For molecules with strong **magnetoanisotropy**, and high-spin (S) ground states, +S and -S microstates will be separated by an energy barrier. This barrier will result in slow magnetization relaxation. Such molecules can exhibit hysteresis. Relaxation occurs by **thermal activation** (over barrier) or by **tunneling** (through barrier).

Barrier = $S^2|D|$ for integer-spin systems and $(S^2 - 1/4)|D|$ for half-integer spin systems.

For MSQ complexes, $D_{\text{complex}}$ is calculated as:

$$D_{\text{complex}} = d_1D_M + d_2D_{SQ} + d_3D_{MSQ}$$

$$D_{MSQ} = D_{\text{dip}} + D_{\text{ex}} \text{ (often } D_{\text{ex}} \gg D_{\text{dip}}\text{)}$$

$$D_{\text{ex}} = J(e_M,g_{SQ}) \sum_{e_M} \left| <g_M|L|e_M> \right|^2 \frac{\lambda_M^2}{\Delta_M^2} + J(e_{SQ},g_M) \sum_{e_{SQ}} \left| <g_{SQ}|L|e_{SQ}> \right|^2 \frac{\lambda_{SQ}^2}{\Delta_{SQ}^2}$$

$D_M$ is based on single ion anisotropy. Ions that are subject to Jahn-Teller distortions will have large $D_M$ (1-10 cm$^{-1}$). Ions that are orbital singlets will often have comparatively smaller $D_M$ (0.1-0.01 cm$^{-1}$). Of course, there are exceptions.

For some papers on single-molecule magnetism, see the following: