Resolving the Contribution Due to Förster-Type Intramolecular Electronic Energy Transfer in Closely Coupled Molecular Dyads

Mohammed A. H. Alamiry, Jerry P. Hagon, Anthony Harriman, Thomas Bura and Raymond Ziessel

SUPPORTING INFORMATION

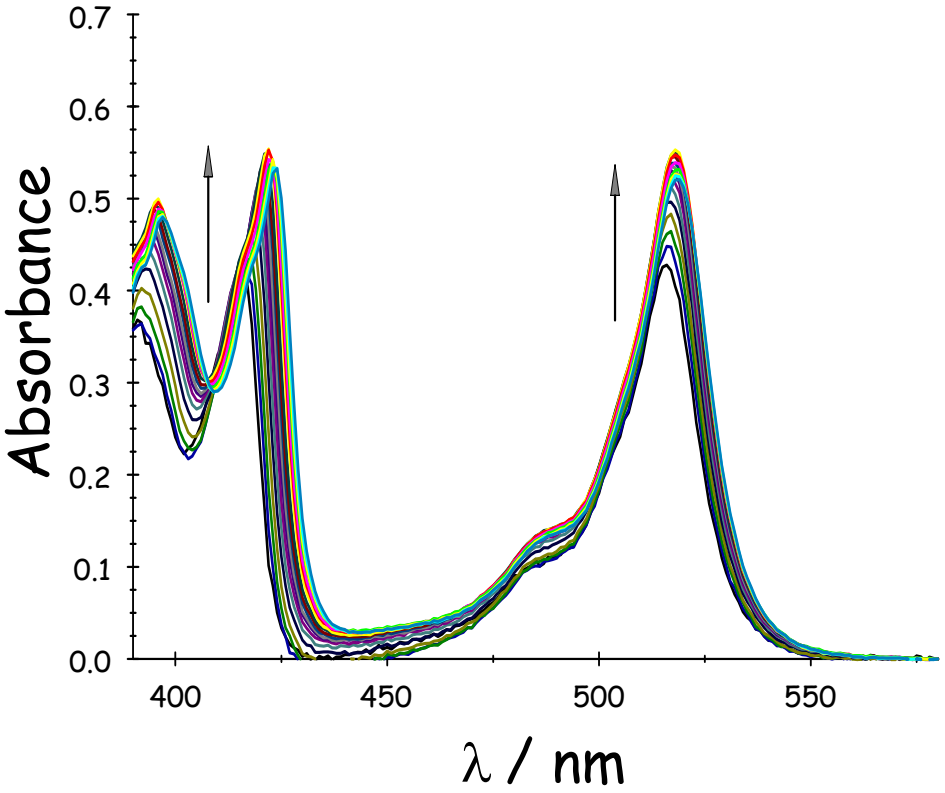

Figure S1. Effect of applied pressure on the absorption spectral profile recorded for PyBPy in MTHF at 20 ^{0}C. The pressure was increased sequentially from atmospheric pressure to 550 MPa.

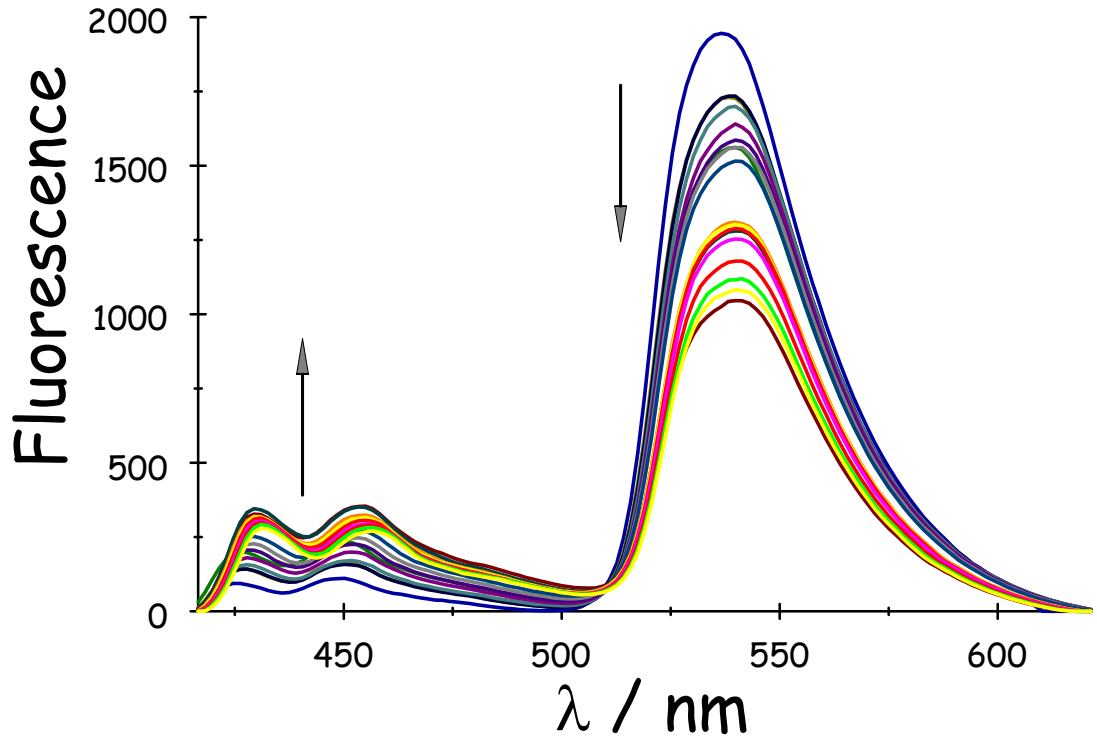

Figure S2. Effect of increasing pressure on the fluorescence spectral profile recorded for PyBPy in MTHF at 20 ^{0}C. The pressure was increased successively from atmospheric pressure to 550 MPa.

Parameters used in the calculations of EET rates

For the ideal dipole approximation:

property	pyrene	perylene
J_{DA} / cm	1.2×10^{-4}	7.8×10^{-4}
R_{CC} / Å	15.1	16.8
κ^2	3.5×10^{-4}	1.3×10^{-4}
μ_D / D	2.0	3.6
μ_A / D	4.7	4.7
V_{DA} / cm^{-1}	0.65	0.84
S	0.608	0.608

For the extended dipole approximation:

Property	pyrene	perylene
Donor dipole length / Å	9.67	11.43
Acceptor dipole length / Å	8.91	8.91
V_{DA} / cm^{-1}	1.76	1.28
$R_{D+,A+}$ / Å	9.12	9.11
$R_{D-,A-}$ / Å	18.73	20.26
$R_{D+,A-}$ / Å	17.05	19.32
$R_{D-,A+}$ / Å	9.12	9.11