Supporting Information

Effects of cucurbit[*n*]uril (*n* = 7, 8, 10) hosts on the formation and stabilization of naphthalenediimide (NDI) radical anion

Xiran Zhao,[a] Fengbo Liu,[a] Zhiyong Zhao,[a] Hakim Karoui,[b] David Bardelang,*[b] Olivier Ouari*[b] and Simin Liu*[a]

a. The State Key Laboratory of Refractories and Metallurgy, School of Chemistry and Chemical Engineering, Wuhan University of Science and Technology, Wuhan 430081, China.

b. Aix Marseille Univ., CNRS, Institut de Chimie Radicalaire, UMR 7273, 13013 Marseille, France.

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Materials & Methods

CB[*n*] (*n* = 7, 8), CB[10] and **NDI** derivate (**NDI**$^{2+}$ as chloride salt) were prepared by the corresponding literature procedures.[1-3] Other materials were obtained from commercial suppliers and were used without further purification. ^{1}H NMR spectra were recorded on an Agilent 600 MHz apparatus (water suppression was used in some cases). EPR (Electron Paramagnetic Resonance) experiments were performed at room temperature using a computer-controlled Bruker EMX ESR spectrometer (Bruker, Wissembourg, France) at 9.5 GHz (X-band) employing 100 kHz field modulation. UV/Vis were performed on a SHIMADZU UV-3600 instrument with 1 cm pathlength cells at 298 K. Fluorescence spectra were measured on a PerkinElmer LS-55 machine, with excitation and emission monochrometer bandpasses set at 10 nm and an excitation wavelength of 360 nm. The UV irradiation process was carried out with a high-pressure mercury lamp (CLE-M500/M350, China, 500 mW. Cyclic voltammograms tests were conducted on an electrochemical workstation (CHI 660, China) under computer control, using a single-compartment glass cell fitted with a working glassy carbon electrode (0.071 cm^2), a Pt auxiliary electrode and an Ag/AgCl reference electrode. DFT calculations were performed using the Gaussian09 Rev.D01 package with B3LYP/6-31G(d) and CPCM as a water continuum model.

1. A. I. Day, A. P. Arnold, R. J. Blanch, B. Snushall. *J. Org. Chem.* **2001**, *66*, 8094–8100.
2. X. Yang, Z. Zhao, X. Zhang, S. Liu. *Sci. China Chem.* **2018**, DOI: 10.1007/ s11426-017-9173-4.
3. L. Chen, Y.-M.Zhang, L.-H. Wang, Y. Liu. *J. Org. Chem.* **2013,** *78*, 5357–5363.

The K_a measurements for the CB[7]-NDI^{2+} complex

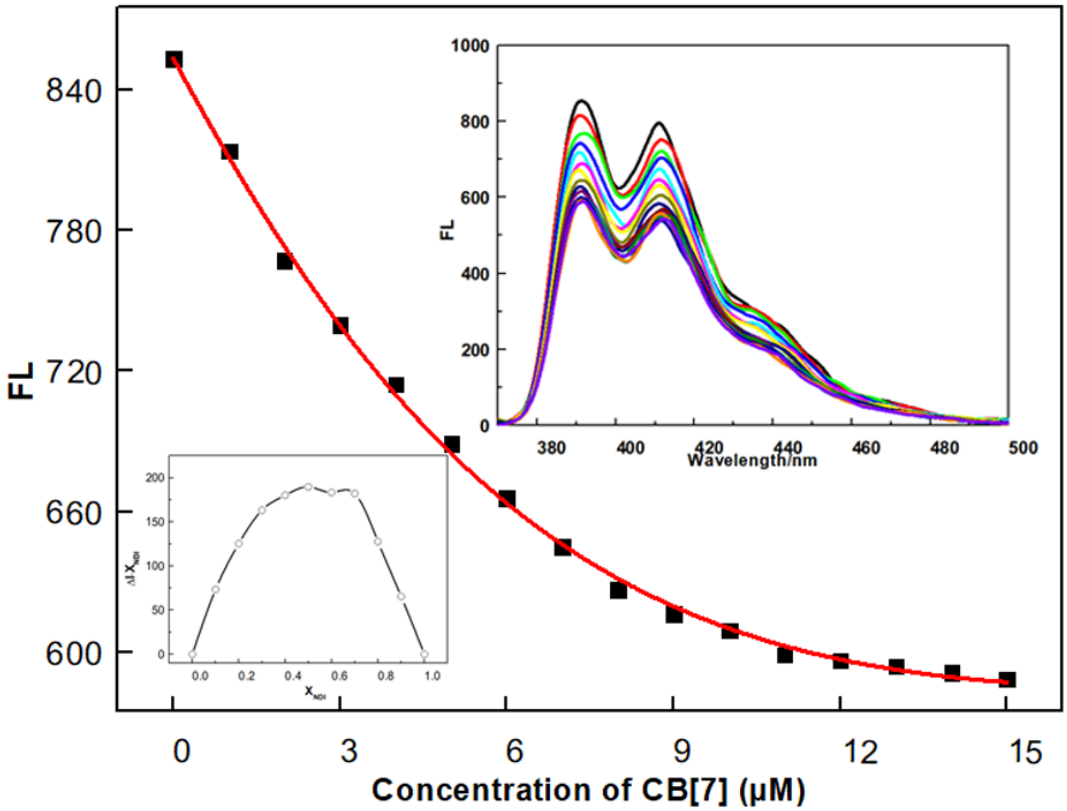


Figure S1 Job's plot and nonlinear least-squares fitting of data (Fl. Intensity) at 391 nm for the CB[7]-**NDI**$^{2+}$ complex ([**NDI**$^{2+}$] = 5.0 μM). The binding constants K_{a1} and K_{a2} are 5.14 × 10^4 and 1.06 × 10^5 M^{-1} respectively.

