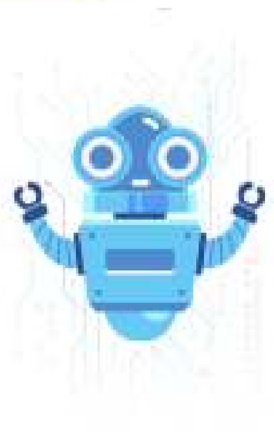
I'm not a bot



Concept of chromophore and auxochrome pdf

Chromophore and auxochrome examples. Chromophores and auxochromes. Chromophore and auxochrome pdf.

Molecular Coloration TheoryExploring the world of chromophores and auxochromes!A chromophore is essentially a "color-bearer" in Greek, referring to any isolated group that exhibits unique electromagnetic radiation absorption. This phenomenon occurs within the UV or visible spectrum, showcasing its distinct color-contributing properties.Chromophores are responsible for molecules absorbing specific wavelengths of light while reflecting others, resulting in the color we experience. The energy difference between two chemical orbitals within a chromophore falls within the visible spectrum region. When exposed to light, chromophores change conformation, influencing their interaction with electromagnetic radiation.Molecules requiring more than one chromophore to impart color are classified as dependent chromophores. For instance, acetone's single ketone group renders it colorless, whereas diacetyl's two ketone groups imbue a yellow hue.Chromophores can be categorized into two types: those containing only π electrons and undergoing π-π* transitions, such as ethylenic and acetylenic groups; and those containing both π and n (nonbonding) electrons, responsible for n-π* and π-π* transitions, like nitro, azo, carbonyl, and nitrite groups.These chromophores are saturated and unsaturated groups consisting of one or more non-bonded electron pairs. Linked to the chromophore, auxochromes assist in wavelength variation by increasing absorption intensity and shifting max wavelengths.Auxochromes enhance a molecule's color without imparting it themselves. Examples include OH, NH2, NHR, and NR2 groups. When combined with chromophores, auxochromes induce bathochromic shifts (redshifts), whereas their removal causes hypsochromic shifts (blueshifts). The introduction of auxochromes also results in a hyperchromic effect, increasing the intensity of absorption maxima.Bathochromic and hypsochromic shifts refer to the changes in absorption wavelengths. A bathochromic shift occurs when an auxochrome or solvent change causes absorption to shift towards longer wavelengths (redshift), whereas a hypsochromic shift happens when conjugation is removed or polarity increases, shifting absorption towards shorter wavelengths (blueshift). The hypochromic effect is observed when the extinction coefficient Emax decreases, often due to the introduction of a group that distorts the molecular geometry. This distortion leads to an increase in delocalization, which stabilizes the molecule and reduces its energy state. As a result, there is a shift in wavelength towards longer wavelengths, known as redshift. Conjugated double bonds, such as those found in 1,3-butadiene and 1,2-butadiene, absorb at higher wavelengths due to their increased delocalization. Similarly, aromatic rings with conjugated systems, like naphthalene and anthracene, exhibit longer absorption wavelengths. The polarity of the solvent can also influence the position and intensity of absorption bands. In particular, the presence of a polar hydrolytic solvent causes a hypsochromic shift in the n- -π* transition by decreasing the energy state of the autochrome's lone pair of electrons. Conversely, the π- π* transition is stabilized more in the presence of a polar solvent, leading to a bathochromic shift due to the lower energy gap between the HOMO and LUMO orbitals. The hypochromic effect can be understood using Beers' Law and Lambert's Law, which describe the relationship between the intensity of radiation passing through an absorbing medium. According to these laws, the rate of decrease in intensity is proportional to the concentration of the absorbing substance and the thickness of the absorbing medium. The extinction coefficient Emax plays a critical role in determining the position and intensity of absorption bands in a sample. Absorption Coefficient Calculations and Chromophore Concept: The intensity of incident radiation, Io, can be defined as Io - I, where I is the intensity after passing through the medium. The absorption intensity, Iabs, can be calculated using the formula: Iabs = Io - I. Additionally, the intensity of transmitted light, I, can be expressed as Io * 10^(-a'cx), where a' is the extinction coefficient and c is the concentration of the absorbing medium. Absorption laws may exhibit deviations due to various factors such as non-linear relationships between absorbance and concentration or