HOW SIDE REACTIONS CAN INFLUENCE POLY(2-OXAZOLINE) SYNTHESIS FOR POLYMER THERAPEUTICS AND HYDROGELS

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Poly(2-oxazolines) (PAOx) are an interesting bioinspired class of polymers whose biocompatibility allows for drug, protein and gene delivery applications. PAOx are available through cationic ring-opening polymerization (CROP) of 2-oxazolines representing an easy and key strategy for the synthesis of well-defined polymers with controlled average polymer composition, narrow size exclusion chromatography (SEC) trace and suitable end-group functionalities. Due to the living nature of CROP and by the incorporation of the correct 2-oxazoline comonomer, a wide variety of linear as well as branched/network (co)polymers can be synthesized with well-tailored structures and less abrupt transitions from one comonomer type to the other. Even so, a key challenge to be dealt with consists of evaluating the PAOx synthesis success at the molecular level, hence, beyond experimentally accessible average CROP characteristics.

In this contribution [1-3], a combination of an advanced kinetic Monte Carlo modeling technique with meticulous experimental analysis is covered, allowing the kinetic analysis of CROP of 2-oxazolines, with specific focus on functionality design per chain length and the effect of side reactions such as chain transfer to monomer (*b*-elimination) and macropropagation. A novel parameter tuning is introduced with for the first time reliable macropropagation rate coefficients based on complete SEC data. Model-based design is shown to be an effective strategy to identify optimal synthesis conditions that maximize the functionality efficiency for both low and high targeted chain lengths.

References

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