

## MS31 Unconventional interactions or symmetries for optimized and new properties, including chirality

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Interactions of aromatic ligands in sandwich and half-sandwich compounds

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### Abstract

Aromatic rings in sandwich and half-sandwich compounds can form the same types of interactions as non-coordinated aromatic molecules. However, in organometallic compounds, because of the coordination, the electrostatic potential of the aromatic ring can be changed, causing some changes in the interactions [1,2].

Stacking interaction between coordinated and uncoordinated benzene has the energy of -4.40 kcal/mol, while the calculated staking between two coordinated benzenes has the energy of -4.01 kcal/mol. These energies are significantly stronger than stacking between two uncoordinated benzenes (-2.73 kcal/mol). In crystal structures coordinated benzene and coordinated cyclopentadienyl anion form stacking interactions that dominantly have large horizontal displacements (more than 4.5 Å). This dominance is caused by the relatively strong stacking interactions at large displacements [1].

Electrostatic potential surfaces of aromatic ligands in half-sandwich compounds are entirely positive, making them capable of forming strong anion- $\pi$  and C-H/anion interactions [2,3,4] Our calculations of energies of interactions between half-sandwich compounds and halide anions showed that aromatic ligands in half-sandwich compounds can bind to anions. Anion- $\pi$  interactions with half-sandwich compounds are stronger than with most of organic aromatic compounds, while C-H/anion interactions are even stronger than anion- $\pi$  interactions [2].

Our studies show that transition metal coordination makes aromatic moieties suitable for strong stacking interactions, as well as strong interactions with anions and gives new insights into the molecular design.

### References

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