Supporting Information

The Role of Fluoride in the Anion-π Interaction with Naphthalene Diimide

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Experimental Section

General Procedures

All reagents were purchased from Sigma Aldrich. 2,6-Dibromo-*N*,*N*'-bis(2-ethylhexyl)-1,8:4,5-naphthalenetetracarboxylic diimide (Br_2-NDI) was purchased from TCI. N,N'-bis(2-ethylhexyl)-1,4,5,8-naphthalenetetracarboxylic diimide (NDI) was synthesized according to literature.[1] 1H, 19F and 13C{1H} NMR were performed on JEOL 500MHz NMR system with chemical shifts referenced to the deuterated solvent. ESI-MS measurements were performed on Shimadzu LCMS-IT-TOF, isotope distribution patterns were used as a composition proof in addition to *m/z* signal. Elemental analysis was carried out using CHNS FlashEA 1112 Elemental Analyzer from Thermo Fisher Scientific. UV-Vis-NIR absorption spectra were recorded on a Shimadzu UV-3101PC UV-VIS-NIR Spectrophotometer. Cyclic voltammetry (CV) experiments were performed using Autolab potentiostat (model PGSTAT30) by Echochimie. All CV measurements were recorded in dry THF with 0.1 M tetra-n-butylammonium hexafluorophosphate as supporting electrolyte (scan rate of 100 $mV \bullet s^{-1}$), glassy carbon disk as working electrode, gold disk as counter electrode and Ag/AgCl as reference electrode. Ferrocene was used as external standard (HOMO = oxidation onset = –4.80 eV). HOMO/LUMO values of the compounds were calculated using the formula: –4.80 – (oxidation/reduction onset of compound). Continuous wave X- band ESR spectra were obtained with a JEOL (FA200) spectrometer at room temperature using dry THF as solvent. Microwave frequency, 9.1938 GHz; power, 6.39 mW; modulation frequency, 100 kHz

Reaction between NDI and TBAF in THF with bubbling of compressed dry air

NDI-OH: 100 mg (0.20 mmol) of NDI, 257 mg (0.81 mmol) of TBAF and 50 mL of anhydrous inhibitor-free THF were added to a round bottom flask. The reaction was stirred at 25 °C with continuous bubbling of compressed dry air for 2 hours. The reaction mixture was poured into DI water and extracted using dichloromethane. The organic layer was collected, dried using anhydrous sodium sulphate, filtered and concentrated. Pure NDI-OH was obtained as light yellow solid by preparative thin-layer chromatography (silica gel matrix) using dichloromethane as eluent. Yield = 5 – 10%. ^{1}H NMR (500 MHz, Methylene Chloride-d_2) δ 12.95 (s, 1H), 8.70 (d, *J* = 7.7 Hz, 1H), 8.53 (d, *J* = 7.7 Hz, 1H), 8.26 (s, 1H), 4.17-4.05 (m, 4H), 1.98-1.86 (m, 2H), 1.41-1.29 (m, 16H), 0.95-0.86 (m, 12H). ^{13}C{^{1}H} NMR (126 MHz, Methylene Chloride-d_2) δ 169.45, 165.00, 163.78, 163.52, 163.17, 132.19, 129.88, 128.36, 127.83, 127.41, 125.17, 124.95, 121.84, 105.98, 54.00, 45.03, 44.53, 38.50, 38.41, 31.20, 31.18, 29.17, 29.14, 24.53, 24.52, 23.60, 23.59, 14.40,

10.91, 10.90. Anal. Calcd for $C_{30}H_{38}N_2O_5$: C, 71.12; H, 7.56; N, 5.53; O, 15.79. Found: C, 71.01; H, 7.75; N, 5.43. HR-ESI-MS *m/z*: 507.2859; calcd for $C_{30}H_{38}N_2O_5+H^+$ = 507.2853.

Reaction between Br_2-NDI and TBAF in THF

Br-NDI-OH: 259 mg (0.40 mmol) of Br_2-NDI, 505 mg (1.60 mmol) of TBAF and 100 mL of anhydrous inhibitor-free THF were added to a round bottom flask. The reaction was stirred at 25 ^oC for 2 hours. The reaction mixture was poured into DI water and extracted using dichloromethane. The organic layer was collected, dried using anhydrous sodium sulphate, filtered and concentrated. Pure Br-NDI-OH was obtained as yellow solid by column chromatography (silica gel) using 100% hexane $\rightarrow$ 30% hexane + 70% dichloromethane as eluent. Yield = 67%. ^1H NMR (500 MHz, Chloroform-*d*) δ 12.89 (s, 1H), 8.94 (s, 1H), 8.37 (s, 1H), 4.21 – 4.08 (m, 4H), 1.99 – 1.88 (m, 2H), 1.35 (m, 16H), 0.97 – 0.85 (m, 12H). $^{13}C\{^1H\}$ NMR (126 MHz, Chloroform-*d*) δ ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 168.62, 164.23, 162.05, 161.81, 161.48, 139.22, 128.86, 127.06, 125.57, 124.32, 124.27, 124.25, 123.39, 105.62, 77.16, 45.25, 44.42, 37.96, 37.89, 30.78, 30.75, 28.69, 28.67, 24.12, 23.23, 23.16, 14.22, 10.74, 10.69. Anal. Calcd for $C_{30}H_{37}BrN_2O_5$: C, 61.54; H, 6.37; Br, 13.65; N, 4.78; O, 13.66. Found: C, 61.35; H, 6.51; N, 4.71. HR-ESI-MS *m/z*: 585.1955; calcd for $C_{30}H_{37}BrN_2O_5+H^+$ = 585.1959.

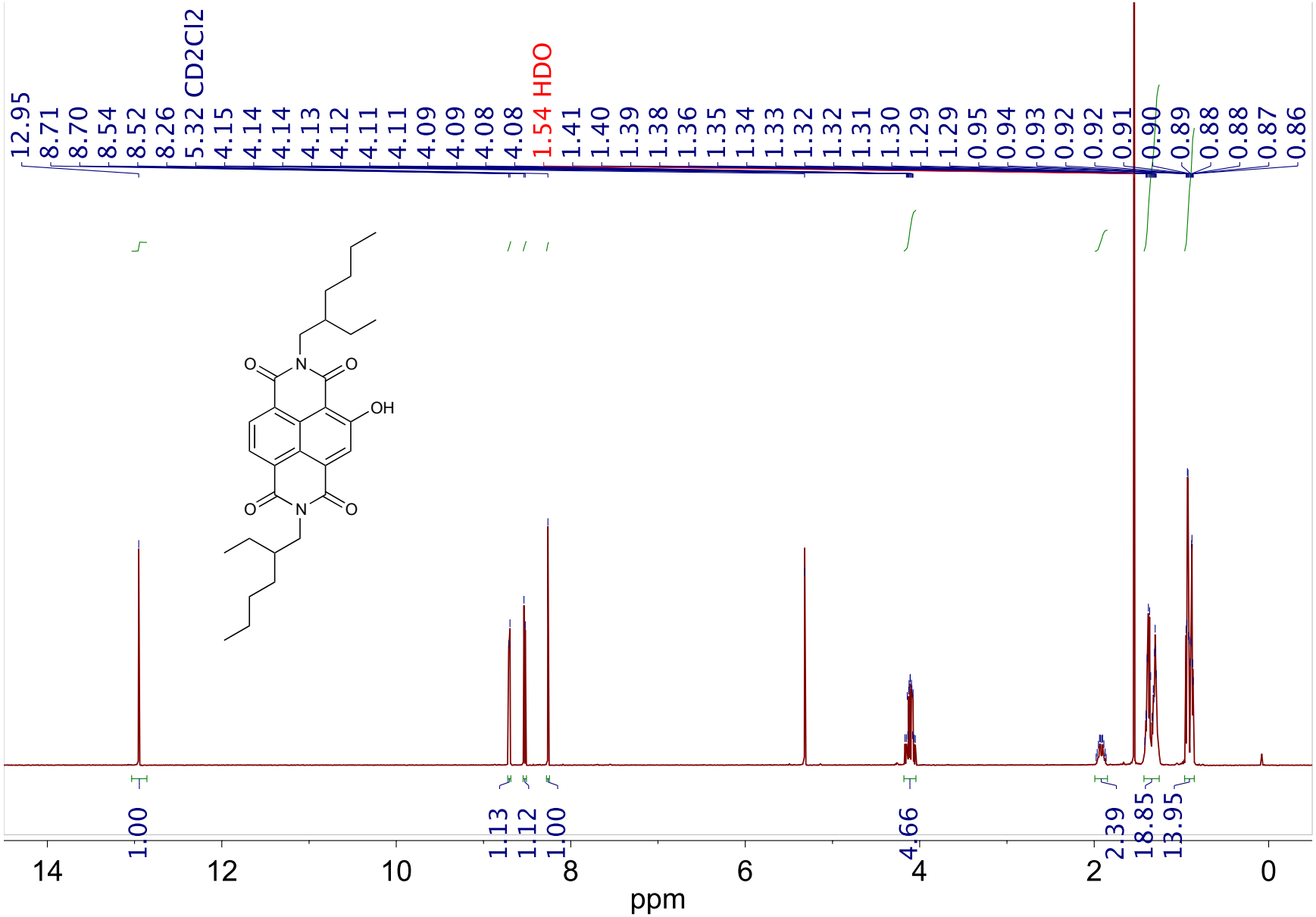


Figure S1. ^{1}H NMR of NDI-OH.

