5 - Cationic ring-opening polymerization of 2-propyl-2-oxazolines: Understanding structural effects on polymerization behavior based on molecular modeling

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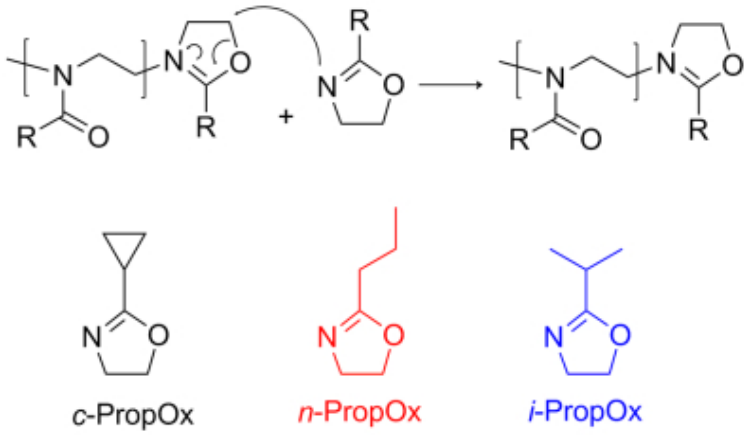
In recent years poly(2-alkyl-oxazolines) - regarded to be pseudo-polypeptides - have received considerable attention for, amongst others, biomedical applications. The living cationic ring opening polymerization (CROP) leads to good control over dispersity and end group fidelity while by variation of the monomer structure a broad range of polymer properties is easily accessible.[1]



Poly(2-propyl-2-oxazoline)s are known to exhibit interesting thermo responsive behavior.[2] Therefore the polymerization kinetics of *n*-PropOx, *i*-PropOx and the missing analogue 2-cyclopropyl-2-oxazoline (*c*-PropOx) were investigated. The polymerization rate constant (k_p) was found to decrease in the order *c*-PropOx > *n*-PropOx > *i*-PropOx.[3] Theoretical free energy calculations confirmed the trend for k_p. Studies of a set of DFT-based reactivity descriptors, electrostatics and frontier molecular orbitals revealed that the observed reactivity is dictated by electrostatic effects.[4] Consequently the copolymerization of *c*-PropOx and 2-ethyl-2-oxazoline yields gradient copolymers which cloud points can be tuned by variation of the composition.

1. O. Sedlacek, B. D. Monnery, S. K. Filippov, R. Hoogenboom, M. Hruby, *Macromol. Rapid Commun.*, **2012** , *33*, 1648.

2. C. Weber, R. Hoogenboom, U. Schubert, *Prog. Polym. Sci.*, **2012** , *37*, 686.

3. M. M. Bloksma, C. Weber, I. Y. Perevyazko, A. Kuse, A. Baumgärtel, A. Vollrath, R. Hoogenboom, U. S. Schubert, *Macromolecules* **2011** , *44*, 4057.

4. H. Goossens, S. Catak, M. Glassner, V. R. de la Rosa, B. Monnery, F. De Proft, V. Van Speybroeck, R. Hoogenboom, *ACS Macro Lett.* **2013** , *2*, 651.

Sunday, August 10, 2014 10:25 AM
Poly(2-Oxazoline)s and Polypeptoids (08:00 AM - 11:55 AM)
Location: Hilton San Francisco Union Square
Room: Golden Gate 6

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