^{1}H NMR of the NDI^{2+} with CB[8]/CB[10]

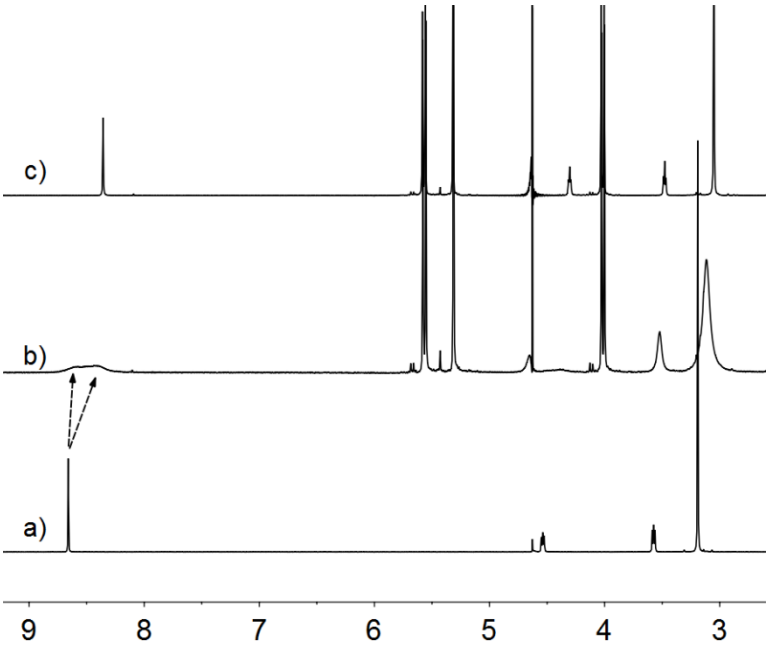


Figure S2 ^{1}H NMR spectra (D_2O, 298 K) of: a) **NDI**$^{2+}$ (2.0 mM); b) **NDI**$^{2+}$ with 0.5 eq CB[8]; c) **NDI**$^{2+}$ with 1.1 eq CB[8].

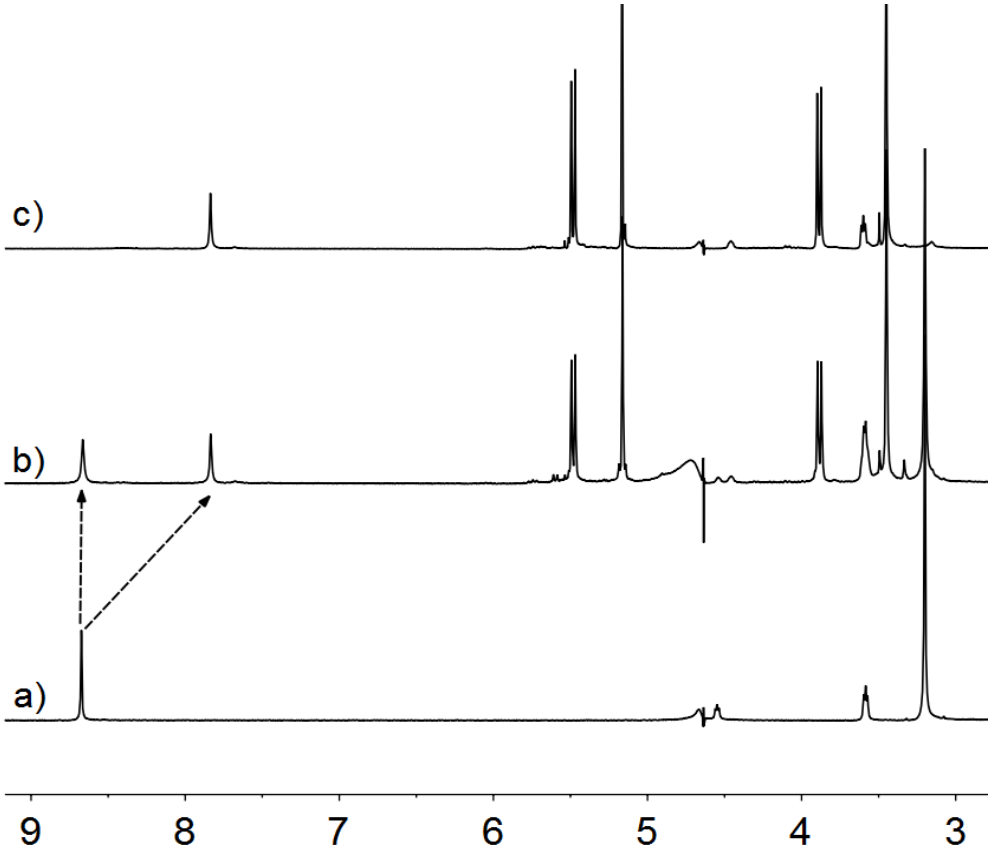


Figure S3 ^{1}H NMR spectra (D_2O, 298 K) of: a) **NDI**$^{2+}$ (2.0 mM); b) **NDI**$^{2+}$ with 0.25 eq CB[10]; c) **NDI**$^{2+}$ with 0.5 eq CB[10].

