-}$ in the absence of light, but did so after irradiation. Subsequent addition of an oxidizing agent, $NOBF_4$ completely regenerated NDI's H_A signals. Less basic anions, such as Br^-, I^-, and PF_6^- did not change the NDI spectra (Figure S12).

EPR Spectroscopy

EPR spectra (Figure S13) was obtained from a Bruker Elexsys-500 spectrometer, at the X-band, microwave frequency 9.3902 GHz; microwave power 1 mw; and modulation amplitude 1 Gauss (G) at 298 K. The microwave frequency was measured with a built-in digital counter and the magnetic field was calibrated using 2,2-diphenyl-1-picrylhydrazyl (DPPH; g = 2.0037). Modulation amplitude and microwave power were optimized for high signal-to-noise ratio and narrow peaks.[S3] In the presence of 1 equiv. of F^-, the EPR spectrum of the paramagnetic $NDI^{\bullet-}$ radical anion showed hyperfine splitting and g = 2.0030. The experimental EPR spectrum is identical to the simulated one, confirming an $NDI^{\bullet-}$ formation.

Isothermal Titration Calorimetric (ITC) Analysis

ITC studies were conducted on a Microcal VP-ITC ultra-sensitive isothermal titration microcalorimeter. The VP-ITC unit, equipped with a precise temperature control set at 25.0±0.1°C, directly measures the heat evolved or absorbed in solution as a result of infection of reactant. The reference cell was filled with *o*-dichlorobenzene (ODCB). All titrations were run at 25°C. Before each experiment the sample was degassed at 25°C for 10 minutes using the Thermovac (a vaccum thermostating system). Each of 40 injections of 6 μL of a tetrabutylammonium fluoride (TBAF, 10 mM) solution was delivered into a solution of NDI (0.5 mM) over 12s by a syringe spinning at 270 rpm, with a 240 s equilibriation time between injections. The instrument was controlled by Microcal Observer software comprising a 16-bit A/D converter board for data acquisition and a second interface board for calorimetric control. Data from control experiments in which ODCB was injected into the NDI solutions of ODCB were subtracted from the data obtained from receptor-anion titration experiments to account for heat of dilution.

Electrospray Ionization Mass Spectrometry (ESI-MS)

ESI-MS (Figure S14) were recorded on a JEOL AccuTOF JMS-T100LC mass spectrometer using negative ionization mode for the detection of the complexes of NDI receptor and F^-, AcO^-, and $H_2PO_4^-$ ions. ESI-MS shows *m*/*z* signals of 1:1 NDI•anion complexes.

Energy Minimized Structures of NDI/Anion Complexes

Electrostatic potential map of NDI shows (Figure S15a) that the imide rings are the most electron deficient parts (deep blue) of the molecule. The energy minimization of NDI molecules and NDI/anion complexes were carried out applying the density functional theory (DFT) with the Becke three-parameter hybrid exchange functional in concurrence with the Lee-Yang-Parr gradient-corrected correlation function (B3LYP functional) with the 6-31+G** basis set [B3LYP/6-31+G**] using Gaussian 03 program.[S4] B3LYP/6-31+G** energy minimized structures (Figure S15b–i) of the NDI•anion complexes show that the anions are preferentially located above an imide ring of NDI, which are the most electron deficient areas of the π-acceptor. For instance, in NDI **5**•F^- complex, F^- is located 1.69 Å above the carbonyl carbon, forming an ∠O=C···F angle of 111.3˚. For comparison, a typical C–F covalent bond length is much shorter at 1.30–1.34 Å. In NDI **5**•AcO^- complex, AcO^- is located 2.91 Å above the carbonyl carbon, whereas, a typical C–O covalent bond length is 1.2–1.4 Å. In NDI **5**•Cl^- complex, Cl^- is located 3.14 Å above the carbonyl carbon, whereas, a typical C–Cl covalent bond length is ca. 1.7 Å. These calculations show that the anions are considerably far apart from the NDI planes and do not involve in covalent bond formation.

References

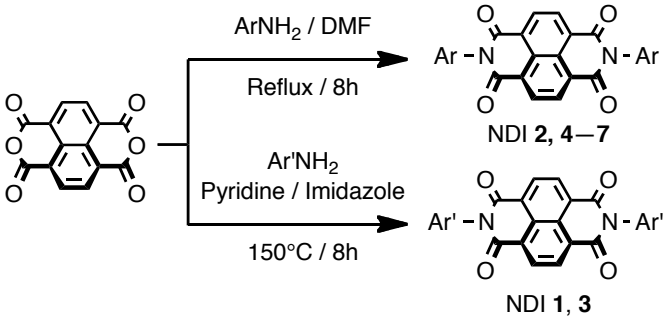
(S1) (a) Roger, C.; Würthner, F. *J. Org. Chem.* **2007**, *72*, 8070–8075. (b) Sakai, N.; Mareda, J.; Vauthey, E.; Matile, S. *Chem. Commun.* **2010**, *46*, 4225–4237.

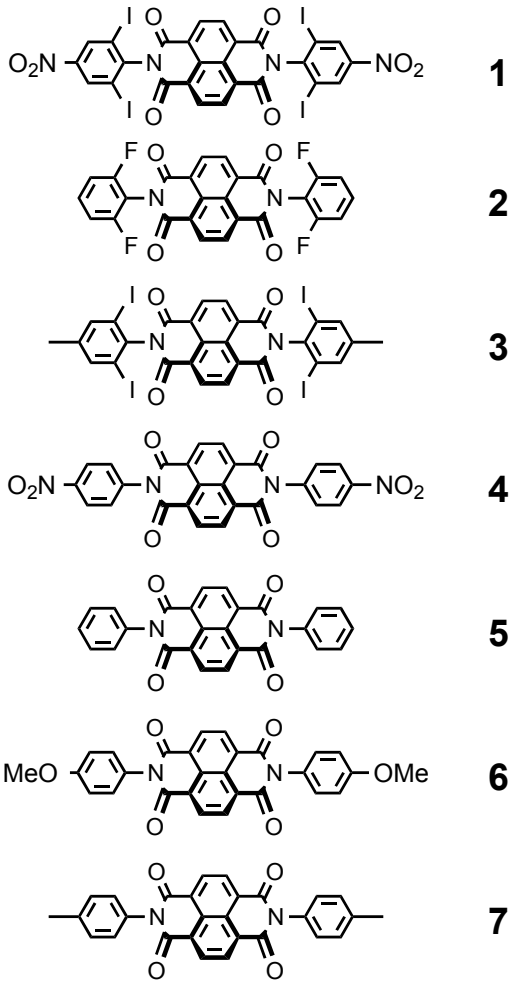
(S2) (a) Benesi, H. A.; Hildebrand, J. H. *J. Am. Chem. Soc.* **1949**, *71*, 2703–2707. (b) Chifotides, H. T.; Schottel, B. L.; Dunbar, K. R. *Angew. Chem. Int. Ed.* **2010**, *49*, 7202–7207.

(S3) (a) Andric, G.; Boas, J. F.; Bond, A. M.; Fallon, G. D.; Ghiggino, K. P.; Hogan, C. F.; Hutchison, J. A.; Lee, M. A. -P.; Langford, S. J.; Pilbrow, J. R.; Troup, G. J.; Woodward, C. P. *Aust. J. Chem*. **2004**, *57*, 1011–1019. (b) Guha, S.; Saha, S. *J. Am. Chem. Soc.* **2010**, *132*, 17674–17677.

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

Supporting Information:
Schemes and Figures





Scheme S1. Synthesis and chemical structures of NDIs **1**–**7**.

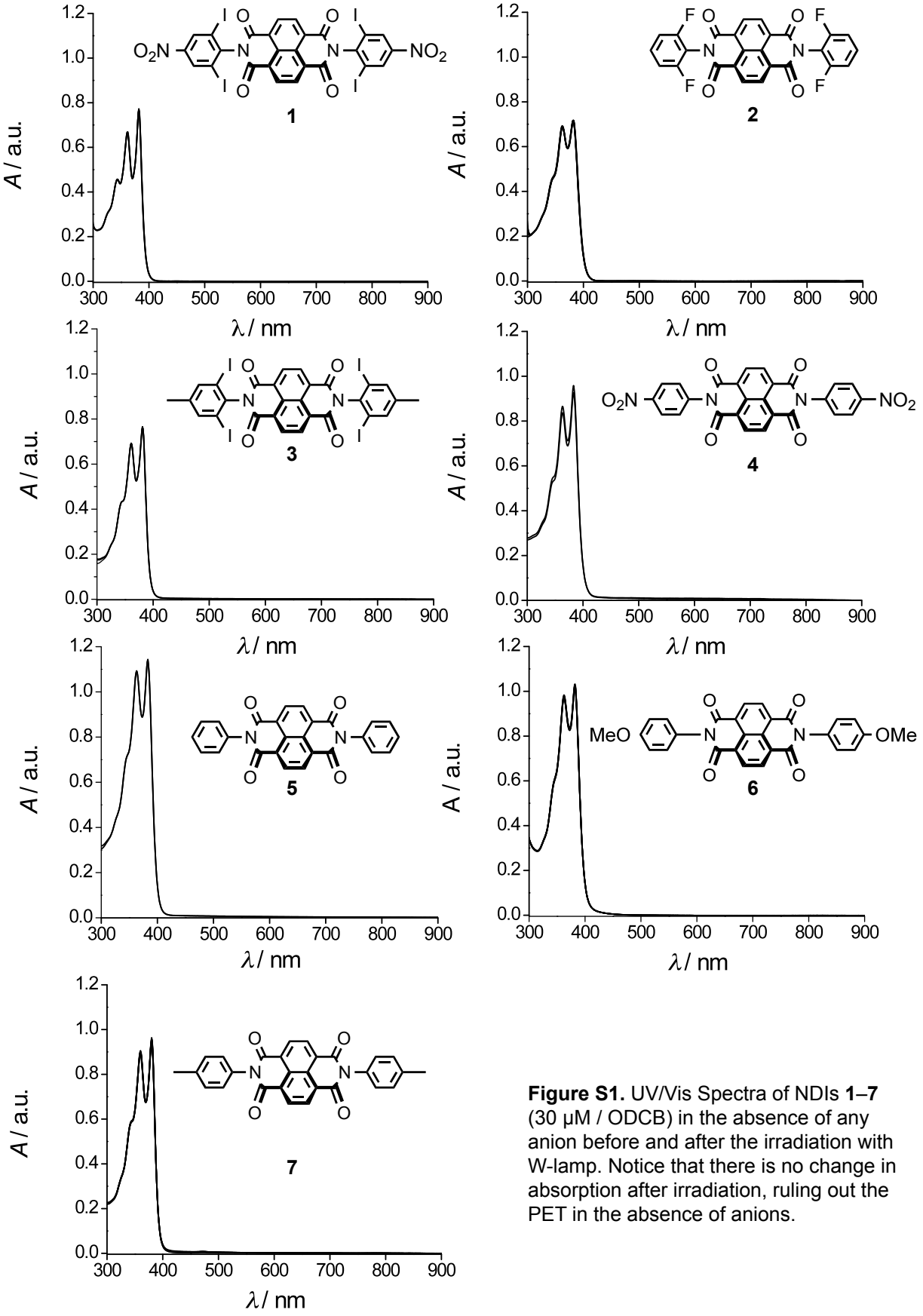


Figure S1. UV/Vis Spectra of NDIs **1**–**7** (30 μM / ODCB) in the absence of any anion before and after the irradiation with W-lamp. Notice that there is no change in absorption after irradiation, ruling out the PET in the absence of anions.

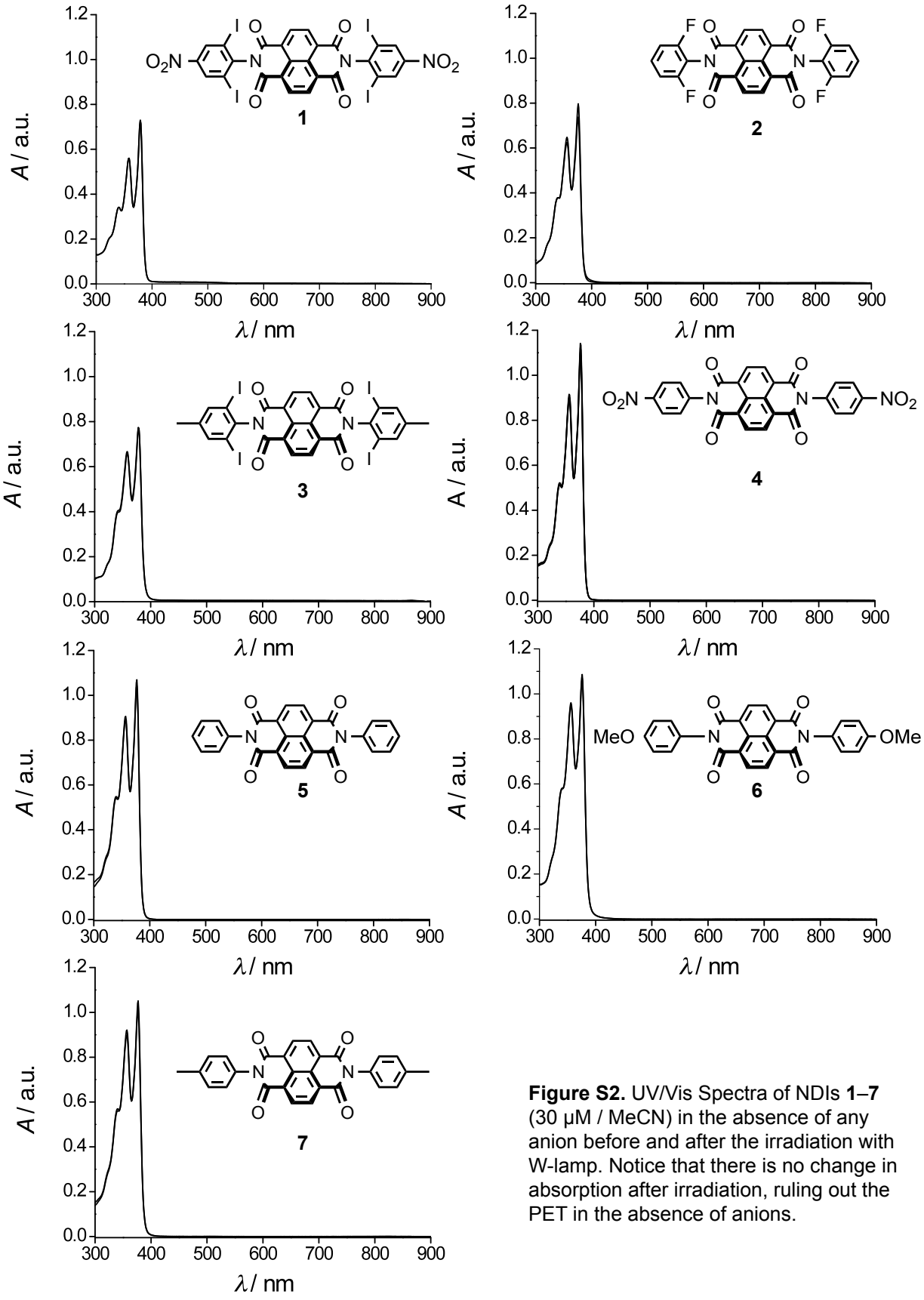


Figure S2. UV/Vis Spectra of NDIs **1**–**7** (30 μM / MeCN) in the absence of any anion before and after the irradiation with W-lamp. Notice that there is no change in absorption after irradiation, ruling out the PET in the absence of anions.

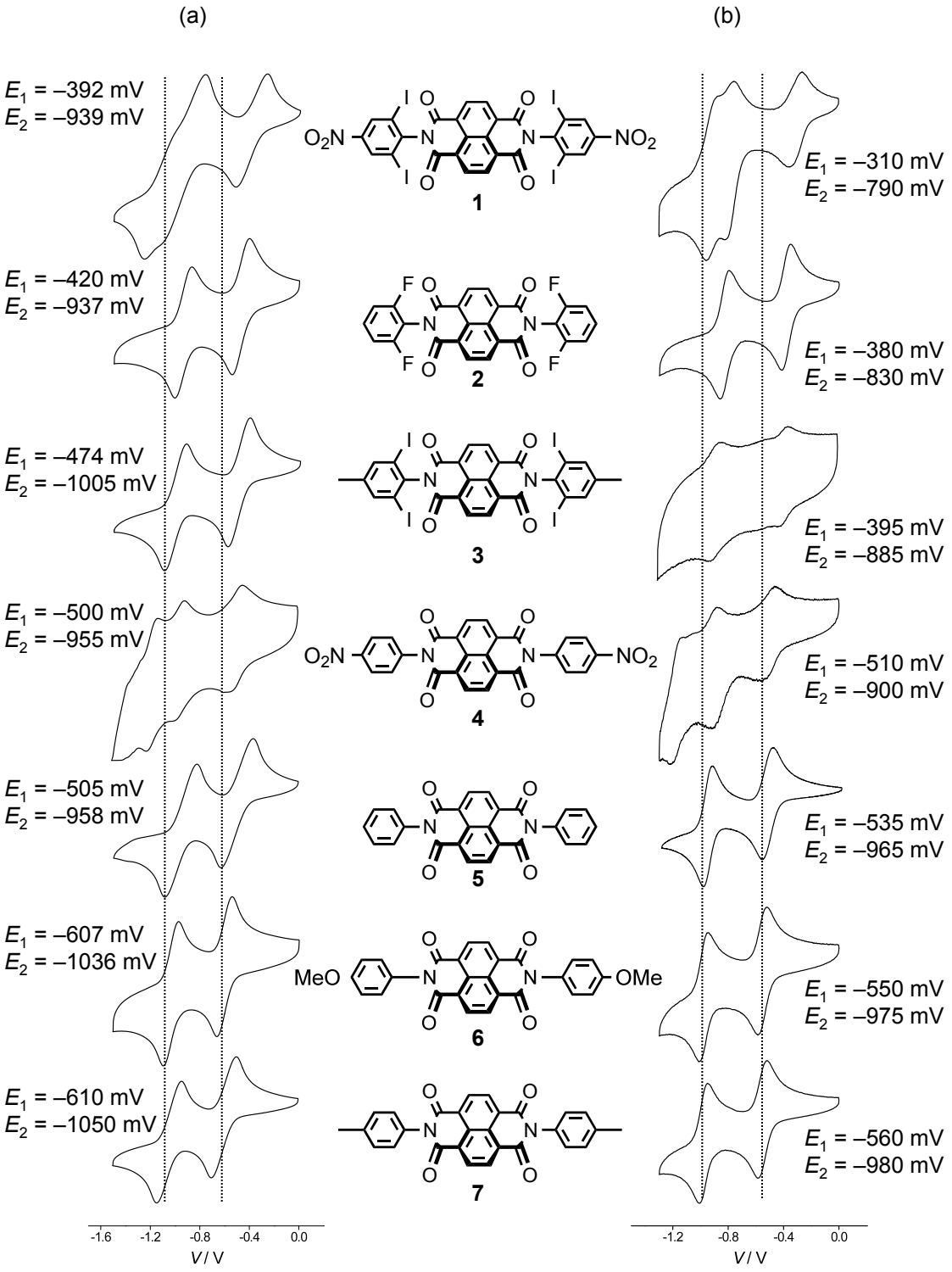


Figure S3. Cyclic voltammogram of NDIs **1**–**7** (vs. Ag/AgCl): (a) 0.5 mM / 0.1 M $TBAPF_6$ in ODCB and (b) 0.5 mM / 0.1 M $TBAPF_6$ MeCN.

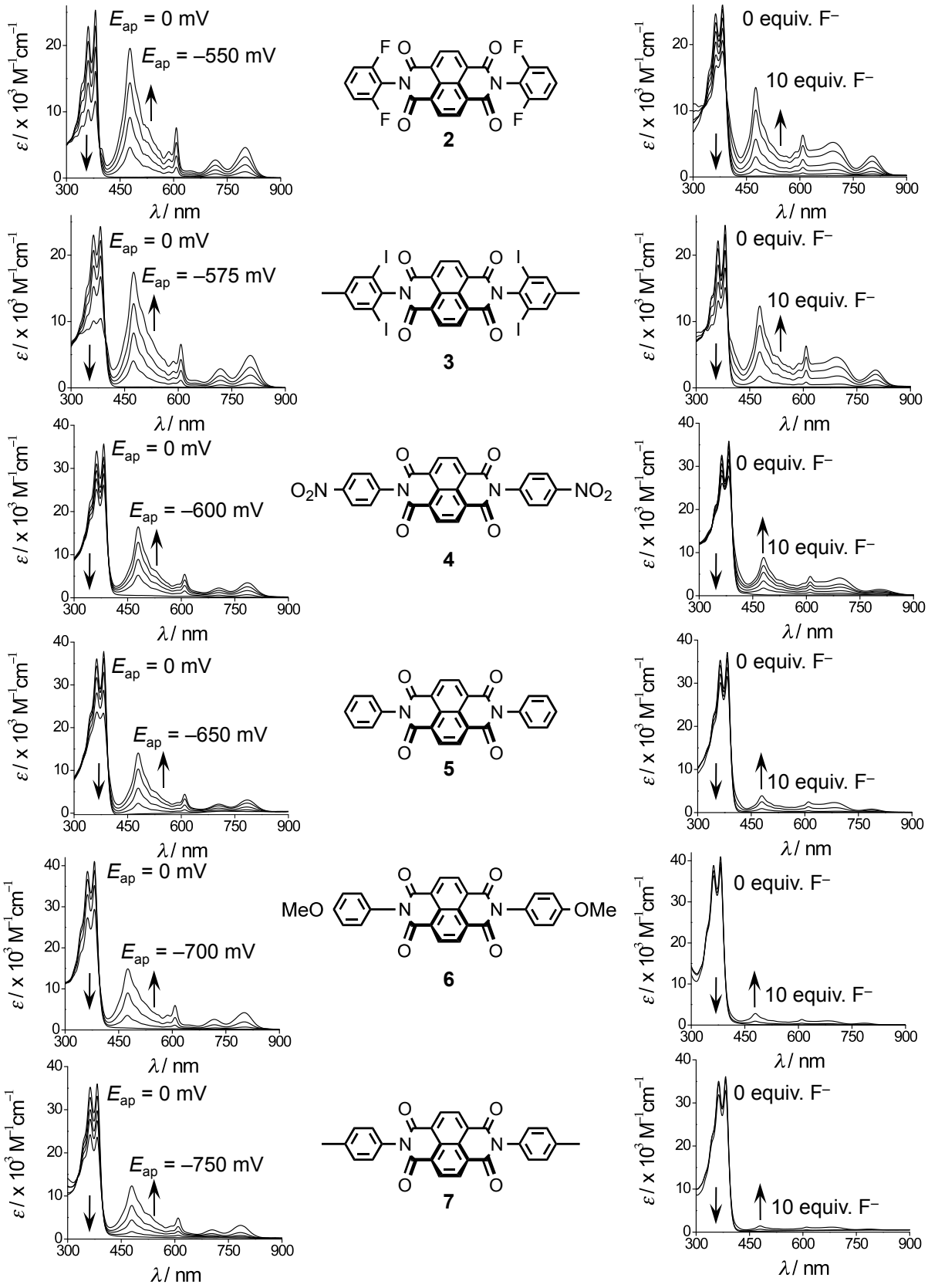


Figure S4. UV/Vis spectroscopic changes of NDIs **2**–**7** in ODCB upon corresponding $NDI^{\bullet-}$ radical anion formation under electrochemical reductions vs. Ag/AgCl (left panels) and with 0–10 equiv. of TBAF (right panels). In each case, ca. 10 equiv. F^- produced the maximum $NDI^{\bullet-}$ signals.

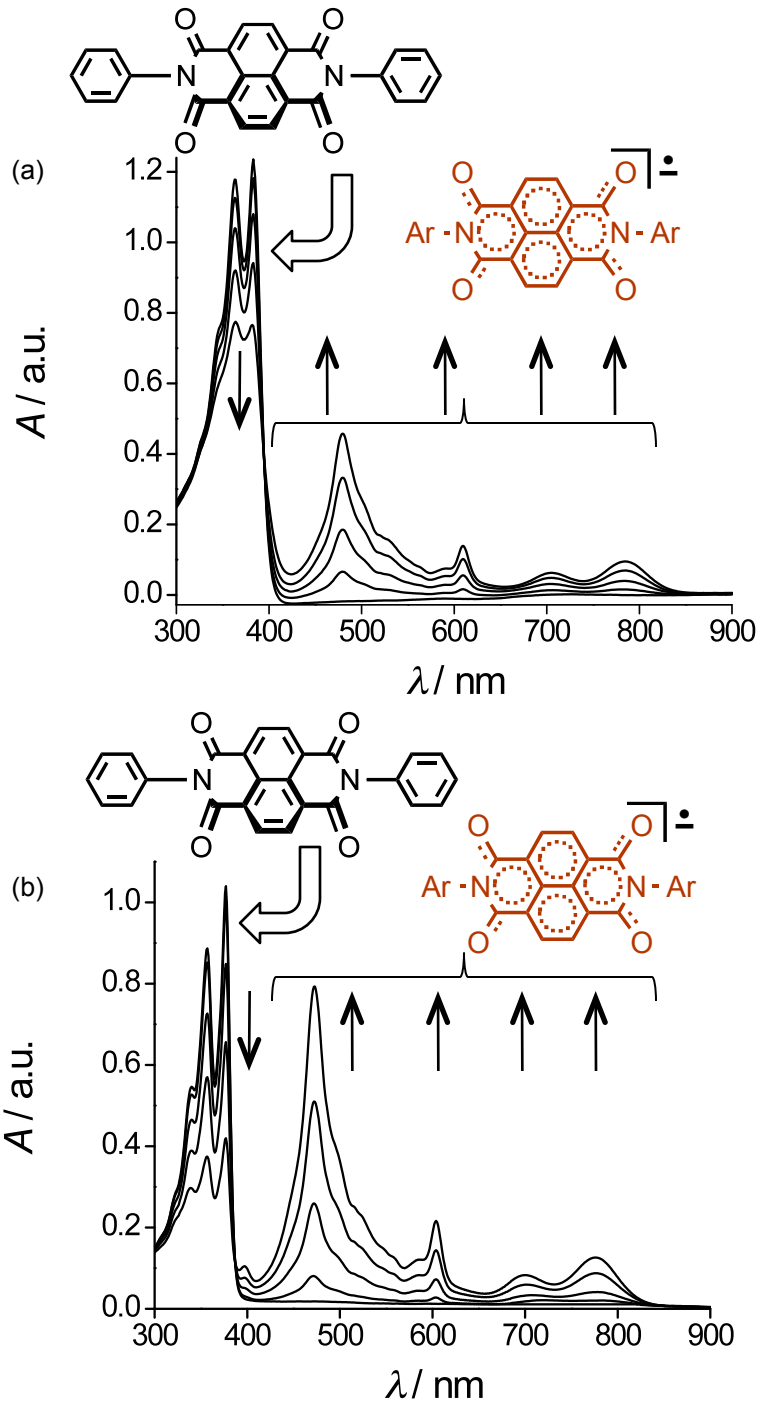


Figure S5. UV/Vis spectroscopic changes of reference NDI **5** at 0 to –650 mV applied potentials (vs. Ag/AgCl) in (a) 0.5 mM / 0.1 M $TBAPF_6$ in ODCB and (b) 0.5 mM / 0.1 M $TBAPF_6$ MeCN, demonstrating the $NDI^{\bullet-}$ radical anion formation. Notice that the isosbestic point in MeCN (386 nm) is 8 nm blue-shifted from that in ODCB (394 nm). The maximum intensity of the $NDI^{\bullet-}$ absorption is higher in MeCN than in ODCB. The spectra and isosbestic points of electrochemically generated $NDI^{\bullet-}$ radical anion are very similar to the spectroscopic changes when anion→NDI ET interactions produce the $NDI^{\bullet-}$ radical anions.

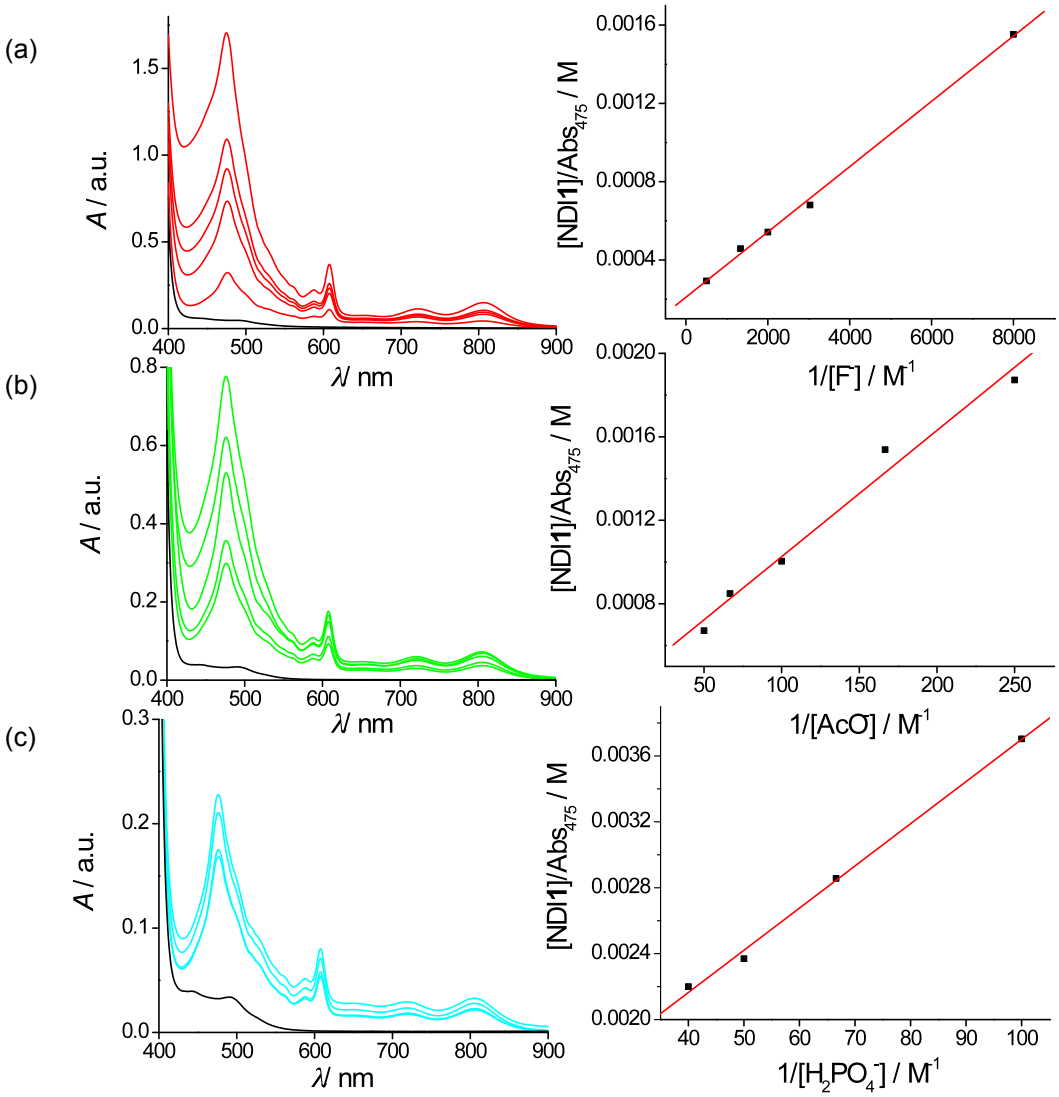
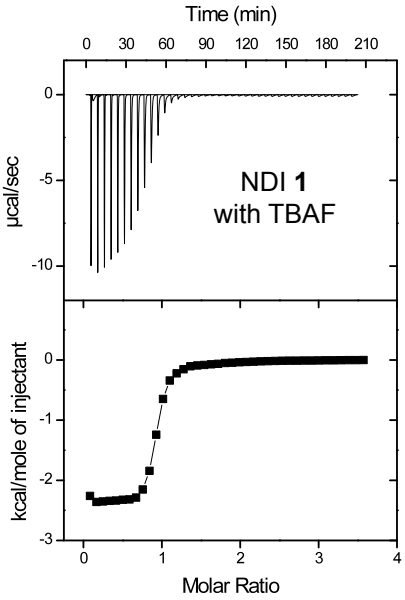
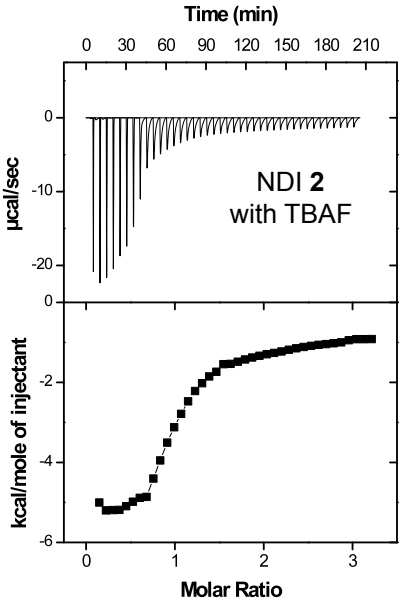


Figure S6. UV/Vis spectroscopic changes of NDI **1** (0.5 mM / ODCB) with increasing concentrations of (a) TBAF (0.0, 0.125, 0.33, 0.5, 0.75, and 2 mM), (b) TBAAcO (0, 4, 6, 10, 15, and 20 mM), and (c) $TBAH_2PO_4$ (0, 10, 15, 20, and 25 mM). The corresponding Benesi-Hildebrand plots of $[NDI]/Abs_{475}$ (y-axis) vs 1/[anion] (x-axis) show excellent linear fit for 1:1 complex with ±10% error, which provide K_as (y-intercept/slope) of NDI•anion complexes.

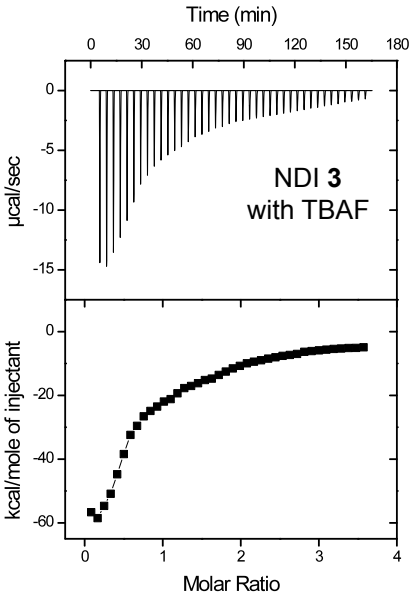
NDI	NDI/F⁻ Ratio	K_a (M^{-1})	ΔG_1 (kcal/mol)
1	1:1	1230	–4.24
2	1:1	1080	–4.15
3	1:1	923	–4.07
4	1:1	708	–3.91
5	1:1	528	–3.74



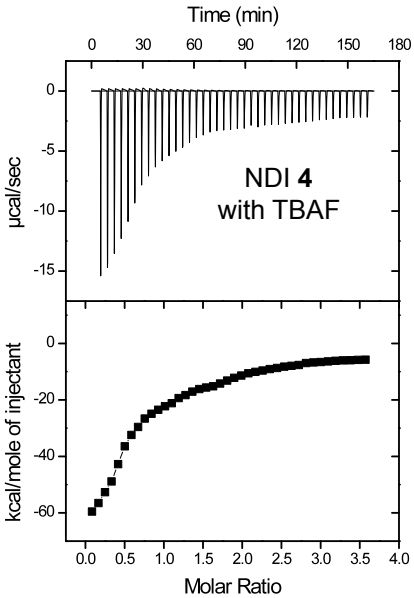
K_a = 1.23 x 10^3 ± 15 M^{-1}
ΔH = –9.88 ± 0.017 kcal/mol
TΔS = –5.64 kcal/mol
ΔG = –4.24 kcal/mol



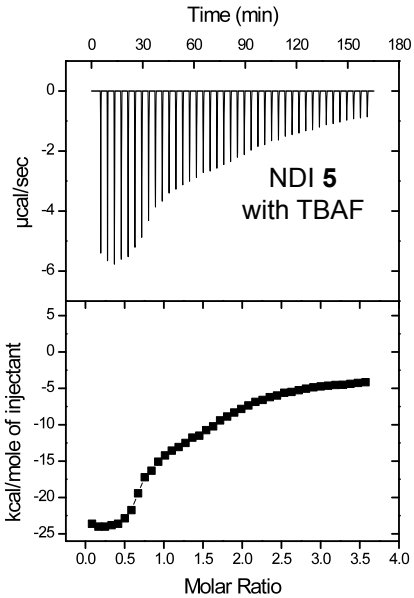
K_a = 1.08 x 10^3 ± 11 M^{-1}
ΔH = –7.85 ± 0.013 kcal/mol
TΔS = –3.70 kcal/mol
ΔG = –4.15 kcal/mol



K_a = 923 ± 6 M^{-1}
ΔH = –6.75 ± 0.011 kcal/mol
TΔS = –2.68 kcal/mol
ΔG = –4.07 kcal/mol



K_a = 708 ± 7 M^{-1}
ΔH = –4.595 ± 0.006 kcal/mol
TΔS = –0.69 kcal/mol
ΔG = –3.91 kcal/mol



K_a = 528 ± 4 M^{-1}
ΔH = –4.90 ±0.007 kcal
TΔS = –1.16 kcal/mol
ΔG = –3.74 kcal/mol

Figure S7. ITC isotherms showing 1:1 interactions between NDIs **1**–**5** and F^- in ODCB at 298 K. K_as and ΔG are summarized in a table.

