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Dissipation in an electric field-driven synthetic rotary caltropbased molecular motor CORINA BARBU, VINCENT CRESPI, The Pennsylvania State University — A molecular caltrop has a three-legged base for attachment to a substrate and a vertical molecular shaft functionalized with a dipole-carrying molecular rotor at the upper end. The desired rotational motion of the rotor can generate dissipation when the motor is driven at frequencies which are close to the natural frequencies of soft vibrational modes in the structure or librational of the rotator about field direction. Classical molecular dynamics simulations elucidate the role of these resonances and investigate motor performance under external drive.

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