Quantum Mechanics_molar absorptivity

The **molar absorption coefficient**, **molar extinction coefficient**, or **molar absorptivity** (*ϵ*), is a measurement of how strongly a chemical species absorbslight at a given wavelength. It is an intrinsic property of the species; the actualabsorbance, *A*, of a sample is dependent on the pathlength, ℓ, and the concentration, *c*, of the species via the Beer–Lambert law, $A = \varepsilon c \ell$.

The SI units for ϵ are m^2/mol, but in practice, they are usually taken as M^{-1} cm^{-1}or L mol^{-1} cm^{-1}. In older literature, cm^2 mol^{-1} is sometimes used with corresponding values 1000 times larger. These units may look different, but it is just a matter of expressing volume in cm^3 or in L.

Different disciplines have different conventions as to whether absorbance isNapierian (e-based) or decadic (10-based), i.e., defined with respect to the transmission via natural logarithm (ln) or common logarithm ($\log_{10}$). The molar absorption coefficient is usually decadic,[1] but when ambiguity exists it is best to qualify it as such.

In biochemistry, the extinction coefficient of a protein at 280 nm depends almost exclusively on the number of aromatic residues, particularly tryptophan, and can be predicted from the sequence of amino acids.[2] If the extinction coefficient is known, it can be used to determine the concentration of a protein in solution.

When there is more than one absorbing species in a solution, the overall absorbance is the sum of the absorbances for each individual species (X, Y, etc.):

$$A = (\varepsilon_{\mathrm{X}} c_{\mathrm{X}} + \varepsilon_{\mathrm{Y}} c_{\mathrm{Y}} + \cdots)\ell,$$

The composition of a mixture of *N* components can be found by measuring the absorbance at *N* wavelengths (the values of ϵ for each compound at these wavelengths must also be known). The wavelengths chosen are usually the wavelengths of maximum absorption (absorbance maxima) for the individual components. None of the

wavelengths must be an *isosbestic point* for a pair of species. For *N* components with concentrations c_i and wavelengths λ_i, absorbances $A(\lambda_i)$ are obtained:

$$A(\lambda_i) = \ell \sum_{j=1}^{N} \varepsilon_j(\lambda_i) c_j$$

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This set of simultaneous equations can be solved to find concentrations of each absorbing species.

The molar extinction coefficient ε (if expressed in units of L mol^{-1} cm^{-1}) is directly related to the Absorption cross section, σ, (in units of cm^2) via theAvogadro constant:[3]

$$\sigma = 1000 \ln(10) \frac{\varepsilon}{N_A} = 3.82 \times 10^{-21} \varepsilon$$

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The molar absorptivity is also closely related to the mass attenuation coefficient, by the equation

(mass attenuation coefficient)×(Molar mass) = (Molar absorptivity).

References

1. ^ [1][2][3]
2. ^ Gill, SC; von Hippel, PH (1989), "Calculation of protein extinction coefficients from amino acid sequence data", *Analytical Biochemistry* **182** (2): 319–26,doi:10.1016/0003-2697(89)90602-7, PMID 2610349
3. ^ Lakowicz, Joseph R (2006), *Principles of Fluorescence Spectroscopy* (3rd ed.), New York: Springer Science+Business Media, LLC, p. 59