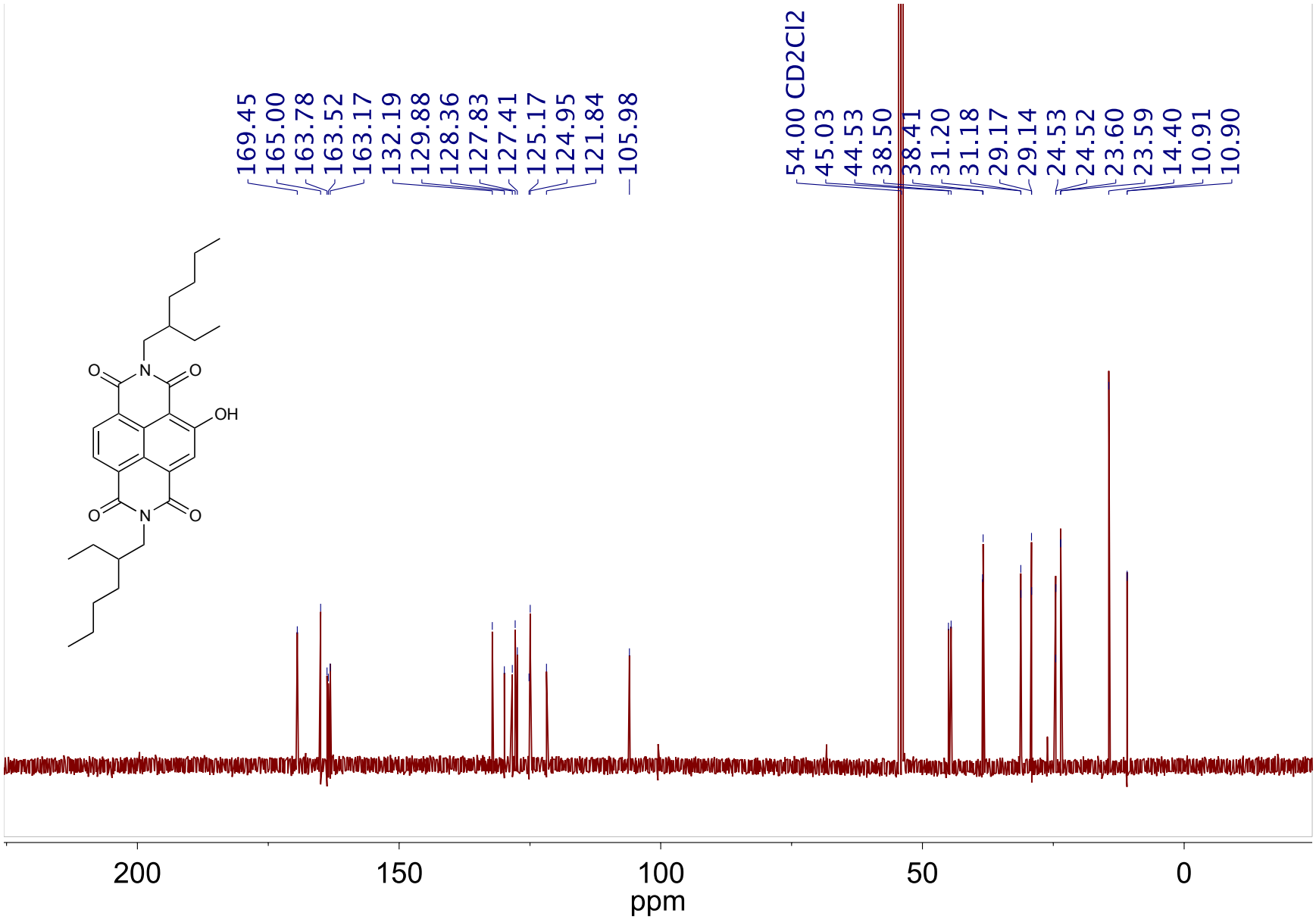


Figure S2. $^{13}C\{^{1}H\}$ NMR of NDI-OH.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	m/z	err [ppm]	rdb	e⁻ Conf	N-Rule
507.2859	1	C 30 H 39 N 2 O 5	507.2853	-1.0	12.5	even	ok

