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ERRATUM

Erratum to: Theoretical Study of the Electronic Excited States and Fluorescence Spectra of Squaraine in Solution

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The original version of this article unfortunately contained a typo in Table 2. In the column headings of Table 2, ΔG(p–p) should be changed to ΔG(t–t), also the table caption is modified. The corrected table is given below as:

Table 2 S_0/S_1 energy gaps {ΔG(t–t)} and the heats of reaction {ΔG(p–t)} from the common planar (B_{1u}) state to each of the twisted structures in CH_2Cl_2 and MeOH solvents (and in vacuum); the dihedral angles ω_1–ω_4 are defined with respect to the central four-membered ring in unit of degrees

Number	ω_1	ω_2	ω_3	ω_4	ΔG(t–t) (eV[a])	ΔG(p–t) (eV[a])
1	0	90	0	90	2.09, 2.12 (1.85)	1.57, 1.68 (0.744)
2	90	90	90	90	1.24, 1.25 (1.09)	0.857, 0.921 (0.371)
3	90	0	90	0	1.44, 1.46 (1.21)	2.09, 2.18 (1.39)
4	0	90	0	0	2.26, 2.23 (2.03)	0.946, 0.975 (0.246)
5	90	90	0	0	2.11, 2.15 (1.72)	0.709, 0.798 (0.0559)
6	90	0	0	0	2.26, 2.31 (1.82)	1.33, 1.44 (0.567)

[a] 1 eV = 96.5 kJ·mol^{-1}

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