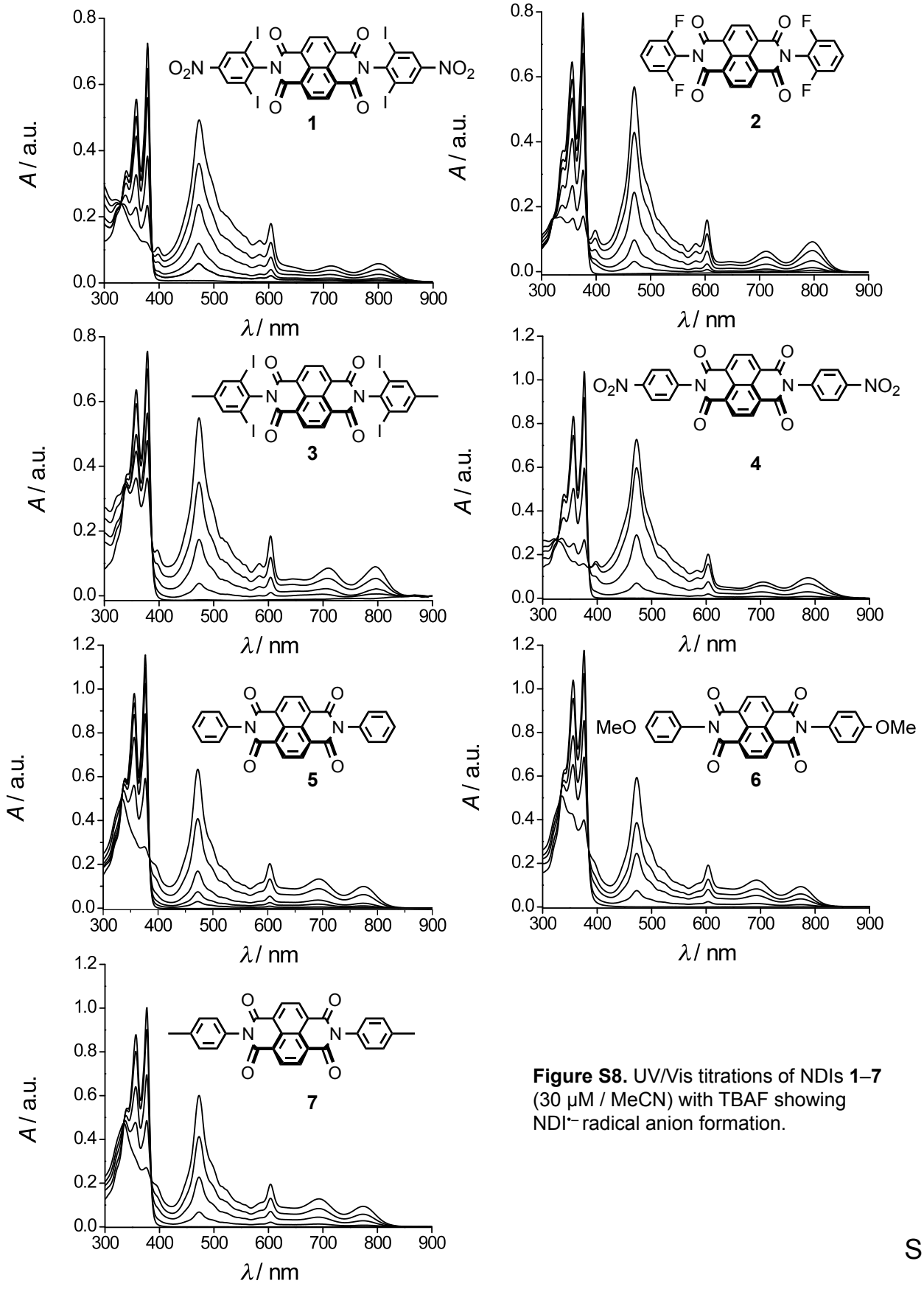


Figure S8. UV/Vis titrations of NDIs **1**–**7** (30 µM / MeCN) with TBAF showing $NDI^{\bullet-}$ radical anion formation.

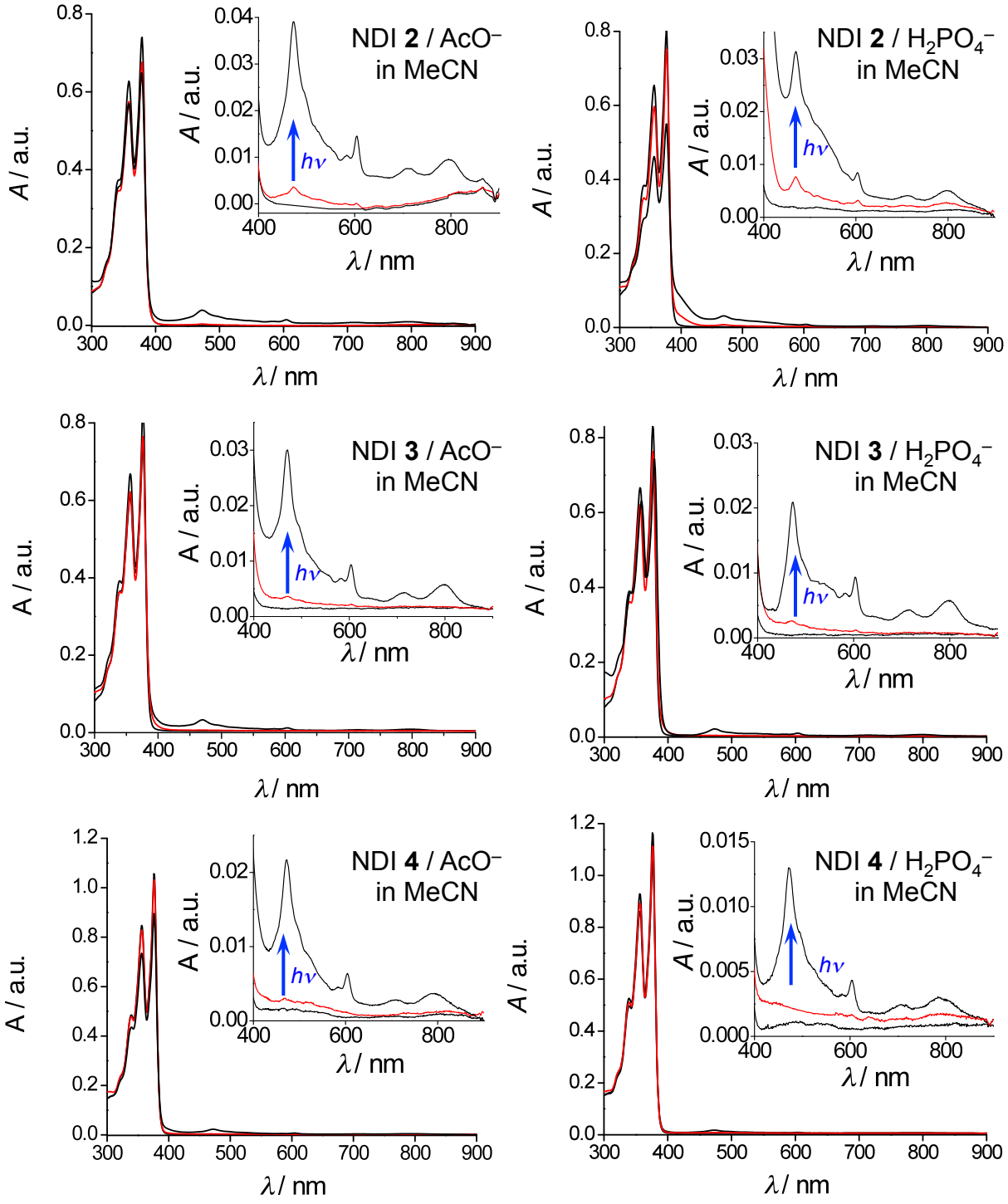


Figure S9. UV/Vis spectra of NDIs **2**, **3**, and **4** (30 μM / MeCN, bottom black traces) with TBAAcO and $TBAH_2PO_4$ in the absence of light (red lines) and after irradiation (top black lines). In each case, extremely weak, if any, $NDI^{\bullet-}$ signal was observed before irradiation (red traces). Intensities of these signals improved significantly after irradiation (top black traces), indicating anion→^{1*}NDI PET. Insets: Magnified 400–900 nm region clearly shows amplification of $NDI^{\bullet-}$ absorptions after irradiations.

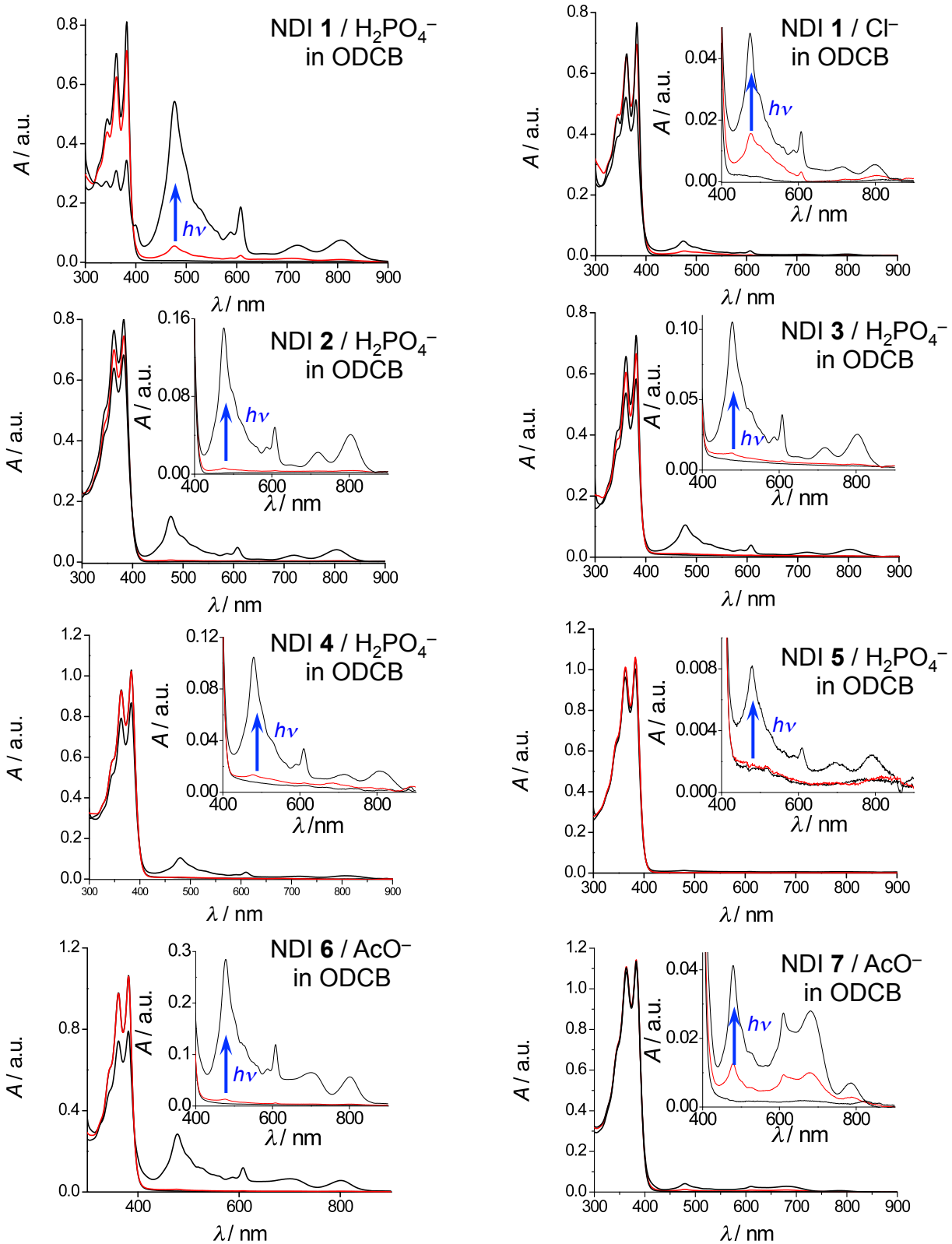


Figure S10. UV/Vis spectra of NDI **1** (30 μM / ODCB) with $TBAH_2PO_4$ and TBACl; NDIs **2**, **3**, **4**, and **5** (30 μM / ODCB) with $TBAH_2PO_4$; and NDIs **6** and **7** (30 μM / ODCB) with TBAAcO before (red traces) and after irradiations (top black traces), showing $NDI^{\bullet-}$ signal amplification through anion→^{1*}NDI PET when direct anion→NDI ET processes are weak or turned OFF. Insets: Magnified 400–900 nm region clearly shows $NDI^{\bullet-}$ absorptions.

