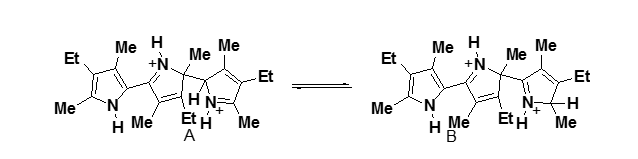
**FROM MONOMERS TO ”POLYMERS”. A THEORETICAL NMR STUDY INVOLVING CHARGED ALKYLPYRROLES.**

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Pyrroles may be polymerized e.g. by treatment with acid or by electrochemical oxidation.[[1]](#endnote-1) The latter may lead to the trimer~~s~~ shown in Figure 12 and to further polymerization.



**Figure 1.**

In order to help in the identification of the dimers, trimers and oligomers we have looked into the possibility of calculating 1H and 13C chemical shift substituent effects for both the neutral species and protonated ones. This is based on a study of the monomers as shown in Figure 2.



**Figure 2.** Monomers.

Calculation of NMR chemical shifts in charged systems will be discussed both with respect to solvent, counter ions, functional, basis sets and electron correlation. This seemingly trivial task turned out to pose great challenges.

1. 1 G.H. Hansen, R.M.Henriksen, F.S.Kamounah, T. Lund and O. Hammerich, Electrochim. Acta 50 (2005) 4936-4955.

   2 Andreas Wagner Tholl, Ole Hammerich, unpublished work. [↑](#endnote-ref-1)