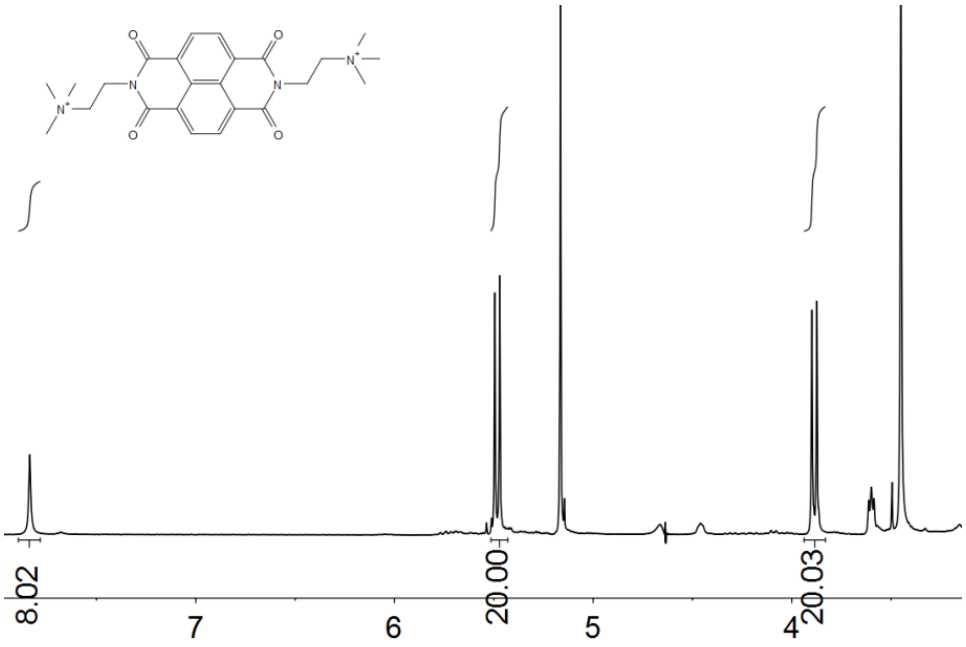


Figure S4 ^{1}H NMR spectra (D_2O, 298 K) of **NDI**$^{2+}$ (2.0 mM) with 0.5 eq CB[10] with integrals.

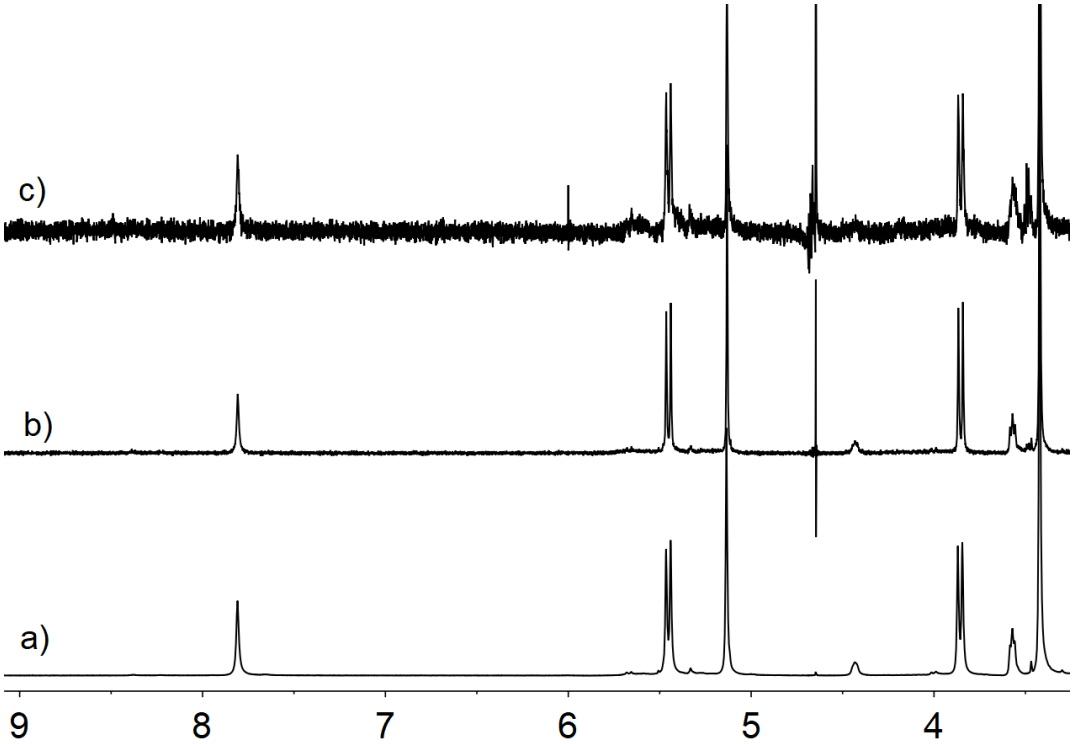


Figure S5 ^{1}H NMR (D_2O, 298 K) spectra for CB[10]·2**NDI**$^{2+}$ at the concentration of: a) 2.0 mM; b) 0.2 mM; c) 0.02 mM. Based on no obvious observation of free guest signals (the signal of protons on aromatic ring was supposed to be 8.65 ppm) by diluting 2.0 mM CB[10]·2**NDI**$^{2+}$ down to 0.02 mM, we assume that the amount of free guest was less than 10% in the solution. A K_a value larger than 10^{12} M^{-2} for the complex can be estimated.

The DFT calculations of the NDI^{2+}/CB[*n*] (*n* = 8, 10)

a) b)

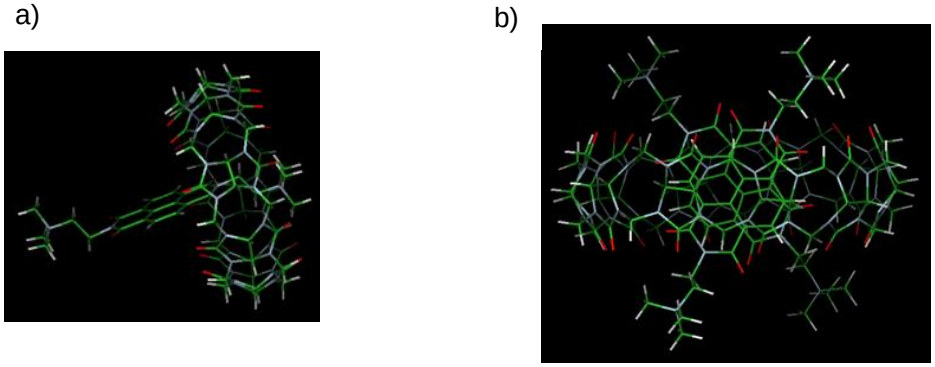


Figure S6 the structure of the DFT minimized complex: a) CB[8]·**NDI**$^{2+}$; b) CB[10]·2**NDI**$^{2+}$.

Table S1 the data of the DFT calculations.