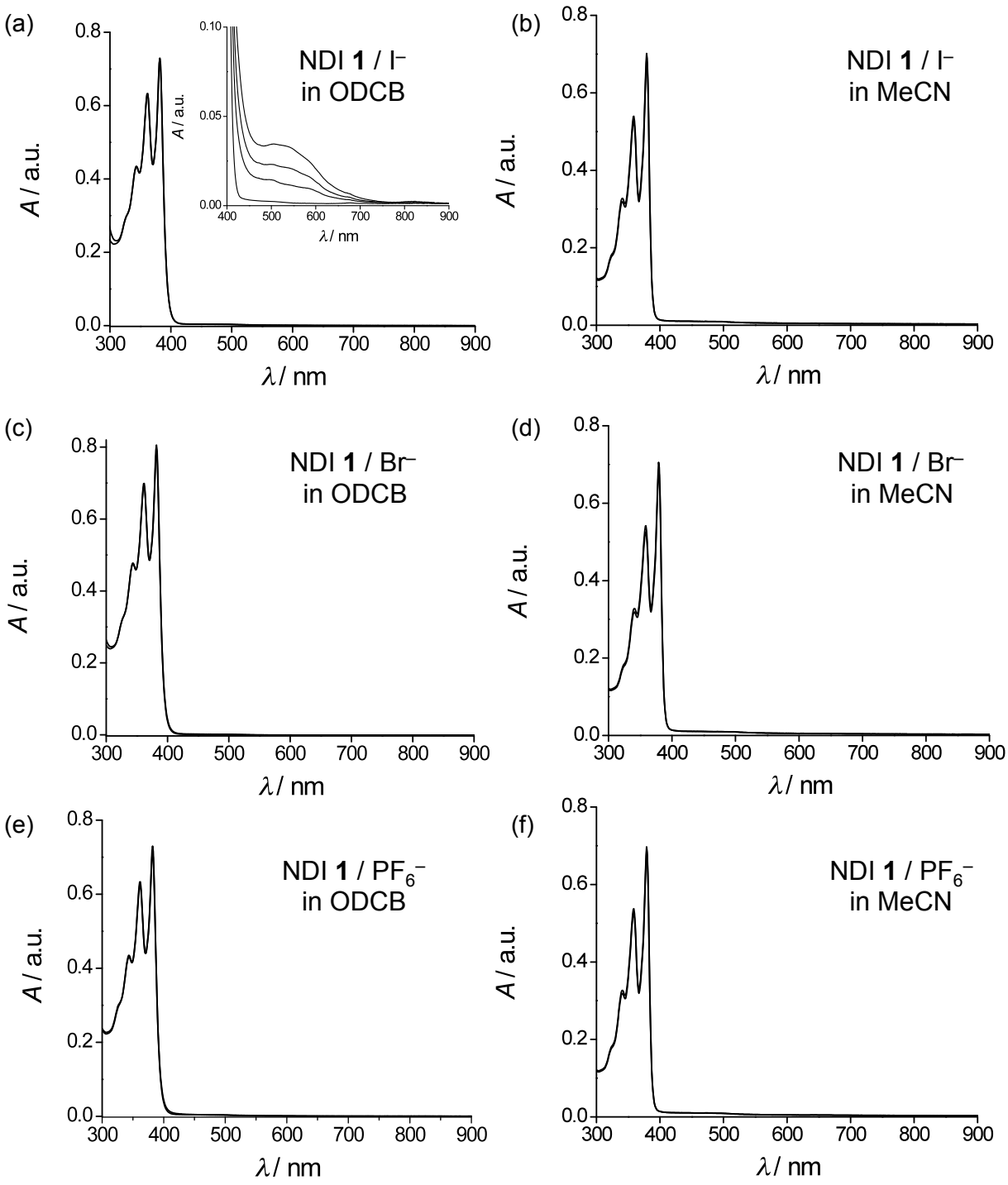


Figure S11. UV/Vis spectra of NDI **1** (30 μM) with TBAI (a,b), TBABr (c,d), and $TBAPF_6$ (e,f) in ODCB and MeCN showing no $NDI^{\bullet-}$ formation even after irradiations. At high NDI **1** concentration (0.5 mM) and excess I^- (100 equiv.) a broad CT band appears: inset in (a).

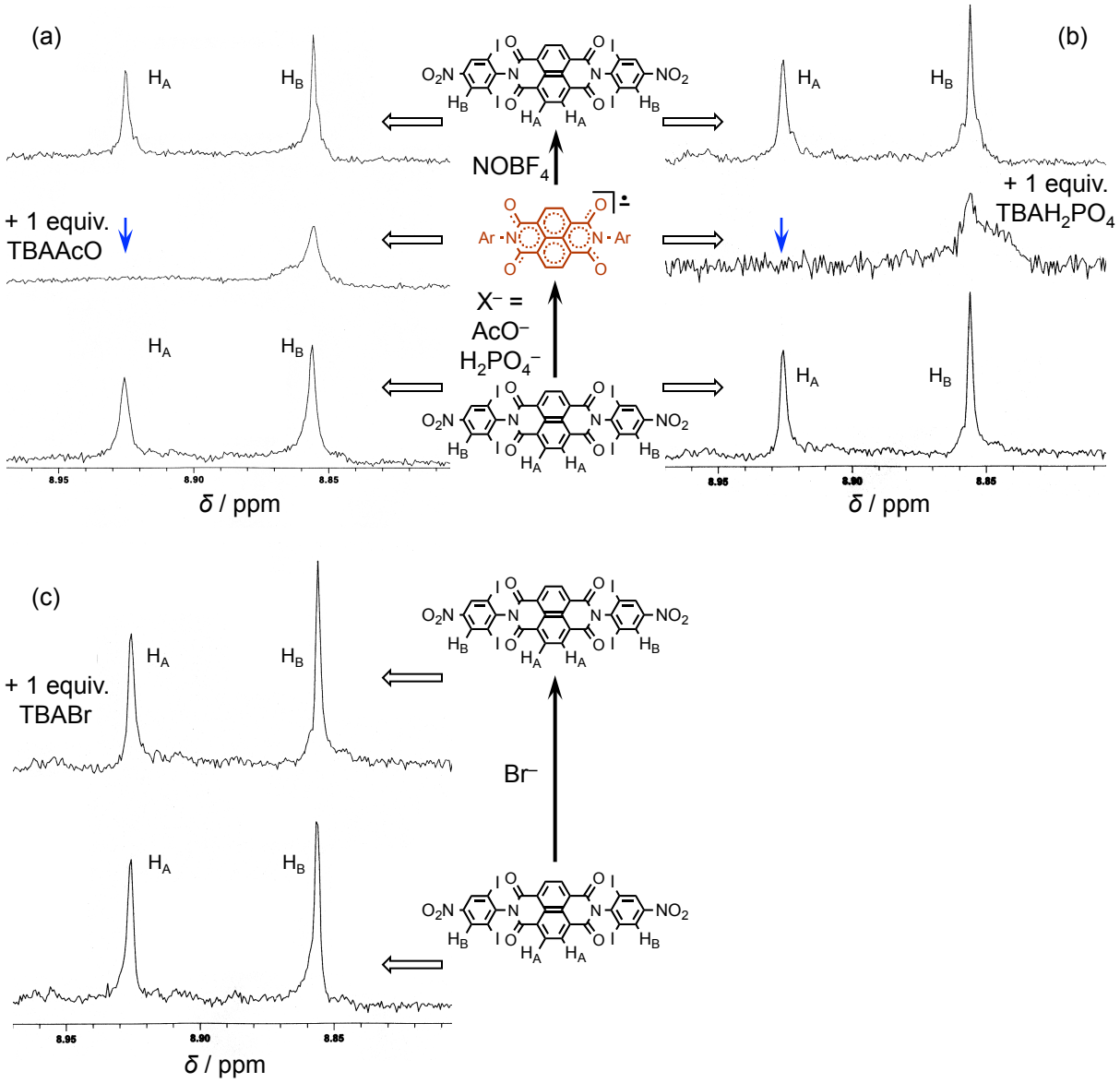


Figure S12. ^{1}H NMR (CD_3CN, 298 K) studies of NDI **1** with (a) TBAAcO, (b) $TBAH_2PO_4$, and (c) TBABr. While AcO^- and $H_2PO_4^-$ produced $NDI^{\bullet-}$ radical anions with through formal anion→NDI ET, Br^- ion did not produce any $NDI^{\bullet-}$ as the spectrum did not change. Oxidation of $NDI^{\bullet-}$ with $NOBF_4$ regenerated the original NDI **1** spectrum in (a) and (b).

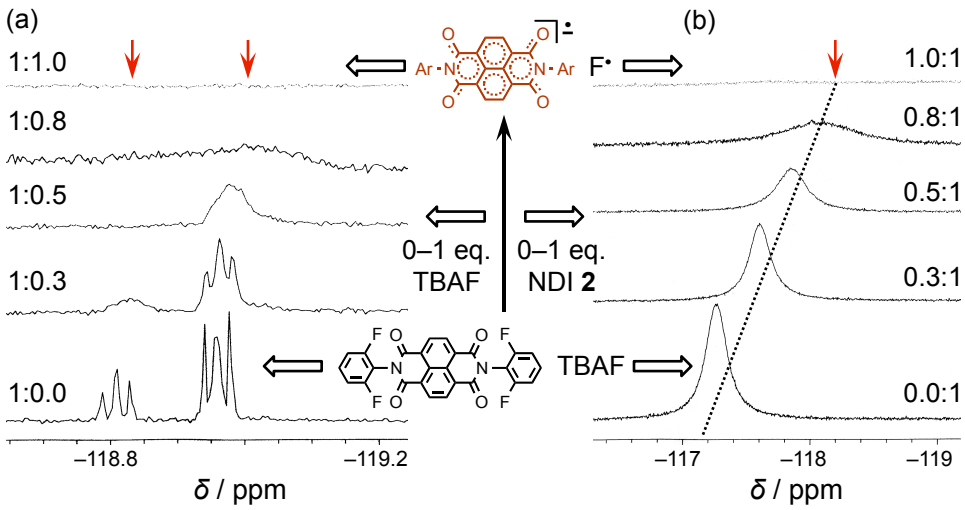


Figure S13. ^{19}F NMR titrations (CD_3CN, 298 K) of (a) NDI **2** with TBAF (0–1 equiv.) showing **2**$^{\bullet-}$ formation and (d) TBAF with NDI **2** (0–1 equiv.) showing F$^{\bullet}$ formation, as the respective ^{19}F signals disappeared. NDI **2** (all NDIs for that matter) can have two major conformers based on the dihedral angles (+/–ϕ) between the two *N*-aryl groups and core NDI plane. For instance, two *N*-aryl groups can be either parallel to each other forming the same ϕ (+/+: eclipsed in the Newman projection along the molecular axis) or they can form opposite ϕ (+/–: staggered in the Newman projection), giving rise to two triplets in the ^{19}F NMR spectrum of NDI **2**. Two *N*-aryl groups could form slightly different ϕ with the NDI core.

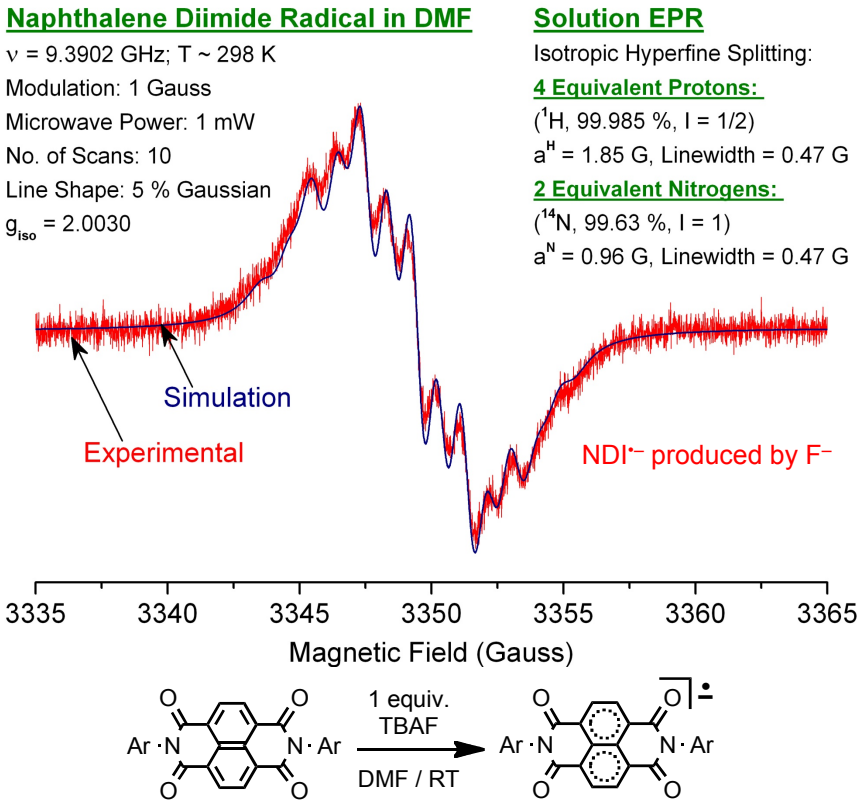


Figure S14. EPR spectrum of NDI•– radical anion generated by TBAF in DMF (298 K).[S3b]

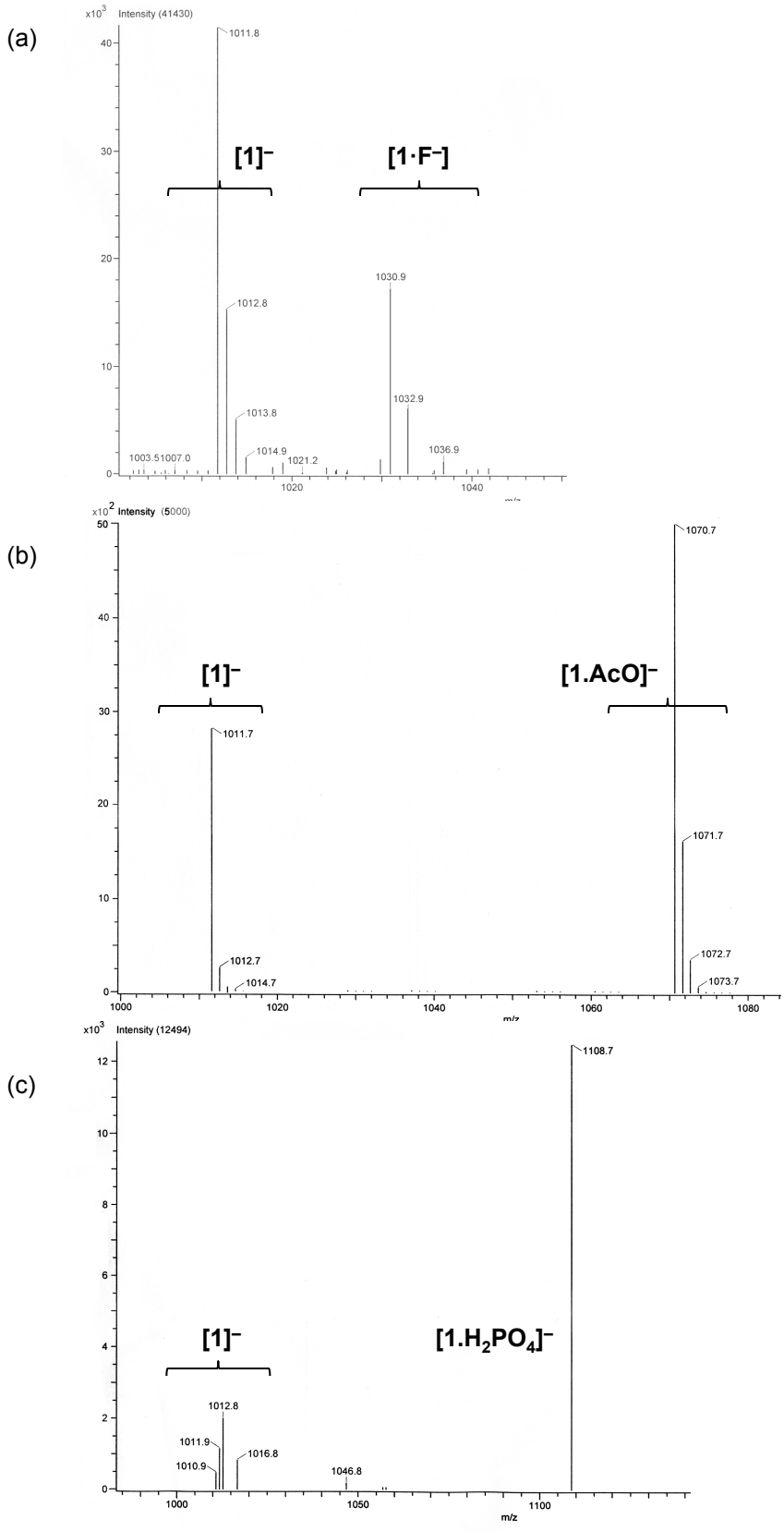


Figure S15(a–c). ESI-MS shows the presence and isotope distribution patterns of (a) [**1**]$^-$ and [**1**·F$^-$], (b) [**1**]$^-$ and [**1**·AcO$^-$], and (c) [**1**]$^-$ and [**1**·$H_2PO_4^-$].

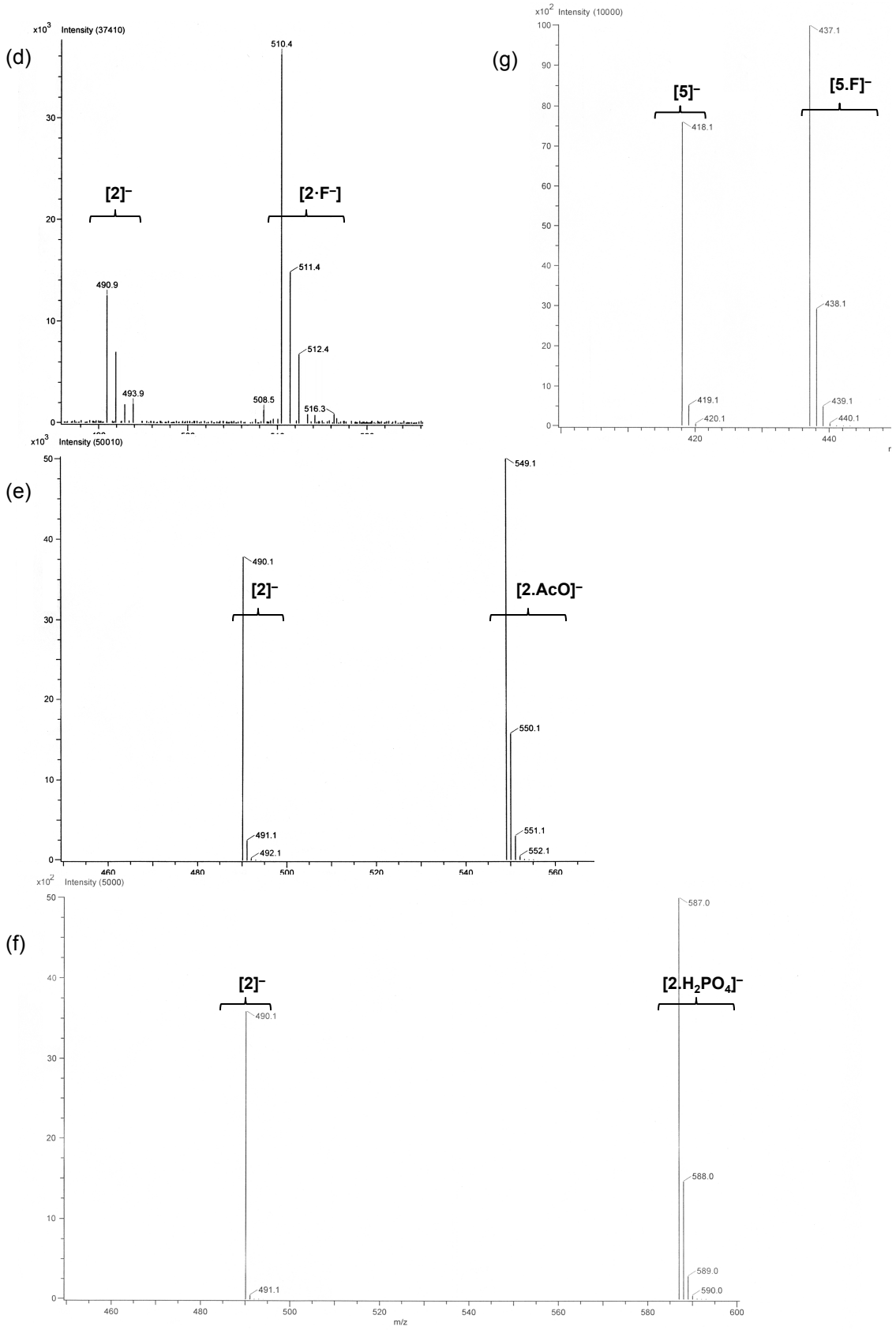
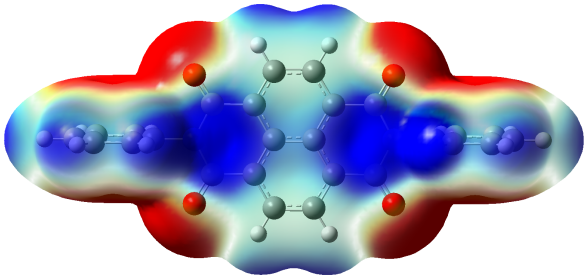


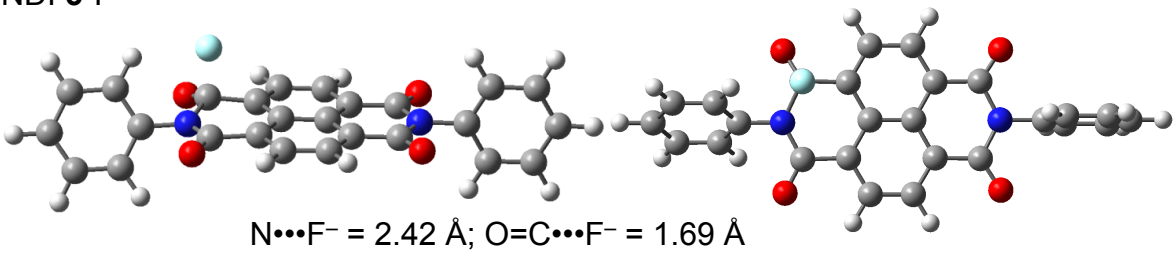
Figure S15(d–g). ESI-MS shows the presence and isotope distribution patterns of (d) [**2**]$^-$ and [**2**·F$^-$], (e) [**2**]$^-$ and [**2**·AcO$^-$], (f) [**2**]$^-$ and [**2**·$H_2PO_4^-$] and (g) [**5**]$^-$ and [**5**·F$^-$].

(a)



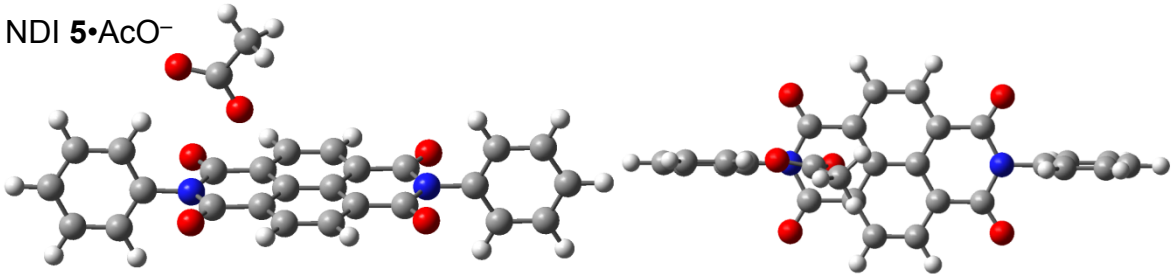
Side View **Top View**

(b) NDI **5**•F^-



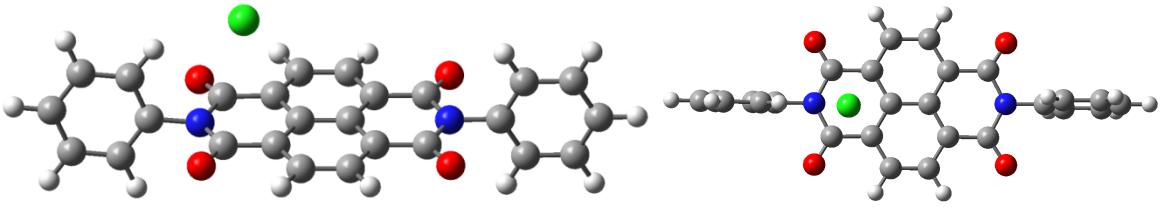
N•••F^- = 2.42 Å; O=C•••F^- = 1.69 Å
∠O=C•••F^- = 111.3°

(c) NDI **5**•AcO^-



N•••AcO^- = 3.05 Å; O=C•••OAc^- = 2.92 Å
∠O=C•••OAc^- = 119.5°

(d) NDI **5**•Cl^-



N•••Cl^- = 3.37 Å; O=C•••Cl^- = 3.14 Å
∠O=C•••Cl^- = 110.4°

Figure S16a–d. B3LYP/6-31+G** calculations show (a) electrostatic potential (ESP) map of NDI **5** and the energy minimized structures of (b) NDI **5**•F^-, (c) NDI **5**•AcO^-, and (d) NDI **5**•Cl^- complexes. ESP map of NDI **5** shows that the imide rings are the most electron deficient areas of NDI, which favors anion binding.

