

Information-thermodynamics analysis of a biological molecular machine in experiments

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Biomolecular motors are high-performance nanomachines that function within cells, and it is expected that their performance has been improved through evolution. The F-ATPase (F motor) studied in this research is a rotary biomolecular motor. When isolated, it hydrolyzes ATP molecules as fuel and rotates its central rotor in one direction; however, within cells, the rotor is rotated in the opposite direction by other motors to synthesize ATP. Thus, F is a reversible motor. Although it has been experimentally demonstrated that this motor rotates efficiently, the mechanism underlying its high performance remains poorly understood.

Since the F motor operates through interactions between its rotor and the stator surrounding it, we expect that a detailed understanding of these interactions will lead to elucidation of its mechanism. In particular, because molecular motors are nanosized engines, a thermodynamic understanding is essential. However, while conventional thermodynamics imposes constraints on the energy balance of the motor as a whole, it is difficult to conduct a thermodynamic analysis of the interactions within the motor. This is because the rotor and stator move in a correlated manner and cannot be treated as independent subsystems.

On the other hand, by employing "information thermodynamics," we can quantitatively evaluate the interactions between the shaft and the stator and further derive the thermodynamic laws that each subsystem must satisfy. This enables thermodynamic discussions with higher resolution at the subsystem level, such as analyzing the operational efficiency of each subsystem. Furthermore, not only has the relation corresponding to the second law been derived, but constraints involving speed have also been established.

In this study, we combined single-molecule experiments of the F motor with information thermodynamic analysis to investigate the energy- and information-mediated interactions within the motor, aiming to elucidate the mechanisms underlying its high performance. In the analysis, we regarded the rotor angle trajectories, which are observed by single-molecule experiments, and the discrete chemical states, which are estimated from the angle trajectories, as the bipartite subsystems and evaluated the energy and information flow between them as well as the heat and work flow. We present the results obtained and discuss their physical and biological significance. In particular, we wish to discuss how information thermodynamics can serve as a powerful framework for understanding complex systems composed of numerous interconnected subsystems, such as biological phenomena.