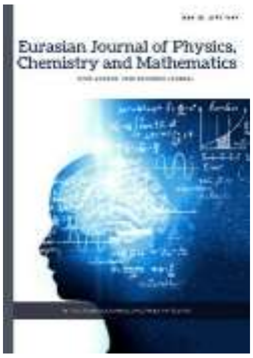

Identification of Typical Functional Groups in Organic Molecules in Absorption Spectroscopy

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ABSTRACT

Spectroscopy is one of the many significant techniques that are employed in the study of physical phenomena. The term "spectrometre" refers to the devices that are utilised in the process of determining the spectra of various chemicals. They are utilised on the compound itself, and there is also the potential for them to be utilised in the analysis of the fragments that are acquired during the degradative process. There are many other kinds of spectroscopy, including ultraviolet, infrared, visible electron spin resonance, nuclear magnetic resonance (NMR), and mass spectroscopy; however, absorption spectroscopy only applies to ultraviolet, visible, and infrared spectroscopy. Molecules that contain double or triple bonds have stable excited states that, when stimulated, give rise to spectra in the near ultraviolet range. As a result, the presence of such a spectrum assists us in detecting and determining the presence of unsaturation. Molecules that are saturated with hydrocarbons, alcohals, ethers, and other substances are see-through in the near ultraviolet. Compounds like acetone and acetic acid, which only have a single multiple bond, are examples.

Keywords: *Organic , Molecules, spectrometer , Absorption , Spectroscopy*

Introduction

Spectrophotometric Studies of the Metal Complexes-

Up until quite recently, structural conclusions were virtually always relied only on data that was chemical in nature. In today's world, physical approaches are regarded as indispensable instruments for clarifying structural details. They are utilised on the compound itself, and there is also the potential for them to be utilised in the analysis of the fragments that are acquired during the degradative process. Spectroscopy is one of the many significant techniques that are employed in the study of physical phenomena. The term "spectrometre" refers to the devices that are utilised in the process of determining the spectra of various chemicals. There are many other kinds of spectroscopy, including ultraviolet, infrared, visible, electron spin resonance, nuclear magnetic resonance (NMR), and mass spectroscopy; however, absorption spectroscopy only applies to ultraviolet, visible, and infrared spectroscopy.

Absorption Spectroscopy:-

Absorption Spectroscopy is one of the scientific subfields that dates back to the beginning of the discipline. In the early years of the eighteenth century, Newton presented the optical principles necessary for spectroscopic investigations. A few years later, Bouguer published his observations on the change in intensity of a beam as it passes through various thicknesses of absorbing material. Both of these men made significant contributions to the field of spectroscopy. century the century During the second half of the nineteenth century, spectroscopists working with emission and absorption techniques made discoveries that laid the ground work for the early twentieth century theories of atomic and molecular structure. Recent refinements of these theories have been based primarily upon modern spectroscopic measurements.

Herschel discovered the infrared zone for the first time in the year 1800, and Coblentz was the first scientist of the current century to devote a great deal of attention to researching it. A realisation of the occurrence of "characteristic frequencies" for absorption by functional groups in organic molecules emerged as a direct result of these findings. These radiations are measured not only in wave length (expressed in micron =1 =10-4 cm or 10-4) but also considered in frequency, which is expressed not in cycles per second but in wave numbers cm, which is also known as reciprocal centimetres. The ultraviolet radiation ranges from 2000-4000° A, while the visible radiation ranges from 4000-7500 A, and the infrared radiation ranges from 1-33. The wave number is equal to the reciprocal of the wave length in centimetres and is defined as the number of waves that occur for every centimetre.

Ultraviolet (200-400 $m\mu$) and visible spectra (400-750$m\mu$):

Although it is possible to identify a small number of functional groups, this portion of the spectrum is most beneficial when it comes to determining the presence and form of unsaturation, particularly in conjugated systems. The analysis of the absorption at and the position of the maxima provides us with helpful information that enables the identification of typical functional groups found in organic compounds. Molecules that contain double or triple bonds have stable excited states that, when stimulated, give rise to spectra in the near ultraviolet range. As a result, the presence of such a spectrum assists us in detecting and determining the presence of unsaturation. Molecules that are saturated with hydrocarbons, alcohals, ethers, and other substances are see-through in the near ultraviolet. Compounds with only one multiple bond, such as acetone, acetic acid, and others, have absorbance intensities that are extremely low and are thus not nearly acceptable for identification. When there are two or more double bonds (or triple bonds) in a molecule that are separated by two or more single bonds, the absorbance is nearly additive. On the other hand, if two multiple bonds are separated from one other by a single bond, which is the case with conjugated bonds, a very high absorbance is the consequence.

