



## University of Groningen

## Electrochemistry, Spectroscopy and Electrogenerated Chemiluminescence of Perylene, Terrylene, and Quaterrylene Diimides in Aprotic Solution

Lee, Sang Kwon; Zu, Yanbing; Herrmann, Andreas; Geerts, Yves; Müllen, Kläus; Bard, Allen J.

Published in: Journal of the American Chemical Society

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version Publisher's PDF, also known as Version of record

Publication date: 1999

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA): Lee, S. K., Zu, Y., Herrmann, A., Geerts, Y., Müllen, K., & Bard, A. J. (1999). Electrochemistry, Spectroscopy and Electrogenerated Chemiluminescence of Perylene, Terrylene, and Quaterrylene Diimides in Aprotic Solution. Journal of the American Chemical Society, 121(14), 3513-3520.

### Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

Take-down policy If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): http://www.rug.nl/research/portal. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

# **Figure Captions**

- Figure S1. The scan rate dependence of the redox peak currents of TDI (a) and QDI(b).
- Figure S2 UV-vis spectra changes on reduction of PDI-1, (a) decreasing neutral, (b) increasing radical anion and (c) increasing dianion response during the reduction in CH<sub>3</sub>CN (electrolyte: 0.1 M TBAPF<sub>6</sub>).
- Figure S3 UV-vis spectra changes on reduction of TDI, (a) decreasing neutral and
  (b) increasing radical anion response during the reduction in CH<sub>3</sub>CN
  (electrolyte: 0.1 M TBAPF<sub>6</sub>).

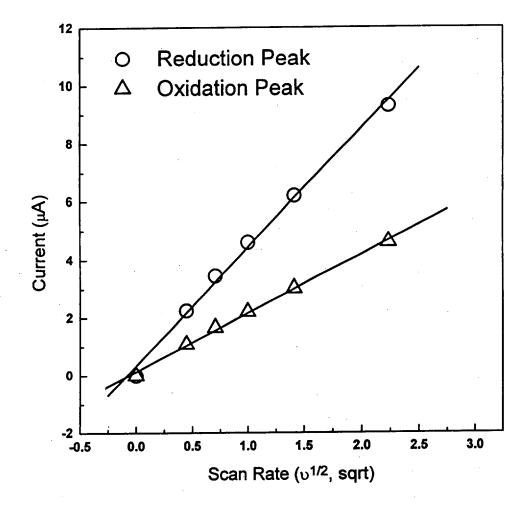


Fig. SIG

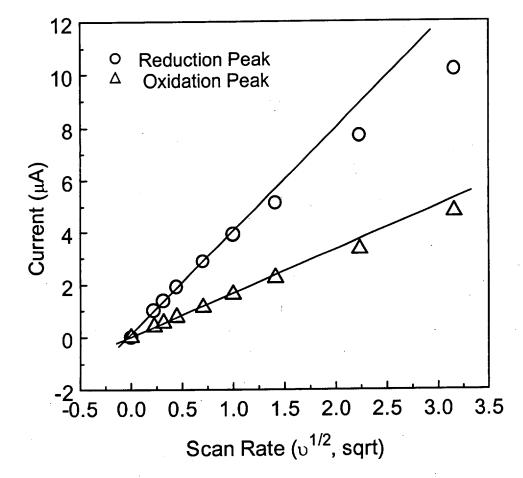


Fig. SIb

© 1999 American Chemical Society, J. Am. Chem. Soc., Lee ja984188m Supporting Info Page 4

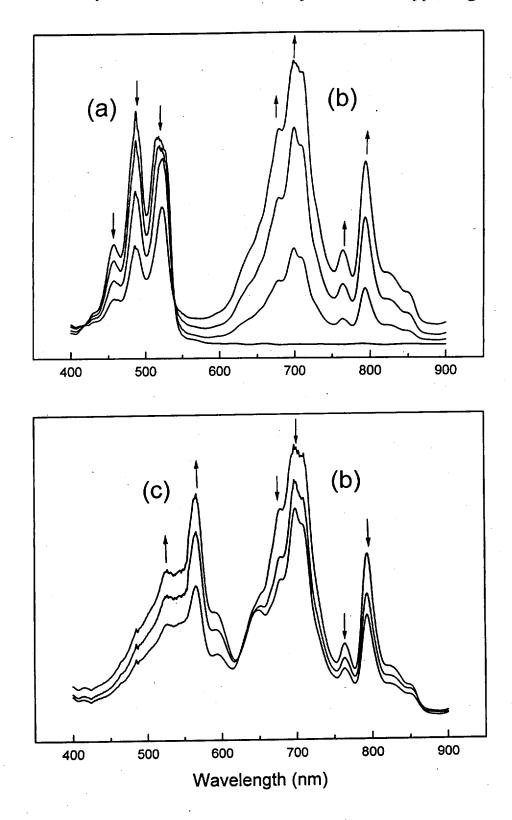


Fig. Sz

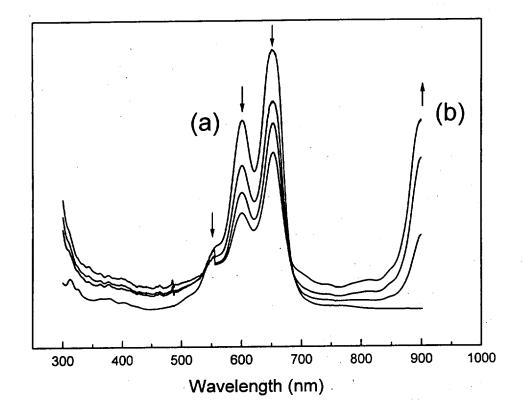


Fig. S3

Table S1. PM3 Calculated Fractional Electron Densities at the Carbonyl Oxygen Atoms  $(\delta_o)$  in the Diimide Molecules With Different Net Charge  $(\delta)$ 

|               | $\delta_{o}$ (PDI-1) | δ <sub>o</sub> (TDI) <sup>a</sup> | $\delta_{o}$ (QDI) |
|---------------|----------------------|-----------------------------------|--------------------|
| $\delta = 0$  | -0.406               | -0.414                            | -0.418             |
| $\delta = -1$ | -0.486               | -0.48                             | -0.473             |
| δ = -2        | -0.567               | -0.547                            | -0.530             |

<sup>a</sup>The electron density at oxygen atom in imide group with N-2,6-di-*iso*-propyphenyl substituent.