Chem 654, Spring 2003
Handout

PS#1 revised, 01/27/03

Problem Set 1. due 02/03/03

1. Draw the repeating unit chemical structures of the linear polymers made from the following ingredients and describe their preparation methods.
   a) Alternating copolymer of styrene and maleic anhydride
   b) Polyurethane from toluene di-isocyanate and butanediol
   c) Polycarbonate from bisphenol A and phosgene
   d) Poly(3-hexylthiophene)
   e) Polyimide from pyromellitic anhydride and phenylene diamine

2. Draw the local chemical structures of the networks resulting from the following chemicals.
   a) Pentaerythritol and phthalic anhydride
   b) Phenol and formaldehyde
   c) Urea and formaldehyde
   d) Epichlorohydrin, bisphenol A and hexamethylene diamine

3. Identify principal components with structures for the following trade name polymers.
   a) Nylon 6,6
   b) Orlon
   c) Dacron
   d) Kapton
   e) Mylar
   f) Formvar
   g) Plexiglas
   h) Tygon
   i) Neoprene

4. a) For the following discrete binary mixture of monodisperse polymers, determine the number average, weight average, z-average and (z+1)-average molar masses:

i	**w_i / g**	**M_i/ (kg/mol)**
1	10	1
2	1	10

   b) For the following discrete ternary mixture of monodisperse polymers, determine the number average, weight average, and z-average molar masses:

i	**w_i / g**	**M_i/ (kg/mol)**
1	3	10
2	2	20
3	1	30

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PS#1-2

5. Consider polycondensation products of an α,ϖ-hydroxyacid, HO-R-COOH, to form a polyester. The chain length distribution can be derived to be continuous, commonly known as the most probable distribution, and the weight fraction of x-mer at an extent of reaction p is given by

$$W_x = xp^{x-1}(1-p)^2 \qquad (1)$$

a) Show that the z-fraction of x-mer is given by

$$Z_x = x^2 p^{x-1}(1-p)^3(1+p)^{-1} \qquad (2)$$

and both W_x and Z_x are normlized over $1 \le x \le \infty$.

Notes on binomial expansions:

$$(1 \pm p)^{-n} = 1 \mp np + \frac{n(n+1)p^2}{2!} \mp \frac{n(n+1)(n+2)p^3}{3!} + \frac{n(n+1)(n+2)(1+3)p^4}{4!} \pm \ldots, \quad (p^2 < 1)$$

$$(1-p)^{-1} = 1 + p + p^2 + p^3 + p^4 + p^5 + \ldots$$

$$(1-p)^{-2} = 1 + 2p + 3p^2 + 4p^3 + 5p^4 + 6p^5 + \ldots$$

$$(1-p)^{-3} = 1 + 3p + 6p^2 + 10p^3 + 15p^4 + 20p^5 + \ldots$$

$$\sum_{x=1}^{\infty} x^2 p^{x-1} = 1 + 4p + 9p^2 + 25p^3 + \ldots, \quad (p^2 < 1)$$

$$= \frac{1 + p}{(1 - p)^3}$$

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b) Find the extent of reaction p at which the weight fraction of 1000-mer is the greatest in the polymerization mixture; find p which gives W_{1000} the maximum in a profile of W_x vs. x.

c) Find the extent of reaction p when the weight fraction of 500-mer is the greatest during the entire course of the polymerization reaction; find p which gives W_{500} the maximum in a profile of W_{500} vs. p.

d) Plot W_x vs. x for p = 0.990, 0.995, 0.998, 0.999 over a range, $0 \le x \le 6000$.

e) Plot W_x vs. p for x = 300, 400, 500, 700, 900 over a range, $0.990 \le p < 1.000$.