Interaction between metallocene units

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Previously it was revealed very frequent occurrence of the specific ferrocene-ferrocene dimers in the ferrocene containing crystal structures [1]. Thus, the analysis of the Cambridge Structural Databank (CSD) showed that nearly 60% of monosubstituted ferrocene derivatives form robust ferrocene dimers composed of two Fc units in parallel orientation (see Figure 1). Formation of the dimer is based on an excellent electrostatic complementarity between the Fc units (Figure 1). A subsequent theoretical study [2] revealed the significant stabilization energy of −5.7 kcal/mol for this specific interaction with dispersion as the most important attractive contribution.

In the present work, we have used the CSD to explore the same interaction between metallocene units but this time analyzed in all metallocene based crystal structures. We have found that all metallocenes equally as ferrocene derivatives are able to form the dimers with very similar geometrical parameters. In addition, we have investigated the supramolecular aggregation of the dimers into chains of different geometry.

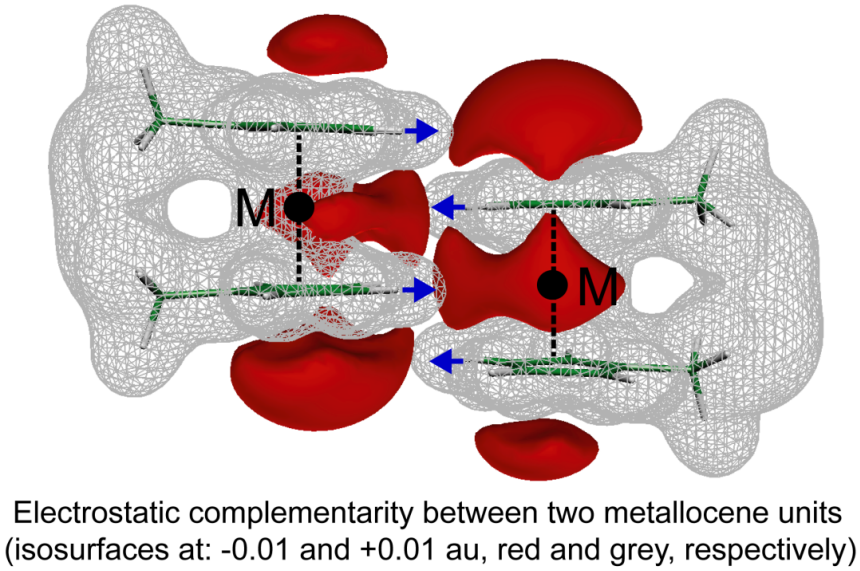

Figure 1. Electrostatic complementarity between two metallocene units.

[1] Bogdanović, G. A. & Novaković, S. B. (2011). CrystEngComm 13, 6930-6932.

[2] Vargas-Caamal, A. et al. (2016). Phys. Chem. Chem. Phys. 18, 550-5564.

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