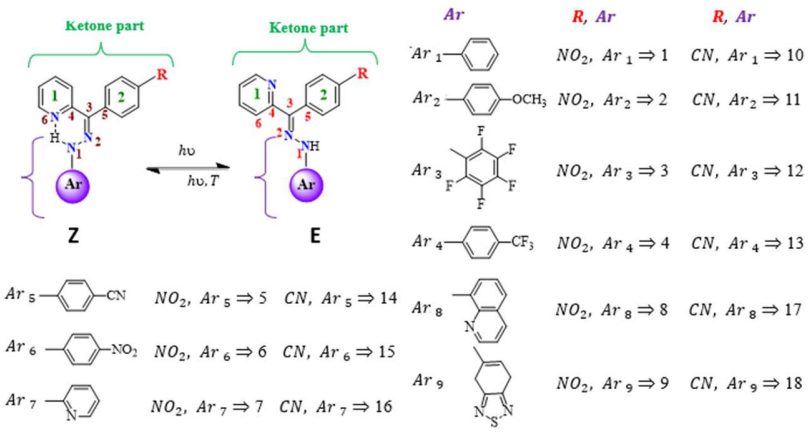
The effect of resonance-assisted hydrogen bond on the 2nd order NLO properties of pyridine hydrazone photoswitches

MERIEM ZAIDI[1], NOUREDDINE KHELFAOUI[1], DOUNIAZED HANNACH[2], DIHA YAHIAOUI[1], SALIMA LAKEHAL[3], CHRISTOPHE MORELL[4] and HENRY CHERMETTE [4]

[1]*Faculté des Sciences, Département de Chimie, Université de Setif-1, Algérie*
[4]*Institut des Sciences Analytiques, Université Claude Bernard Lyon 1, UMR CNRS 5280, 69622 Villeurbanne Cedex, France*
henry.chermette@univ-lyon1.fr, h_douniazed@yahoo.fr

ABSTRACT

In this study, we investigate a selection of 18 E/Z pyridine hydrazone photoswitch molecules to explore the impact of resonance-assisted hydrogen bond (RAHB) on the NLO properties in the E/Z isomers.



Our results demonstrated that the delocalization strength of the electrons and NLO properties of the Z isomers are significantly enhanced by the presence of a RAHB. The Z-isomer exhibited a lower $\Delta E_{0\rightarrow1}$, weaker E_{gap}, smaller BLA, larger $\Delta\mu_{0\rightarrow1}$, higher $\Phi_{E\rightarrow Z}$, and electron delocalization at the quasi-cycle closed (RAHB) compared to the E-isomer. The β_{HRS} value increases as the λ of the incident light decreases and the dispersion has less effect at λ = 1064 and 1340 nm. We note a strong relation between the $\Phi_{E\rightleftarrows Z}$ and β_0, where $\Phi_{E\rightleftarrows Z}$ is proportional to β_0 of the second isomer and inversely proportional to β_0 of the first isomer, this attributed to the electron-withdrawing on the Ar ring. By understanding the influence of HB on the delocalization strength of the electrons (RAHB) and the shape-dependent NLO performance, we gain the ability to design and synthesize novel photoswitch molecules with enhanced NLO characteristics.

Reference: Hannachi, D.; Khelfaoui, N.; Zaidi, M.; Yahiaoui, D.; Lakehal, S.; Morell, C.; Chermette, H. The effect of resonance-assisted hydrogen bond on the second-order nonlinear optical properties of pyridine hydrazone photoswitches: a quantum chemistry investigation. *New J. Chem.,* 2023, 47, 18359–18373.