Additions and Corrections

2006, Volume 18

Andrew C.-A. Chen, Marcel B. Madaras, Kevin P. Klubek, Jason U. Wallace, Simon K.-H. Wei, Lichang Zeng, Thomas N. Blanton, and Shaw H. Chen*: Light-Emitting Organic Materials with Variable Charge Injection and Transport Properties.

Please note the following corrections to this article (*Chem. Mater.* **2006**, *18*, 204–213).

This communication is intended to correct the errors associated with the reduction scans in Figure 6a,b and the resultant half-wave potentials, $E_{1/2}(\text{red})$, presented in Table 1 of the paper in question. In the figure, the reduction peaks at -1.01 and -0.99 V were incorrectly attributed to **TRZ-F(MB)3** and **TRZ-F(MB)5** when in fact these peaks were due to impurities in tetrabutylammonium tetrafluoroborate, TBAF, which was used as received from a commercial source. Purification of the electrolyte by recrystallization from ethanol/water prevented the previously encountered experimental difficulty. The use of acetonitrile and toluene at a 1:1 volume ratio as a mixed solvent coupled with a glassy carbon working electrode resulted in a wide enough

electrochemical window to observe the reduction of the hybrid compounds. This solvent system also avoided peroxides where THF was involved, which seems to have limited the useful window. The corrected values for the core of **TRZ-F(MB)3** and **TRZ-F(MB)5** are presented in Table 1: the reduction potentials vs SCE (i.e., saturated calomel electrode), the reduction potentials vs ferrocene, and their LUMO levels. Moreover, note the negative sign accompanying the LUMO and HOMO levels with reference to the vacuum level. The LUMO levels attributed to the TRZ core in Table 1 fall within the range from -2.5 to -2.7 eV reported for materials containing 1,3,5-triphenyltriazine.⁸²

Further details of the experimental procedures for the electrochemical characterization are described in what follows. An electrochemical analyzer (model CHI660, CH Instruents, Inc., Austin, TX) was employed to perform the cyclic voltammetric measurements. A glassy carbon electrode was adopted as the working electrode to take advantage of its electrical potential window wider than that of the Pt electrode. This electrode ($A = 0.071 \, \mathrm{cm}^2$) was cleaned and activated by electrochemical treatment prior to use. A platinum wire served as the auxiliary electrode. A saturated

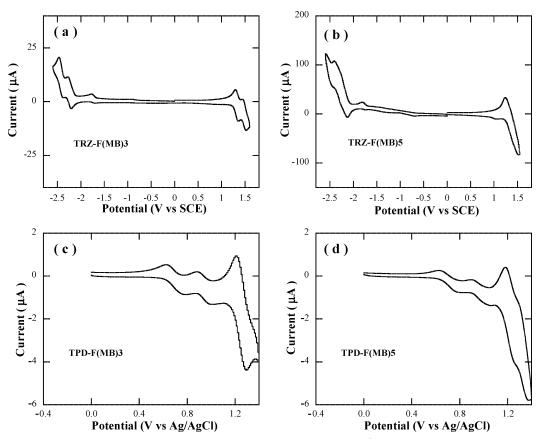


Figure 6. Cyclic voltammetric reduction and oxidation scans of (a) TRZ-F(MB)3 at 2.5×10^{-4} M and (b) TRZ-F(MB)5 at 1.0×10^{-3} M, both in acetonitrile and toluene at a 1:1 volume ratio with 0.1 M tetrabutylammonium tetrafluoroborate as the supporting electrolyte using a glassy carbon electrode; oxidation scans of (c) TPD-F(MB)3 and (d) TPD-F(MB)5, both at 2.5×10^{-4} M in anhydrous CH₂Cl₂ with 0.1 M tetraethylammonium tetrafluoroborate as the supporting electrolyte using a platinum electrode.

Table 1. Electrochemical Characterization in Dilute Solutions by Cyclic Voltammetry

compound		E _{1/2} (red) ^a vs SCE (V)	$E_{1/2}(ox)^a$ vs SCE (V)	E _{1/2} (ox) ^a vs Ag/AgCl (V)	$E_{1/2}(\text{red})^b$ vs Fc (V)	$E_{1/2}(ox)^b$ vs Fc (V)	LUMO ^c (eV)	HOMO ^c (eV)
TRZ-F(MB)3	core	-1.73	_	-	-2.23	_	-2.57	_
	pendent	_	1.33	_	_	0.83	_	-5.63
TRZ-F(MB)5	core	-1.80	_	_	-2.29	_	-2.51	_
	pendent	_	1.30	_	_	0.80	_	-5.60
TPD-F(MB)3	core	_	_	0.71	_	0.25	_	-5.05
	pendent	_	_	1.25	_	0.79	_	-5.59
TPD-F(MB)5	core	_	_	0.72	_	0.26	_	-5.06
	pendent	_	_	1.21	_	0.75	_	-5.55

 $[^]a$ Half-wave potentials, $E_{1/2}$, determined as the average of forward and reverse reduction and oxidation peaks shown in Figure 6. b Relative to ferrocene/ferrocenium with an oxidation potential at 0.50 V vs SCE in acetonitrile and toluene at a 1:1 volume ratio and 0.46 V vs Ag/AgCl in anhydrous CH₂Cl₂. 82 c Relative to ferrocene's HOMO level of -4.8 eV. 82

calomel electrode was used as a quasi-reference electrode to complete a standard three-electrode electrochemical cell. The supporting electrolyte, tetrabutylammonium tetrafluoroborate (>98%, Fluka), was purified by dissolution in a minimum amount of ethanol for treatment with activated charcoal followed by filtration through Celite powder and addition of water (twice the volume of the ethanol) for

recrystallization at 0 °C. Recrystallization was repeated until the oxidation and reduction scans attributable solely to the electrolyte were observed.

CM062382Z

10.1021/cm062382z Published on Web 11/14/2006