Chemical bonding in supermolecular flowers

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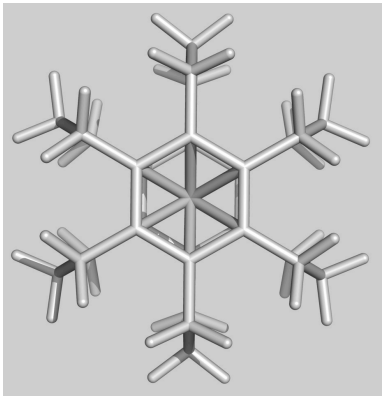
Metal-ligand bonding patterns play an important role in the stability of transition-metal complexes and their spin state preferences. In previous studies[1,2,3] we have looked at several TM-complexes, and found that covalent bonding is often the most important factor to distinguish different metals, and different spin states. In terms of bonding energy, the electrostatic interactions and Pauli repulsion contributed significantly, but these contributions were more or less constant for different metals.

The past studies focused on metallocenes,[1] metalloporphyrins[2] and dibenzene-species.[3] Here we extend the series by looking at several supermolecules, which have the form of ice-flowers (see Figure). We have investigated the stability, electronic structure and spin ground-state for a number of alkaline-earth and transition metals using the recently developed SSB-D functional.[4] The supermolecules show resemblances to the systems studied before, but also some striking differences were observed. Similar to our previous study,[2] we have also investigated how the metal-ligand interactions influence the aromaticity of these interesting clusters.



References

[1] M. Swart, *Inorg. Chim. Acta* ("Inorganic Chemistry - The Next Generation" issue) **2007**, *360*, 179-189

[2] F. Feixas, M. Solà, M. Swart, *Can. J. Chem.* (Tom Ziegler issue) **2009**, *87*, 1063-1073

[3] M.P. Johansson, M. Patzschke, *Chem. Eur. J.* **2009**, *15*, 13210-13218

[4] M. Swart, M. Solà, F.M. Bickelhaupt, *J. Chem. Phys.* **2009**, *131*, 094103