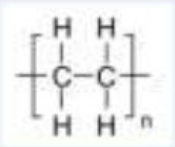
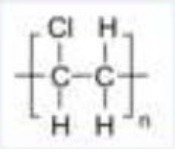
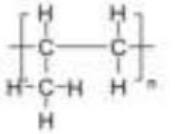
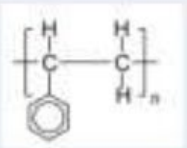
Tutorial Sheet 6

Week 6

Polymer (Abbreviation)	Repeat Unit Structure	Carbon Atoms	Hydrogen Atoms	Fluorine Atoms	Chlorine Atoms	Molar mass (g/mol)
Polyethylene (PE)		2	4	0	0	28.052
Polytetrafluoroethylene (PTFE)		2	0	4	0	100.02
Poly(vinyl chloride) (PVC)		2	3	0	1	62.494
Polypropylene (PP)		3	6	0	0	42.078
Polystyrene (PS)		8	8	0	0	104.144

Question 2

Analysis of a sample of polypropylene showed the molecular weight distribution given in following table. From this information determine:

a) The number-average molecular mass, $\bar{M}n$
b) The weight-average molecular mass, $\bar{M}w$
c) The number-average degree of polymerization, DPn
d) The weight-average degree of polymerization, DPw

Molecular Weight Range (g/mol)	Number Fraction x_i	Weight Fraction w_i
8,000 - 16,000	0.05	0.02
16,000 -24,000	0.16	0.10
24,000 - 32,000	0.24	0.20
32,000 - 40,000	0.28	0.30
40,000 - 48,000	0.20	0.27
48,000 – 56,000	0.07	0.11

Polypropylene (from previous, molecular mass of repeat unit $\bar{m} = 42.078\ g/mol$)

a) $\bar{M}_n = \frac{\sum_i Ni\,Mi}{Ni}$

b) $\bar{M}_w = \frac{\sum_i Wi\,Mi}{Wi}$

c) $DP_n = \frac{\bar{M}n}{\bar{m}}$

d) $DP_w = \frac{\bar{M}w}{\bar{m}}$

Molecular Weight Range (g/mol)	Mean	Number Fraction x_i	Weight Fraction w_i
8,000 - 16,000	$\frac{8000 + 16000}{2} = 12{,}000$	0.05	0.02
16,000 -24,000	20,000	0.16	0.10
24,000 - 32,000	28,000	0.24	0.20
32,000 - 40,000	36,000	0.28	0.30
40,000 - 48,000	44,000	0.20	0.27
48,000 – 56,000	52,000	0.07	0.11

Molecular Weight Range (g/mol)	mean M_i	Number Fraction x_i	x_iM_i	Weight Fraction w_i	w_iM_i
8,000 - 16,000	12,000	0.05	600	0.02	240
16,000 -24,000	20,000	0.16	3200	0.1	2000
24,000 - 32,000	28,000	0.24	6720	0.2	5600
32,000 - 40,000	36,000	0.28	10080	0.3	10800
40,000 - 48,000	44,000	0.2	8800	0.27	11880
48,000 – 56,000	52,000	0.07	3640	0.11	5720
		Sum	33040		36240

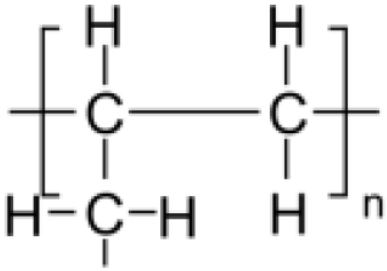
$$\overline{M}_n = \sum x_i M_i = 33{,}040 \text{ g/mol}$$

$$\overline{M}_w = \sum w_i M_i = 36{,}240 \text{ g/mol}$$

b

Polypropylene:

- Repeat unit contains 3 carbon atoms
- (prop = 3)
- One carbon atom sits as a side group with 3 of its own hydrogen atoms
- Molar mass $= 3\times12.01+6\times1.008\ \frac{g}{mol} = 42.078\frac{g}{mol}$



$$DP = \frac{\overline{M}_n}{m} = \frac{33{,}040\ \text{g/mol}}{42.08\ \text{g/mol}} = 785$$

Question 5

For a linear polymer molecule, the total chain length L can be determined from the bond length between chain atoms d, the total number of bonds in the molecule N, and the angle between adjacent chain atoms θ, as follows:

$$L = Nd \sin\left(\frac{\theta}{2}\right)$$

Additionally, the average end-to-end distance r for a polymer molecule can be calculated using:

$$r = d\sqrt{N}$$

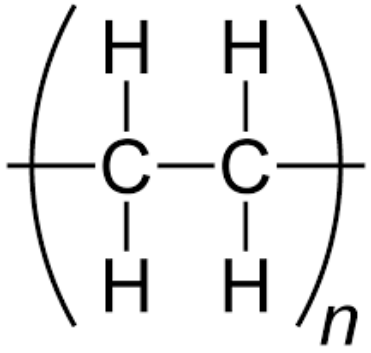
A linear polyethylene has a number average molecular weight o 300,000 g/mol. Determine:

a) the number-average degree of polymerisation, DP_n
b) the average total chain length, L
c) the average end-to-end distance, r

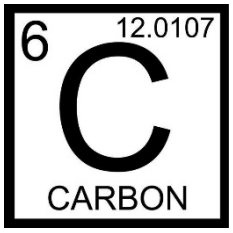
Question 3

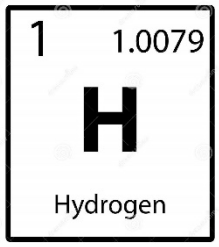
a) Calculate the average of **total chain length**, L, for a linear polyethylene polymer with a average molecular weight ($\bar{M}_n$) of 300,000 g/mol?

$$L = nd.\sin(\frac{\theta}{2})$$



n= $DP = \frac{\bar{M}_n}{m_a}$





$m_{a(PE)}$ = 12*2(C)+1*4(H) = 28 g/mol

(H) —— 1.008 g/mol

(C) —— 12.01 g/mol

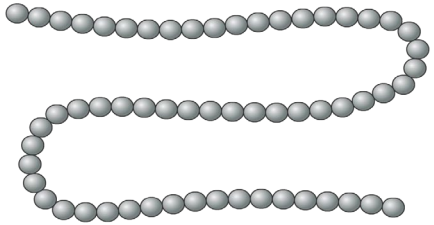
$$DP = \frac{M_n}{m} = \frac{300{,}000}{28} = \mathbf{10{,}714}$$

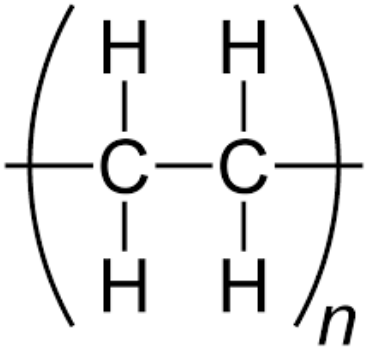
The number of repeating units along the chain

Two C – C in each monomer, there will be a total of (2*10,714 = 21,428) chain bonds in the molecule n.

Given in question
C – C = 0.154 nm,
θ= 109º for PE

$$L = nd.\sin(\frac{\theta}{2})$$





$$L = 10{,}714 * 2 * 0.154.\ \sin(\frac{109}{2})$$

$$L = 2686\ nm$$

b) The average end-to-end distance for a series of polymer molecules r is equal to

$$r = d\sqrt{n}$$

$$r = 0.15\ 4(nm)\sqrt{\ 21{,}428} = 22.5\ nm$$