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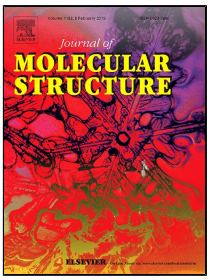

Spectroscopic and first principles investigation on 4-[(4-pyridinylmethylene)amino]-benzoic acid bearing pyridyl and carboxyl anchoring groups

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1. The Photoisomerization of the bi-anchoring molecule 4-[(4-pyridinylmethylene)amino]-benzoic can occur in ambient conditions under visible light.
2. DFT/TDDFT calculations suggest that the cis-to-trans photoisomerization occurs in such conditions. The potential energy surface is constructed, with moderate barrier energy from the cis isomer to the trans isomer.
3. Considering the bi-anchoring groups and the conjugated π system embedded in the molecule, we anticipate it can molecular engineer the TiO_2/perovskite interface in perovskite solar cell or functionalize the halide perovskite material toward motion-related applications.