

## Step-Growth Polymerization: A Single Difunctional Monomer

Difunctional monomers may react to form polymer chains. For example, hydroxy acids may polymerize upon heating:



During this polymerization, every monomer and growing chain has one -OH functionality and one -COOH functionality. We will simulate this polymerization using identical paper clips, one paper clip representing one monomer unit of mass 1 and neglecting the mass of the water.

### Initial Configuration

Place 100 identical paper clips on a piece of paper to represent the monomer units and label each *position* with one number, 1 through 100.

### Polymerization

Use a random number generator (die, tables, calculator, computer) to generate two random numbers between 1 and the maximum number of molecules in your sample (or between 1 and 100, discarding the results with no associated molecule). Join the two molecules selected by the random number generator. This joining leaves one space vacant every time it occurs. Form linear polymer chains through the sequential generation of pairs of random numbers

### 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 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  $w(i)$ . What would be different in a real polymerization with  $10^{23}$  monomer units?
2. How does  $\bar{M}_n$  vary with the extent of reaction? Can you derive an equation that gives  $\bar{M}_n$  as a function of  $X$ ? How does this compare with your results?

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