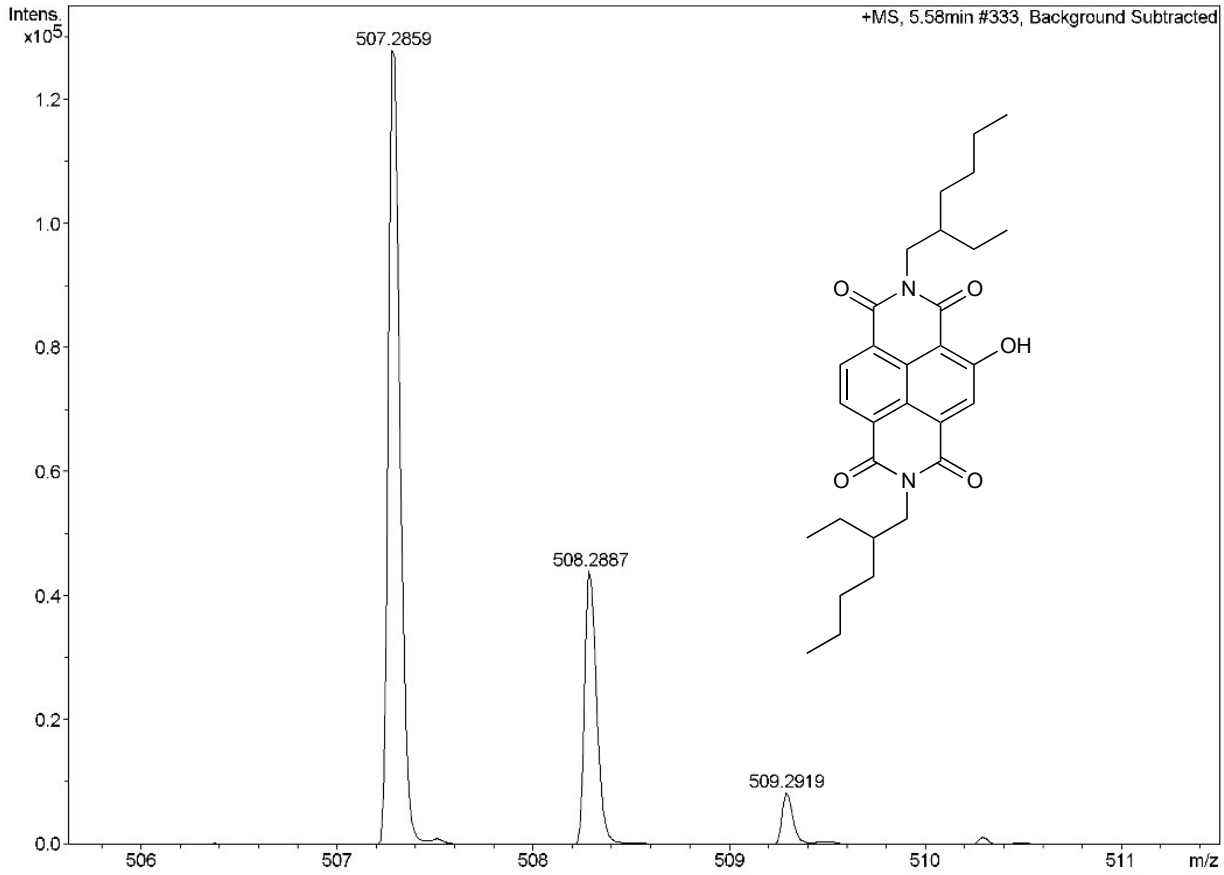


Figure S3. HR-ESI-MS (positive mode) of NDI-OH

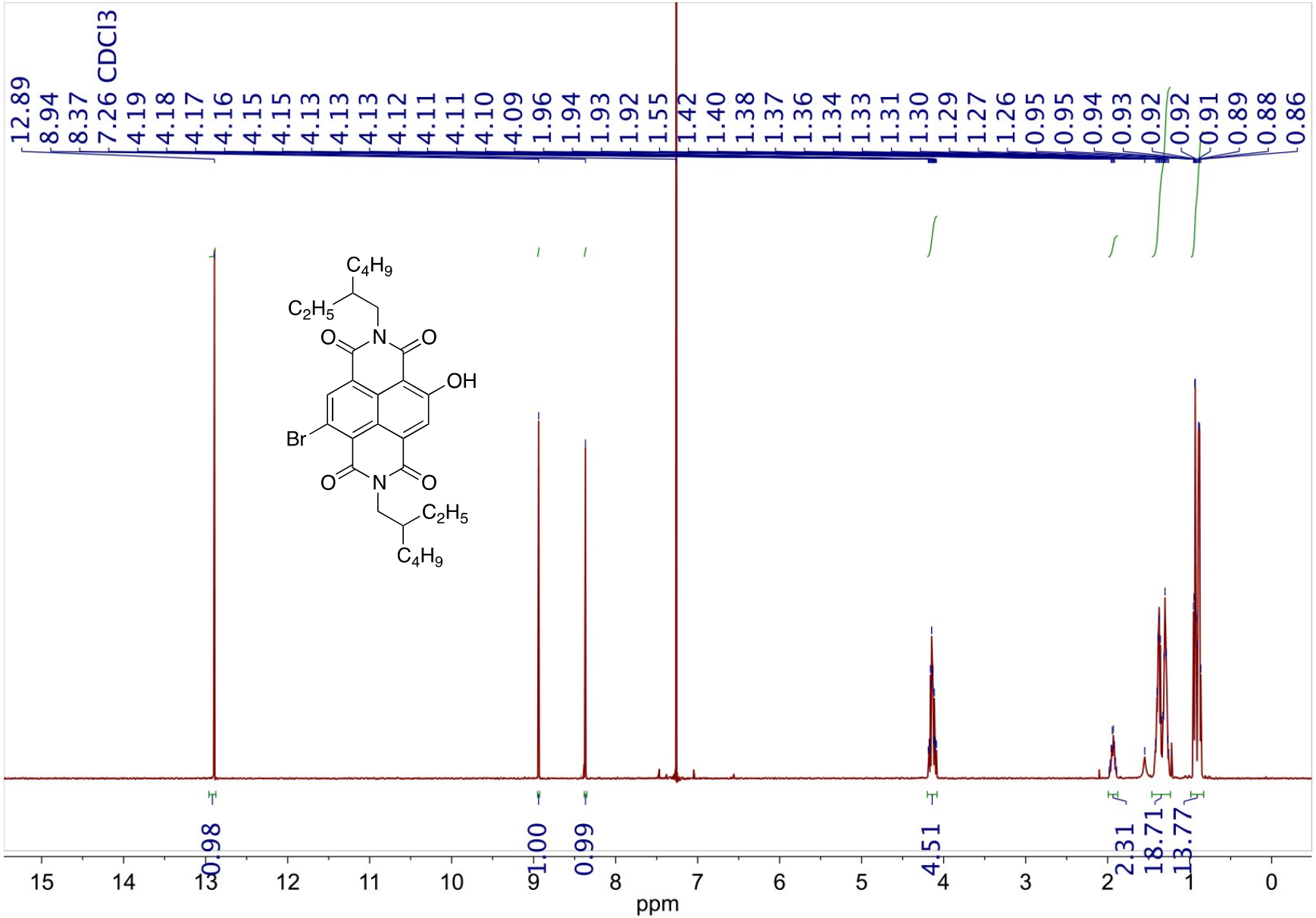


Figure S4. ^{1}H NMR of Br-NDI-OH.

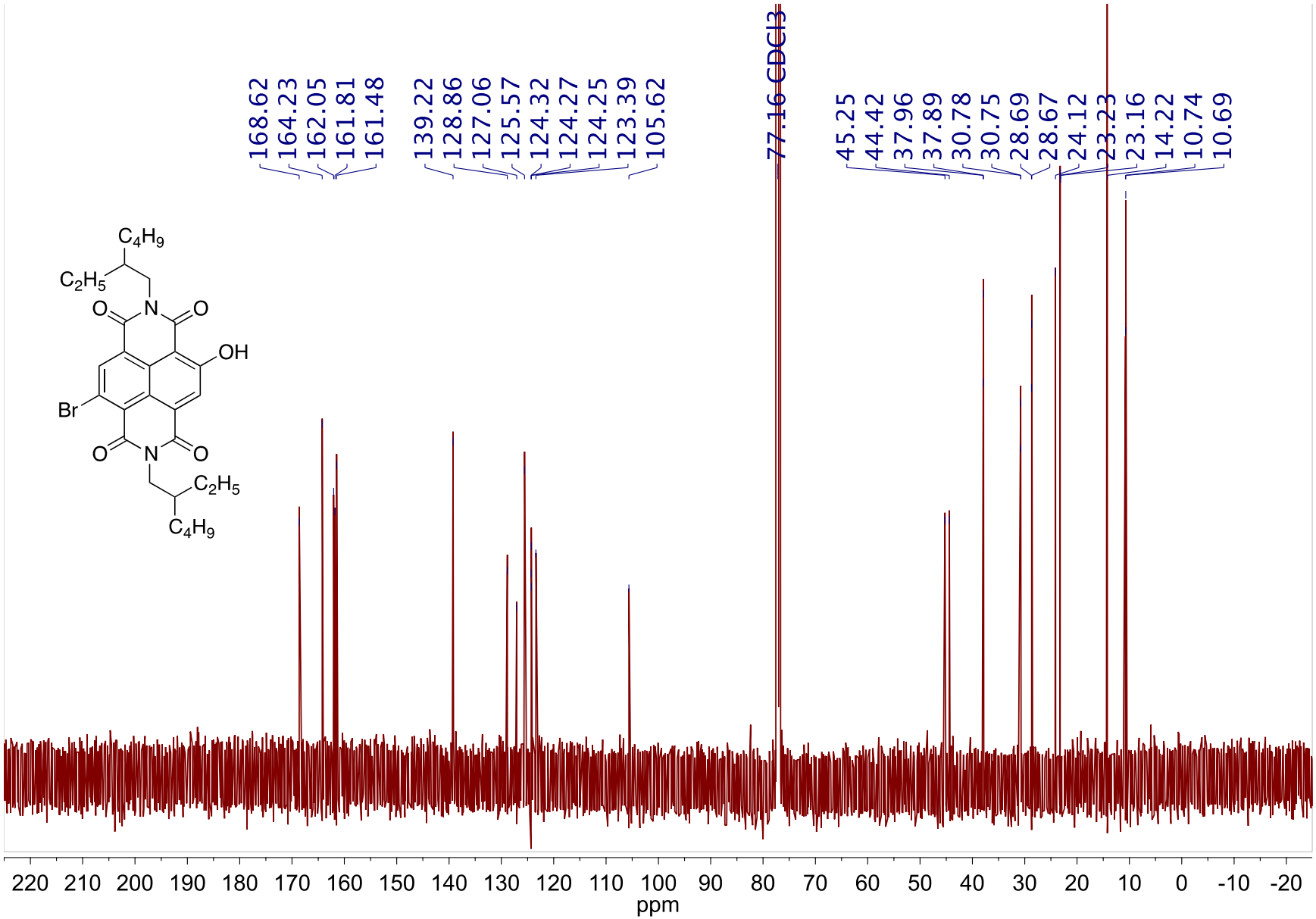


Figure S5. $^{13}C\{^{1}H\}$ NMR of Br-NDI-OH.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	m/z	err [ppm]	rdb	e⁻ Conf	N-Rule
585.1955	1	C 30 H 38 Br N 2 O 5	585.1959	0.7	12.5	even	ok

