Theoretical study of hydrogen bonding in disubstituted ferrocene peptides using AIM theory and NBO analysis

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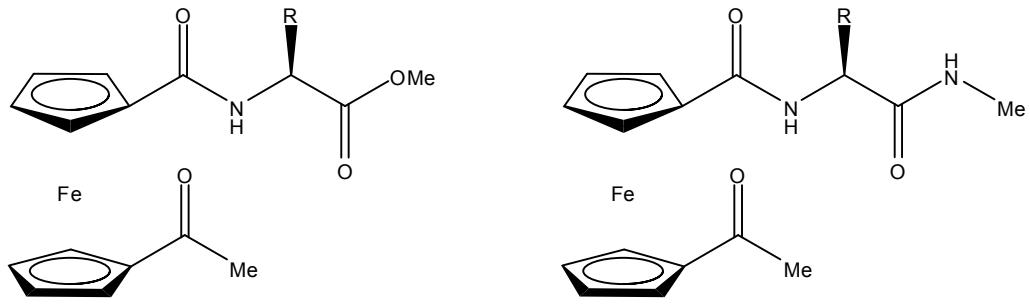
Ferrocene-containing derivatives of asymmetrically substituted 1,1'-dicarboxylic acid with natural amino acids can create hydrogen-bonded structures that result in organised helical ferrocene units in solution.[1,2] In this study we present the results of theoretical investigations of interactions within previously synthesized asymmetrical 1,1'-disubstituted ferrocene peptides of type I, MeCO-Fn-CO-AA-OMe, and type II conjugates, MeCO-Fn-CO-AA-NHMe (Fn = ferrocene-1,1'-diyl, AA = L-α-amino acid, Gly, Ala or Val).

A detailed population analysis of the several most stable conformers of each model type was performed with natural bond orbitals (NBO) and atoms in molecules (AIM) methods on previously optimized geometries with B3LYP/6-311G(d,p) and LanL2DZ basis set at Fe atom. Molecules were classified by the criteria of similarity of the inherent hydrogen bonds. Geometrical, topological and energetic properties of hydrogen bonds at the bond critical points (BCP) were compared. With few exceptions, observed proper N−H···O and improper C−H···O hydrogen bonds can be classified as weak bonds. Relative stability of equivalent conformers does not depend on specific amino acid and can be correlated with the number and type of hydrogen bonds.



[1] L. Barišić, M. Čakić, K. A. Mahmoud, Y. Liu, H.-B. Kraatz, H. Pritzkow, Srećko I. Kirin, N. Metzler-Nolte and V. Rapić, *Chem. Eur. J.*, **19** (2006) 4965.

[2] J. Lapić, D. Siebler, K. Heinze and V. Rapić, *Eur. J. Inorg. Chem.*, **14** (2007) 2014.