Supplementary data for New Journal of Chemistry

π–Conjugation Effect on the Aggregation–Induced Emission of Extended Viologens

Murat Tonga [a, b]

[a] *Department of Chemistry, University of Massachusetts, Amherst, MA 01003, USA*

[b] *Present Address: Polnox Corporation, 225 Stedman St Suite 23, Lowell, MA 01851, USA*

e-mail: murattonga@gmail.com; mtonga@Polnox.com

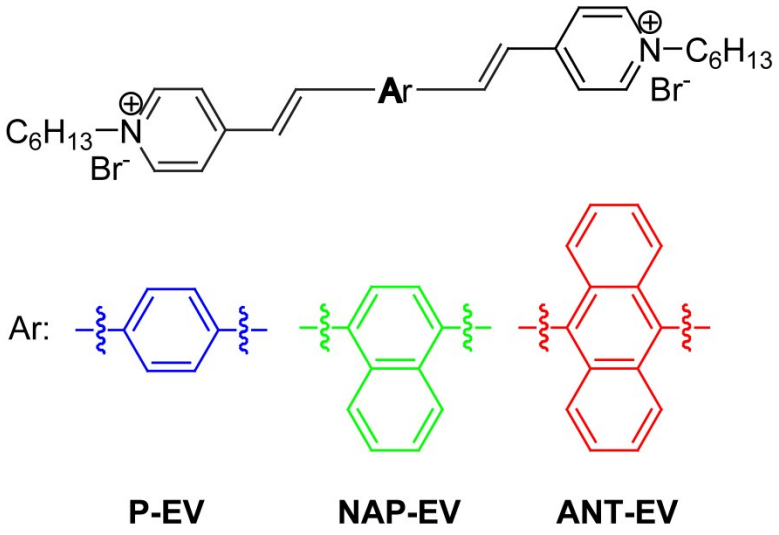
Phone: 1-413-545-2291, Fax: 1-413-545-4490

Contents

1. General methods

All chemicals and solvents were purchased from Fisher Scientific or Sigma–Aldrich and used without further purification unless otherwise indicated. UV–vis spectra and photoluminescence spectra were obtained in 1 cm path length quartz cuvettes at room temperature using a Shimadzu UV–2600 spectrophotometer and a Cary Eclipse photoluminescence spectrophotometer, respectively. The samples were excited at their λ_{max} of absorbance and collected with 1 nm bandwidth. The slit width was 10 nm for both excitation and emission. All computations were performed using the Wavefunction program Spartan04 for Windows using default settings. Geometries were optimized using hybrid DFT methods, B3LYP/6–311G* level.

2. Structures of the EV luminogens



Scheme S1. Structures of the EV luminogens.

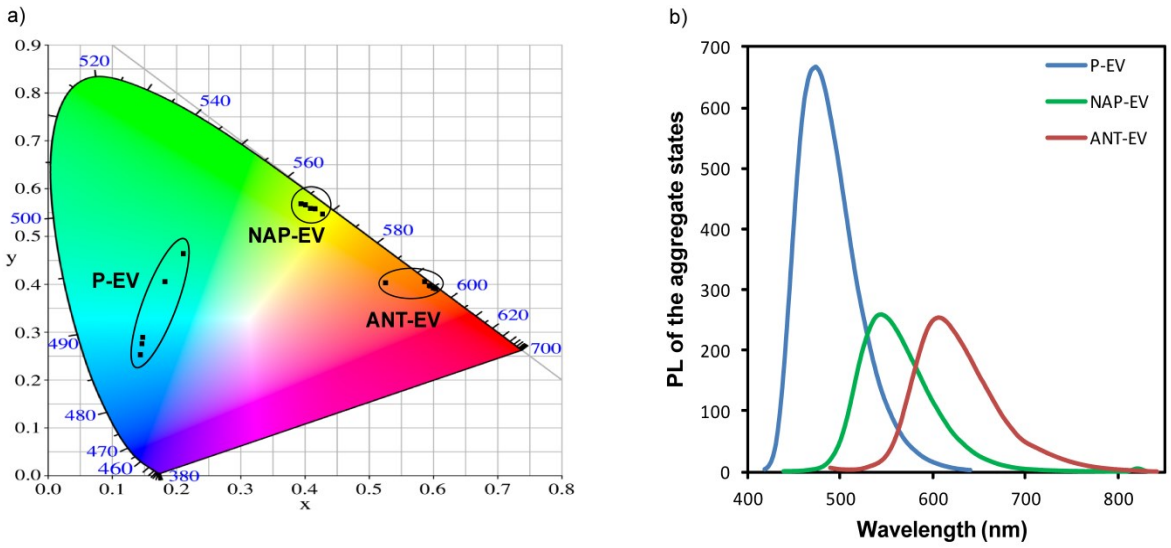


Figure S1. (a) The CIE coordinates of the EV luminogens at the aggregate states, (b) the PL spectra at the maximum intensity resulted with added $f_{toluene}$ = 10%, $f_{toluene}$ = 50%, and $f_{toluene}$ = 90% for **P–EV**, **NAP–EV**, and **ANT–EV**, respectively.

Table S1. Computational data of the luminogens.

	α (°)	**β** (°)	**γ** (°)	**Δδ[a]** (Å)	**E_{HOMO}** (eV)	**E_{LUMO}** (eV)	**E_g^{DFT}** (eV)
P–EV	1.3	2.4	4.7	3.3/3.3	–5.27	–3.17	2.1
NAP–EV	30.6	10.9	41.4	3.31/3.96	–4.68	–3.62	1.06
ANT–EV	46.2	7.5	61.9	3.28/3.94	–4.65	–3.53	1.12