Intermolecular interactions in coordination compounds and their relevance for molecular materials¹

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Coordination compounds are characterized by metals and ligands, as well as by non-coordinated counter ions and/or solvent molecules. When ligands have more than one donor atom in non-chelating orientation, or mono-atomic ligands with more than one lone-pair, the ligands can be bridging between two or more metals. The result may be 1D-, 2D-, or even 3D-bridged coordination compounds. When the metal ions carry unpaired electrons, communication between the metals may be possible via de ligand bridges. This may result in magnetically interesting materials.

The communication between the metals is not necessarily maintained via the ligand bridges, also hydrogen bonding and halogen-halogen interaction, as well as pi-pi stacking may facilitate such communication.

In the last few years also anion-pi and even lone-pair interactions have been recognized as important supramolecular interactions, although magnetic communication between metals via such interactions are not likely to be significant. A possible exception could be the fine-tuning of spin transitions in iron compounds. In such cases subtle variations in metal ligand angles, influenced by supramolecular interactions in the lattice, may cause dramatic shifts in the spin-transition temperatures. Examples of metal-metal communication will be illustrated for several Cu and Fe compounds.

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