Caterina Baccini, 11/10/2023

Monodirectional Photocycle Drives Proton Translocation

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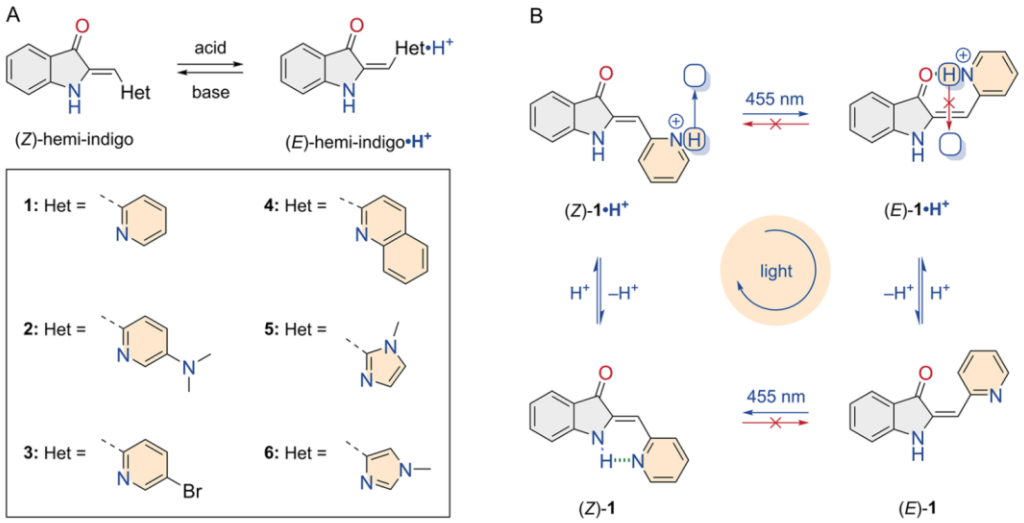
J. Am. Chem. Soc., **2023**, 145, 21020−21026



Who are the corresponding authors and what are their research areas?

Sander J. Wezenberg: Sander studied Chemistry at the University of Nijmegen. He established his independent research group at Leiden University in 2019 and was promoted to Associate Professor in 2022. His main research interests are in the areas of molecular switches, ion recognition and transport, and dynamic supramolecular systems.

What is the main claim of the article?

The authors report a novel unidirectional and repetitive proton translocation, which controls the photoisomerization process of N-heterocycles. Z to E isomerization is allowed when the pyridyl ring is protonated, while reverse isomerization occurs in the neutral state.

How is it demonstrated?

The authors used NMR measurements and Uv-vis analysis to demonstrate photo- and thermal isomerization. The isomerization process was followed by 1H NMR, while a more detailed study was obtained by 2D NOESY and NOE-DIFF spectra. For the calculation of quantum yields for the Z → E isomerization induced at 455 nm and backward they used an actinometer. Finally, DFT calculations were performed to support the experimental evidence.

What are the typical experimental conditions?

^{1}H NMR: from 5.7 to 6.7 mM in $CDCl_3$

Uv-vis: for thermal isomerization: from 0.28 to 0.89 mM in degassed $CHCl_3$, 1mm cuvette. For photoisomerization: from 0.028 to 0.088 mM in degassed $CHCl_3$, 1 cm quarz cuvette.

Quantum yield measurements: 455 nm irradiation in $CHCl_3$ at 273 K in a 1 cm quartz cuvette.

DFT calculation: Gaussian 09, geometry optimization were performed at the B3LYP 6-311++G(d,p) level of theory. UV-Vis spectra were calculated by TD-DFT on the B3LYP 6-311++G(d,p) level of theory

Which are the key related papers?

1. V. Josef, F. Hampel, H. Dube, *Angew. Chem.Int. Ed.,* **2022**, 61, 1-8.
2. S.M. Landge, I. Aprahamian, *J. Am. Chem. Soc.,* **2009**, 131, 51, 18269–18271.