Optical Purity Worksheet

1. A solution has 80% (R)-2-bromobutane and 20% (S)-2-bromobutane
2. What is the “enantiomeric excess” of (R)-2-bromobutane?

80% - 20% = 60% excess of (R)-2-bromobutane

1. If pure (R)-2-bromobutane rotates light 100º to the right, how much rotation would occur for a solution with 80% (R)-2-bromobutane and 20% (S)-2-bromobutane

80º - 20º = 60º, 60%optical purity

1. If a solution has a 50/50 mixture of (R)- and (S)-2-bromobutane, what would be the enantiomeric excess and the optical purity?

ZERO!!

1. If a solution has a 50% ee, what would be the ratio of enantiomers?

a. 50% R, 50% S or

**b. 75% R, 25% S**

1. A 0.44 g/mL sample of codeine is put in a 1.5-cm polarimeter tube. The D-line of sodium was used to measure the rotation of the sample. The observed rotation was -9.0°. Using this data, find the specific rotation of codeine.

**specific rotation of codeine = observed rotation / [(concentration in g / mL)(tube length in dm)]**

**= -9.0° / [(0.44 g/mL)(0.15 dm)]**

**= -136°**

**(which is at a concentration of 1 g/mL and a path length of 1dm)**

1. If optically pure (S)-2-deuterobutane is known to have a specific rotation of [a] = +10°, and the final product is observed to have [a] = -9°, what can be concluded about the product with respect to its

**a) optical purity = 90%**

**b) enantiomeric excess = 90%**

**c) composition in % (R) and % (S) = 95% (R) + 5% (S)**

1. A mixture of two enantiomers has as observed rotation of -18°. The specific rotation of the (-) enantiomers is -27°. Find the % of the two enantiomers in the solution.

**The -18° tells you immediately that there is more of the (-) enantiomer. The excess of the (-) enantiomer is -18°/-27° x 100 = 66.7%, so the remaining 33.3% of the enantiomers present is divided equally between the (-) and (+) enantiomers. This means there is 33.3 / 2 = 16.7 % of the (+) enantiomer and 66.7 + 16.7 = 83.3% of the (-) enantiomer.**

**Another way to calculate these two values is by using**

**ee = 100 \* |d-l| / |d+l| , where d is the % of the (+) enantiomer and l is the % of the (-) enantiomer**

**66.7 = 100 \* |d-l| / |d+l|**

**66.7d + 66.7 l = 100 l – 100 d (l had to be put first because it is larger than d)**

**166.7d = 33.3 l But, l + d = 100%, so d = 100-l**

**166.7(100-l) = 33.3 l**

**16670-166.7 l = 33.3 l**

**l = 16670/200 = 83.3%, d = 100 – l = 16.7%**