Synthesis and Electrochromic Behavior of a Multi-Electron Redox-Active N-Heteroheptacenequinone

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Identification code	C48 H62 N8 O7 S
CCDC	1871181
Empirical formula	C48 H62 N8 O7 S
Formula weight	895.11
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	<i>P</i> -1
Unit cell dimensions	$a = 8.996(9)$ Å $\alpha = 87.116(15)^{\circ}$
	$b = 13.612(14) \text{ Å} \beta = 82.877(16)^{\circ}$
	$c = 20.05(2)$ Å $\gamma = 77.657(15)^{\circ}$
Volume	2379(4) Å ³
Ζ	2
Density (calculated)	1.250 mg/m ³
Absorption coefficient	0.127 mm^{-1}
<i>F</i> (000)	956
Crystal size	0.200 x 0.080 x 0.020 mm ³
Theta range for data collection	1.864 to 25.027°
Index ranges	-6<=h<=10, -16<=k<=16, -23<=l<=23
Reflections collected	11147
Independent reflections	8199 [<i>R</i> (int) = 0.1277]
Completeness to theta = 25.242°	95.1%
Data / restraints / parameters	8199 / 88 / 612
Goodness-of-fit on F^2	0.853
Final <i>R</i> indices $[I > 2\sigma(I)]$	$R_1 = 0.0892$, w $R_2 = 0.2121$
R indices (all data)	$R_1 = 0.2268, wR_2 = 0.2828$
Largest diff. peak and hole	$0.406 \text{ and } -0.407 \text{ e.}\text{\AA}^{-3}$

Table S1. Crystal data and structure refinement for $C_6OAHCQ \cdot (DMSO)$



Figure S1. DFT calculations of HOMO, HOMO+1, and HOMO+2 of \mathbf{COAHCQ} .



Figure S2. Cyclic voltammogram of C₆OAHCQ at 1.0 mM in CH_2Cl_2 solution of nBu_4NPF_6 (0.10 M) at scanning velocity of 100 mVs⁻¹.



Figure S3. UV-vis absorption spectrum of C_6OAHCQ at applied voltage of 0 V after applying voltage of -1.2 V in a 0.10 M solution of nBu_4NPF_6 in CH_2Cl_2 .



Figure S4. Photographs of spectroelectrochromic cell setup.

We carried out spectroelectrochemical experiments to investigate redox-active stability of C_6OAHCQ upon applying at -0.70 (Figure S1) and -2.20 V (Figure S2), respectively. Redox-active stabilities for C_6OAHCQ at -0.70 and -2.20 V were much lower than that at -1.20 V because initial UV-vis absorption spectra could not recovered by returning the potential to 0 V.



Figure S5. Time-dependent UV–vis absorption spectra of C_6OAHCQ at an applied voltage of -0.70 V in a 0.10 M solution of nBu_4NPF_6 in CH_2Cl_2 .



Figure S6. Time-dependent UV–vis absorption spectra of C_6OAHCQ at an applied voltage of -2.20 V in a 0.10 M solution of nBu_4NPF_6 in CH_2Cl_2 .



Figure S7. Predicted molecular structures in the reduction process for C_6OAHCQ . We speculated the reduction mechanism.



Figure S8. ¹H NMR spectrum of C₆OAHCQ.



Figure S9. ¹³C NMR spectrum of C₆OAHCQ.