

Calculation of nmr parameters in paramagnetic metal-organic materials

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Presentation plan

- 1 MOFs = Metal—organic frameworks

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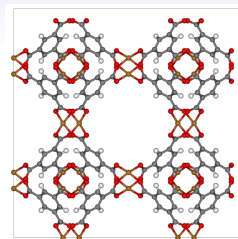
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- 3 NMR parameter calculation
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- 5 Preliminary results

MOF = METAL-ORGANIC FRAMEWORK

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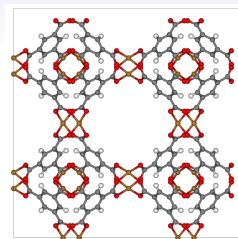
- crystal structure: central metallic ions + organic ligands



● carbon ● copper
● oxygen ○ hydrogen

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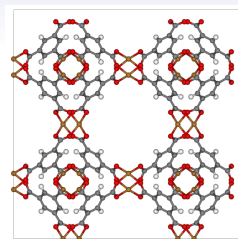
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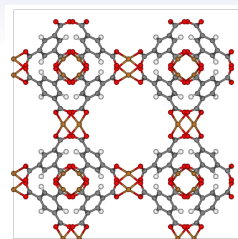
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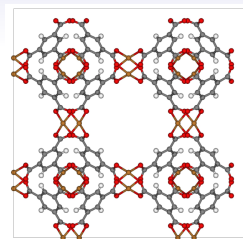
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- NMR spectra feature large shifts caused by unpaired electrons



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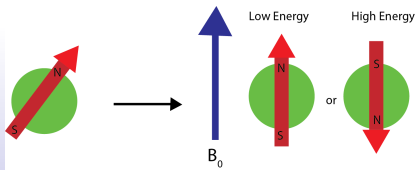
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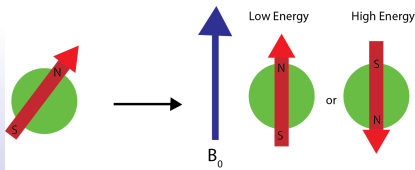
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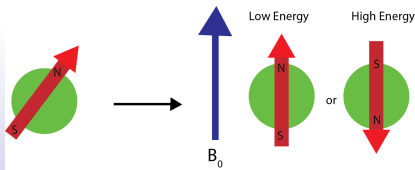
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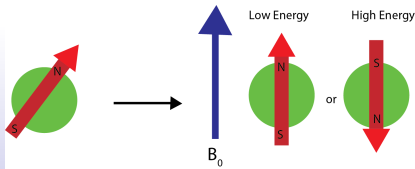
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- radio frequency spectrum: excitations from low to high energy states
- absorption peak at $\Delta E = \hbar\omega_{res}$
- ω_{res} depends on $B_{eff}(\text{observed nucleus})$



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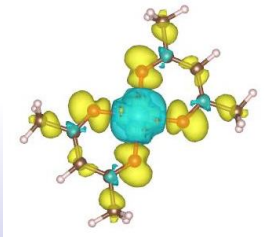
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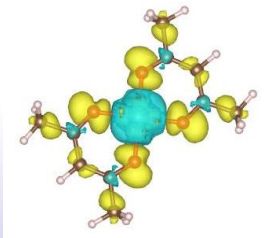


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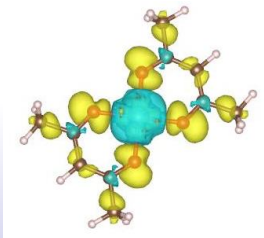


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Total shift tensor $\underline{\underline{\sigma}}$ is defined by:

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Two sources of chemical shifts:

- electron density change caused by applied external magnetic field
- depends on electron density $n(\vec{r})$
- coupling between unpaired electron and observed nuclei
- depends on spin density $n_{\uparrow}(\vec{r}_{nuclei}) - n_{\downarrow}(\vec{r}_{nuclei})$

Calculation of NMR parameters:
accurate electronic wave function needed.