physiochemical changes in solutions. These deviations can be categorized into positive, negative, instrumental, and physiochemical types. The concept of chromophore is essential in understanding absorption spectra. Chromophores are isolated covalently bonded groups that show characteristic absorption in the UV/Visible region. They can be classified based on electronic transitions, including π to π* transitions, n to π* and π to π* transitions, and σ to σ* and n to σ* transitions. Chromophoric structures can exhibit varying absorption wavelengths depending on their specific group composition. For instance, carbonyl groups are associated with absorption near 280 nm, while conjugated dienes show absorption near 233 nm. The presence of auxochromes can influence chromophore behavior by shifting the absorption band towards longer wavelengths. Auxochromes do not act as primary chromophores but enhance coloration by extending conjugation and sharing nonbonding electrons with the chromophore. This interaction leads to the formation of a new chromophore with distinct absorption characteristics. Benzene – 255nm (εmax - 203) Aniline – 280nm (εmax- 1430), the auxochrome group is – NH2 Examples of such groups include – OH, - OR, -NH2, -NHR, -NR2, -SH etc. Substituents can affect a chromophore in four ways: i. Bathochromic shift (red shift) – a shift to longer wavelength; lower energy ii. Hypsochromic shift (blue shift) – shift to shorter wavelength; higher energy iii. Hyperchromic effect – an increase in intensity iv. Hypochromic effect – a decrease in intensity Chromophore 200 nm 700 nm e Hypochromic Hypsochromic Hyperchromic Bathochromic Absorption and intensity shifts: Bathochromic shift: absorption shifted towards longer wavelength, change of solvent/auxochrome, red shift/bathochromic shift n to * transition for carbonyl compounds experiences bathochromic shift when the polarity of the solvent is decreased. Hypsochromic shift or effect: - Shift towards shorter wavelength – blue shift/hypsochromic shift - Change of solvent towards higher polarity or removal of conjugation Hyperchromic shift: - Shift due to increase in intensity - εmax increase - Due to the introduction of auxochrome, ex: Pyridine - 257 nm and εmax is 2750; 2 – methyl pyridine 262 nm and εmax is 3560 Hypochromic shift: - Inverse of hyperchromic shift – i.e., decrease of intensity - introduction of any group to the compounds which is going to alter the molecular pattern of the compound results in a hypochromic shifts, ex: biphenyl absorption is at 250 nm and 19000 εmax - Whereas 2–methyl biphenyl has an absorption of 237 nm and 10250 εmax Here's a rewritten version of the text with increased burstiness: The study of DNA and RNA bases has led to significant advances in understanding their stacking and cation binding properties. A 2007 review by Hannon (1) highlighted the importance of supramolecular DNA recognition, which has far-reaching implications for fields such as biomedicine and materials science. In terms of determining guanine plus cytosine content, researchers have employed various methods, including ultraviolet absorbance-temperature profiles. For example, Mandel and Marmur's work (2) in 1968 demonstrated the effectiveness of using UV absorbance-temperature profiles for determining the G+C content of DNA. Beyond DNA, researchers have also explored the use of ultraviolet absorption spectroscopy to study protein stability and folding. Mach et al.'s (3) 1995 review highlighted the importance of this technique in understanding protein structure and function. In addition to these findings, Wetlaufer's (4) 1963 work on ultraviolet spectra of proteins and amino acids provided valuable insights into protein chemistry. The study of aromatic residues in proteins has also been an active area of research. Levine and Federici's (5) 1982 paper demonstrated the use of model compounds for second-derivative spectroscopy to quantify aromatic residues. Furthermore, researchers have investigated insulin self-association, including spectrum changes and thermodynamics. Lord et al.'s (6) 1973 study provided valuable insights into this phenomenon. In recent years, scientists have developed new methods for determining protein and nucleic acid content of viruses using UV absorbance. Porterfield and Zlotnick's (7) 2010 paper presented a simple and general method for accomplishing this task. Lastly, the location of abnormal tyrosines in actin has been studied by researchers such as Mihashi and Ooi (8). Their work highlighted the importance of understanding protein structure at the molecular level.