Supporting Information

Mechanical Bond-Protected Air-Stable Radicals

Junling Sun,¹,² Zhichang Liu,*,¹,² Wei-Guang Liu,³ Yilei Wu,¹ Yuping Wang,¹
Jonathan C. Barnes,¹,⁴ Keith R. Hermann,¹ William A. Goddard III,³ Michael R. Wasielewski,¹,²
and J. Fraser Stoddart¹,*

¹Department of Chemistry and ²Argonne-Northwestern Solar Energy Research (ANSER) Center,
Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA

³Materials and Process Simulation Center, California Institute of Technology, Pasadena,
California 91125, USA

⁴Department of Chemistry, Washington University, One Brookings Drive, St. Louis, MO 91125, USA

*E-mail: zhichang-liu@northwestern.edu, stoddart@northwestern.edu

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Section A. General Methods

All reagents were purchased from commercial suppliers and used without further purification. Compounds MDAP•2PF₆, DB•2PF₆, CBPQT•4PF₆, and DAPQT•4PF₆ were prepared according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60 F254 (E. Merck). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). C-18 Columns were used for analytical and preparative reverse-phase high-performance liquid-chromatography (RP-HPLC) on Agilent 1260 infinity LC equipped with Agilent 6120 LC/MS electrospray system and Shimadzu Prominence LC-8a instruments, respectively, eluted with H₂O/MeCN (0.1 % v/v TFA) and monitored using a UV detector (λ = 360 nm). UV/Vis Spectra were recorded at room temperature on a Shimadzu UV-3600 spectrophotometer. Nuclear magnetic resonance (NMR) spectra were recorded on Agilent DD2 500 as well as on Bruker Avance III 400 and 500 spectrometers, with working frequencies of 400 and 500 MHz for ¹H, as well as 100 and 125 MHz for ¹³C nuclei, respectively. Chemical shifts were reported in ppm relative to the signals corresponding to the residual non-deuterated solvents (CD₃CN: δ_H = 1.94 ppm and δ_C = 118.26 ppm for ¹³CN). High-resolution mass spectra (HR-ESI) were measured on a Finnigan LCQ iontrap mass spectrometer. Electron paramagnetic resonance (EPR) measurements at X-band (9.5 GHz) were performed with a Bruker Elexsys E580, equipped with a variable Q dielectric resonator (ER-4118X-MD5-W1). All samples were prepared in an Argon-filled atmosphere. Samples were loaded into quartz 1.4 mm tubes and sealed with a clear ridged UV doming epoxy (IllumaBond 60-7160RCL) and used immediately after preparation. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) experiments were carried out at room temperature in argon-purged MeCN solutions with a Gamry Multipurpose instrument (Reference 600) interfaced to a PC. CV Experiments were performed using a glassy carbon working electrode (0.071 cm²). The electrode surface was polished routinely with 0.05 μm alumina-water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was Ag/AgCl electrode. The concentration of the supporting electrolyte tetrabutylammonium hexafluorophosphate (NH₄PF₆) was 0.1 M.
Section B. Synthetic Protocols

