# Chain Growth Polymerization: A Living Polymerization

Polystyrene may be produced by the polymerization of styrene monomer with an initiator. At the beginning of this polymerization, the initiator rapidly generates active sites onto which monomer units add sequentially. During this polymerization, every polymer chain starts with an initiator fragment and has an active site at its end.

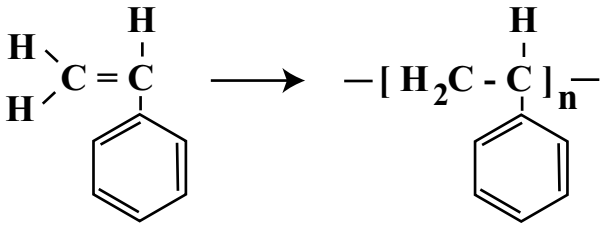

Figure 1: The polymerization of styrene to form polystyrene.

We will simulate this polymerization using red paper clips to represent the initiator fragments and silver paper clips to represent the monomer units. Each monomer unit has a mass 1 and the mass of the initiator fragment is neglected.

## Initial Configuration

Place ten red initiator fragments on a piece of paper and label them with the numbers 1 to 10. Count out and have available 100 hundred monomer units to react.

## Polymerization

Use a random number generator (die, tables, calculator, computer) to generate a random number between 1 and 10, inclusive. Add a monomer unit to the chain indicated by the random number. Form linear polymer chains through sequential generation of random numbers and addition of clips to the chain .

## Quantification of the Molecular Weight

At the start, and at regular intervals after approximately five reactions, calculate the following for your mixture:

- the extent of reaction
- the number average molecular weight of the growing chains (unreacted monomers are not included in this average)

Think carefully about the most simple and efficient way to do each calculation.

## Questions

1. What are the final $\bar{M}_n$ and $\bar{M}_w$ for this polymerization? What is the polydispersity? Sketch the molecular weight distribution $w(i)$. In a real polymerization where the concentration of initiator is very small (about 0.1 % rather than the 10 % used here) what would the polydispersity be?

2. How does $\bar{M}_n$ of the growing chains vary with the extent of reaction? Can you derive an equation which gives $\bar{M}_n$ as a function of $X$ and the initiator concentration? How does this compare to your results?

3. The title indicates a "living" polymerization where the reaction continues indefinitely as long as there is monomer present. Does your polymerization procedure replicate this? Why or why not? What are the advantages of this type of polymerization? How could you use this type of polymerization in order to synthesize a block copolymer?