

## Extended Fe-4 butterfly complexes: theoretical analysis of magnetic properties and magnetostructural maps

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R�sum� en anglais	<p>The inclusion of additional metal atoms in Fe-4 butterfly complexes drastically modifies their magnetic properties. Exchange interactions of a Fe<sub>4</sub>Y<sub>2</sub> complex have been calculated using theoretical methods based on density functional theory. The calculated values are in good agreement with experimental data showing that the change in the nature of bridging ligands induces a dramatic decrease of the antiferromagnetic wing-body interaction while the body-body interaction between the two central iron atoms is ferromagnetic. Finally, we propose a new tool to facilitate the understanding of the magnetic properties in polynuclear iron complexes. Magnetostructural maps allow us to correlate the calculated exchange coupling constants with metal-metal distances for the dinuclear or polynuclear iron complexes that we have studied.</p>
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### Liens

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