

Theoretical study of photochromism in (E)-2-methoxy-6-(pyridine-3-yliminomethyl)phenol

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Photochromic compounds such as N-Salicylideneanilines (SA) undergo reversible color change when exposed to light of different wavelengths [1]. The accepted mechanism is proton transfer to the nitrogen (cis-keto form), followed by isomerisation to the trans-keto form [2]. We present here the results obtained in a theoretical study of photochromism process in a SA derivative, (E)-2-methoxy-6-(pyridine-3-yliminomethyl)phenol (PYV3), using a methodology that combines electronic structure calculations and quantum nuclear dynamics [3]. Curvilinear atomic displacement coordinates are employed to construct a quasi diabatic Hamiltonian that combine the description of excited state intramolecular proton transfer (ESIPT) process and cis-trans isomerism [4, 5]. With help of quantum nuclear dynamics and critical points on the potential energy surfaces such as conical intersections and transition states, we present the time scales of the processes involved in photochromism of PYV3.

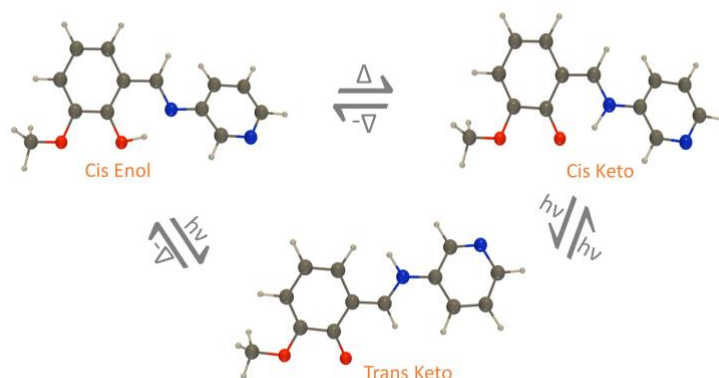


Figure 1. Photochromism in PYV3

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