CB[8]·**NDI**$^{2+}$	BSSE 1st fragment considered: **NDI**$^{2+}$ 2nd fragment considered: CB[8] Counterpoise corrected energy = -6266.214467169158 BSSE energy = 0.014851712148 sum of monomers = -6266.099534327011 complexation energy = -81.44 kcal/mole (raw) complexation energy = -72.12 kcal/mole (corrected)
CB[10]·2**NDI**$^{2+}$	BSSE 1st fragment considered: 1st **NDI**$^{2+}$ 2nd fragment considered: 2nd **NDI**$^{2+}$ 3rd fragment considered: CB[10] Counterpoise corrected energy = -8921.747696534798 BSSE energy = 0.040740033275 sum of monomers = -8921.696017209570 complexation energy = -57.99 kcal/mole (raw) complexation energy = -32.43 kcal/mole (corrected)

More details about the Atomic coordinates for the DFT minimized structures are given in the last supplementary data.

The fluorescence spectra of NDI^{2+}/CB[*n*] (*n* = 8, 10) under UV irradiation

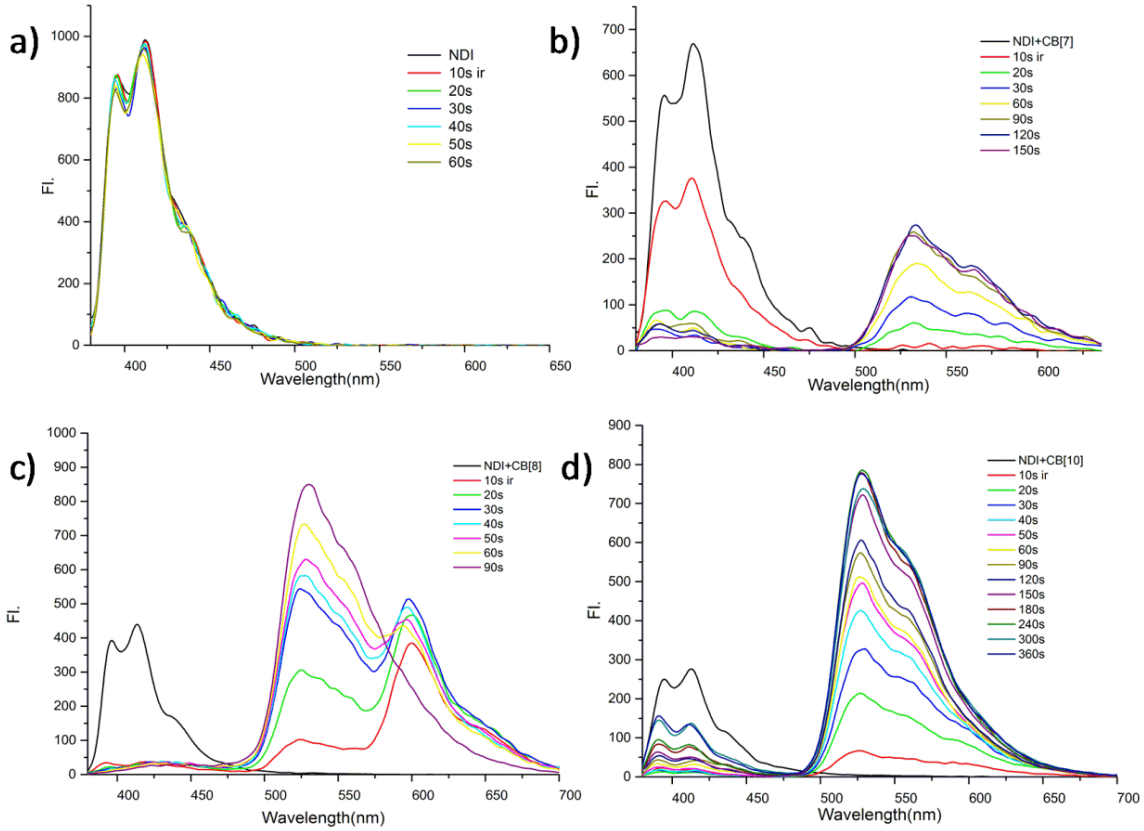


Figure S7 Fluorescence spectra of NDI^{2+} (0.05 mM) in the presence of CB[*n*] (*n* = 7, 8, 10) with different UV irradiation time: a) NDI^{2+} alone ; b) NDI^{2+} with 2.2 eq CB[7]; c) NDI^{2+} with 1.1 eq CB[8]; d) NDI^{2+} with 0.5 eq CB[10].

^{1}H NMR changes of NDI^{2+} in the presence of CB[*n*] as a function of irradiation time

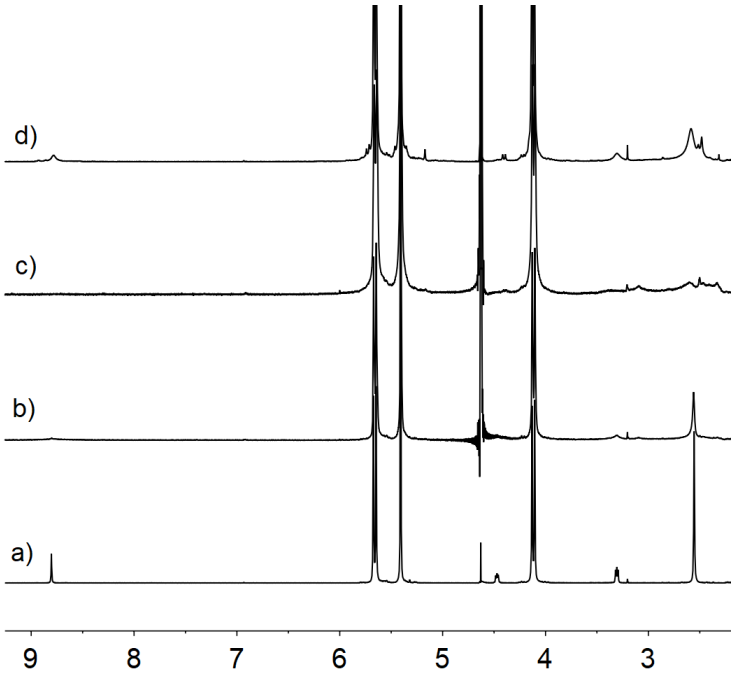


Figure S8 ^{1}H NMR spectra (D_2O, 298 K) of: a) **NDI^{2+}** (2.0 mM) with CB[7] (2.2 eq); b) irradiated for 10 s; c) irradiated for 30 s; d) solution in air for 2 days after irradiation.

