Calculation of nmr parameters in paramagnetic metal-organic materials

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Presentation plan

1. NMR — what and why

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2. MOFs = Metal—organic frameworks

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3. NMR parameter calculation

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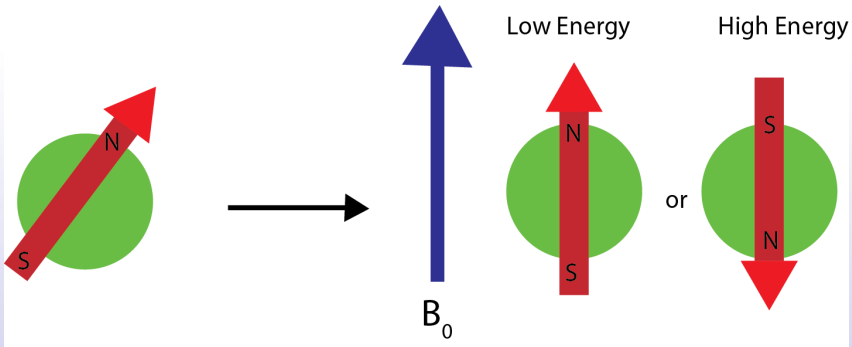
Nuclei and external magnetic field

- strong external magnetic field: several T
- nuclei with magnetic moment: lowest energy state splits
- two new states ΔE apart
- radio frequency spectrum: excitations from low to high energy states
- absorption peak at $\Delta E = \hbar\omega_{res}$
- ω_{res} depends on $B_{eff}(observednucleus)$



Several parameters affect $B_{eff}(nucleus)$ and ω_{res}:

- electronic structure – shielding of external magnetic field
- spin–spin coupling to nearby nuclei and unpaired electrons
- unpaired electrons: large paramagnetic shifts