Molecules **2015**, *20*, 19027-19029; doi:10.3390/molecules201019027

OPEN ACCESS

molecules

ISSN 1420-3049

www.mdpi.com/journal/molecules

Correction

Correction: Gomez, T., *et al.* Imaging the Ultrafast Photoelectron Transfer Process in Alizarin-TiO_2. *Molecules* 2015, *20*, 13830–13853

Tatiana Gomez [1,*], Gunter Hermann [2], Ximena Zarate [1], Jhon Fredy Pérez-Torres [2] and Jean Christophe Tremblay [2,*]

[1] Dirección de Postgrado e Investigación, Universidad Autónoma de Chile, Llano Subercaceaux 2801, San Miguel, Santiago, Chile; E-Mail: ximena.zarate@uautonoma.cl

[2] Institut für Chemie und Biochemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany; E-Mails: gunter.hermann@fu-berlin.de (G.H.); jperez@zedat.fu-berlin.de (J.F.P.-T.)

* Authors to whom correspondence should be addressed; E-Mails: tatiana.gomez@uautonoma.cl (T.G.); jc.tremblay@fu-berlin.de (J.C.T.); Tel./Fax: +56-02-661-8570 (T.G.); Tel.: +49-30-838-58150 (J.C.T.); Fax: +49-30-838-54792 (J.C.T.).

Academic Editor: Derek J. McPhee

Received: 10 October 2015 / Accepted: 12 October 2015 / Published: 20 October 2015

The author wishes to make the following correction to this paper [1]. Due to mislabeling, please replace:

Table 1. Calculated (Calc.) and experimental (Exp. [14]) excitation energies in eV, active molecular orbitals (MO) and their contributions in %. Top panel: time-dependent density functional theory (TDDFT)/Becke three-parameter-Lee-Parr-Yang (B3LYP); bottom panel: TDDFT/Perdew-Burke-Ernzerhof (PBE).

Alizarin			**Alizarin-$(TiO_2)_{15}$**		
Calc.	Exp. [14]	MO (%)	Calc.	Exp.	MO (%)
2.82	2.88	HOMO→LUMO (97.7)	2.66	2.47	HOMO→LUMO+2 (95.5) HOMO-1→LUMO+1 (35.3)
			3.35	3.54	HOMO-1→LUMO+2 (25.8) HOMO-1→LUMO+5 (6.9) HOMO→LUMO+4 (11.7)
			3.74	3.54	HOMO-4→LUMO+2 (43.9) HOMO-4→LUMO+1 (9.4) eHOMO-4→LUMO+5 (9.5) HOMO→LUMO+20 (7.8) HOMO→LUMO+22 (9.7)

Table 1. *Cont.*

Alizarin			Alizarin-$(TiO_2)_{15}$		
Calc.	Exp. [14]	MO (%)	Calc.	Exp.	MO (%)
2.29 3.28	2.88 3.82	HOMO→LUMO (95.1) HOMO-4→LUMO (58.3) HOMO→LUMO+1 (35.0)	2.16	2.47	HOMO→LUMO+2 (25.6) HOMO→LUMO+4 (11.3) HOMO→LUMO+11 (17.6) HOMO→LUMO+12 (24.0)
			2.91	3.54	HOMO-5→LUMO+3 (18.9) HOMO-6→LUMO+2 (7.2) HOMO-4→LUMO+2 (10.7) HOMO-6→LUMO+4 (6.5) HOMO-4→LUMO+7 (11.7) HOMO→LUMO+26 (17.7)

With this corrected table:

Table 1. Calculated (Calc.) and experimental (Exp. [14]) excitation energies in eV, active molecular orbitals (MO) and their contributions in %. Top panel: time-dependent density functional theory (TDDFT)/Becke three-parameter-Lee-Parr-Yang (B3LYP); bottom panel: TDDFT/Perdew-Burke-Ernzerhof (PBE).

Alizarin			Alizarin-$(TiO_2)_{15}$		
Calc.	Exp. [14]	MO (%)	Calc.	Exp.	MO (%)
2.82	2.88	HOMO→LUMO (97.7)	2.66	2.47	HOMO→LUMO+2 (95.5)
			3.35	3.54	HOMO-1→LUMO+1 (35.3) HOMO-1→LUMO+2 (25.8) HOMO-1→LUMO+5 (6.9) HOMO→LUMO+4 (11.7)
			3.74	3.54	HOMO-4→LUMO+2 (43.9) HOMO-4→LUMO+1 (9.4) HOMO-4→LUMO+5 (9.5) HOMO→LUMO+20 (7.8) HOMO→LUMO+22 (9.7)
2.29 3.28	2.88 3.82	HOMO→LUMO (95.1) HOMO-4→LUMO (58.3) HOMO→LUMO+1 (35.0)	2.16	2.47	HOMO→LUMO+2 (25.6) HOMO→LUMO+4 (11.3) HOMO→LUMO+11 (17.6) HOMO→LUMO+12 (24.0)
			2.91	3.54	HOMO-5→LUMO+3 (18.9) HOMO-6→LUMO+2 (7.2) HOMO-4→LUMO+2 (10.7) HOMO-6→LUMO+4 (6.5) HOMO-4→LUMO+7 (11.7) HOMO→LUMO+26 (17.7)

The authors would like to apologize for any inconvenience caused to the readers by these changes. We will update the paper [1] and the original will remain available on the article webpage.

References

1. Gomez, T.; Hermann, G.; Zarate, X.; Pérez-Torres, J.F.; Tremblay, J.C. Imaging the Ultrafast Photoelectron Transfer Process in Alizarin-TiO_2. *Molecules* **2015**, *20*, 13830–13853.