

# Following the Ultrafast Dynamics of a Bistable Intramolecular H-Transfer Switch

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Bistable intramolecular H-transfer systems are of substantial interest for photochromic molecular switches as the electronic deactivation happens on an ultrafast timescale and thus excludes possible undesired side reactions. Here, we report on the electronic lifetimes involved in the reaction and deactivation pathway of the bistable H-transfer switch N-(3-pyridinyl)-2-pyridine-carboxamide (NPPCA, Fig. 1).

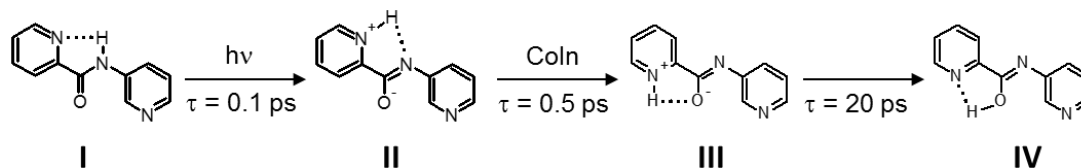


FIG. 1. Reaction scheme of H-transfer in NPPCA upon photoexcitation.

We verify the H-transfer pathway by means of structurally sensitive time-resolved vibrational absorption spectroscopy (TVAS). As the excited-state intermediate structures I and II decay on an ultrafast timescale, only vague features could be observed in the transient spectra. However, in agreement with *ab initio* frequency calculations, the formation of the final H-transferred species IV could be unambiguously identified by following the incomplete bleach recovery of the C=O band of I at  $1690\text{ cm}^{-1}$  and the rise of the C=N band of IV at  $1675\text{ cm}^{-1}$  (Fig. 2).

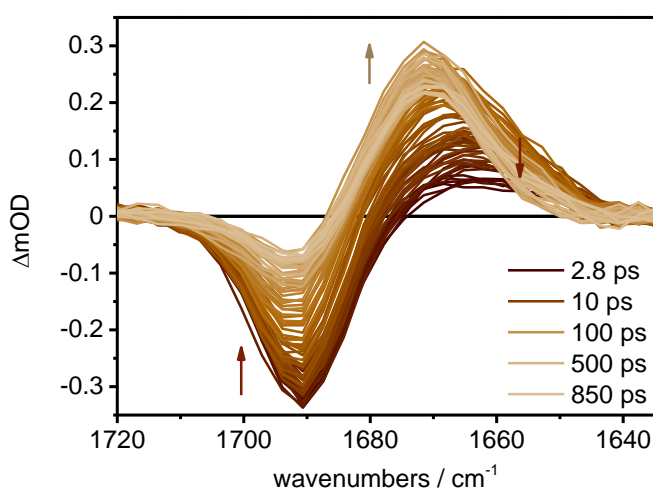


FIG. 2. Transient vibrational absorption spectra of the H-transfer switch NPPCA upon photo-excitation over time.