

Correction to “Excitation Energy Transfer between Higher Excited States of Photosynthetic Pigments: 1. Carotenoids Intercept and Remove B Band Excitations”

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In our article titled “Excitation Energy Transfer between Higher Excited States of Photosynthetic Pigments: 1. Carotenoids Intercept and Remove B Band Excitations” (DOI: [10.1021/acsomega.3c05895](https://doi.org/10.1021/acsomega.3c05895)),^{4,5} we computationally approximated the fluorescence yields of chlorophylls (Chls) and carotenoids (Crts). During the calculations of the theoretical values, an input/output error in the code resulted in reading the absorption spectrum twice instead of reading the emission and absorption spectrum.

Consequently, the values reported in Table 2 of the first part of the article series have to be corrected. The new values generally agree much better with the experiments for all tested states and pigments. The approach is thus shown to be a very reliable tool to access the properties of biomolecular excitations that are otherwise inaccessible, provided an emission spectrum can be obtained.

Of the erroneous values, only one (the yield for the B band of Chl *b*) entered our subsequent Förster model calculations; the experimentally reported values were used otherwise. The resulting changes in the model are thus minute and even further strengthen our interpretation: that emission from Chl *b* states is a process that might be biologically harmful and, thus,

suppressed. Therefore, we are issuing a correction to our published article to incorporate these updates with an explanation of any changes to the interpretation. We apologize for the oversight and any inconvenience it may have caused.

Table 2A is the table from the originally published article, and Table 2B is the corrected table.

COMMENTS

Regarding the fluorescence yield parameters for our Förster-type model, we chose the lowest values available to bias against EET between higher energy states. After correction of the computed values, only two choices are affected: Chl *a*, B band, for which the error will not be considered further (0.88×10^{-4} instead of 1×10^{-4}), and the Chl *b* B band for which the yield has changed from 0.92×10^{-4} to 0.36×10^{-4} ; this needs to be accounted for when donating from the B band of Chl *b*. Due to the radius being affected with the sixth root of the donor's quantum yield, the effect is minimal: Chl *b* B–B homo-exchange radii remain virtually unchanged ($\kappa^2 = 2/3$) or become 16.4 from 16.5 Å ($\kappa^2 = 4$) and radii to Crts also change by about 0.1–0.2 Å. The error is thus negligible, not resulting in new figures or an update to the model.

Table 2A. Computed and Experimentally Known^{1–3} Values for the Fluorescence Yields of Chl and Crt States⁴

band	Chl <i>a</i>		Chl <i>b</i>		Bcr	Lut	Neo	Per	Vio	Zea
	Q	B/ 10^{-4}	Q	B/ 10^{-4}	S ₂ / 10^{-4}					
theory	0.58	2.95	0.27	0.92	3.01	3.02	3.04	1.72	2.64	2.74
Exp. ^{2,3}	0.32	less than 1	0.117	less than 1	1.5	see Bcr	see Bcr	see Bcr	see Bcr	see Bcr

⁴For the Crts, the S₂ state lifetime for Bcr (163 fs) was used in all cases. Bold values are the ones used throughout this article for calculations.

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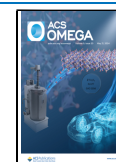


Table 2B. Computed (for Two Different Refractive Indices n , 1.4 for Protein and 1.36 for Acetone) and Experimentally Known^{1–3} Values for the Fluorescence Yields of Chl and Crt States^a

Band	Chl <i>a</i>		Chl <i>b</i>		Bcr	Lut	Neo	Per	Vio	Zea
	Q	B/10 ⁻⁴	Q	B/10 ⁻⁴						
$n = 1.4$	0.45	0.88	0.209	0.36	1.64	1.79	1.88	0.39	1.61	1.60
$n = 1.36$	0.42	0.83	0.197	0.34	1.55	1.69	1.78	0.37	1.52	1.51
Exp. ^{2,3}	0.32	less than 1	0.117	less than 1	1.5	see Bcr	see Bcr	see Bcr	see Bcr	see Bcr

^aFor the Crts, the S₂ state lifetime for Bcr (163 fs) was used in all cases. Bold values are the ones used throughout this article for further calculations; for Chl b, B band, 0.92×10^{-4} was used due to a computational error with virtually no consequences for our model (see correction comments).

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