

Correction to Tetraphenylhexaazaanthracenes: 16π Weakly Antiaromatic Species with Singlet Ground States

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Due to a typographical error in the equation used to calculate the optical band gaps (E_g^{onset}) for TPHA-1, TPHA-2, and TPHA-3, the values reported in Table 2 of the main paper and the data in Table S4 in the Supporting Information are incorrect. The correct data should be as follows:

Table 2. Absorption [$\lambda_{\text{max}}(\text{abs})$ ($\log \epsilon$)], Optical Band Gap [E_g^{onset}], Fluorescence [$\lambda_{\text{max}}(\text{PL})$] Maxima, and Quantum Yield (Φ_f) of TPHA-1–TPHA-3 in DCM

	$\lambda_{0-0}(\text{abs})$ ($\log \epsilon$) [nm]	E_g^{onset} (eV)	$\lambda_{\text{max}}(\text{PL})$ [nm]	Φ_f ($\lambda_{\text{exc}} = 473 \text{ nm}$)
TPHA-1	589 (4.23)	1.99	622	0.0995 ± 0.005
TPHA-2	496 (4.35), 624 (3.48)	1.85	653	<0.002
TPHA-3	503 (4.32), 687 (3.66)	1.68	655	<0.008

Table S4. Experimental (UV–Vis) and Computational [DFT UB3LYP 6-311G(2d)] Optical Band Gaps of TPHA-1–TPHA-3

	TPHA-1		
	λ (nm)	E_g^{onset} (eV)	E_g^{DFT} (eV)
optical band gap	622	1.99	
HOMO–LUMO	540		2.30
HOMO–LUMO+1	574		2.62
	TPHA-2		
	λ (nm)	E_g^{onset} (eV)	E_g^{DFT} (eV)
optical band gap	671	1.85	
HOMO–LUMO	576		2.15
HOMO–LUMO+1	471		2.63
	TPHA-3		
	λ (nm)	E_g^{onset} (eV)	E_g^{DFT} (eV)
optical band gap	738	1.68	
HOMO–LUMO	674		1.84
HOMO–LUMO+1	484		2.56

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