Description for the general public

Introduction. General information on polymers:

The purpose of this project is to elaborate a novel method of polymer syntheses.

The major materials used today are metals, ceramics and polymers. Polymers are either natural or synthetic. Among the natural ones are e.g. wood (cellulose) and biopolymers vital for living species as well as for plants. Chemists working in the area of useful polymers are interested first of all in the polymer syntheses. Indeed, today, when we compare the volume of produced synthetic materials, the polymers are on the second place, only after concrete; metals are on the third place (metals are much heavier than polymers). Besides, the importance of polymers stems from versatility of their properties and related applications – from the packaging materials to the blood vessels.

All of the polymers are prepared in the processes of polymerization. One of these is so called ring-opening-polymerization (ROP). It is called this way, since chemical compounds (monomers) in ROP are cyclic. Such a cyclic compound in the polymerization process is opening the cycle (ring) and then, these opened structures are joined together thousands of times in the identical reactions-polymerizations. The formed chains resemble the connected series of pearls and have to be long enough to have the required properties.

The aim and importance of the present project:

Polymers are prepared in the catalyzed polymerization processes. Catalysts are indispensable for polymerization. Particularly important today are catalysts without metals, so called organocatalysts. Metals are harmful, at least in such areas as biomedicine or electronics. Therefore the organocatalysts, not containing metals are being actively developed. However, organocatalysts, applied in polymerization, in order to have sufficient control over a process, require additionally initiators. Thus, the catalytic system is composed of two different chemical compounds. Then, initiators are becoming, during polymerization, integral parts of polymer molecules and catalytic components, often toxic strong base, are left free in polymer.

This was one of the reasons to undertake research that should provide chemical compounds that could simultaneously perform catalytic and initiating functions (“two in one”). We are calling these compounds of a dual role INICATs. In contrast to the two components systems INICATs are entirely becoming parts of the polymer molecules and, therefore, no low molar mass compound is being left in polymer. Compounds attached to macromolecules are often becoming much less toxic then when are in the free-state. Finding the proper INICATs, and finding conditions of polymerization leading to high polymers require extensive basic (fundamental) research.

To accomplish the presented above research program first of all synthesis of INICATs is necessary. Thus, the group able to initiate polymerization has to be introduced into the known and already used basic catalyst. In the preliminary experiments several INICATs have already been prepared and at least two have been shown to polymerize selected monomers in the process, in which the expected molar masses and structures have been obtained. However, the resulting molar masses are still not of the order of million times higher than the mass of hydrogen atom. Such a property is the most desirable for polymers.

Two monomers will be studied the most extensively: L-lactide (LLA) and ε-caprolactone (CL). The resulting polymers are biodegradable; besides LLA is biobased.

Thus, the planned research with INICATs will concentrate on the studies of kinetics and mechanisms of polymerization and then in using these results in finding proper conditions of high polymers preparation. Perhaps it will we found out that in chosen INICATs there are some molecular fragments that lead to the side reactions, not permitting high molar mass polymers formation. Following these results improved INICATs will be synthetized (with a help of competent organic chemists). Thorough understanding of the process requires studies of kinetics and mechanisms of polymerizations, since polymerization with INICATs differs from the known until now polymerization reactions. Besides, using INICATs it is also planned to prepare star-like and highly branched polymers. INICATs, based on esters of the acids of phosphorus (phosphates and phosphonates with hydroxyl groups) will provide ionic-hydrophilic segments. Polymers of similar structures have properties typical for hydrophilic - hydrophobic copolymers. Polymers with INICATs should give a novel generation of micelles. These micelles will be biodegradable and may contain in their hydrophobic cores bioactive compounds.