Communication: the dark singlet state as a doorway state in the ultrafast and efficient intersystem crossing dynamics in 2-thiothymine and 2-thiouracil. [1]

Enviado por Carlos E Crespo-Hernández [2] el 28 septiembre 2014 - 9:48am

 [2]

Título	Communication: the dark singlet state as a doorway state in the ultrafast and efficient intersystem crossing dynamics in 2-thiothymine and 2-thiouracil.
Publication Type	Journal Article
Year of Publication	2014
Autores	Pollum, M [3], Crespo-Hernández, CE [4]
Journal	J Chem Phys
Volume	140
Issue	7
Pagination	071101
Date Published	2014 Feb 21
ISSN	1089-7690

Abstract	Femtosecond broadband transient absorption experiments are reported for 2-thiothymine and 2-thiouracil in aqueous buffer solution and in acetonitrile. It is shown that the S1(n?*) state acts as a doorway state in the ultrafast and efficient population of the T1(??*) state upon 316 nm excitation. A sequential kinetic model is presented to explain the excited-state dynamics in 2-thiothymine and 2-thiouracil upon UVA excitation: S2(??*) ? S1(n?*) ? T1(??*). The experimental results are also used to scrutinize the excited-state relaxation pathways recently predicted for 2-thiouracil at the CASPT2//CASSCF level of theory [G. Cui and W. Fang, J. Chem. Phys. 138, 044315 (2013)]. The efficient population of the T1(??*) state for both 2-thiothymine and 2-thiouracil in a few hundreds of femtoseconds lends further support to the emerging idea that thiobase derivatives exhibit photo-toxic properties that can be effectively harnessed in photo-chemotherapeutic applications.
DOI	10.1063/1.4866447 [5]
Alternate Journal	J Chem Phys
PubMed ID	24559331 [6]

Links
[1] https://www.cienciapr.org/es/communication-dark-singlet-state-doorway-state-ultrafast-and-efficient-intersystem-crossing-dynamics?language=en [2] https://www.cienciapr.org/es/user/ccrespo?language=en [3] https://www.cienciapr.org/es/biblio?language=en&f%5Bauthor%5D=4388 [4] https://www.cienciapr.org/es/biblio?language=en&f%5Bauthor%5D=4390 [5] http://dx.doi.org/10.1063/1.4866447 [6] https://www.ncbi.nlm.nih.gov/pubmed/24559331?dopt=Abstract