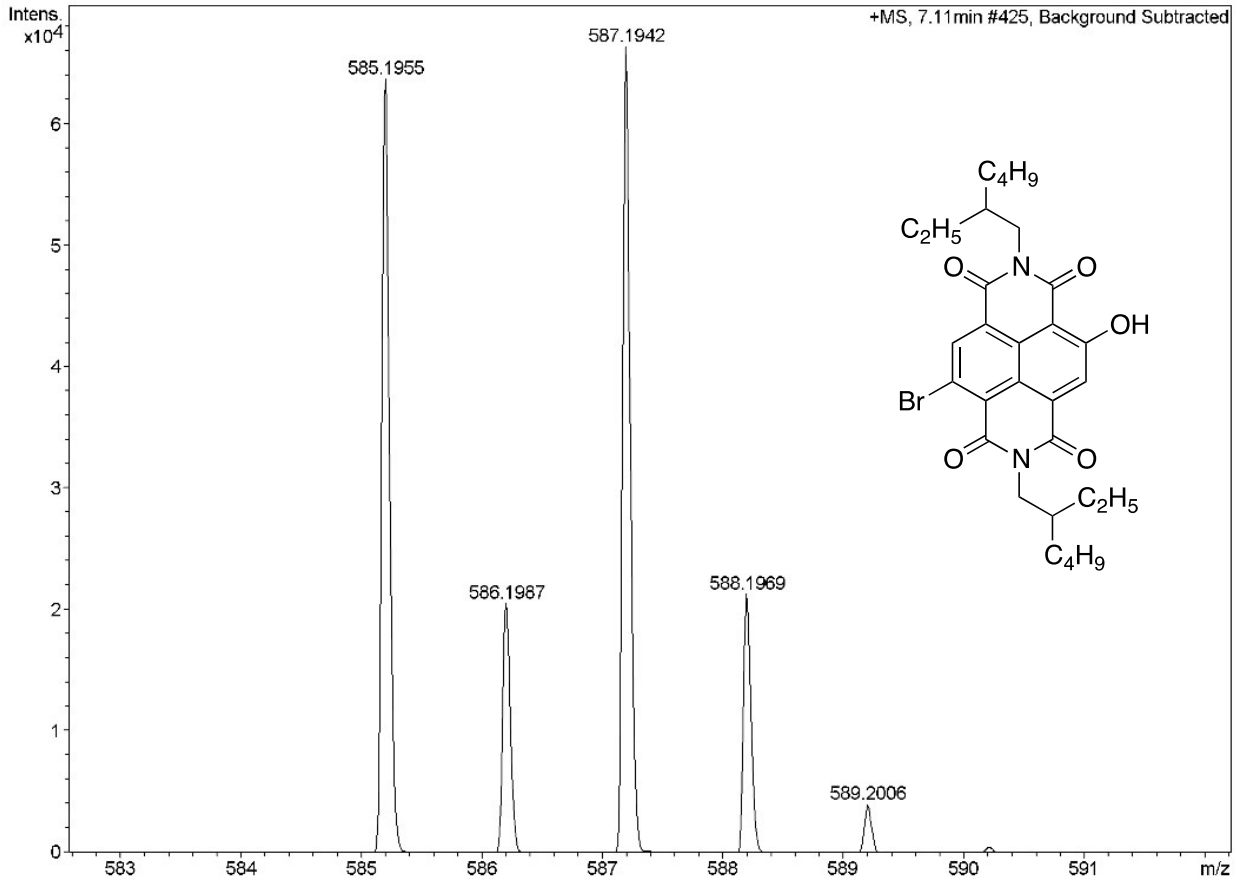


Figure S6. HR-ESI-MS (positive mode) of Br-NDI-OH.

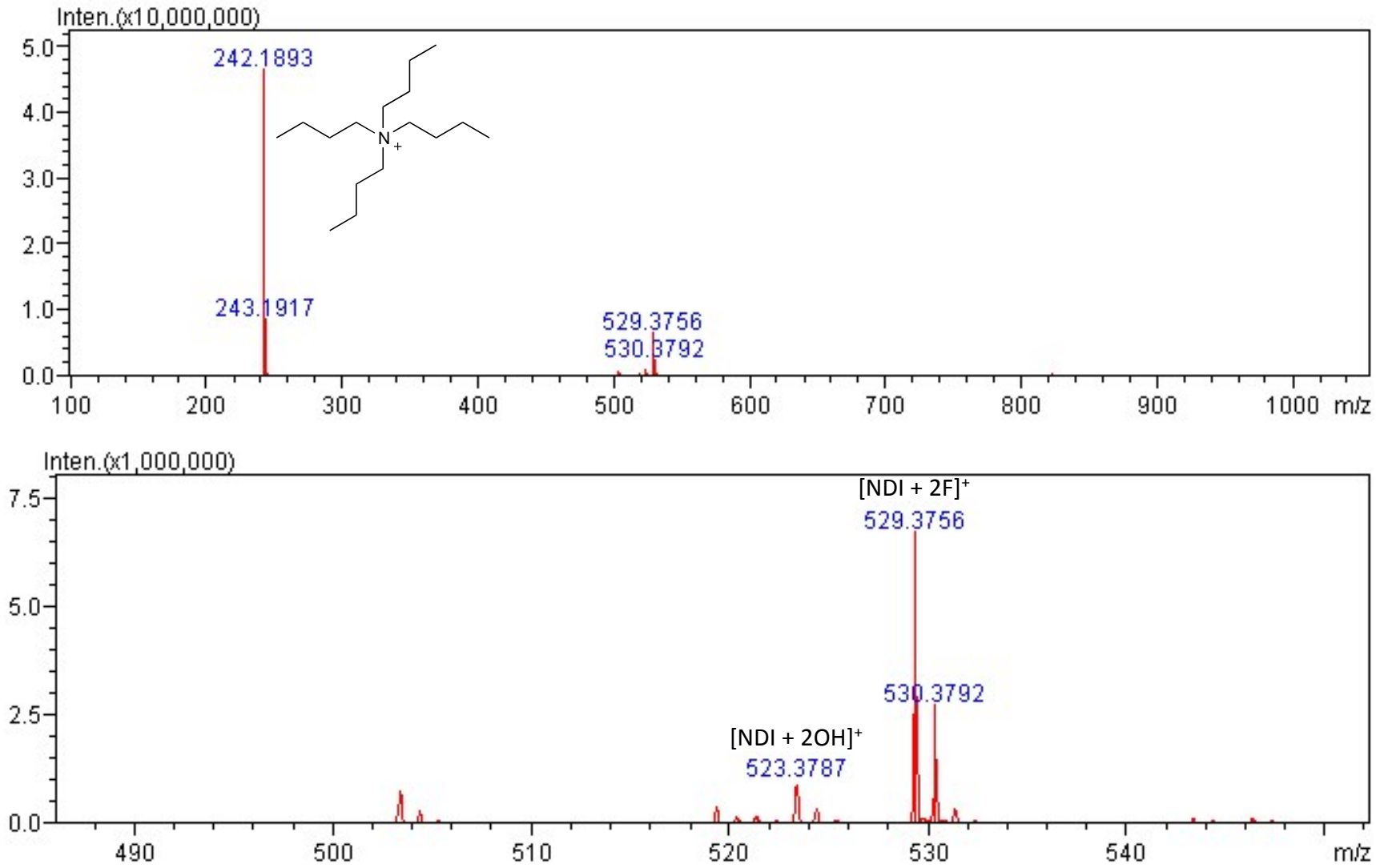


Figure S7. ESI-MS (positive mode) of the reaction between NDI and TBAF in THF. Top: zoom out. Bottom: zoom in.

