Abstract Submitted
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Group transfer theory of single molecule imaging experiments in the F-ATPase biomolecular motor[1] SANDOR VOLKAN-KACSO, RUDOLPH MARCUS, California Insitute of Technology — I describe a chemo-mechanical theory to treat single molecule imaging and "stalling" experiments on the F-ATPase enzyme. This enzyme is an effective stepping biomolecular rotary motor with a rotor shaft and a stator ring. Using group transfer theoretical approach the proposed structure-based theory couples the binding transition of nucleotides in the stator subunits and the physics of torsional elasticity in the rotor. The twisting of the elastic rotor domain acts as a perturbation upon the driving potential, the Gibbs free energy. In the theory, without the use of adjustastable parameters, we predict the rate and equilibrium constant dependence of steps such as ATP binding and phosphate release as a function of manipulated rotor angle. Then we compare these predictions to available data from stalling experiments. Besides treating experiments, the theory can provide guides for atomistic simulations, which could calculate the reorganization parameter and the torsional spring constant. The framework is generic and I discuss its application to other single molecule experiments, such as controlled rotation and other biomolecular motors, including motor-DNA complexes and linear motors.[PNAS, Early Edition, Oct. 19, 2015, doi: 10.1073/pnas.1518489112]

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