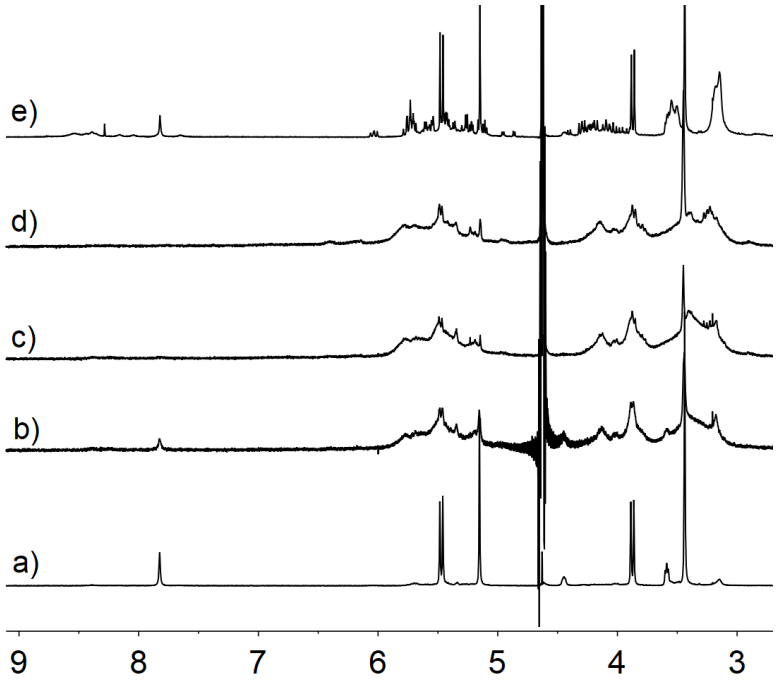


Figure S9 ^{1}H NMR spectra (D_2O, 298 K) of: a) **NDI^{2+}** (2.0 mM) with CB[10] (0.5 eq); b) irradiated for 10 s; c) irradiated for 30 s; d) irradiated for 60 s; e) solution in air for 2 days after irradiation.

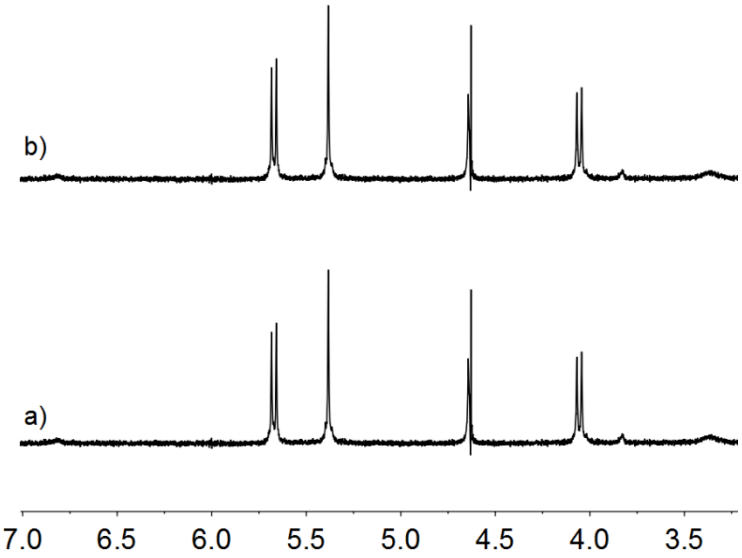


Figure S10 ^{1}H NMR spectra (D_2O, 298 K) of: a) 1,4-Benzenedimethanamine (2.0 mM) with CB[10] (~ 0.5 mM); b) after UV irradiation for 5 mins.

The EPR spectroscopy of NDI^{2+}/CB[*n*] with different irradiation time

Aqueous solutions were prepared by weighting the components in the relevant ratio (for CB[7], guest:host 1:2.2, for CB[8], guest:host 1:1.1 and for CB[10], guest:host 2:1) before ultrasound (cleaner) exposure for 10 seconds and vortexing for 30 seconds prior to filtrations through 0.2 or 0.45 µm cut-off nylon membrane filters. Finally the solutions were degassed for 120 seconds by bubbling argon before introducing 300 µL of the relevant solution in a quartz flat cell (≈ 1 mm) and sealing prior to irradiation and measurements. EPR spectra were recorded at room temperature using a computer-controlled Bruker EMX ESR spectrometer (Bruker, Wissembourg, France) at 9.5 GHz (X-band) employing 100 kHz field modulation. The UV photolysis was performed by a 1000 W xenon-mercury Oriel lamp selecting 300 W as the working power. The experimental conditions used to record the EPR spectra under irradiation (4 scans, Figure 6 of the paper) were the following: power, 10 mW; receiver gain, 2.10^5; modulation amplitude, 0.025 mT and sweep time, 21 s.

For the signal decay experiments (Figures S12-S14), solutions were prepared as mentioned before for EPR but the cell was flushed by argon prior to introducing the argon bubbled solution and sealing to avoid oxygen. The irradiation source had to be changed since optical fibers resulted in localized radical generation over the rectangle surface of the quartz flat cell and probable artificial signal decay due to diffusion or oxygen. We thus used a Rayonet UV reactor (model RPR-200) using 14 light bulbs and irradiating for 180 s at 350 nm the whole quartz flat cell prior to setting the cell in the spectrometer and monitoring signal over time. We noted almost immediate signal (and color) loss when the solution was exposed to air or shaked under air.