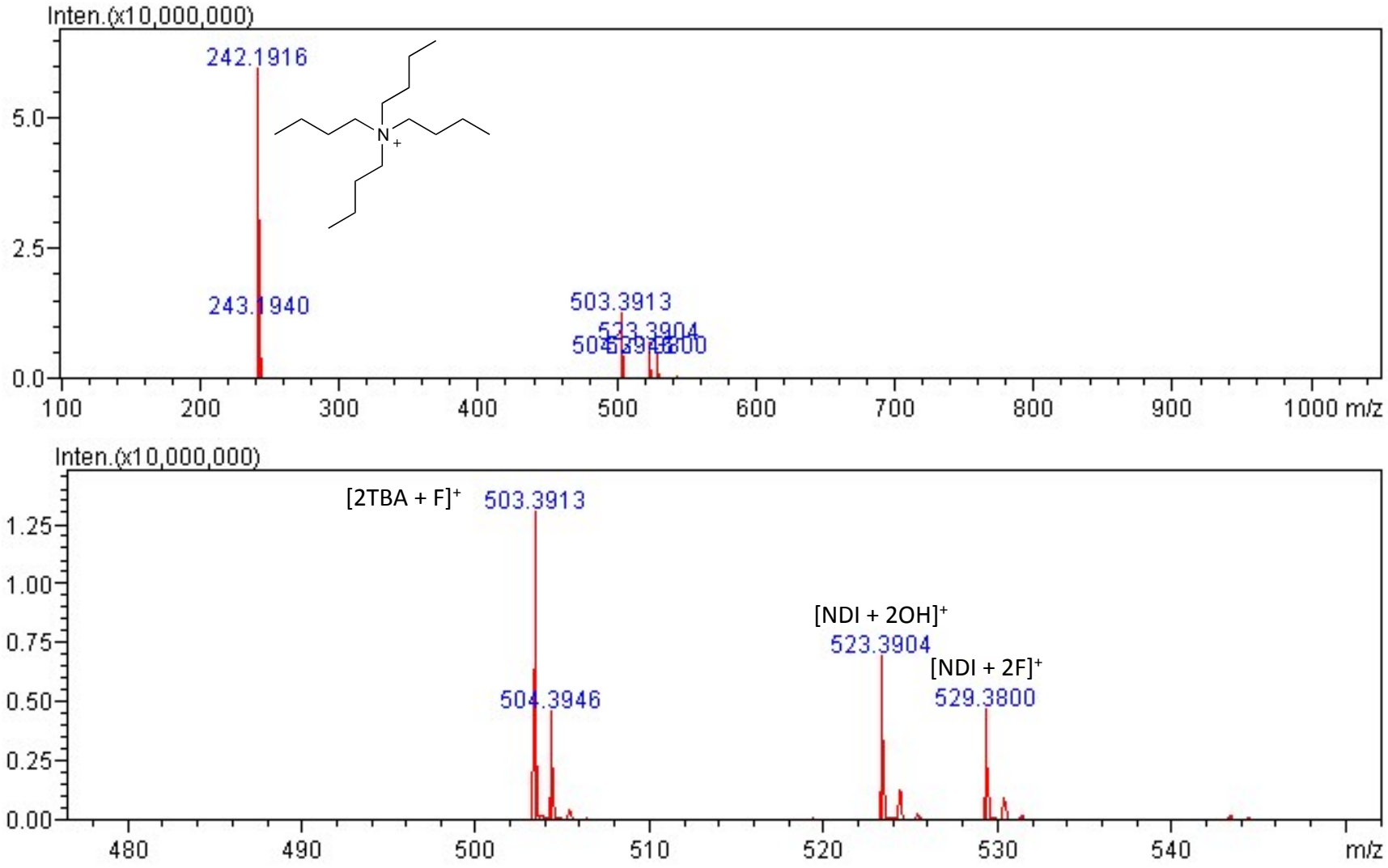


Figure S8. ESI-MS (positive mode) of the reaction between NDI and TBAF in THF with bubbling of CDA. Top: zoom out. Bottom: zoom in.

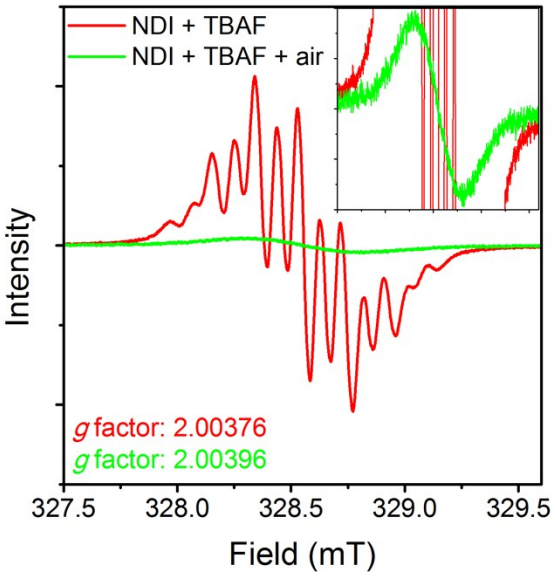


Figure S9. EPR of freshly prepared deaerated NDI with the addition of 4 equivalence of TBAF in anhydrous THF, followed by bubbling with CDA for 2 hours. Inset: magnification of EPR signal of the latter.

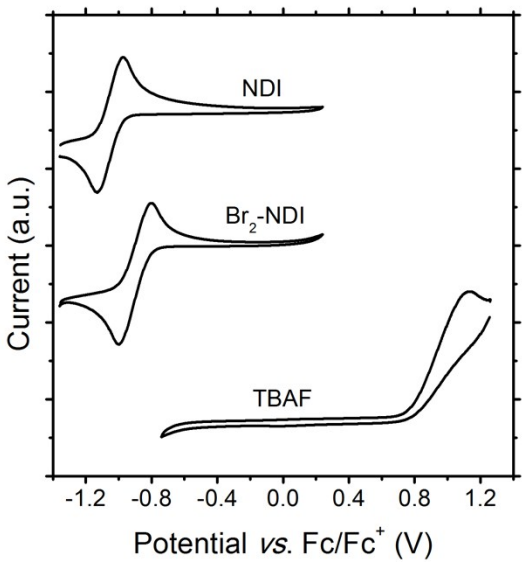


Figure S10. Cyclic voltammogram of NDI, Br_2-NDI and TBAF in THF.

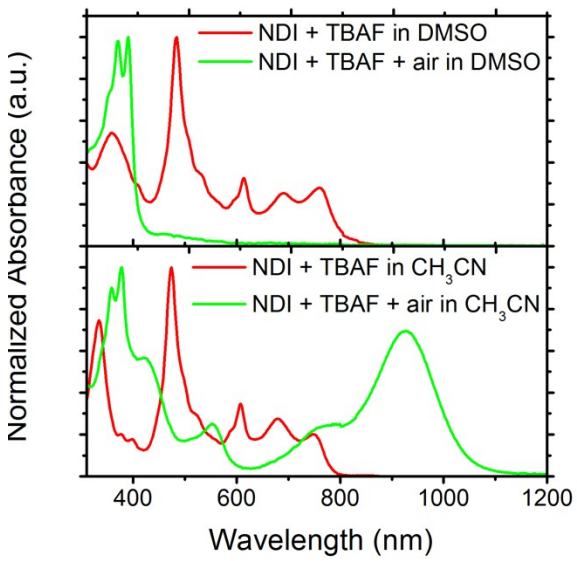


Figure S11. Solution UV-Vis of NDI + TBAF in DMSO (top) and acetonitrile (bottom) before and after bubbling with air.

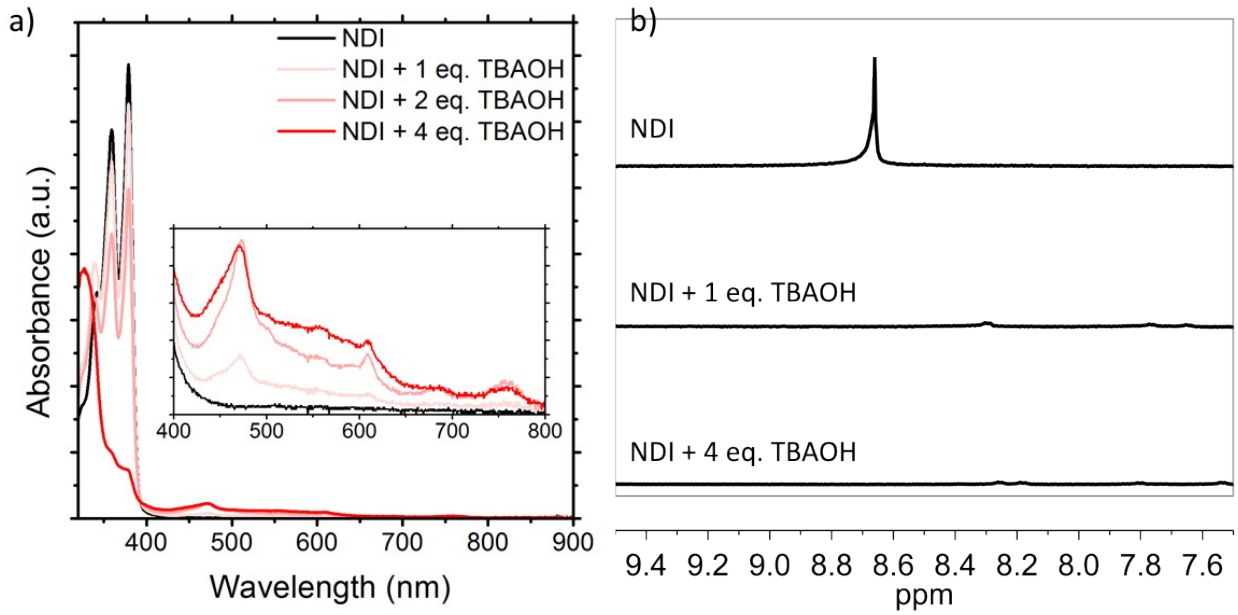


Figure S12. a) Solution UV-Vis absorption spectra of NDI upon addition of tetrabutylammonium hydroxide 30-hydrate (TBAOH) and b) ^{1}H NMR of NDI, followed by addition of TBAOH.

DFT calculations

DFT calculations were carried out using the Gaussian 09 program suite.[2] Geometry optimization was carried out in the gas-phase using CAM-B3LYP 6-311G+ (d,p) for the NDI unit and LanL2DZPD[3] for F^-/OH^-. Frequency checks were carried out to ensure all geometries are global minimum structures. Single-point calculation was carried out on the optimized geometry using the keyword counterpoise=2 to obtain the BSSE corrected interaction energy. For the enthalpy of electron transfer between NDI and F^-/OH^-, these structures were optimized using solvation model IEF-PCM (THF) and frequency checks were performed to ensure these geometries are global minimum. No global minimum could be found for the complexes when various` solvation model was applied.

