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Title:	The curious case of the photochemistry of 2-hydroxyphenylazo-3,5-dimethylisoxazole: unravelling the process among tautomerization, photoisomerization, and conformational changes
Authors:	Sah, Chitranjan (/jspui/browse?type=author&value=Sah%2C+Chitranjan) Mahadevan, Anjali (/jspui/browse?type=author&value=Mahadevan%2C+Anjali) Kumar, Pravesh (/jspui/browse?type=author&value=Kumar%2C+Pravesh) Venkataramani, Sugumar (/jspui/browse?type=author&value=Venkataramani%2C+Sugumar)
Keywords:	curious case of the photochemistry 2-hydroxyphenylazo-3,5-dimethylisoxazole tautomerization, photoisomerization
Issue Date:	2022
Publisher:	Royal Society of Chemistry
Citation:	Physical Chemistry Chemical Physics, 24(13), 7848-7855.
Abstract:	Considering the growing interest in azoheteroarene photoswitches, the molecular level process underlying photochemistry is intriguing. In our earlier investigation on phenylazo-3,5-dimethylisoxazole, besides E–Z photoisomerization, we also observed light-induced phase transition that supports the possible conformational changes under neat conditions. Furthermore, hydrogen bond-forming groups such as –OH, at the ortho position to the azo chromophore, can potentially hamper the isomerization through tautomerism. All of them develop a curiosity in the photochemical outcome of 2-hydroxyphenylazo-3,5-dimethylisoxazole (HPAI, 1). Herein, we report the photochemistry of HPAI in an argon matrix at 4 K, followed by infrared spectroscopy. Through experiments and computations, we identified the E–Z photoisomerization in HPAI as the only observed channel among the above-mentioned possibilities.
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