Aromatic compounds have many absorption bands; for instance, benzene absorbs light at 184 (E,60000), 204 (E,7400), and 254 (E, 200) nm. All are $\pi \rightarrow \pi$ transitions, and the band with a wavelength of 254 nanometers is referred to as the benzenoid band. This band is distinguished by having an exceptionally high degree of fine structure. In the benzenoid band, benzene derivatives are typically found. between 250 and 280 nm, however for polynuclear aromatics it shifts to longer wave lengths as the number of rings grows, moving to bigger values as the number of rings increases.

Objectives of the Study

1. To study on Absorption Spectroscopy
2. To study on Infra red absorption spectrophotometry

Infra red absorption spectro-photometry:

The analysis of infrared spectra can yield a significant amount of information, such as the existence of a variety of functional groups and the strength of hydrogen bonds (intra molecular and inter molecular). The determination of the conformational orientations of cis and trans isomers, the orientation of aromatic compounds, and so on. In order for a substance to be able to absorb in the infrared region, it is necessary for the vibrations in the molecule to give birth to an asymmetrical charge distribution. This is the key need. Because of this, it is not required that the molecules have a dipole moment that is stable throughout time. The portion of the form 2.5 that is of interest for the purposes of analysis μ to a wave number of 25 or between 4000-400 (waves per centimetre, cm). The typical optical materials, such as glass or quartz, have a high absorption coefficient in the infrared spectrum. As a consequence of this, the instrumentation used for measuring spectra in the infra red area is noticeably dissimilar to that utilised for the visible and ultra violet regions. The many patterns of vibration and rotation that occur within a molecule are what give rise to its infrared spectrum. When wave lengths are less than 2.5 μ , Changes in the vibrational and rotational levels of the molecule can be brought about as a result of the rotation since it possesses enough energy to do so. Pure rotating spectra of molecules may only be observed at wave lengths that are significantly longer than the long wave length limit (2.5). μ) in the case of the majority of infrared spectrophotometers.

Infra Red Spectra (4000-650 Cm^1)

The environment of the molecule as a whole has an effect on the frequency of the individual bonds that make up the molecule. Nevertheless, some bonds exhibit characteristics that set them apart from other bonds. are more stable than single bonds, and X-H type bonds (N-H, O-H, C-H, etc.) feature the very light hydrogen atoms at the terminals of the molecule. These are equivalent to springs that are exceptionally powerful, or these are the connecting balls for terminals that are really light. And much like the spring-ball system, the vibrations of these bands are only moderately impacted by the motions of the rest of the molecules. Therefore, the stretching frequencies of these particular bands appear within a range that is typical for their separate types of bands; taken as a whole, these frequencies appear in the range of 3600 cm to 1500 cm.

In the region below 1600 xxcm, these bands emerge because of the stretching of single bonds, such as C-C, C-N, C-O, C-halogen, etc., as well as those bands that appear because of the bending of various bands. Single bonds have bond stretching of about the same order, and in addition to this, they are typically connected cumulatively, such as C-C-C-0. Single bonds have bond stretching of roughly the same order. Because of this, there is a stronger reciprocal interaction between the bands, a larger variety of appearances for the bands, and a significant sensitivity of band positions to even modest changes in the structure. The portion of the infrared spectrum with lower frequencies, between 1300 and 650 cm, is referred to as the finger print region, and within this region, each chemical has its own unique pattern. Infrared spectroscopy offers a way for comparing compounds that is superior to the more common approach of calculating the melting point of a combination.

The infrared spectrum can tell us the structure of a novel substance by identifying which groups of atoms are present in the molecule and which ones are missing. The characteristic absorption bands, or frequencies, that a given compound absorbs light of are almost always the same from one compound to the next. These bands are caused by a particular collection of atoms. At 3200-3600 cm cm, the OH group of alcohols has the strongest absorption, followed by the C=O group of ketones between 1700 cm, and the CH group at 1450 and 1375 Cm. the The stretching frequencies grow in the sequence from 700 to 1500 cm but are dropped to 2630 cm when the band strength increases from a single bond to a double bond to a triple bond. In the case of the 0-0 bond, the band strength is unaltered; the only change is an increase in the mass. Because of the fact that the C-0 stretching frequency arises between 2000 and 1500 cm-1 and is particularly sensitive to variations in structure and environment, the corbonyl group absorptions are extremely valuable in the field of organic chemistry.