1) Synthesis of the [2]Catenane AC•7PF₆

Scheme S1. Synthesis of the [2]Catenane AC•7PF₆

**AC•7PF₆**: DAPQT•4PF₆ (432 mg, 0.38 mmol) and DB•2PF₆ (306 mg, 0.38 mmol) were dissolved in degassed MeCN (140 mL) in a 250-mL round-bottomed flask in a glovebox. An excess of Zn dust (~100 mg) was added under vigorous stirring to this solution. After 30 min, the solution turned from colorless to a deep purple color, an observation which is indicative of the formation of the hetero-trisradical complex (DB⊂DAPQT)•3PF₆. The excess of Zn dust was filtered off. The purple filtrate was collected in another round-bottomed flask and 4,4'-bipyridine (62 mg, 0.40 mmol) was added to it. The resulting mixture was allowed to stand for 2 weeks at room temperature before being removed from the glovebox and the solvent evaporated off under vacuum. The resulting deep purple solid was subjected to RP-HPLC (H₂O / MeCN 0.1% TFA / 0 → 100% in 40 min). Pure fractions were collected, concentrated, added to a saturated NH₄PF₆ solution (ca. 20 mL), and filtered to afford AC•7PF₆ as a purple solid (59 mg, 8%). For NMR spectroscopic characterization, AC•7PF₆ (2 mg) was oxidized to AC•8PF₆ by the addition of an excess (1 mg) of NO•PF₆. ¹H NMR (500 MHz, CD₃CN, 298 K) of AC•8PF₆: δ = 10.06 (s, 4H), 8.96 (d, J = 6.7 Hz, 4H), 8.78 (d, J = 6.7 Hz, 4H), 8.66 (d, J = 7.1 Hz, 4H), 8.49 (s, 4H), 8.35 (d, J = 8.4 Hz, 4H), 8.21 (d, J = 8.3 Hz, 4H), 8.16 (d, J = 8.3 Hz, 4H), 8.05 (d, J = 8.3 Hz, 4H), 7.71
(d, J = 6.7 Hz, 4H), 6.42 (s, 4H), 6.07 (s, 4H), 5.89 (s, 4H), 4.08 (d, J = 6.7 Hz, 4H), 3.62 (d, J = 6.7 Hz, 4H). $^{13}$C NMR (125 MHz, CD$_3$CN, 298 K) of AC•8PF$_6$: $\delta_C = 148.7, 148.1, 142.9, 141.9, 140.3, 140.0, 138.5, 138.2, 132.9, 132.8, 132.3, 132.1, 131.8, 131.3, 130.1, 128.5, 128.3, 128.1, 122.3, 121.6, 67.8, 67.3, 67.2, 65.7, 65.3, 65.1, 63.4, 48.0, 36.9, 32.6, 31.7, 30.9, 30.3, 30.1, 29.8, 23.4, 22.9, 14.4, 9.2. ESI-HRMS for AC•7PF$_6$: Calcd for C$_{76}$H$_{64}$F$_{42}$N$_8$P$_7$: m/z = 1958.3099 [M – PF$_6$]$^+$; found: 1958.3109.

2) Synthesis of the [2]Catenane SC•7PF$_6$

Scheme S2. Synthesis of the [2]Catenane SC•7PF$_6$

SC•7PF$_6$: Following a procedure similar to that described for the synthesis of AC•7PF$_6$, the reaction of a mixture composed of DAPQT•4PF$_6$ (200 mg, 0.17 mmol), DB•2PF$_6$ (142 mg, 0.17 mmol) and 2,7-diazapyrene (36 mg, 0.17 mmol) afforded SC•7PF$_6$ as a purple solid (18 mg, 5%). For NMR spectroscopic characterization, SC•7PF$_6$ (2 mg) was oxidized to SC•8PF$_6$ by the addition of an excess (1 mg) of NO•PF$_6$. $^1$H NMR (500 MHz, CD$_3$CN, 298 K) of SC•8PF$_6$: $\delta_H = 9.97$ (s, 8H), 8.44 (s, 8H), 8.35 (d, J = 5.8 Hz, 8H), 8.24 (d, J = 7.8 Hz, 8H), 8.06 (d, J = 7.8 Hz, 8H), 6.41 (s, 8H), 5.97 (s, 8H), 3.45 (d, J = 5.8 Hz, 8H). $^{13}$C NMR (125 MHz, CD$_3$CN, 298 K) of SC•8PF$_6$: $\delta_C = 147.9, 144.1, 141.9, 141.6, 138.3, 132.9, 132.1, 131.7, 130.0, 126.2, 121.5, 67.7, 31.0. ESI-HRMS for SC•7PF$_6$: Calcd for C$_{80}$H$_{64}$F$_{36}$N$_8$P$_6$: m/z = 2006.3099 [M – PF$_6$]$^+$; found: 2006.3102.
Section C. NMR Spectroscopy

1) \(^1\)H NMR Spectra of AC•8PF\(_6\)

Since AC•7PF\(_6\) is a paramagnetic compound, its oxidized form—namely, AC•8PF\(_6\)—was characterized by NMR spectroscopy. The \(^1\)H NMR spectrum (Figure S1) of AC•8PF\(_6\) was recorded in CD\(_3\)CN at 298 K. It reveals that two proton resonances of β2 and β3 are very much shifted to high field on account of the ‘shielding effect’ enforced by the mechanical bond.

![1H NMR Spectrum](image)

**Figure S1.** \(^1\)H NMR Spectrum (500 MHz, CD\(_3\)CN, 298 K) of AC•8PF\(_6\).

The assignments of proton resonances have been made based on \(^1\)H–\(^1\)H gCOSY (Figure S2) obtained in CD\(_3\)CN at room temperature. The key correlation peaks are labeled in the 2D NMR spectrum.
2) $^1$H NMR Spectra of SC•8PF$_6$

SC•7PF$_6$ was oxidized with NO•PF$_6$ before being subjected to NMR spectroscopic analysis. In the $^1$H NMR spectrum (Figure S3) of SC•8PF$_6$, the upfield shift of the resonance for the $\beta$ proton indicates the formation of the mechanically interlocked structure. In addition, compared with the resonance for the $\alpha$ proton in the two central BIPY$^{2+}$ units in AC$^{8+}$, those in SC$^{8+}$ are shifted to higher field because the additional 2,7-diazapyrenium unit in SC$^{8+}$ exerts a stronger ‘shielding effect’. Again, the assignments have been made based on $^1$H–$^1$H gCOSY (Figure S4) obtained in CD$_3$CN at room temperature. The key correlation peaks are labeled in the spectrum.
Figure S3. $^1$H NMR Spectrum (500 MHz, CD$_3$CN, 298 K) of SC•8PF$_6$.  