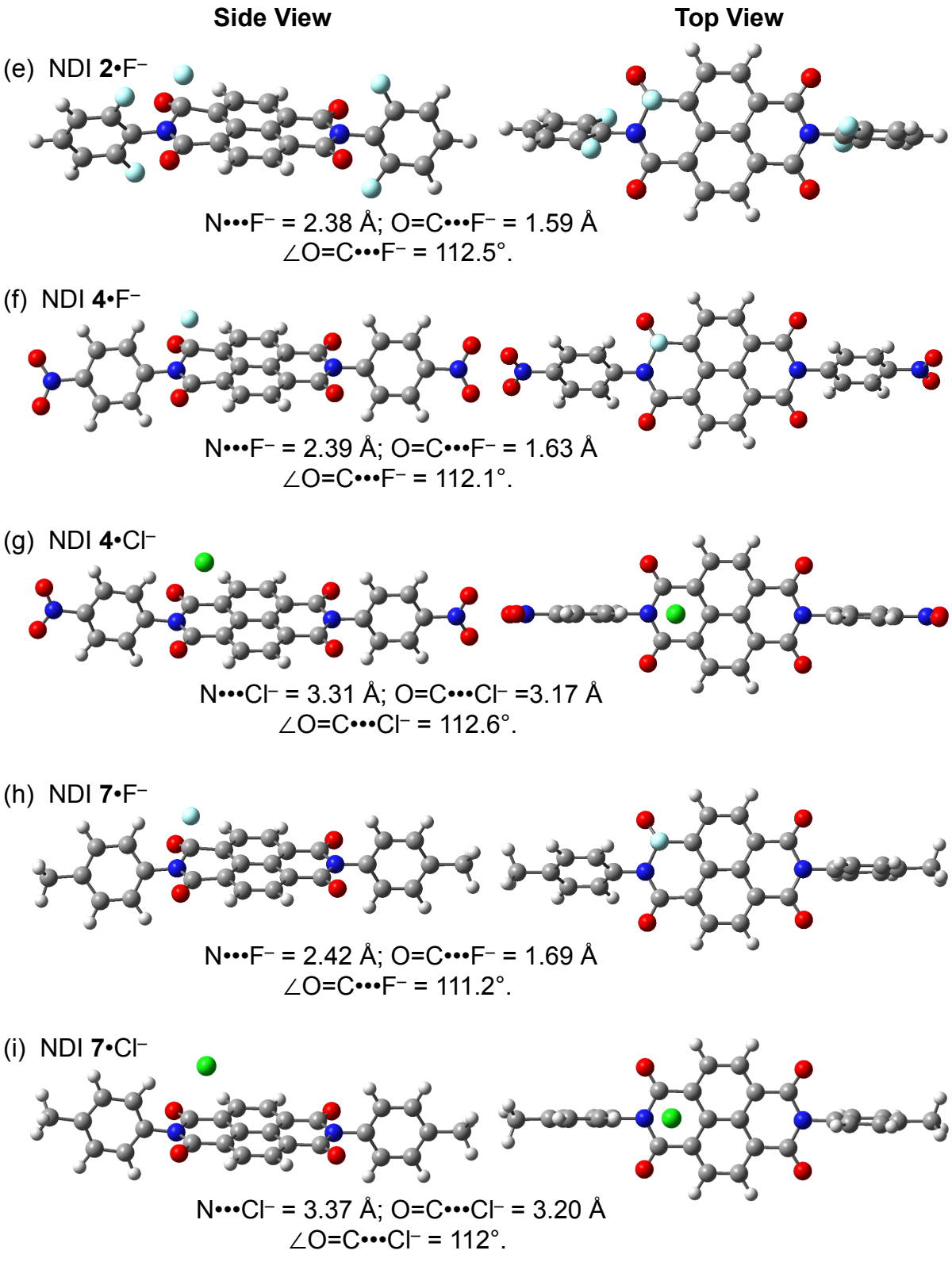


Figure S16d–i. B3LYP/6-31+G** calculations show (e) NDI **2**•F⁻, (f) NDI **4**•F⁻, (g) NDI **4**•Cl⁻, (h) NDI **7**•F⁻, and (i) NDI **7**•Cl⁻ complexes.

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

NDI **5**•F^-

N	3.43784500	0.11905200	0.07084400
C	2.78572200	1.30518100	-0.14745100
C	1.28509500	1.24758500	-0.21531500
C	0.58929500	0.02169000	-0.06413200
C	1.29769400	-1.19781300	0.06394300
C	2.80635700	-1.24417600	-0.05974800
C	0.57749300	2.43047100	-0.37466300
C	-0.83716200	0.02176300	-0.03058200
C	-1.53491900	1.24676100	-0.18909300
C	-0.82804800	2.42948500	-0.36946700
C	-3.01224900	1.26842700	-0.16172000
N	-3.65139200	0.02429500	0.03628100
C	-2.99787800	-1.22575000	0.20458200
C	-1.52712700	-1.20264300	0.16062700
C	-0.80262800	-2.38117100	0.31648500
C	0.60071000	-2.37782800	0.26962600
H	1.17253400	-3.29254500	0.38110900
H	-1.34963900	-3.30610000	0.46983200
H	1.13763300	3.35192300	-0.48848900
H	-1.38499400	3.35258400	-0.49297800
O	3.43008100	-2.18923700	0.44241700
O	3.35753400	2.39851800	-0.22497200
O	-3.66562900	-2.24044800	0.37598400
O	-3.67897400	2.28959400	-0.29815400
C	4.86850000	0.13548600	0.17283800
C	5.48809800	0.84789100	1.20379900
C	6.88033000	0.86145900	1.30741800
C	7.66094500	0.15511000	0.38746700
C	7.03613600	-0.56143400	-0.63807400
C	5.64466400	-0.57133700	-0.75236800
H	7.35354500	1.42178100	2.10997500
H	8.74504900	0.16163100	0.47056900
H	7.63402400	-1.11784900	-1.35561600
C	-5.09597100	0.02309400	0.07428600
C	-5.75705400	0.23611200	1.28367900
C	-7.15268500	0.23584700	1.31972200
C	-7.88457600	0.02204800	0.14831900
C	-7.21562600	-0.19129000	-1.06017200
C	-5.81997700	-0.19048100	-1.09840100
H	-7.66689800	0.40217100	2.26215200
H	-8.97076100	0.02144200	0.17716500
H	-7.77888400	-0.35868400	-1.97390600
H	5.13977800	-1.12499700	-1.53518300
H	4.87764700	1.39416200	1.91455700
H	-5.17713300	0.40075900	2.18619600
H	-5.28849700	-0.35599500	-2.03009700
F	2.79739000	-1.34311600	-1.74633200

Total energy = −1509.6741098

NDI **5**•AcO^-

N	3.18363000	-0.76501700	0.17007800
C	2.54710300	-0.31663600	1.34149700
C	1.06130500	-0.20744900	1.30357700
C	0.35548800	-0.50635800	0.11521500
C	1.04901800	-0.87437800	-1.06051100
C	2.53753100	-0.97658900	-1.05477000
C	0.37094100	0.16179100	2.44696100
C	-1.06327200	-0.41716500	0.09679700
C	-1.74912300	-0.03468700	1.27767400
C	-1.03189200	0.25094900	2.43297900
C	-3.22309500	0.06397600	1.27960200
N	-3.87380600	-0.23230700	0.05717600
C	-3.23569000	-0.62083800	-1.14394700
C	-1.76001700	-0.70715600	-1.10378100
C	-1.05528800	-1.06846700	-2.24507400
C	0.34805200	-1.15288300	-2.22330900
H	0.90520400	-1.42370800	-3.11326700
H	-1.61032600	-1.27990900	-3.15294600
H	0.93665000	0.39272100	3.34264400
H	-1.57757000	0.54663800	3.32283000
O	3.16244500	-1.29373200	-2.05777000
O	3.18203500	-0.11074000	2.36482400
O	-3.90121500	-0.86665700	-2.14308800
O	-3.88115700	0.37883500	2.26409800
C	4.63385300	-0.79062900	0.17347000
C	5.29605900	-2.00361800	0.35743800
C	6.69260800	-2.03063000	0.35659800
C	7.41046700	-0.84431100	0.17512500
C	6.72914900	0.36353700	-0.00543700
C	5.33178300	0.40384600	-0.00918400
H	7.21568500	-2.97298200	0.49719000
H	8.49776500	-0.86284000	0.17498300
H	7.28328800	1.28769200	-0.14563900
C	-5.31587900	-0.12732600	0.03511600
C	-6.09718100	-1.24368200	0.33161300
C	-7.48918000	-1.13873200	0.30959100
C	-8.09564700	0.07991700	-0.00752800
C	-7.30570600	1.19431600	-0.30324900
C	-5.91349400	1.09189500	-0.28265800
H	-8.09830100	-2.00819300	0.54003100
H	-9.17900200	0.16074600	-0.02400200
H	-7.77150400	2.14408700	-0.54994900
H	4.78709400	1.34319500	-0.14664100
H	4.72103200	-2.91454100	0.49561800
H	-5.61385100	-2.18415400	0.57642100
H	-5.28858100	1.94966600	-0.50982400
C	2.52748200	2.97398100	-0.63553400
O	3.76098200	3.14114100	-0.45218900
O	1.85628800	1.92116400	-0.39642000

C	1.72183300	4.16266800	-1.20811100
H	1.20219600	3.85163800	-2.12218700
H	0.95194200	4.46363800	-0.48719300
H	2.37123400	5.01542200	-1.42544800

Total energy = –1638.3316696

NDI **5**•Cl^-

N	-3.36189100	0.15905900	-0.41882600
C	-2.72400400	-1.08921700	-0.60327400
C	-1.23933700	-1.10338800	-0.50123400
C	-0.53114900	0.10111300	-0.26372200
C	-1.21995100	1.31797700	-0.05788300
C	-2.70952700	1.35553200	-0.10078700
C	-0.54586300	-2.28314700	-0.72841900
C	0.89073900	0.08313900	-0.21771100
C	1.57742800	-1.13993000	-0.43113900
C	0.85673300	-2.30183800	-0.68574800
C	3.05099000	-1.17890300	-0.39154400
N	3.70506300	0.04895200	-0.11507800
C	3.06827100	1.29155500	0.09740800
C	1.58985800	1.28908700	0.03969400
C	0.88872500	2.47125000	0.24519000
C	-0.51505000	2.48614300	0.19405600
H	-1.07117800	3.40185400	0.36118900
H	1.44780500	3.37841900	0.44825000
H	-1.11161200	-3.18907900	-0.91271300
H	1.40309800	-3.22524700	-0.84621900
O	-3.33499800	2.39216500	0.08505100
O	-3.36730700	-2.07304600	-0.93413500
O	3.73358400	2.29839200	0.31332400
O	3.71227300	-2.19294800	-0.58362100
C	-4.80689400	0.14623800	-0.33525100
C	-5.40216200	-0.31709200	0.83913700
C	-6.79573500	-0.32945200	0.92897300
C	-7.57971000	0.11900800	-0.13914800
C	-6.96799900	0.58152300	-1.30811700
C	-5.57460800	0.59399500	-1.40839900
H	-7.26858300	-0.69090500	1.83810200
H	-8.66410300	0.10796000	-0.06166500
H	-7.57249000	0.93204600	-2.14051200
C	5.14892700	0.02582500	-0.04511600
C	5.77520500	-0.29320900	1.15937100
C	7.16945100	-0.31596400	1.22848700
C	7.93315900	-0.01864300	0.09634400
C	7.29812600	0.30089700	-1.10707800
C	5.90404500	0.32259000	-1.17932500
H	7.65726400	-0.56589000	2.16631800
H	9.01815200	-0.03608000	0.15146900
H	7.88664200	0.53308800	-1.99021600
H	-5.08321300	0.95201200	-2.30779200

H	-4.76052600	-0.66153600	1.64862900
H	5.17050800	-0.52336000	2.03070800
H	5.39865800	0.56994300	-2.10743400
Cl	-2.23759100	-1.08978400	2.49798100

