Optical Rotation problems Key

1. The optical rotation of a sample composed of only 2-butanol is determined. \( \alpha_{\text{obs}} = -0.45^\circ \). \([\alpha]_D\) is known to be 13.52\(^\circ\)ml/g dm for (+)-2-butanol. If the cell pathlength was 0.6 dm and the concentration of 2-butanol in the sample was 0.15 g/ml what is the enantiomeric excess (EE)? Calculate the percentage of the (+) and (-) isomers.

\[
\frac{0.45}{(0.6)(0.15)} = 5.0 = \alpha_{\text{obs}} \text{ adjusted for concentration and pathlength}
\]

\[
\frac{5.0}{13.5} = 37\% \quad (+)\% = 68.5\% \quad (-)\% = 31.5\%
\]

2. A sample of pure (d)-borneol is found to produce an \( \alpha_{\text{obs}} = 10.1^\circ \). What must be the concentration if \([\alpha]_D = 37.7^\circ\)ml/g dm assuming a 1 dm pathlength?

\[
10.1 = [\alpha]_D \cdot c \cdot l \\
\[\quad c = \frac{10.1}{37.7} = 0.26 \text{ g/ml}\]
\]

3. A sample of an unknown enantiomerically pure compound produces an \( \alpha_{\text{obs}} = -120^\circ \) when \( c = 1.0 \text{ g/ml} \). Upon diluting the sample to 0.5 g/ml the \( \alpha_{\text{obs}} = +120^\circ \). Explain.

\([\alpha]_D = +240^\circ\) and only appeared to be -120\(^\circ\) when first measured. Dilution by half must produce a 50% smaller optical rotation not a change of sign!

4. A sample has a 50% EE and \( \alpha_{\text{obs}} = 20^\circ \) for a concentration of 0.4g/ml and \( l = 0.5\text{ dm} \). What is \([\alpha]_D\) for the pur isomer?

\[
\frac{20}{(0.4)(0.5)} = \alpha_{\text{corr}} = 100^\circ \\
\frac{100}{[\alpha]_D} = 50\% \quad \text{therefore} \quad [\alpha]_D = 200^\circ
\]