<u>Spectrometer settings for CB[10] solution:</u>
10 mW as the power, 1.0×10^4 as the receiver gain, 0.1 mT as the modulation amplitude and 42 s as the time sweep, 172 spectra (2 hours kinetics).
<u>Spectrometer settings for CB[7] and CB[8] solutions:</u>
20 mW as the power, 2.5×10^5 as the receiver gain, 0.1 mT as the modulation amplitude and 42 s as the time sweep, 150 spectra (1 hour and 45 minutes kinetics).

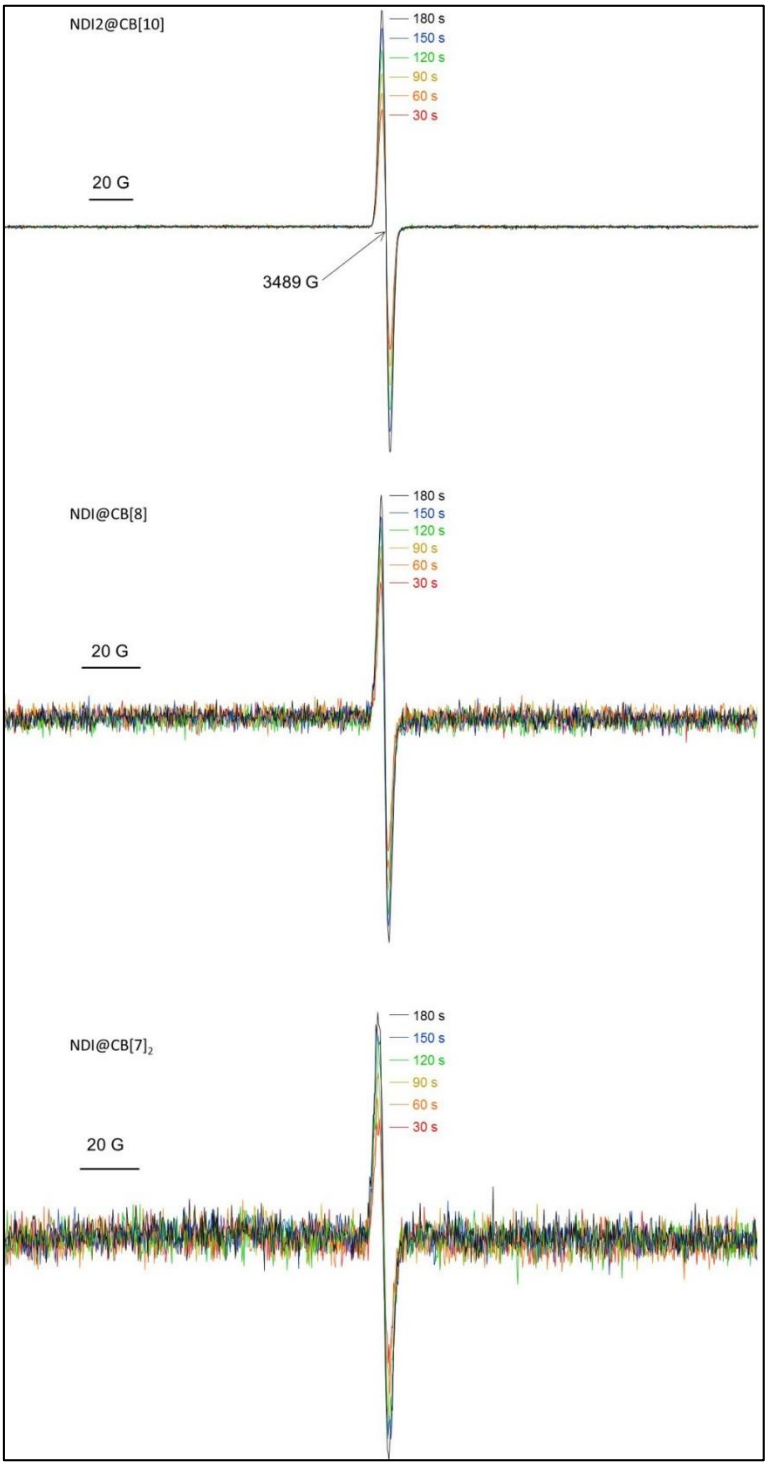


Figure S11 CB[*n*]-dependent, time monitoring of the EPR signal intensity with irradiation time ([**NDI**$^{2+}$] = 3.0 mM).