F^- close-shell singlet RCAM-B3LYP LanL2DZPD
G energy (IEFPCM, THF) = -99.989901

$F^\bullet$ open-shell doublet UCAM-B3LYP LanL2DZPD
G energy (IEFPCM, THF) = -99.747372

OH^- close-shell singlet RCAM-B3LYP LanL2DZPD
G energy (IEFPCM, THF) = -75.915416

$OH^\bullet$ open-shell doublet RCAM-B3LYP LanL2DZPD
G energy (IEFPCM, THF) = -75.742616

NDI close-shell singlet RCAM-B3LYP 6-311G+ (d,p)
G energy (IEFPCM, THF) = -1025.836838

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.410667	0.710017	0.000000
2	6	0	1.223059	1.399749	0.000000
3	6	0	2.415005	-0.694484	0.000000
4	6	0	-0.002330	0.704162	0.000000
5	6	0	1.223059	2.882337	0.000000
6	6	0	1.232081	-1.392819	0.000000
7	1	0	3.349864	-1.238757	0.000000
8	6	0	-1.232081	1.392819	0.000000
9	6	0	0.002330	-0.704162	0.000000
10	7	0	-0.012907	3.521856	0.000000
11	8	0	2.247146	3.533211	0.000000
12	6	0	1.249718	-2.877266	0.000000
13	6	0	-1.249718	2.877266	0.000000
14	6	0	-2.415005	0.694484	0.000000
15	6	0	-1.223059	-1.399749	0.000000
16	6	0	0.017068	4.986156	0.000000
17	7	0	0.012907	-3.521856	0.000000
18	8	0	2.286946	-3.505873	0.000000
19	8	0	-2.286946	3.505873	0.000000
20	6	0	-2.410667	-0.710017	0.000000
21	1	0	-3.349864	1.238757	0.000000
22	6	0	-1.223059	-2.882337	0.000000
23	1	0	-1.006075	5.343818	0.000000
24	1	0	0.540092	5.343341	0.885545
25	1	0	0.540092	5.343341	-0.885545
26	6	0	-0.017068	-4.986156	0.000000
27	8	0	-2.247146	-3.533211	0.000000
28	1	0	-0.540092	-5.343341	-0.885545
29	1	0	1.006075	-5.343818	0.000000
30	1	0	-0.540092	-5.343341	0.885545
31	1	0	3.342101	1.260262	0.000000
32	1	0	-3.342101	-1.260262	0.000000

NDI$^{\bullet-}$ open-shell doublet UCAM-B3LYP 6-311G+ (d,p)
G energy (IEFPCM, THF) = -1025.975742

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.694088	2.436486	0.000022
2	6	0	-1.405557	1.225223	0.000010
3	6	0	0.681156	2.440006	0.000021
4	6	0	-0.713970	-0.001867	-0.000003
5	6	0	-2.857208	1.229721	0.000012
6	6	0	1.400194	1.232714	0.000011
7	1	0	1.233876	3.370131	0.000028
8	6	0	-1.400194	-1.232714	-0.000019
9	6	0	0.713970	0.001867	0.000000
10	7	0	-3.496011	-0.010608	0.000003
11	8	0	-3.537660	2.255592	0.000027
12	6	0	2.852800	1.252993	0.000009
13	6	0	-2.852800	-1.252993	-0.000025
14	6	0	-0.681156	-2.440006	-0.000031
15	6	0	1.405557	-1.225223	-0.000009
16	6	0	-4.955961	0.018590	0.000007
17	7	0	3.496011	0.010608	0.000017
18	8	0	3.511947	2.292204	0.000003
19	8	0	-3.511947	-2.292204	-0.000051
20	6	0	0.694088	-2.436486	-0.000026
21	1	0	-1.233876	-3.370131	-0.000045
22	6	0	2.857208	-1.229721	-0.000002
23	1	0	-5.312158	-1.005419	-0.000002
24	1	0	-5.317984	0.543693	0.883354
25	1	0	-5.317989	0.543708	-0.883330
26	6	0	4.955961	-0.018590	0.000025
27	8	0	3.537660	-2.255592	-0.000009
28	1	0	5.317994	-0.543667	-0.883334
29	1	0	5.312158	1.005419	0.000065
30	1	0	5.317979	-0.543734	0.883350
31	1	0	-1.251766	3.363738	0.000032
32	1	0	1.251766	-3.363738	-0.000033

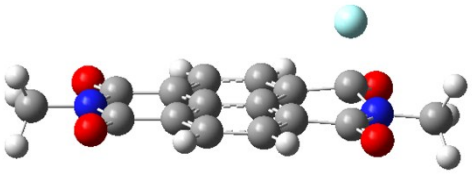
NDI close-shell singlet RCAM-B3LYP 6-311G+ (d,p)
G energy (gas phase) = -1025.823890

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.410813	0.711036	0.000000
2	6	0	1.222910	1.400249	0.000000
3	6	0	2.415678	-0.693839	0.000000
4	6	0	-0.002592	0.704415	0.000000
5	6	0	1.225722	2.884863	0.000000
6	6	0	1.232950	-1.392493	0.000000
7	1	0	3.346775	-1.245655	0.000000
8	6	0	-1.232950	1.392493	0.000000
9	6	0	0.002592	-0.704415	0.000000
10	7	0	-0.014238	3.522727	0.000000
11	8	0	2.247597	3.532532	0.000000
12	6	0	1.254400	-2.878876	0.000000
13	6	0	-1.254400	2.878876	0.000000
14	6	0	-2.415678	0.693839	0.000000
15	6	0	-1.222910	-1.400249	0.000000
16	6	0	0.014238	4.986297	0.000000
17	7	0	0.014238	-3.522727	0.000000
18	8	0	2.289934	-3.503599	0.000000
19	8	0	-2.289934	3.503599	0.000000
20	6	0	-2.410813	-0.711036	0.000000
21	1	0	-3.346775	1.245655	0.000000
22	6	0	-1.225722	-2.884863	0.000000
23	1	0	-1.011003	5.340259	0.000000
24	1	0	0.540874	5.344141	0.883517
25	1	0	0.540874	5.344141	-0.883517
26	6	0	-0.014238	-4.986297	0.000000
27	8	0	-2.247597	-3.532532	0.000000
28	1	0	-0.540874	-5.344141	-0.883517
29	1	0	1.011003	-5.340259	0.000000
30	1	0	-0.540874	-5.344141	0.883517
31	1	0	3.338016	1.269516	0.000000
32	1	0	-3.338016	-1.269516	0.000000

NDI$^{\bullet-}$ open-shell doublet UCAM-B3LYP 6-311G+ (d,p)
G energy (gas phase) = -1025.915074

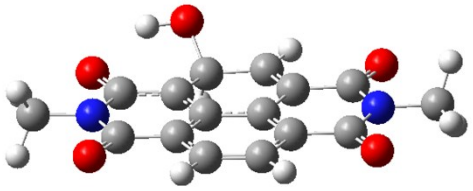
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.437257	0.694723	0.000000
2	6	0	1.225797	1.405490	0.000000
3	6	0	2.441318	-0.680362	0.000000
4	6	0	-0.002127	0.714562	0.000000
5	6	0	1.234352	2.858250	0.000000
6	6	0	1.234352	-1.399579	0.000000
7	1	0	3.367029	-1.240955	0.000000
8	6	0	-1.234352	1.399579	0.000000
9	6	0	0.002127	-0.714562	0.000000
10	7	0	-0.011792	3.494225	0.000000
11	8	0	2.254500	3.541477	0.000000
12	6	0	1.259819	-2.853106	0.000000
13	6	0	-1.259819	2.853106	0.000000
14	6	0	-2.441318	0.680362	0.000000
15	6	0	-1.225797	-1.405490	0.000000
16	6	0	0.016112	4.950255	0.000000
17	7	0	0.011792	-3.494225	0.000000
18	8	0	2.294117	-3.514454	0.000000
19	8	0	-2.294117	3.514454	0.000000
20	6	0	-2.437257	-0.694723	0.000000
21	1	0	-3.367029	1.240955	0.000000
22	6	0	-1.234352	-2.858250	0.000000
23	1	0	-1.011339	5.299959	0.000000
24	1	0	0.546514	5.313150	0.880977
25	1	0	0.546514	5.313150	-0.880977
26	6	0	-0.016112	-4.950255	0.000000
27	8	0	-2.254500	-3.541477	0.000000
28	1	0	-0.546514	-5.313150	-0.880977
29	1	0	1.011339	-5.299959	0.000000
30	1	0	-0.546514	-5.313150	0.880977
31	1	0	3.359674	1.260912	0.000000
32	1	0	-3.359674	-1.260912	0.000000

[NDI···F]$^{-}$ close-shell singlet RCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for F
G energy (gas phase) = -1125.395851