Figure S4. $^1$H-$^1$H gCOSY NMR Spectrum (500 MHz, CD$_3$CN, 298 K) of SC•8PF$_6$. 
Section D. UV-Vis-NIR Absorption Spectroscopy

1) UV-Vis-NIR Absorption of MV$^+$ and MDAP$^{++}$

The UV-Vis-NIR absorption spectra (Figure S5) of MV$^{++}$ and MDAP$^{++}$, which were obtained by reducing the corresponding MV$^{2+}$ and MDAP$^{2+}$ dications using Zn dust, reveal that both of them exhibit characteristic radical absorption bands centered around 600 nm, despite the fact that the molar absorption coefficient of MDAP$^{++}$ is much lower than that of MV$^{++}$.

![Figure S5. UV-Vis-NIR Absorption Spectra (50μM, MeCN, optical length: 1 cm) of MV$^+$ and MDAP$^{++}$.](image)

2) UV-Vis-NIR Absorption of MDAP$^{++}$+CBPQT$^{2(++)}$, MV$^+$⊂CBPQT$^{2(++)}$ and MV$^+$⊂DAPQT$^{2(++)}$.

The UV-Vis-NIR absorption spectra (Figure S6) show that the methyl viologen MV$^{++}$ radical cation can form trisradical complexes with both CBPQT$^{2(++)}$ and DAPQT$^{2(++)}$ supported by the
absorption bands centered on 920 and 1100 nm, respectively. The mixture of \textbf{MDAP}^{+} and \textbf{CBPQT}^{2(++)}, however, fails to form the corresponding trisradical complex as indicated by the lack of the NIR absorption bands. This observation can be explained by the fact that the cavity of \textbf{CBPQT}^{2(++)} is not large enough to accommodate \textbf{MDAP}^{+}.

\textbf{Figure S6.} UV-Vis-NIR Absorption Spectra (50μM, MeCN, optical length: 1 cm) of \textbf{MDAP}^{+} + \textbf{CBPQT}^{2(++)}, \textbf{MV}^{+} ⊂ \textbf{CBPQT}^{2(++)} and \textbf{MV}^{+} ⊂ \textbf{DAPQT}^{2(++)}.

\textit{2) Association Constant Determination}

The measurement of the association constant ($K_a$) for the formation of the hetero trisradical complex between the \textbf{DB}^{++} radical cation and the \textbf{DAPQT}^{2(++)} bis(radical cation) in MeCN was
carried out under Ar in a glovebox. An excess of Zn (20 mg) dust was added separately to solutions of \( \text{DB}^{2+} \) (15 mM) and \( \text{DAPQT}^{4+} \) (0.5 mM) in degassed MeCN (5 mL) contained in two separate vials. After both reaction mixtures had been stirred for 30 min and the reduction was complete, they were filtered into another two vials to give solutions (5 mL × 2) of \( \text{DB}^{+} \) (15 mM) and \( \text{DAPQT}^{2+} \) (0.5 mM), respectively. The concentrated solution of \( \text{DB}^{+} \) was added incrementally to the solution of \( \text{DAPQT}^{2+} \). The UV-Vis spectra were recorded one after the other. The stacked spectra (Figure S7a) show that, upon the addition of \( \text{DB}^{+} \), a new absorption band centered on 920 nm emerges and reaches a maximum when ca. 3 equiv of \( \text{DB}^{+} \) has been added. From the UV-Vis-NIR titration experiment, a plot (Figure S6b, black dot) of absorption intensity at 920 nm against the equiv of \( \text{DB}^{+} \) was obtained and a non-linear least squares data treatment\(^2\) (Figure S7b, red line) gave an association constant of \((8.9 \pm 2.8) \times 10^3 \text{ M}^{-1}\).

![Figure S7](image.png)

**Figure S7.** a) Stacked UV-Vis-NIR spectra obtained by titrating \( \text{DB}^{+} \) into a solution of \( \text{DAPQT}^{2+} \); b) Binding isotherm simulation.
Section E. Electrochemistry

Figure S8. Differential pulse voltammograms of a) SC•7PF₆, b) HC•7PF₆, and c) AC•7PF₆.

