DOI: 10.1002/ejoc.200600667

Tuning the Photochromic Properties of a Flavylium Compound by pH

Margarida C. Moncada,[a,b] Fernando Pina,*[a] Ana Roque,[a] A. Jorge Parola,[a] Mauro Maestri,*[c] and Vincenzo Balzani[c]

Keywords: Flavylium / NMR spectroscopy / Photochromic properties / Multistate/multifunctional systems

Concerning the original article,[1] *we regret to inform that due to an unfortunate exchange of labels on the flasks during the course of the experimental work leading to this manuscript, all experimental results published in this article refer to 7-hydroxy-4′-methoxyflavylium perchlorate and not to 4′-(dimethylamino)-7-hydroxyflavylium perchlorate. According to this, each designation "4′-(dimethylamino)-7-hydroxyflavylium" should be substituted by "7-hydroxy-4′-methoxyflavylium". In particular, all chemical structures in Scheme 2 on page 305 should contain* OCH_3 *instead of* $N(CH_3)_2$*. The only part of the manuscript that does not concern 7-hydroxy-4′-methoxyflavylium is the first paragraph of the Experimental Section on page 312, that should be substituted by the following:*

7-Hydroxy-4′-methoxyflavylium chloride was prepared[26] from the condensation of 4′-methoxyacetophenone (0.78 g, 5.2 mmol) and 2,4-dihydroxybenzaldehyde (0.81 g, 5 mmol), by dissolving the reagents in acetic acid (10 mL), followed by addition of HBF_4 and acetic anhydride. The red solid that precipitated was recrystallized by dissolving it in 3% (v/v) HCl and then adding concentrated HCl, which allowed us to isolate the product (0.35 g, 20%). $C_{16}H_{13}ClO_3 \cdot 1.4H_2O$ (314.0): calcd. C 61.21, H 5.07; found C 61.33, H 4.94. EI-MS: *m*/*z* (%) = 252 (100) $[M - H - ClO_4]^+$. ^1H NMR: see Table 1.

We apologize to all readers for any confusion that this error might have caused. In our opinion, the work is still useful for the scientific community taking into account that it refers to the compound "7-hydroxy-4′-methoxyflavylium", all the studies carried out being actual. It is true that at the time we noticed that the NMR signal corresponding to the methyl group integrated less than expected, but it was then explained by partial loss of intensity due to irradiation to suppress the water peak. We recently synthesized 4′-(dimethylamino)-7-hydroxyflavylium perchlorate to be used in undergoing studies in our laboratory and only then did we notice that the absorption spectra were different. That took us to a full investigation to identify the discrepancies until we finally synthesized 7-hydroxy-4′-methoxyflavylium chloride and confirmed that the labels were unfortunately exchanged.

The Authors

[1] M. C. Moncada, F. Pina, A. Roque, A. J. Parola, M. Maestri, V. Balzani, *Eur. J. Org. Chem.* **2004**, 304–312.
[26] A. R. Katritzky, P. Czerney, J. R. Levell, W. Du, *Eur. J. Org. Chem.* **1998**, 2623–2629..

Received: August 1, 2006
Published Online: August 24, 2006

[a] Departamento de Quimica, CQFB-*Requinte*, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Quinta da Torre, 2829-516 Monte de Caparica, Portugal
E-mail: fjp@dq.fct.unl.pt
[b] Instituto Superior de Ciências da Saúde, 2825 Monte de Caparica, Portugal
[c] Dipartimento di Chimica "G. Ciamician", Università di Bologna, Via Selmi 2, 40126 Bologna, Italy
E-mail: mmaestri@ciam.unibo.it

