



ϵ : Molar Absorption Coefficients (UV-VIS)

These spectral properties are tricky to find in reference materials. First, some definitions:

Molar absorption coefficient (ϵ)

Synonyms: Molar extinction coefficient, Molar absorptivity)

"The recommended term for the absorbance for a molar concentration of a substance with a path length of l cm determined at a specific wavelength. Its value is obtained from the equation $\epsilon = A / cl$

Strictly speaking, in compliance with SI units the path length should be specified in meters but it is current general practice for centimeters to be used for this purpose. Under defined conditions of solvent, pH and temperature the molar absorption coefficient for a particular compound is a constant at the specified wavelength."

-- R.C. Denney, Dictionary of Spectroscopy, 2nd ed. (Wiley, 1982), p.119-20.

Molar absorptivity

Synonym: Molar (decadic) absorption coefficient.

Decadic absorbance divided by the path-length l and mole concentration c , of the absorbing material. $\epsilon = A_{10}/cl$. The molar absorptivity is a Beer-Lambert absorption coefficient. SI unit: $m^2 mol^{-1}$.

-- Handbook of Vibrational Spectroscopy, v.5 p.3772 (Wiley, 2002)

Extinction coefficient

A term that has been widely used for the molar absorptivity, unfortunately often with values given in ill-defined units. Use of this term has been discouraged since the 1960s, when international agreement with non-chemical societies reserved the word "extinction" for diffusion of radiation, i.e. the sum of the effects of absorption, scattering, and luminescence.

-- *ibid.*, p.3760

Where to Find Them - Print

Values of ϵ and $\log\epsilon$ can be found scattered through spectral and general reference sources, although they are not always clearly marked. They generally appear near wavelength numbers (λ_{\max}). Much depends on the type of substance you're looking for. Here are some suggested places to look. All in the Spectra Section unless otherwise noted.

Atlas of spectral data and physical constants for organic compounds.

QD 257.7 G7 1975 (6 vols., 2nd ed., CRC, 1975)

Molar absorption coefficients appear in parentheses next to the wavelengths in the Ultraviolet column.

CRC handbook of biochemistry and molecular biology.

QP 514.2 H34 1975 Reference (CRC, 1975-)

Vol. A2, pp.383-545, table titled "Molar absorptivity and $A(1\%1\text{cm})$ values for proteins at selected wavelengths of the ultraviolet and visible region."

Data for biochemical research.

QP 520 D37 1986 Reference (Oxford, 1986)

ϵ or $\log\epsilon$ is occasionally given in parentheses next to the λ_{\max} in the General Remarks column in the chapters on amino acids, amines, amides, peptides; carboxylic acids, alcohols, aldehydes, ketones; phosphate esters; vitamins and coenzymes, etc.

Handbook of data on organic compounds. (HODOC)

Handbook Table (7 vols., 3rd. ed., CRC, 1994)

Molar absorption coefficients when available are given in parentheses next to major bands in the UV section of the entry.

Handbook of ultraviolet and visible absorption spectra of organic compounds.

QD 291 H5 (Plenum, 1967)

$\log \epsilon$ appears in the column next to the λ_{\max} .

Merck index.

Handbook Table

ϵ is given in parentheses next to the UV max in the properties paragraph of some entries.

Organic electronic spectral data.

QC 437 O65 (Wiley, 1946-89)

$\log\epsilon$ is given in parentheses next to the λ_{\max} . There is no cumulative index to this series, which is a big drawback.

Practical handbook of spectroscopy.

QD 95 P73 1991 (CRC, 1991)

The UV table (pp.565-646) data are sorted into groups based on the intensity of the strongest band, then in decreasing order by wavelength of the strongest band. If you already have ϵ you can identify an unknown this way.

Sadtler ultraviolet spectra.

Sadtler Alcove

Molar absorptivities are provided in the spectrum's data table for many compounds, denoted as a_m . Use the main index set to locate the compound, as described on the **Sadtler** page.

Ultraviolet spectra of aromatic compounds.

QC 459 F7 (Wiley, 1951)
600 spectra plotted by $\log \epsilon$ as a function of wavelength.

UV-VIS atlas of organic compounds.

QC 462.85 P47 1992 (2nd ed., VCH, 1992)
Exact values of ϵ_{\max} are indicated on the spectral traces.

Where to Find Them - Online

There are not many online resources where this kind of data is available or searchable, short of doing a full literature search. In SciFinder Scholar, the best approach is to search for the compound by registry number, then refine the results by topic, using the phrase "molar absorption coefficient". This might result in some articles that contain the data, but the original documents will have to be consulted. In Beilstein Crossfire, the UV.EAC field contains numerically searchable extinction/absorption coefficient data.

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