The electrochemistries of both SC•7PF₆ and AC•7PF₆ were investigated and compared with that of HC•7PF₆. Differential pulse voltammetry (DPV) reveals (Figure S8) that AC•7⁺ exhibits (Figure S8c) six redox processes and seven discrete redox states, whereas SC•7⁺ has (Figure S8a) only four redox processes and five redox states on account of its higher symmetry. In contrast, there are five redox processes and six redox states in the differential pulse voltammogram (Figure S8b) of HC•7PF₆. The introduction of the DAP²⁺ units to replace the BIPY²⁺ units in this octacationic [2]catenane system modulates the stereoelectronic structures and hence achieves a consecutive series of five, six, and seven redox states in the resulting SC•7PF₆ (0, 4+, 6+, 7+, and 8+), HC•7PF₆ (0, 2+, 4+, 6+, 7+, and 8+), and AC•7PF₆ (0, 1+, 2+, 4+, 6+, 7+, and 8+), respectively, which make these catenanes ideal for applications as memory devices.

Section F. Crystallographic Characterization

All crystallographic data are available free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
1) \(\text{DB} \subset \text{DAPQT} \cdot 4\text{PF}_6\)

a) Methods. Single crystals of \(\text{DB} \subset \text{DAPQT} \cdot 4\text{PF}_6\) were grown in a glovebox under Ar by preparing a 1 mL solution of 0.5 mM \text{DAPQT} \cdot 4\text{PF}_6\) and 0.5 mM \text{DB} \cdot 2\text{PF}_6\) in MeCN, followed by the addition of an excess of Zn dust. The resulting suspension was filtered and the filtrate divided between four culture tubes. Slow vapor diffusion of \(\text{iPr}_2\text{O}\) into the MeCN solutions led to the formation of purple crystals during a three-week period. A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa Apex2 diffractometer. The crystal was kept at 100 K during the data collection. Using Olex2\textsuperscript{S3}, the structure was solved with the XT\textsuperscript{S4} structure solution program using direct methods and refined with the ShelXL\textsuperscript{S5} refinement package using least squares minimization. The solid-state superstructure of \((\text{DB} \subset \text{DAPQT})^{2+}\) is shown in Figure S9.

b) Crystal data. Monoclinic, space group \(P2_1/m\) (no. 11), \(a = 11.0874(5)\), \(b = 17.3630(7)\), \(c = 18.0711(8)\) Å, \(\beta = 97.398(3)\)°, \(V = 3449.9(3)\) Å\(^3\), \(Z = 2\), \(T = 100.0\) K, \(\mu(\text{CuK}\alpha) = 3.408\) mm\(^{-1}\), \(D_{\text{calc}} = 1.689\) g mm\(^{-3}\), 6312 reflections measured (7.088° \(\leq \theta \leq 133.578°\)), 6312 unique (\(R_{\text{sigma}} = 0.0273\)) which were used in all calculations. The final \(R_1\) was 0.0705 (\(I > 2\sigma(I)\)) and \(wR_2\) was 0.2137 (all data).

c) Refinement details. The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell\_Now (Sheldrick, 2005), and the data were processed using both orientation matrices with SAINT. The exact twin matrix identified by the integration program was found to be (0.515 0.001 –0.488 / 0.003 –1.000 –0.001 / –1.506 –0.001 –0.515). The second domain is rotated from first domain by 180° about the reciprocal lattice \(a–c\) axis. The absorption correction was carried out using TWINABS V2008/4 (Sheldrick, 2008) to create an HKLF 5 file, which was used in all refinements. The twin fraction refined to a value of 0.173(2).
**Figure S9.** Solid-state superstructure of (DB⊂DAPQT)\(^{2+4+}\). a) A perspective view showing the distances between stacked units and the torsional angle of A and B units. b) Space-filling representation. c) A side-on view showing the angle of tilt between the A and B units. d) Part of the solid-state superstructure showing that there are 8 PF\(_6^-\) anions surrounding two 1:1 complexes. Solvent molecules are omitted for the sake of clarity.
2) AC•7PF₆

a) Methods. Single crystals of AC•7PF₆ were grown on the bench-top by slow vapor diffusion of iPr₂O into a 1.0 mM solution in MeCN over the course of a week. A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa Apex2 diffractometer. The crystal was kept at 100 K during data collection. Using Olex2⁵³, the structure was solved with the XM⁵⁴ structure solution program using dual space and refined with the XL⁵⁵ refinement package using least squares minimization. The solid-state structure of AC•7PF₆ is shown in Figure S10.

