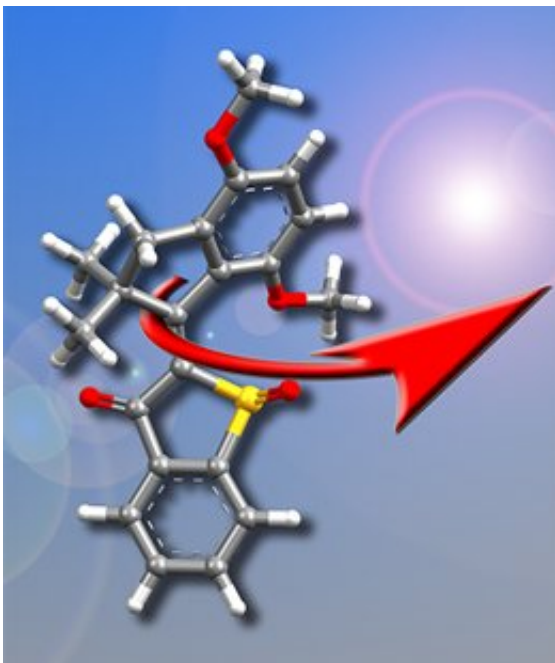


Molecular motor: Four states of rotation

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Four states of rotation. Credit: Ludwig Maximilian University of Munich

With the help of ultrafast spectroscopy and quantum mechanical calculations, Ludwig-Maximilians-Universitaet (LMU) in Munich researchers have characterized the complete rotational cycle of the light-driven, chemical motor molecule hemithioindigo.

Chemist Dr. Henry Dube, heading an Emmy Noether Junior Research Group, has developed a molecular machine based on the molecule hemithioindigo (HTI). It exhibits unidirectional rotational motion about a specific chemical bond when exposed to light. In collaboration with

Prof. Eberhard Riedle of BioMolekulare Optik and physicist Regina de Vivie-Riedle, he has now resolved the dynamics of the entire rotational mechanism. The findings appear in the *Journal of the American Chemical Society (JACS)*.

Hemithioindigo contains a central carbon-carbon double bond ($C=C$). This type of bond is capable of undergoing a reversible, light-dependent structural change known as photo-isomerization, which is normally not directional. In previous work, Dube had shown that HTI can serve as the basis for a molecular motor whose motion can be controlled precisely. In the HTI-based molecular motor, a succession of photo-isomerization and thermal helix-inversion steps causes the central double bond to rotate unidirectionally at a rate of up to 1 kHz at room temperature. While most other chemical motors require high-energy ultraviolet light to power them, the HTI motor can be driven with visible light. This feature extends its range of application and increases its potential for use in biological and medical contexts.

The team has now characterized the dynamics of unidirectional [rotation](#) in the HTI motor using a variety of ultrafast spectroscopic techniques to distinguish the intermediate states in the rotation cycle. By comparing these results with detailed [quantum mechanical calculations](#) of the possible reaction pathways, they were able to construct a precise quantitative model of the operation of this nanomachine. The results show that the rotation remains unidirectional even at room temperature, and reveal how the rate of rotation can be most effectively upgraded. The full rotation cycle resolves into four conformational and energy states, and the probabilities and rates of the transitions between them were determined for the first time. The relevant timescales for these transitions vary from picoseconds (10^{-12} s) to milliseconds (10^{-3} s). All the relevant steps were successfully monitored spectroscopically under the same conditions, i.e. over a range spanning nine orders of magnitude.

"Our comprehensive analysis yields unprecedented functional insight into the operation of such molecular motors. We now have a complete picture of the rotational motion of this molecule, which we can exploit to develop novel approaches to [motor](#) design that make better use of light energy and are thus more efficient," says Dube.

More information: Roland Wilcken et al, Complete Mechanism of Hemithioindigo Motor Rotation, *Journal of the American Chemical Society* (2018). [DOI: 10.1021/jacs.8b02349](https://doi.org/10.1021/jacs.8b02349)

Provided by Ludwig Maximilian University of Munich

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