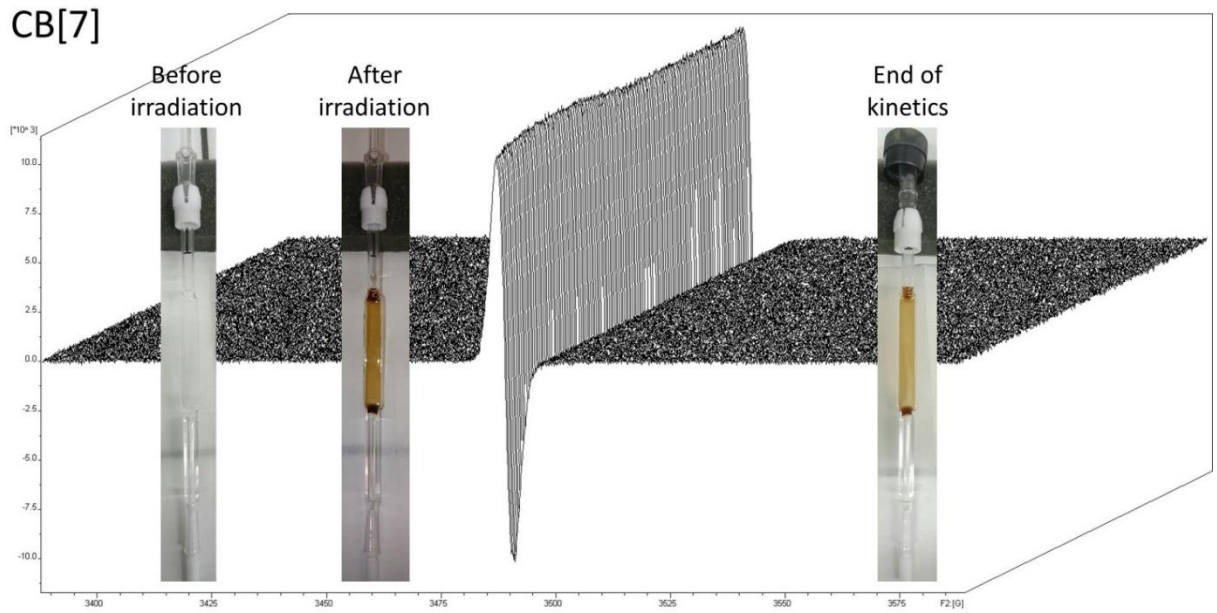


Figure S12 Time monitoring of the EPR signal intensity of a solution of **NDI** with CB[7] (2.2 eq.) for 105 minutes after shutting down irradiation (prior irradiation time was 180 s at 350 nm) ([**NDI**$^{2+}$] = 3.0 mM, intense signals due to improved spectrometer settings for monitoring).

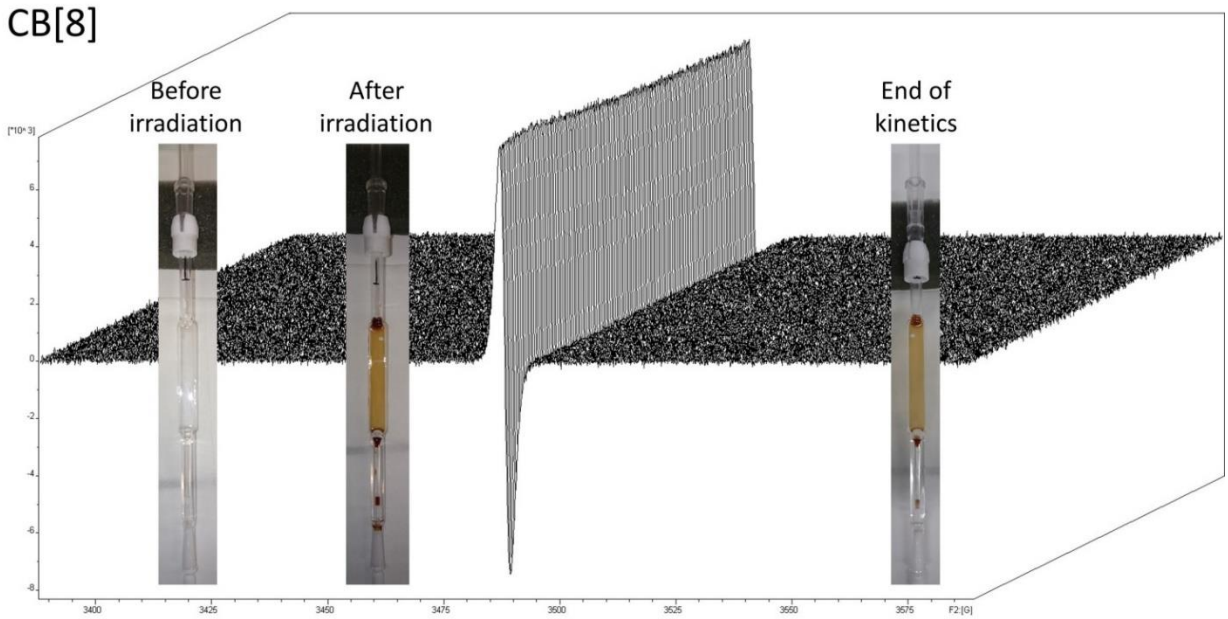


Figure S13 Time monitoring of the EPR signal intensity of a solution of **NDI** with CB[8] (1.1 eq.) for 105 minutes after shutting down irradiation (prior irradiation time was 180 s at 350 nm) ([**NDI**$^{2+}$] = 3.0 mM, intense signals due to improved spectrometer settings for monitoring).

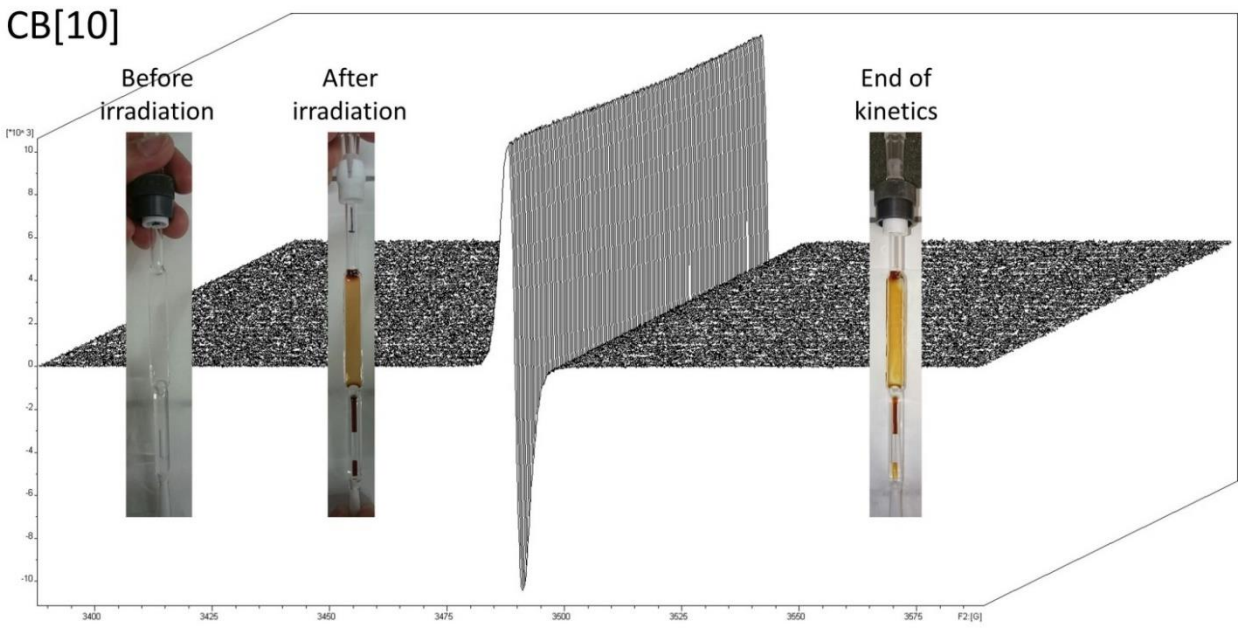


Figure S14 Time monitoring of the EPR signal intensity of a solution of **NDI** with CB[10] (0.5 eq.) for 120 minutes after shutting down irradiation (prior irradiation time was 180 s at 350 nm) ([**NDI**$^{2+}$] = 3.0 mM).