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.920304	2.446650	0.077437
2	6	0	1.594579	1.243624	0.031532
3	6	0	-0.482217	2.480169	0.036431
4	6	0	0.872893	0.029333	-0.038588
5	6	0	3.060430	1.213320	0.050287
6	6	0	-1.205649	1.310340	-0.031005
7	1	0	-1.024742	3.412936	0.041206
8	6	0	1.536477	-1.218288	-0.100823
9	6	0	-0.540156	0.063577	-0.046233
10	7	0	3.675547	-0.039252	-0.011336
11	8	0	3.766084	2.238518	0.115587
12	6	0	-2.688559	1.369989	-0.157677
13	6	0	2.997819	-1.269267	-0.092392
14	6	0	0.794303	-2.382164	-0.180509
15	6	0	-1.272190	-1.143574	-0.094947
16	6	0	5.139946	-0.049738	0.008527
17	7	0	-3.352175	0.195591	-0.282254
18	8	0	-3.271278	2.481523	-0.215738
19	8	0	3.645262	-2.331787	-0.154179
20	6	0	-0.607164	-2.344178	-0.179042
21	1	0	1.323023	-3.322627	-0.235859
22	6	0	-2.769188	-1.124492	-0.001295
23	1	0	5.460184	-1.082511	-0.042904
24	1	0	5.527152	0.513790	-0.836982
25	1	0	5.501585	0.419075	0.920428
26	6	0	-4.801608	0.241782	-0.421016
27	8	0	-3.426083	-2.135273	-0.373158
28	1	0	-5.264904	0.555064	0.514646
29	1	0	-5.071779	0.953909	-1.196632
30	1	0	-5.122247	-0.762174	-0.674237
31	1	0	1.497611	3.357809	0.132899
32	1	0	-1.202467	-3.242644	-0.229340
33	9	0	-2.766557	-1.013705	1.724187

[NDI···OH]$^{-}$ close-shell singlet RCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for OH
G energy (gas phase) = -1101.358460



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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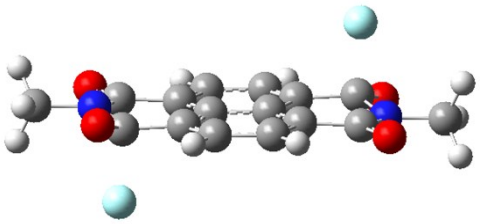
2	6	0	-1.399789	0.963774	-0.140805
3	6	0	0.726746	2.260173	-0.158124
4	6	0	-0.650245	-0.218217	-0.079741
5	6	0	-2.798188	0.918292	-0.091637
6	6	0	1.429716	1.116030	-0.096410
7	1	0	1.251614	3.204913	-0.119376
8	6	0	-1.277058	-1.484920	-0.005746
9	6	0	0.777128	-0.182890	-0.079337
10	7	0	-3.413102	-0.355325	-0.020856
11	8	0	-3.541026	1.965340	-0.090608
12	6	0	2.899215	1.174122	-0.027595
13	6	0	-2.727619	-1.562333	0.014200
14	6	0	-0.511327	-2.659036	0.042512
15	6	0	1.508197	-1.356311	-0.016370
16	6	0	-4.870672	-0.422579	0.028831
17	7	0	3.583965	-0.042340	0.018902
18	8	0	3.551020	2.234948	-0.023043
19	8	0	-3.370247	-2.644945	0.068494
20	6	0	0.864543	-2.610176	0.036925
21	1	0	-1.044215	-3.597655	0.087957
22	6	0	2.976761	-1.308425	0.015607
23	1	0	-5.247610	-0.984467	-0.823835
24	1	0	-5.188257	-0.939491	0.932371
25	1	0	-5.238840	0.595986	0.014560
26	6	0	5.045558	0.032388	0.070466
27	8	0	3.684124	-2.332260	0.048176
28	1	0	5.421273	0.560089	-0.802902
29	1	0	5.357501	0.581849	0.955371
30	1	0	5.424898	-0.981091	0.096746
31	1	0	-0.983966	2.712043	-1.309323
32	1	0	1.470673	-3.501016	0.080370
33	8	0	-1.269629	3.289626	0.632471
34	1	0	-2.242109	3.172796	0.553067

[NDI···2F]$^{2-}$ close-shell singlet RCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for F
G energy (gas phase) = -1225.211787



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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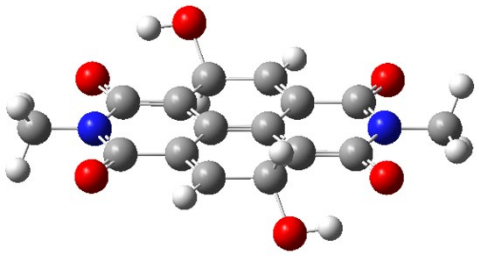
2	6	0	1.820903	-0.252696	0.345510
3	6	0	1.422517	2.052784	-0.258203
4	6	0	0.440844	-0.520171	0.191776
5	6	0	2.767928	-1.347966	0.716626
6	6	0	0.078996	1.814131	-0.437470
7	1	0	1.790382	3.050252	-0.450828
8	6	0	-0.078996	-1.814131	0.437470
9	6	0	-0.440844	0.520171	-0.191776
10	7	0	2.113745	-2.568816	1.168925
11	8	0	3.898250	-1.077466	1.205928
12	6	0	-0.809736	2.888092	-0.930654
13	6	0	0.809736	-2.888092	0.930654
14	6	0	-1.422517	-2.052784	0.258203
15	6	0	-1.820903	0.252696	-0.345510
16	6	0	2.991310	-3.627465	1.641554
17	7	0	-2.113745	2.568816	-1.168925
18	8	0	-0.369404	4.041859	-1.182988
19	8	0	0.369404	-4.041859	1.182988
20	6	0	-2.291213	-1.021383	-0.143369
21	1	0	-1.790382	-3.050252	0.450828
22	6	0	-2.767928	1.347966	-0.716626
23	1	0	2.539663	-4.125958	2.496645
24	1	0	3.154362	-4.366081	0.855837
25	1	0	3.930899	-3.155520	1.906369
26	6	0	-2.991310	3.627465	-1.641554
27	8	0	-3.898250	1.077466	-1.205928
28	1	0	-3.154362	4.366081	-0.855837
29	1	0	-2.539663	4.125958	-2.496645
30	1	0	-3.930899	3.155520	-1.906369
31	1	0	3.347730	1.194728	0.282774
32	1	0	-3.347730	-1.194728	-0.282774
33	9	0	3.030225	-1.907691	-1.008145
34	9	0	-3.030225	1.907691	1.008145

[NDI···2OH]$^{2-}$ close-shell singlet RCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for OH
G energy (gas phase) = -1177.074449



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	1.301931	-1.344229	0.169196
3	6	0	-0.920945	-2.478203	0.433525
4	6	0	0.689195	-0.036853	0.002014
5	6	0	2.779208	-1.442056	0.151797
6	6	0	-1.514257	-1.119514	0.173254
7	6	0	1.514257	1.119514	-0.173254
8	6	0	-0.689195	0.036853	-0.002014
9	7	0	3.484935	-0.273848	0.008953
10	8	0	3.399249	-2.534542	0.278965
11	6	0	-2.888833	-1.034179	0.145976
12	6	0	2.888833	1.034179	-0.145976
13	6	0	0.920945	2.478203	-0.433525
14	6	0	-1.301931	1.344229	-0.169196
15	6	0	4.937007	-0.363563	0.026574
16	7	0	-3.484935	0.273848	-0.008953
17	8	0	-3.702965	-2.044992	0.236207
18	8	0	3.702965	2.044992	-0.236207
19	6	0	-0.571248	2.469171	-0.333213
20	6	0	-2.779208	1.442056	-0.151797
21	1	0	5.308250	0.651212	-0.065425
22	1	0	5.278140	-0.824787	0.953949
23	1	0	5.291791	-0.984834	-0.796782
24	6	0	-4.937007	0.363563	-0.026574
25	8	0	-3.399249	2.534542	-0.278965
26	1	0	-5.278140	0.824787	-0.953949
27	1	0	-5.308250	-0.651212	0.065425
28	1	0	-5.291791	0.984834	0.796782
29	1	0	1.084356	-3.416879	0.422243
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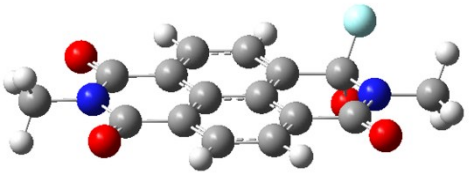
31	1	0	1.212894	2.829051	-1.441680
32	1	0	-1.212894	-2.829051	1.441680
33	8	0	1.464677	3.499406	0.465478
34	1	0	2.428105	3.325882	0.388167
35	8	0	-1.464677	-3.499406	-0.465478
36	1	0	-2.428105	-3.325882	-0.388167

