

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_{complex} is calculated as:

$$D_{\text{complex}} = d_1 D_M + d_2 D_{\text{SQ}} + d_3 D_{\text{MSQ}}$$

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

$$D^{\text{ex}} = \underbrace{J(e_M, g_{\text{SQ}})}_{> 0} \left[\frac{|\langle g_M | L | e_M \rangle|^2}{M^2} \right] + \underbrace{J(e_{\text{SQ}}, g_M)}_{\approx 0} \left[\frac{|\langle g_{\text{SQ}} | L | e_{\text{SQ}} \rangle|^2}{\text{SQ}^2} \right]$$

$e = \text{excited state}$
 $g = \text{ground state}$

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

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

- 1) Barra, A.-L.; Brunel, L.-C.; Gatteschi, D.; Pardi, L.; Sessoli, R. *Acc. Chem. Res.* **1998**, *31*, 460-466.
- 2) Christou, G.; Gatteschi, D.; Hendrickson, D. N.; Sessoli, R. *MRS Bulletin* **2000**, 66-71.

For an $S = 10$ molecule:

