

Biomaterials HW 3

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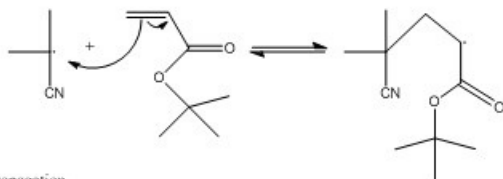
September 28th, 2016

1.

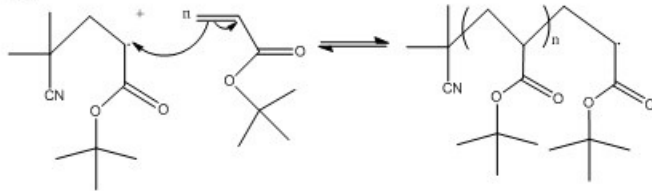
Disassociation



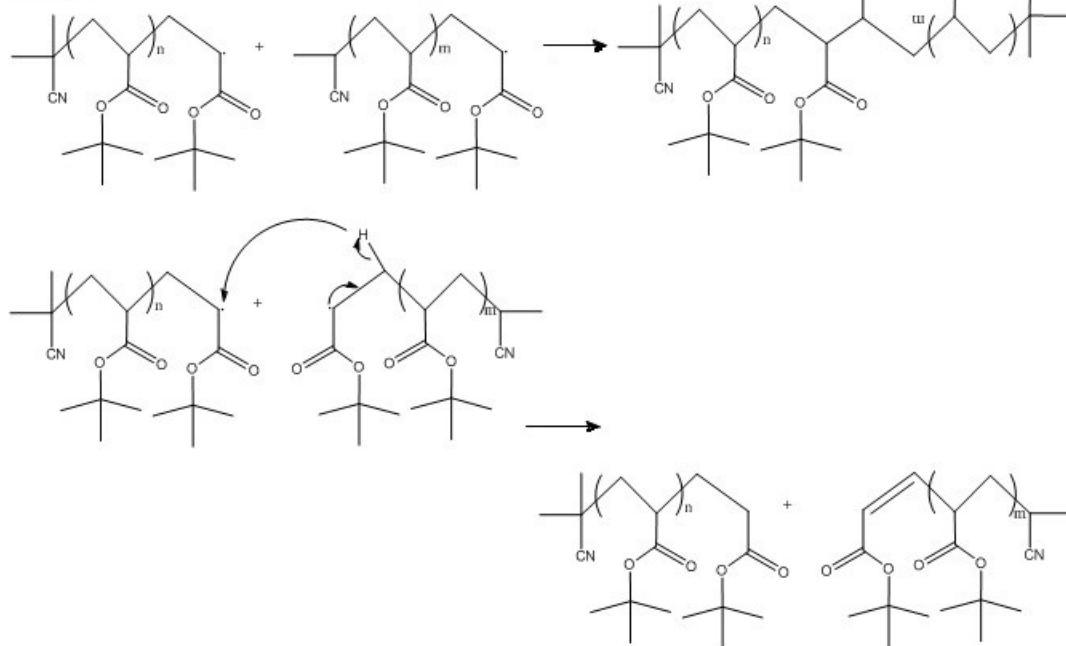
Initiation

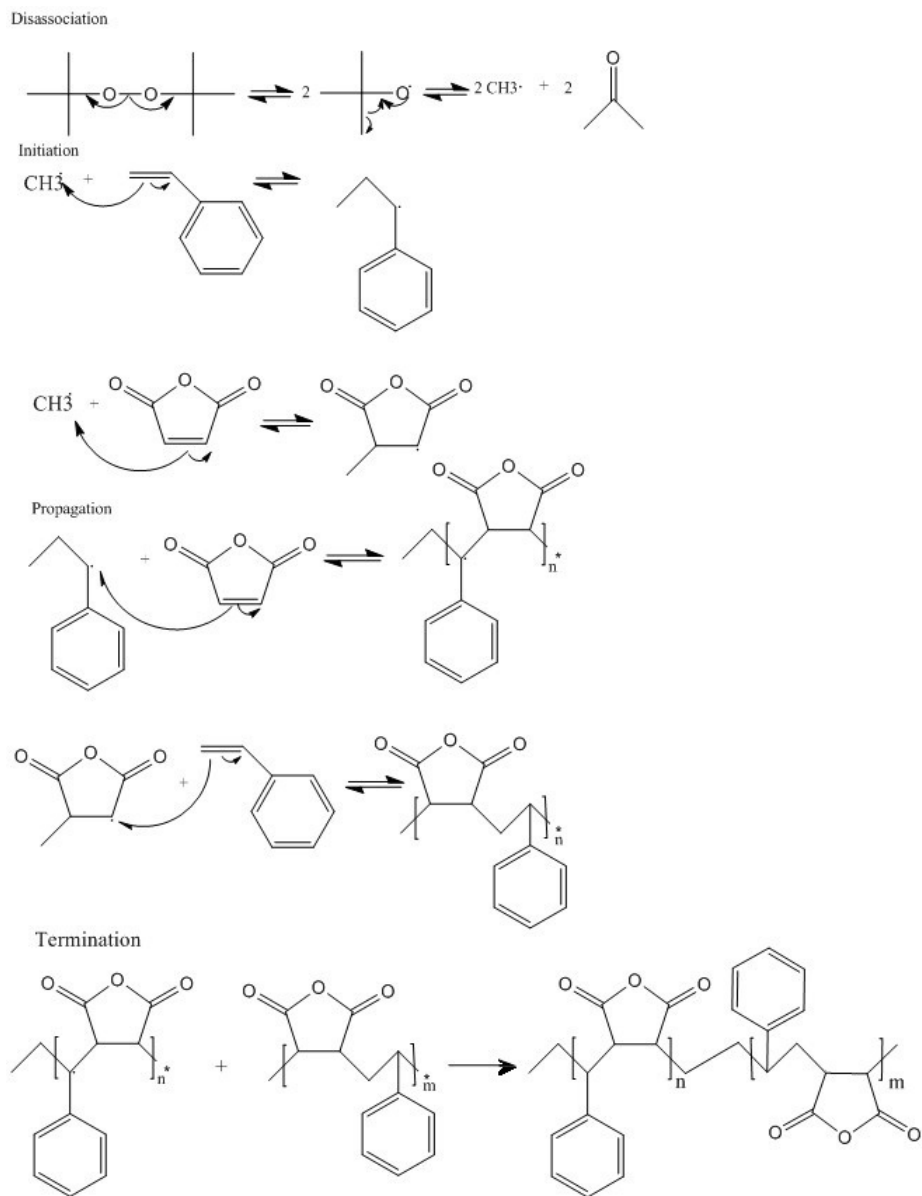


Propagation



Termination





2a. From the problem, we know that

$$k_d = 4.47 \times 10^{-6} \text{ s}^{-1}, \frac{k_p^2}{k_t} = 1 \times 10^{-2} \text{ mol}^{-1} / \text{ s}, f = 0.4$$

First, convert the concentrations of the two chemicals to molar concentrations (Molar mass of methyl methacrylate is 100.14 g/mol and molar mass for benzoyl peroxide is 242.23 g/mol)

$$[\text{benzoyl peroxide}] = [M] = 0.9988 M$$

$$[\text{methyl methacrylate}] = [I] = 0.00411 M$$

Then, since the concentration of I changes over time,

$$-\frac{d[I]}{dt} = 2fk_d[I]_0$$

which, after integrating, becomes

$$[I] = [I]_0 e^{-2fk_d t}$$

The steady state rate of polymerization is

$$R_p = k_p \left(\frac{fk_d}{k_t} \right)^{1/2} [M][I]^{1/2}$$

which, after substituting the previous formula, becomes

$$-\frac{d[M]}{dt} = k_p \left(\frac{fk_d}{k_t} \right)^{1/2} [M] ([I]_0 e^{-2fk_d t})^{1/2}$$

which, after integrating, becomes

$$-ln \frac{[M]}{[M]_0} = k_p \left(\frac{fk_d}{k_t} \right)^{1/2} [I]_0^{1/2} \left(\frac{e^{-fk_d t}}{-fk_d} \right)$$

Since $[M]/[M]_0 = 0.5$, we can solve for t to get

$$t = 24.7 \text{ hours}$$

2b. Then, combining the formula

$$x_n = \frac{k_p[M]}{(1+q)k_t^{0.5}(\frac{R_i}{2})^{0.5}}, q = 1$$

and the formula

$$R_i = 2fk_d[I]$$

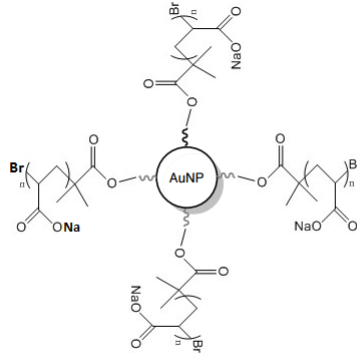
gives

$$x_n = \frac{k_p[M]}{(2k_t^{0.5}(fk_d[I])^{0.5})}$$

We can also substitute the formula for [I] in terms of $[I]_0$ that we found earlier to get

$$x_n = \frac{k_p[M]}{(2k_t^{0.5}(fk_d[I]_0 e^{-2fk_d t})^{0.5})} = 739$$

3a.



3b.