[NDI···F]• open-shell doublet UCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for F
G energy (gas phase) = -1125.243507



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-1.628764	1.250084	0.005417
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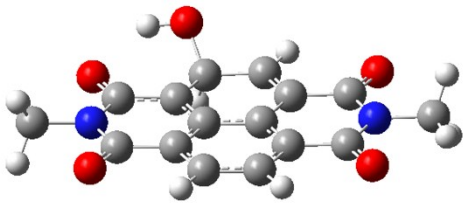
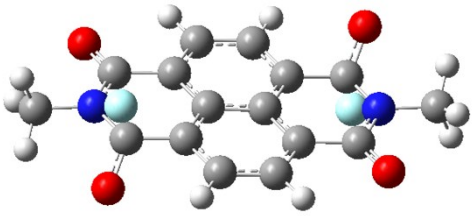
4	6	0	-0.880319	0.052203	0.004592
5	6	0	-3.102699	1.188331	0.003849
6	6	0	1.168475	1.377945	-0.003538
7	1	0	0.934297	3.479071	-0.019166
8	6	0	-1.519337	-1.209489	-0.005796
9	6	0	0.529437	0.118155	0.013434
10	7	0	-3.694917	-0.076859	-0.001644
11	8	0	-3.810123	2.204842	0.007872
12	6	0	2.647589	1.461590	-0.022454
13	6	0	-2.996032	-1.286049	-0.008673
14	6	0	-0.774033	-2.365485	-0.022762
15	6	0	1.268267	-1.084069	-0.002219
16	6	0	-5.164331	-0.113821	-0.002311
17	7	0	3.352726	0.276769	-0.023121
18	8	0	3.228084	2.560225	-0.033714
19	8	0	-3.591946	-2.371889	-0.017035
20	6	0	0.631774	-2.305837	-0.017366
21	1	0	-1.288502	-3.313989	-0.037093
22	6	0	2.768316	-1.029006	0.037357
23	1	0	-5.469810	-1.151933	-0.007183
24	1	0	-5.545155	0.390754	0.881188
25	1	0	-5.544774	0.398729	-0.881373
26	6	0	4.820948	0.320304	0.022660
27	8	0	3.077683	-1.713055	1.222853
28	1	0	5.238360	-0.184597	-0.843448
29	1	0	5.116199	1.362075	0.020002
30	1	0	5.177016	-0.157426	0.934483
31	1	0	-1.582995	3.367243	0.001015
32	1	0	1.214992	-3.212962	-0.031083
33	9	0	3.300705	-1.784307	-1.030223

[NDI···OH]• open-shell doublet UCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for OH
G energy (gas phase) = -1101.239690



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.761454	2.316444	-0.301982
2	6	0	-1.399789	0.963774	-0.140805
3	6	0	0.726746	2.260173	-0.158124
4	6	0	-0.650245	-0.218217	-0.079741
5	6	0	-2.798188	0.918292	-0.091637
6	6	0	1.429716	1.116030	-0.096410
7	1	0	1.251614	3.204913	-0.119376
8	6	0	-1.277058	-1.484920	-0.005746
9	6	0	0.777128	-0.182890	-0.079337
10	7	0	-3.413102	-0.355325	-0.020856
11	8	0	-3.541026	1.965340	-0.090608
12	6	0	2.899215	1.174122	-0.027595
13	6	0	-2.727619	-1.562333	0.014200
14	6	0	-0.511327	-2.659036	0.042512
15	6	0	1.508197	-1.356311	-0.016370
16	6	0	-4.870672	-0.422579	0.028831
17	7	0	3.583965	-0.042340	0.018902
18	8	0	3.551020	2.234948	-0.023043
19	8	0	-3.370247	-2.644945	0.068494
20	6	0	0.864543	-2.610176	0.036925
21	1	0	-1.044215	-3.597655	0.087957
22	6	0	2.976761	-1.308425	0.015607
23	1	0	-5.247610	-0.984467	-0.823835
24	1	0	-5.188257	-0.939491	0.932371
25	1	0	-5.238840	0.595986	0.014560
26	6	0	5.045558	0.032388	0.070466
27	8	0	3.684124	-2.332260	0.048176
28	1	0	5.421273	0.560089	-0.802902
29	1	0	5.357501	0.581849	0.955371
30	1	0	5.424898	-0.981091	0.096746
31	1	0	-0.983966	2.712043	-1.309323
32	1	0	1.470673	-3.501016	0.080370
33	8	0	-1.269629	3.289626	0.632471
34	1	0	-2.242109	3.172796	0.553067

[NDI···2F]$^{\bullet-}$ open-shell doublet UCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for F
G energy (gas phase) = -1225.149688



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-0.504869	2.466309	0.099724
4	6	0	0.708148	-0.055397	-0.003192
5	6	0	2.988037	1.037478	0.047573
6	6	0	-1.303583	1.330559	0.049247
7	1	0	-0.996845	3.426316	0.127451
8	6	0	1.303583	-1.330559	-0.049247
9	6	0	-0.708148	0.055397	0.003192
10	7	0	3.508648	-0.332662	0.116804
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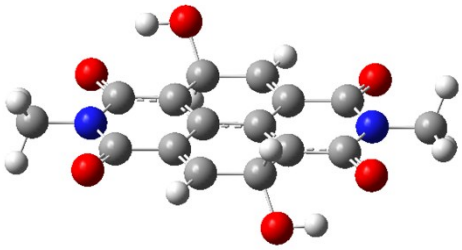
12	6	0	-2.777795	1.473997	-0.003352
13	6	0	2.777795	-1.473997	0.003352
14	6	0	0.504869	-2.466309	-0.099724
15	6	0	-1.496303	-1.111168	-0.038064
16	6	0	4.958786	-0.436140	0.237675
17	7	0	-3.508648	0.332662	-0.116804
18	8	0	-3.310178	2.610491	0.009104
19	8	0	3.310178	-2.610491	-0.009104
20	6	0	-0.882890	-2.358743	-0.107030
21	1	0	0.996845	-3.426316	-0.127451
22	6	0	-2.988037	-1.037478	-0.047573
23	1	0	5.203204	-1.371543	0.729092
24	1	0	5.430864	-0.415520	-0.744280
25	1	0	5.294543	0.415948	0.820955
26	6	0	-4.958786	0.436140	-0.237675
27	8	0	-3.500375	-1.867838	-0.933606
28	1	0	-5.430864	0.415520	0.744280
29	1	0	-5.203204	1.371543	-0.729092
30	1	0	-5.294543	-0.415948	-0.820955
31	1	0	1.517088	3.227979	0.175075
32	1	0	-1.517088	-3.227979	-0.175075
33	9	0	3.402897	1.478096	-1.345250
34	9	0	-3.402897	-1.478096	1.345250

[NDI···2OH]$^{\bullet-}$ open-shell doublet UCAM-B3LYP 6-311G+ (d,p) for NDI, LanL2DZPD for OH
G energy (gas phase) = -1177.124421



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	6	0	0.705334	-0.067183	-0.000121
5	6	0	2.726400	-1.576092	0.054269
6	6	0	-1.543768	-1.031883	0.112810
7	6	0	1.543768	1.031883	-0.112810
8	6	0	-0.705334	0.067183	0.000121
9	7	0	3.489887	-0.425670	-0.037994
10	8	0	3.286605	-2.691410	0.115808
11	6	0	-2.952838	-0.882927	0.111176
12	6	0	2.952838	0.882927	-0.111176
13	6	0	1.015930	2.431987	-0.296456
14	6	0	-1.259096	1.407699	-0.093326
15	6	0	4.942172	-0.589923	-0.046411
16	7	0	-3.489887	0.425670	0.037994
17	8	0	-3.752199	-1.871233	0.165085
18	8	0	3.752199	1.871233	-0.165085
19	6	0	-0.473967	2.496037	-0.193851
20	6	0	-2.726400	1.576092	-0.054269
21	1	0	5.379283	0.399297	-0.100558
22	1	0	5.264240	-1.104871	0.856282
23	1	0	5.245080	-1.191342	-0.901117
24	6	0	-4.942172	0.589923	0.046411
25	8	0	-3.286605	2.691410	-0.115808
26	1	0	-5.264240	1.104871	-0.856282
27	1	0	-5.379283	-0.399297	0.100558
28	1	0	-5.245080	1.191342	0.901117
29	1	0	0.929503	-3.475805	0.215255
30	1	0	-0.929503	3.475805	-0.215255
31	1	0	1.306405	2.791194	-1.298092
32	1	0	-1.306405	-2.791194	1.298092
33	8	0	1.580465	3.365497	0.648958
34	1	0	2.543610	3.233809	0.547203
35	8	0	-1.580465	-3.365497	-0.648958
36	1	0	-2.543610	-3.233809	-0.547203

References

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