



NOMENCLATURE

Current CD spectrometers measure CD in terms of ellipticity Θ , usually expressed in millidegrees. This is, if you want, a rather strange way to express results, since CD is an absorption phenomena. Indeed the French school, which developed first commercial units, was using ΔOD as scale, but Americans took over many years ago and ellipticity Θ is the standard acquisition scale used today. Conversion is however very simple:

$$\Delta A = \Theta/32980$$

where:

ΔA in absorbance units

Θ is ellipticity in mdeg

Literature data are usually reported in **molar ellipticity** $[\Theta]$:

$$[\Theta] = \Theta/(10 \times C \times l)$$

or

$$[\Theta] = (\Theta \times M)/(c \times l \times 10000)$$

where:

Θ is ellipticity in mdeg

C is the molar concentration (mole/l)

l is the cell path in cm

M is molecular weight

c is concentration in g/ml

since obviously

$$C = (1000 \times c)/M$$

$[\Theta]$ is expressed in $\text{deg} \times \text{cm}^2 \times \text{decimole}^{-1}$

For macromolecules such as proteins the mean residue molar ellipticity is used $[\Theta]_{MRW}$:

$$[\Theta]_{MRW} = \Theta/(10 \times C_r \times l)$$

Formula is still the same, but C_r is the mean residue molar concentration

$$C_r = (n \times 1000 \times c_g)/M_r$$

where:

n is the number of peptide bonds (residue)

c_g is the macromolecule concentration (g/ml)

M_r is the molecular weight of the species

Notes:

-the Jasco software is not able to differentiate $[\Theta]$ from $[\Theta]_{MRW}$, so inputting concentration you must divide by the number of amino acids

-Jasco uses molecular ellipticity term in place of molar ellipticity

-most secondary structure estimation programs need $[\Theta]_{MRW}$

Another used way to report data in literature is **molar circular dichroism** $\Delta \epsilon$:

$$\Delta \epsilon = \epsilon_L - \epsilon_R = \Delta A/C \times l$$

simple relations apply:

$$[\Theta] = 3298 \times \Delta \epsilon \quad \text{and} \quad \Delta \epsilon = [\Theta]/3298$$

$\Delta \epsilon_{MRW}$ is often used for macromolecules as mean residue molar circular dichroism, same rules as above

Note:

-Jasco software indicates $\Delta \epsilon$ as molecular CD

Furthermore data are occasionally expressed as anisotropy factor g

$$g = \Delta \epsilon/\epsilon = \Delta A/A$$

which is independent from concentration and linearly related to the enantiomeric excess