b) Crystal data. Triclinic, space group P1̅ (no. 2), a = 13.4859(7), b = 16.4625(8), c = 22.4987(11) Å, α = 86.055(2), β = 88.919(2), γ = 82.503(2)°, V = 4940.3(4) Å³, Z = 2, T = 99.99 K, μ(CuKα) = 2.367 mm⁻¹, Dcalc = 1.580 g mm⁻³, 17492 reflections measured (3.936° ≤ 2θ ≤ 136.69°), 17492 unique (Rint = 0.0000, Rsigma = 0.0321) which were used in all calculations. The final R₁ was 0.0809 (I > 2σ(I)) and wR₂ was 0.2347.

c) Refinement details. The crystal used for this experiment was found to be nonmerohedrally twinned. Although the data were processed through TWINABS, the de-twinned HKLF 4 format file was found to provide a better refinement. Attempts to refine against both twin components gave a twin fraction of approximately 20%. The disordered PF₆⁻ anion was refined with similar distance (SADI) and enhanced rigid bond (RIGU) restraints.

d) Solvent treatment details. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 199.7 Å³ [4.0%] Total electron count / cell = 41.9.
Figure S10. Solid-state structure of AC\textsuperscript{7+}. a) A perspective view showing the distances between stacked units and torsional angles of A–C units. b) Space-filling representation. c) A side-on view showing the dihedral angle between the B and C units. d) A perspective view showing that there are 7 PF\textsubscript{6}\textsuperscript{−} anions surrounding the catenane. Solvent molecules are omitted for the sake of clarity.
3) **SC•7PF$_6$**

*a) Methods.* Single crystals of **SC•7PF$_6$** were grown on the bench-top by slow vapor diffusion of $'Pr_2$O into a 1.0 mM solution in MeCN over the course of a week. A suitable single crystal was selected and mounted in inert oil and transferred to the cold gas stream of a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 100 K during data collection. Using Olex2$^2$, the structure was solved with the XM$^3$ structure solution program using dual space and refined with the XL$^4$ refinement package using least squares minimization. The solid-state structure of **SC•7PF$_6$** is shown in Figure S11.

*b) Crystal data.* triclinic, space group $P\overline{1}$ (no. 2), $a = 13.3492(5)$, $b = 27.9262(13)$, $c = 31.5473(18)$ Å, $\alpha = 73.377(4)$, $\beta = 89.810(4)$, $\gamma = 80.969(3)^\circ$, $V = 11118.6(9)$ Å$^3$, $Z = 4$, $T = 100.03$ K, $\mu$(CuK$_\alpha$) = 2.040 mm$^{-1}$, $D_{calc}$ = 1.286 g mm$^{-3}$, 52846 reflections measured ($9.38^\circ \leq 2\theta \leq 118.244^\circ$), 31303 unique ($R_{int} = 0.0671$, $R_{sigma} = 0.0996$) which were used in all calculations. The final $R_1$ was 0.1428 ($I > 2\sigma(I)$) and $wR_2$ was 0.4038 (all data).

*c) Refinement details.* The disordered PF$_6^-$ counterions were refined with similar distance restraints (SADI) to keep the geometry reasonable. The enhanced rigid bond restraint (RIGU) was applied globally.

*d) Solvent treatment details.* The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 3555.8 Å$^3$ [32.0%] Total electron count / cell = 429.5
Figure S11. Solid-state structure of SC\(^{7+}\). a) A perspective view showing distances between stacked units and torsional angles of A and B units. b) Space-filling representation. c) A side-on view showing the dihedral angle between the A and B units. d) A perspective view showing that there are 7 PF\(_6^-\) anions surrounding the catenane. Solvent molecules are omitted for the sake of clarity.
Section G. DFT Calculations

Calculations were performed using density functional theory (DFT) with the M06 functional, as implemented\textsuperscript{S6} in Jaguar 7.6.110. Geometry optimizations were performed\textsuperscript{S7} using the 6-31G* basis set. Electronic energies (Table S1) were obtained\textsuperscript{S8} using the 6-311++G** basis set. Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for MeCN ($\varepsilon = 37.5$ and $R_0= 2.179$ Å) using\textsuperscript{S9} the PBF module in Jaguar.

Table S1. Calculated Binding Energies ($\Delta E$) of [2]Catenanes

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\textsuperscript{a}The energies are calculated in MeCN.
Figure S12. Spin Densities of a) AC\(^{7+}\) and b) SC\(^{7+}\).

Section H. References


(S6) Jaguar 7.6, Schrödinger, LLC, New York, NY (2006).


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