

SECONDARY STRUCTURAL MOTIFS IN DISUBSTITUTED FERROCENE AMIDES

Saša Opačak, Berislav Perić, Darko Babić, Srećko I. Kirin

Ruder Bošković Institute, Bijenička cesta 54, Zagreb, Croatia

Disubstituted ferrocene amino acids and peptides are known to form well defined secondary structures often mimicking natural motifs, such as β - or γ -turns [1]. When the two chiral substituents are hydrogen bonded, ferrocene rotation is hindered and a new element of helical chirality is evoked enabling characterisation by chiroptic methods.

Ferrocene amides, on the other hand, are also capable of forming interesting secondary structures, but are not well described in the literature. Our current research is inspired by our previous work in enantioselective hydrogenation catalysis with chiral triphenylphosphine Rh complexes [2]. We have synthesised a small series of 1, 1' - disubstituted ferrocene amides and their monosubstituted analogues (**Figure 1**), which are inspired by the structure of precatalytic complexes from our previous work [2]. We have noticed that these compounds form hydrogen bonds and have defined solution structures, different from the ferrocene peptides. It is particularly interesting to mention that these compounds exhibit solvent induced chirality inversion. In this work we characterize our new supramolecular system by various instrumental techniques (NMR, IR, UV-Vis, CD, MS, SC XRD) and DFT calculations in an attempt to ascertain the solution structure and explain supramolecular phenomena.

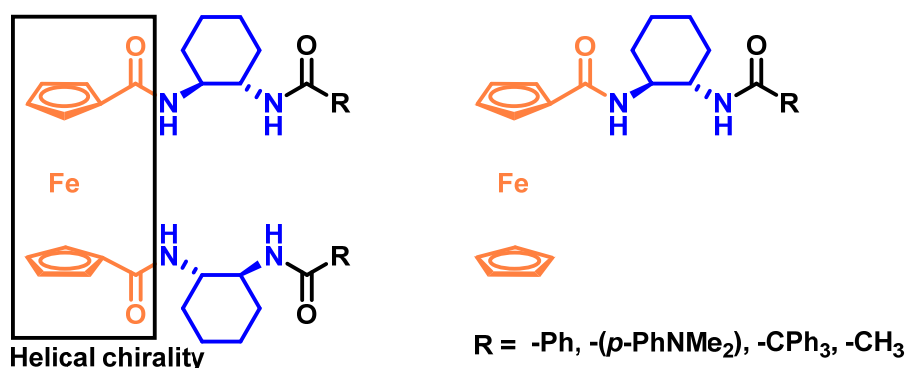


Figure 1 Ferrocene amides presented herein.

[1] S. I. Kirin, H. B. Kraatz, N. M. Nolte, *Chem. Soc. Rev.* **35** (2006) 348-354.

[2] S. Opačak, Z. Kokan, Z. Glasovac, B. Perić, S. I. Kirin, *Eur. J. Org. Chem.* (2019) 2115-2128.