

ADDITIONS AND CORRECTIONS

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Martin Stein, Juergen Keck, Frank Waiblinger, Anja P. Fluegge, Horst E. A. Kramer, Achim Hartschuh, Helmut Port, David Leppard, and Gerhard Rytz: Influence of Polymer Matrices on the Photophysical Properties of UV Absorbers

Corrigendum: In this last paper of a series on UV absorbers of the benzotriazole and the (2-hydroxyphenyl)triazine class, we discussed alternative mechanisms, other than a true ESIPT process, that could contribute to the deactivation of these UV absorber molecules. In this discussion (section 3.3, p 2060), we erroneously quoted a paper of Catalán et al. for “the photophysical behavior of TIN P and related compounds...(being)...determined by aggregates, such as dimers...” (ref 72 in the above paper). The respective paragraph should rather read as follows:

...Another scheme for the explanation of the photophysical behavior of compounds with an intramolecular hydrogen bridge was suggested by Catalán et al.⁷² They have postulated that the photophysical behavior of TIN P and related compounds is not a consequence of an excited-state intramolecular proton transfer (ESIPT). We have already discussed this aspect in an earlier publication;³² the following results are, in fact, fully compatible with a mechanism based on an ESIPT.

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Joseph P. Kenny, Karl M. Krueger, Jonathan C. Rienstra-Kiracofe, and Henry F. Schaefer III*: C₅H₄: Pyramidane and Its Low-Lying Isomers.

Page 7745. A transcription error resulted in erroneous coupled cluster relative energetics in Table 1. Therefore, those same values quoted in Figure 11 are also incorrect. The appropriate corrections, ranging from fractions of kcal/mol to several kcal/mol, do not change the overall qualitative conclusions regarding the features of the C₅H₄ potential energy surface or the viability of the pyramidane isomer.

TABLE 1: Coupled Cluster and DFT Relative Energies (kcal/mol) Including Zero-Point Corrections

structure	CCSD(T)		B3LYP	BP86
	TZ2P	DZP	DZP	DZP
1	0.0	0.0	0.0	0.0
2		19.5	16.6	17.4
3	23.1	22.2	20.8	20.2
4		33.9	31.2	35.1
5		12.5	10.5	15.4
6	29.3	27.6	27.0	32.6
7		10.3	7.2	11.3
8		-17.4	-18.6	-10.4
9		-44.3	-47.7	-37.9
10		-36.3	-45.7	-38.9

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