Total energy = –1870.0581546

NDI **2**•F^-

N	-3.43817400	0.10958600	0.01250200
C	-2.80039200	1.30900800	0.15665200
C	-1.30135300	1.27254500	0.04164400
C	-0.60771700	0.04558100	-0.13362900
C	-1.31152300	-1.16725400	-0.35072300
C	-2.81745800	-1.17153700	-0.57002300
C	-0.59418300	2.45418800	0.20650800
C	0.81867300	0.03500400	-0.07679300
C	1.51539100	1.26009000	0.09471600
C	0.81059500	2.45096900	0.21955700
C	2.98962800	1.27495800	0.14468500
N	3.62437400	0.01597600	0.03001700
C	2.97539700	-1.23947300	-0.13270100
C	1.50825300	-1.20079000	-0.19371400
C	0.78676500	-2.37930200	-0.35950200
C	-0.61495700	-2.36084800	-0.43985200
H	-1.18582900	-3.27138700	-0.58712300
H	1.33474300	-3.31302800	-0.43726800
H	-1.15448300	3.37210800	0.34573200
H	1.36794400	3.37328900	0.34631600
O	-3.46920900	-2.20966100	-0.36528400
O	-3.37738600	2.36072200	0.45253600
O	3.65267700	-2.25808600	-0.21080900
O	3.66568900	2.28907100	0.27728900
C	-4.84413400	0.07075500	0.18871300
C	-5.73992300	0.61336300	-0.73852400
C	-7.12063800	0.54901000	-0.58277900
C	-7.64154300	-0.09024000	0.54344600
C	-6.78885200	-0.64050700	1.50185600
C	-5.41563300	-0.54228000	1.30726100
H	-7.75819500	0.99050900	-1.34071500
H	-8.71730600	-0.15613800	0.67696400
H	-7.16390700	-1.13692300	2.38991300
C	5.05034900	0.00311400	0.08450700
C	5.82886100	0.10691200	-1.06825300
C	7.21776300	0.09611000	-1.04206600
C	7.85987600	-0.02302200	0.19214800
C	7.12307200	-0.12903400	1.37359000
C	5.73639100	-0.11370000	1.29333300
H	7.76828800	0.17975400	-1.97211100
H	8.94454500	-0.03341500	0.23370700
H	7.59916700	-0.22277300	2.34293300
F	5.19887600	0.22276700	-2.25731800

F	5.01510000	-0.21596100	2.43114000
F	-4.60053400	-1.03564100	2.26512000
F	-5.25131800	1.23345900	-1.83074700
F	-2.78976500	-0.76229400	-2.10666000

Total energy = –1906.6241373

NDI **4**•F^-

N	-3.63385000	0.02331100	0.00131400
C	-2.97656600	-1.20902400	-0.28578100
C	-1.50881200	-1.19395300	-0.21637800
C	-0.81865900	0.00211300	0.10651600
C	-1.51451600	1.20778900	0.37806200
C	-2.98931900	1.24083600	0.33661800
C	-0.78721500	-2.35493700	-0.48089500
C	0.60728600	-0.00787000	0.16015800
C	1.31153200	-1.21326600	-0.07519100
C	0.61478500	-2.36331400	-0.41000900
C	2.81837700	-1.29413200	0.08385100
N	3.46307500	0.09802700	0.07468200
C	2.80223800	1.26390400	0.38310200
C	1.30287000	1.19612500	0.43800900
C	0.59653500	2.36010000	0.70650500
C	-0.80827900	2.36445900	0.68637400
H	-1.36386100	3.27257500	0.89575400
H	1.15626800	3.26489800	0.91503500
H	-1.33425500	-3.25696600	-0.73572600
H	1.18484400	-3.26524400	-0.60367300
O	-3.65427200	2.24290100	0.57440100
O	-3.64337400	-2.19601800	-0.57404400
O	3.36931700	2.34656400	0.55936400
O	3.44004900	-2.17390800	-0.53113800
C	-5.07089300	0.03195200	-0.05803600
C	-5.80957100	-0.72324700	0.85774300
C	-7.19989700	-0.72165400	0.80319900
C	-7.83218200	0.04758200	-0.17473000
C	-7.11115800	0.80943500	-1.09535000
C	-5.72140000	0.79501300	-1.03236200
H	-7.79276900	-1.30019100	1.50018200
H	-7.63658500	1.39443400	-1.83944000
C	4.87946800	0.11952000	-0.03563700
C	5.65478400	-0.81636500	0.67018000
C	7.03896700	-0.81134500	0.54678300
C	7.64911800	0.13314400	-0.28423800
C	6.89457500	1.07214200	-0.99387200
C	5.51161700	1.05957800	-0.86642000
H	7.64944400	-1.52390100	1.08711700
H	7.39280900	1.78854000	-1.63477600
H	-5.13776000	1.38154100	-1.73218800
H	-5.29363000	-1.31666100	1.60339800
H	5.15600800	-1.53481700	1.30677900

H	4.91408800	1.78183500	-1.40772300
N	-9.29955500	0.05596200	-0.23692600
O	-9.83871700	0.74300300	-1.10908300
O	-9.91855600	-0.62423000	0.58605100
N	9.10185000	0.14164400	-0.41473600
O	9.75388400	-0.70157300	0.21419800
O	9.62093400	0.99274000	-1.14967500
F	2.82761500	-1.54689000	1.69168000

Total energy = –1918.710081

NDI **4**•Cl^-

N	-3.66889300	0.04433300	-0.15913800
C	-3.02465500	-1.19391400	-0.41023700
C	-1.55180000	-1.16026300	-0.45359000
C	-0.86158500	0.06618800	-0.26680600
C	-1.55423900	1.28161700	-0.03163600
C	-3.03025400	1.29287700	0.02572200
C	-0.83860400	-2.33212300	-0.67811100
C	0.55945200	0.07574700	-0.30804200
C	1.26097300	-1.13800700	-0.51646900
C	0.56489500	-2.32054000	-0.71530700
C	2.74658900	-1.13975400	-0.59023600
N	3.38582400	0.11331000	-0.46347500
C	2.74178300	1.32329500	-0.16241000
C	1.25366200	1.29358400	-0.11898200
C	0.55574700	2.47010400	0.10771700
C	-0.84827500	2.46386400	0.15447900
H	-1.40182800	3.37784200	0.34099900
H	1.11564900	3.38562100	0.26219700
H	-1.38837600	-3.25684600	-0.81730200
H	1.12667100	-3.23377200	-0.87468300
O	-3.70093100	2.29963800	0.21972900
O	-3.69717900	-2.20441100	-0.57632800
O	3.38177200	2.35329900	-0.00345500
O	3.39448300	-2.14193800	-0.84839300
C	-5.10893100	0.02829500	-0.08536800
C	-5.73273600	-0.25785700	1.13063100
C	-7.12229500	-0.27635300	1.21192300
C	-7.86272700	-0.00313100	0.06118300
C	-7.25506400	0.28528900	-1.16140900
C	-5.86493800	0.29846700	-1.22781300
H	-7.63181400	-0.49612800	2.14150800
H	-7.86576300	0.49183800	-2.03109000
C	4.82479800	0.09360100	-0.34792400
C	5.38782200	-0.27270000	0.87726600
C	6.77426700	-0.29705400	1.00710600
C	7.56202100	0.04946600	-0.09388600
C	7.00565500	0.41917400	-1.32024000
C	5.61911400	0.43809700	-1.44192700
H	7.24485900	-0.57696600	1.94118600

H	7.65203100	0.68110400	-2.14809300
H	-5.36213600	0.51957000	-2.16286700
H	-5.12824000	-0.46681400	2.00642400
H	4.72094700	-0.52998800	1.70006000
H	5.15220200	0.72101300	-2.37920000
N	-9.33170600	-0.01990500	0.13850700
O	-9.96810600	0.22751700	-0.88909900
O	-9.85123500	-0.27657200	1.22727900
N	9.02525000	0.02576800	0.03676800
O	9.50849200	-0.30596000	1.12267900
O	9.70349600	0.33772500	-0.94837100
Cl	2.26600400	-0.76489500	2.52035800

Total energy = –2279.0890926

NDI **7**•F^-

N	3.44595900	0.10824600	-0.03984200
C	2.79617100	1.29606500	0.17504700
C	1.29507200	1.24249700	0.23638200
C	0.59680200	0.01814000	0.08436000
C	1.30285300	-1.20312800	-0.04003700
C	2.81065200	-1.25179300	0.08840500
C	0.58944200	2.42711300	0.39178500
C	-0.82947300	0.02137000	0.04616200
C	-1.52518900	1.24789500	0.20108400
C	-0.81611400	2.42919300	0.38219700
C	-3.00261800	1.27256500	0.16979500
N	-3.64455800	0.02995700	-0.02890500
C	-2.99259400	-1.22129300	-0.19445900
C	-1.52174200	-1.20155700	-0.14589500
C	-0.79941600	-2.38179100	-0.29836700
C	0.60382700	-2.38170700	-0.24679300
H	1.17380000	-3.29794800	-0.35521200
H	-1.34809900	-3.30557400	-0.45268300
H	1.15125500	3.34744200	0.50653900
H	-1.37142100	3.35364900	0.50299400
O	3.43523600	-2.19991300	-0.40637100
O	3.37056500	2.38813600	0.25369700
O	-3.66097300	-2.23546000	-0.36693900
O	-3.66655400	2.29592500	0.30375300
C	4.87728300	0.11935500	-0.13170500
C	5.64783400	-0.58162000	0.80336000
C	7.03773500	-0.57706800	0.69889800
C	7.69420100	0.12433400	-0.32447600
C	6.90672400	0.82122000	-1.24887700
C	5.51237000	0.81653200	-1.15972000
H	7.62408900	-1.13228300	1.42892000
H	7.38619800	1.37351600	-2.05464300
C	-5.08855900	0.03078800	-0.06974900
C	-5.82015500	-0.17070900	1.09936800
C	-7.21462400	-0.16879100	1.05595300

C	-7.90184700	0.03189100	-0.14953100
C	-7.14746300	0.23821100	-1.31285800
C	-5.75252600	0.23677200	-1.27747300
H	-7.77612300	-0.32451500	1.97424200
H	-7.65615900	0.40341300	-2.25976600
H	4.91620800	1.36123000	-1.88389400
H	5.13838000	-1.12861200	1.58808300
H	-5.29656700	-0.32628500	2.03737600
H	-5.17673800	0.39866300	-2.18327800
C	9.20414700	0.12412700	-0.41919600
H	9.54706200	0.67984100	-1.29818900
H	9.66302600	0.58528600	0.46485700
H	9.60196600	-0.89573400	-0.49350400
C	-9.41277600	-0.00352900	-0.19765300
H	-9.78002100	-1.02733100	-0.34671100
H	-9.85151100	0.36768400	0.73440200
H	-9.80106700	0.60584600	-1.02018300
F	2.79106900	-1.34730200	1.78030200

Total energy = –1588.3144814

NDI **7**•Cl^-

N	-3.69238500	0.04839900	-0.14129000
C	-3.04293100	-1.19243900	-0.35929700
C	-1.56801800	-1.16129800	-0.40277000
C	-0.87633700	0.06748100	-0.24735100
C	-1.57102700	1.28641300	-0.04534400
C	-3.04963000	1.29729000	0.01139200
C	-0.85325700	-2.33714700	-0.60002400
C	0.54526400	0.07710500	-0.29271100
C	1.24797900	-1.13952500	-0.47367000
C	0.55018600	-2.32608500	-0.64174500
C	2.73381200	-1.13929100	-0.56114800
N	3.37718700	0.11182200	-0.44419900
C	2.72929300	1.32662100	-0.18402500
C	1.23991500	1.29849500	-0.13922900
C	0.53964200	2.47933100	0.05854000
C	-0.86455300	2.47309600	0.10769700
H	-1.41942000	3.39099000	0.26995300
H	1.09940500	3.39899900	0.18730100
H	-1.40356400	-3.26489600	-0.71548500
H	1.11230800	-3.24243500	-0.78064300
O	-3.71050100	2.31631900	0.17692800
O	-3.70579100	-2.21348700	-0.50187800
O	3.36029700	2.36770700	-0.05365400
O	3.37317600	-2.14811000	-0.81774700
C	-5.13560400	0.03243200	-0.06493600
C	-5.76251700	-0.19240500	1.15939400
C	-7.15552700	-0.20827400	1.23262500
C	-7.94389900	-0.00229700	0.09161000
C	-7.29290100	0.22749700	-1.12841400

C	-5.89995700	0.24390900	-1.21054500
H	-7.63567200	-0.38258800	2.19258500
H	-7.88145200	0.39698100	-2.02701500
C	4.82081200	0.09629300	-0.34372700
C	5.40189700	-0.25798600	0.87454000
C	6.79237600	-0.27503000	0.98075200
C	7.61365600	0.06033900	-0.10706700
C	7.00165700	0.40920100	-1.31831300
C	5.60989400	0.42718300	-1.44083000
H	7.24653300	-0.55636500	1.92842600
H	7.61752400	0.66758200	-2.17706000
H	-5.40445100	0.42437900	-2.15931900
H	-5.15980800	-0.35253500	2.04775600
H	4.74989800	-0.51928700	1.70675600
H	5.13971000	0.69792400	-2.38130900
C	-9.45293500	-0.05728000	0.17036800
H	-9.91662200	0.55688400	-0.60831800
H	-9.81830500	-1.08411900	0.03914900
H	-9.81598600	0.29620500	1.14096600
C	9.11974400	0.06930700	0.03541200
H	9.46756500	0.99012800	0.52195300
H	9.46858100	-0.77082100	0.64606400
H	9.61431300	0.00603900	-0.93955000
Cl	2.22036300	-0.81480500	2.57705400

Total energy = –1948.698799