

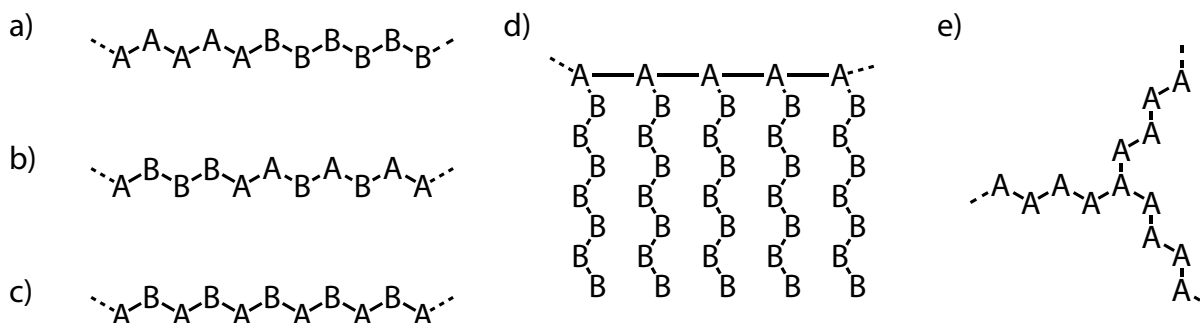
Polymer Science 2024

Exercise 1

- Conventionally, polymers are named according to a source-based or a structure-based convention, or using trade names (see reading recommendations). Draw the chemical structure (Lewis formulae) of the following polymers. Add the commonly used abbreviation and/or trade names where applicable.

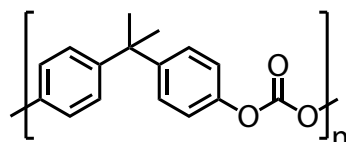
poly(ethylene), poly(vinyl alcohol), poly(tetrafluoroethylene), poly(styrene), poly(propylene), poly(ϵ -caprolactone), nylon 6, poly(ethylene terephthalate), poly(styrene-*b*-isoprene), poly(styrene-*co*-(ethylene oxide)), poly(1-phenylethylene).

- Name the following polymers based on their different architectures if A represents styrene monomers and B represents ethylene monomers. Use the reading recommendations.



- A “model” of a linear poly(ethylene) chain with a molecular weight of 200'000 g/mol is constructed using a paper clip to represent one repeating unit. How many paper clips do you need?
- Why is M_w often preferred over M_n as a measure of molar mass? Consider the hypothetical case of a sample consisting of two chains of molar masses $M_1 \gg M_2$. Discuss M_n and M_w in the limit of $M_2 \rightarrow 0$.
- What is the root mean square of the distance between the ends (R_n) of a chain of polyethylene with a molar mass of 140'000 g/mol?

6. Calculate M_n and M_w for (i) a sample containing equal *masses* of polymers with molecular weights of 5,000 g/mol and 85,000 g/mol, and (ii) a sample containing equal *moles* of polymers with molecular weights of 5,000 g/mol and 85,000 g/mol.
7. Below is the chemical formula for bisphenol A polycarbonate:



Despite its apparently rigid structure (presence of benzene rings in the main chain), the polycarbonate has a C_∞ of 2.2 in methylene dichloride. This is because we consider the benzene group as only one catenary bond instead of 5. The average length of a bond becomes thus approximately $(5 + 5 + 1 + 1) / 4 = 3$ times the length of a single C-C (or C-O) bond. What would the value of C_∞ be if we consider each link separately?

8. Some properties of ideal polymers are independent of the chemical structure. For a simple treatment of all ideal polymers, one might define an equivalent freely jointed chain. This newly defined chain has the same mean-square end to-end distance, R_n , and the same maximum end-to-end distance $R_{\max}$ (projection length) as the actual polymer. Using this concept, a complex chemical structure simplifies to a straight chain of N Kuhn monomers with an effective length b (Kuhn length). Calculate the Kuhn length b of polypropylene. How many monomers make up one Kuhn monomer? Calculate the molecular weight M_0 of the Kuhn monomer.

Hint: For the calculation of $R_{\max}$ use the all-*trans* conformation with a bond angle of $\theta = 68^\circ$.

9. An ideal polymer chain is often referred to as a Gaussian chain or Gaussian coil, because the Gaussian distribution successfully describes its end-to-end distance. Which assumptions are made in the Gaussian approximation? When does this approximation become valid? Can you imagine limitations of this approach?

Tip: Use the reading recommendation.

Reading suggestions:

- P. Hodge *et al.*, *Pure Appl. Chem.* **2020**, 92, 797-813; **A concise guide to polymer nomenclature for authors of papers and reports in polymer science and technology (IUPAC Technical Report).**
- H. N. Cheng, B. A. Howell, *J. Chem. Edu.* **2017**, 94, 1794-1797; **A Primer on Polymer Nomenclature: Structure-Based, Source-Based, and Trade Names.**
- T. Sakai, *Physics of Polymer Gels*. First Edition. Wiley-VCH Verlag GmbH & Co. KGaA (**2020**).

(You can download these documents from the Moodle-folder 'Reading Recommendation'.)