THE JOURNAL OF PHYSICAL CHEMISTRY C
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCC

Addition/Correction

Correction to "Confirmation of the Origins of Panchromatic Spectra in Squaraine Thin Films Targeted for Organic Photovoltaic Devices"

Nicholas J. Hestand, Chenyu Zheng, Anirudh Raju Penmetcha, Brandon Cona, Jeremy A. Cody, Frank C. Spano, and Christopher J. Collison*

J. Phys. Chem. C **2015**, *119* (33), 18964−18974. DOI: 10.1021/acs.jpcc.5b05095

Cite This: *J. Phys. Chem. C* 2022, 126, 11436−11437

Read Online

ACCESS | Metrics & More | Article Recommendations

In our original publication, Table 2 contains the parameters used to simulate the absorption spectra shown in Figure 9. It has come to our attention that this table contains a typographical error and reports an incorrect value for the t_{CT} parameter used for the simulation of the $DBSQ(OH)_2$ aggregate spectrum shown in Figure 9b. The value published is 0.28 eV, but the correct value of 0.34 eV was used in the simulation. The entire Table 2 appears here with the correct value of t_{CT} shown in bold.

Table 2. Parameters for Modeling Squaraine Mixed Solvent Spectra[a]

parameter	$DPrSQ(OH)_2$	$DBSQ(OH)_2$
η_Z	0.69 eV	0.69 eV
t_Z	1.05 eV	1.05 eV
λ^2	1	1
$\hbar\omega_{vib}$	0.16 eV	0.16 eV
η_{CT}	1.42 eV	1.37 eV
t_{CT}	0.55 eV	**0.34 eV**
λ_{CT}^2	0.5	0.5
line width	0.15 eV	0.15 eV
spectral shift	−0.087 eV	0.006 eV

[a]This table replaces Table 2 in the original publication. The corrected value appears in bold.

Additionally, in the original publication our simulations of the aggregate spectra shown in Figure 9 assume that the geometry of the aggregate is the same as the geometry given by the crystal structure. Unfortunately, the geometry used when calculating the $DBSQ(OH)_2$ aggregate spectrum is slightly different than that given by the crystal structure. In the Supporting Information to the original paper, Table S1 contains the geometric parameters used in the simulations. In this table the *x*, *y*, and *z* values listed for $DBSQ(OH)_2$ are inconsistent with the crystal structure. We have reproduced the entire Table S1 here with the correct values (i.e., derived from the crystal structure) for these parameters shown in bold.

We have also recalculated the absorption spectrum for $DBSQ(OH)_2$ using the correct geometric parameters. The results are shown here in Figure 9b. Comparison of the new simulation with the one in Figure 9b of the original publication shows only minor differences. Hence, this error does not alter any of the main results or conclusions of our original publication.

Table S1. Geometric Parameters for $DPrSQ(OH)_2$ and $DBSQ(OH)_2$ (Å)[a]

coordinate	$DPrSQ(OH)_2$	$DBSQ(OH)_2$
l	6.69	6.60
x	3.58	**3.47**
y	1.82	**1.84**
z	3.32	**3.35**

[a]This table replaces Table S1 in the original publication. The corrected values appear in bold.

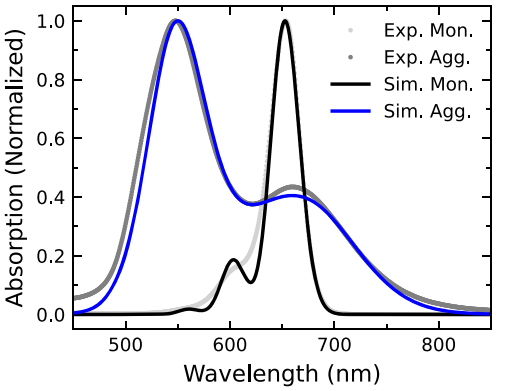
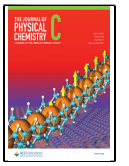


Figure 9b. Simulated spectrum of $DBSQ(OH)_2$ aggregates in 50:50 $DMSO/H_2O$ solvent mixtures using the essential states dimer model including ICT. This figure replaces Figure 9b in the original manuscript.

Published: June 28, 2022



AUTHOR INFORMATION

Corresponding Author

Christopher J. Collison; orcid.org/0000-0003-1301-3401; Email: cjcscha@rit.edu

Authors

Nicholas J. Hestand; orcid.org/0000-0001-7522-2466
Chenyu Zheng; orcid.org/0000-0001-7896-0376
Anirudh Raju Penmetcha
Brandon Cona
Jeremy A. Cody
Frank C. Spano; orcid.org/0000-0003-3044-6727

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jpcc.2c04087

Author Contributions

Brandon Cona is no longer at Rochester Institute of Technology and could not be contacted about publication of this Correction.

https://doi.org/10.1021/acs.jpcc.2c04087
J. Phys. Chem. C 2022, 126, 11436−11437