HOMO–LUMO energy gap estimated by UV/Vis absorption spectrum

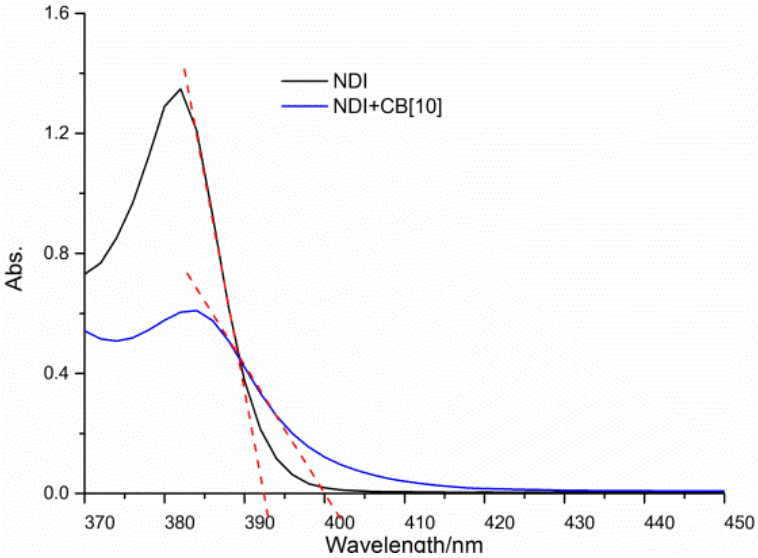
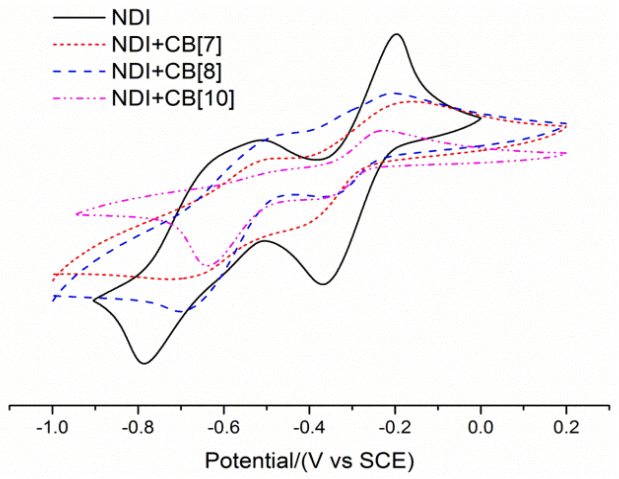


Figure S15 The energy gap estimated by UV/Vis absorption spectra of **NDI**$^{2+}$, **NDI**$^{2+}$ with CB[7] and **NDI**$^{2+}$ with CB[8], ΔE=$\frac{1240}{392}$ = 3.16 eV; **NDI**$^{2+}$ with CB[10], ΔE=$\frac{1240}{399}$ = 3.10 eV.



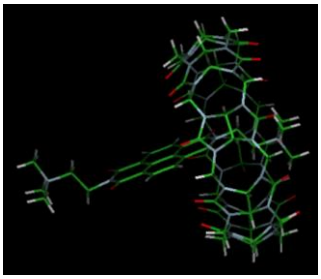
	NDI:	NDI/CB[7]:	NDI/CB[8]:	NDI/CB[10]
LUMO	-3.95 eV	-4.09 eV	-4.05eV	-4.11 eV
HOMO	-7.11 eV	-7.25 eV	-7.21eV	-7.21eV

Figure S16 Cyclic voltammograms and the LUMO and HOMO energy levels of **NDI**$^{2+}$ and **NDI**$^{2+}$ with CB[*n*] (2.0 mM in H_2O).

Supplementary data of the DFT

DFT calculations were performed using the Gaussian09 Rev.D01 package with B3LYP/6-31G(d) and CPCM as a water continuum model. Several starting geometries were considered placing the guest at several positions and letting the system minimizing before comparing their energies without, and with BSSE corrections (counterpoise method). The trends were similar (lowest energy complexes remained complexes with the lowest energy even after BSSE correction). The complexes were frequency checked for true minima. Finally, this structural approach does not consider the extra stabilization afforded by the expected release of high energy water molecules from the cavities of cucurbiturils and this may account for differences when comparing NMR data and modeling.

Atomic coordinates for the DFT minimized CB[8]·**NDI**$^{2+}$ complex



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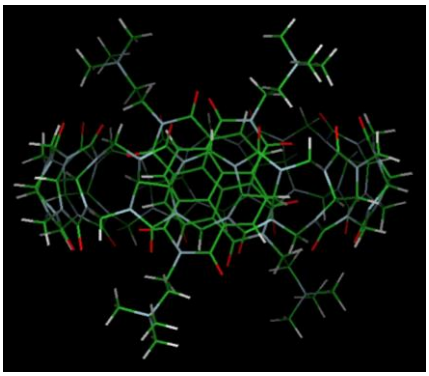
Atomic coordinates for the DFT minimized CB[10]·2**NDI**$^{2+}$ complex



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H	-2.443569	4.408472	-4.431620
H	-1.626485	3.816285	-5.909033
H	-2.934234	1.264744	-6.192414
H	-1.148637	1.453753	-6.182851
H	-1.935798	0.263968	-5.106282
H	-4.206495	1.903889	-4.195149
H	-3.392466	2.772135	-2.861014
H	-3.105157	1.024985	-3.105990