Activating a Light-Driven Molecular Motor by Metal Complexation

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Designing increasingly complex, responsive, and dynamic molecular systems where the actions can be controlled by a combination of cooperative stimuli is a key challenge towards the development of functional systems.[1,2,3,4] We designed and synthesized a light-driven molecular motor, based on the well-known bisoxazoline ligands,[5] of which the motor function can be selectively activated *in situ* by coordination to a metal salt and deactivated in the presence of a competing ligand. The absorption wavelength and the energy barriers in the thermal part of the rotation cycle strongly depend on the choice of metal and the resulting geometry around the metal center. To better understand these observations, we performed DFT calculations to elucidate the mechanism of the thermal part of the rotation cycle. These calculations show how the geometry of the metal center influences the rotational barriers and the possibility to couple the rotary motion with the wagging movement of the metal center. We anticipate that this approach will open new avenues towards more complex, dynamic and coupled molecular systems.

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