Exercise # 7 ANSWERS

Predictions for Alkane Halogenation by Free Radical Substitution

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**Assuming that each of the pentanes below undergoes monochlorination:**

1. Predict the number of unique monochlorination products possible
2. Qualitatively predict the `major’ and `minor’ products
3. Calculate the expected % yield of all the unique monochlorination products assuming

**Site Relative yield/H for radical chlorination [see supplement 7 ]**

**1o 1**

**2o 3.7**

**3o 5.1**



**7.1 n-pentane**

**A minor** number of unique monochlorination products possible \_\_3\_\_\_\_

1. `major’ and `minor’ products (draw them) B major

C major

1. Calculate the expected % yield of all the unique monochlorination products assuming relative yield values above. Relative % yield (calc)

**A=>1o contribution = 6\*1 = 6 ∝ probability of reaction 100\*6/28.2 =21.3**

**B=>2o contribution = 4\*3.7 =14.8 100\*14.8/28.2 = 52.5**

**C=>2o contribution =2\*3.7=7.4 100\*7.4/28,2 =26.2**

**Sum = 28.2 78.7 % of monochlorination at 2o**

**7.2 neopentane**



1. number of unique monochlorination products possible \_\_1\_\_\_\_
2. **`major’** and `minor’ products (draw them)

ONLY ONE PRODUCT

**7.3 isopentane**

1. number of unique monochlorination products possible \_\_4\_\_\_\_
2. `major’ and `minor’ products (draw them)

A B C D



1. Calculate the expected % yield of all the unique monochlorination products assuming relative yield values above.

**A=>3\*1=3 B => 2\*3.7=7.4 C =>1\*5.1=5.1 D=>6\*1 =6 SUM=21.5**

**Rel %=100\*3/21.5 =100\*7.4/21.5 =100\*5.1/21.5 =100\*6/21.5**

**13.9% 34.4 % 23.7% 27.9%**