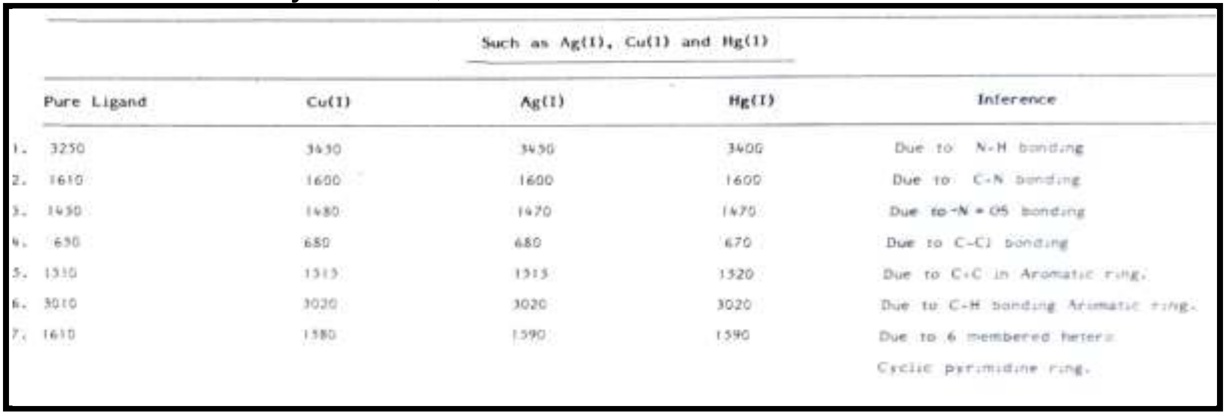
It might be challenging to interpret the bands in an I-R spectrum that have been seen to overlap with other bands. It is possible for the absorption band of a certain group to be displaced by conjugation, neighbouring electrons with drawing substituents, or hydrogen bonding, and it is also possible for this band to be mistaken with the band of a different group.

Research Method

Experimental:

On an automated Perkin-Elmer 577 spectrophoto metre set to NBr phase and slow scan mode, all of the infra red absorption spectra were recorded. The spectrum results suggest that there is a change in the absorption frequencies due to the creation of complexes. The first maxima in all of the ligands can be attributed to N-H bonding and can be found between 3200 and 3400 cm-1. The chelation process is responsible for the shifting of this maximum in the chelates between 3400 cm and 3650 cm. The shifting of the other absorption frequencies in chelates is additional confirmation of the creation of chelates. Table No.1 contains a recording of the numerous absorption frequencies that are associated with the groups and bands that are present in the molecules that make up ligands and complexes.

Table no. 1 Frequencies of Absorption for 2 Chloro, 4 Phenyl Thio Uracil, and 6 Phenyl Pyrimidine, as well as Metal Chelates of Metals

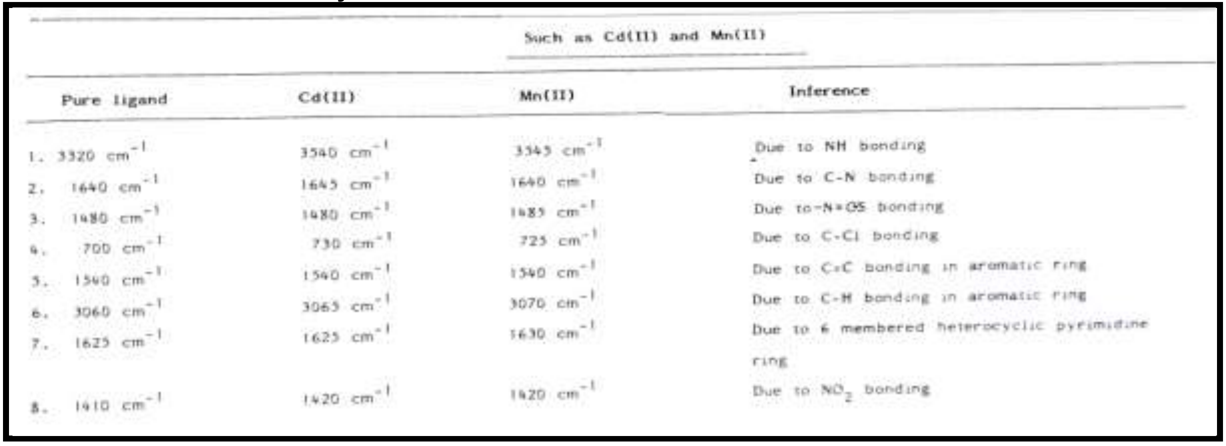


Such as Ag(I), Cu(I) and Hg(I)

Pure Ligand	Cu(I)	Ag(I)	Hg(I)	Inference
1. 3250	3430	3450	3400	Due to N-H bonding
2. 1610	1600	1600	1600	Due to C-N bonding
3. 1450	1480	1470	1470	Due to -N = OS bonding
4. 650	680	680	670	Due to C-Cl bonding
5. 1510	1515	1515	1520	Due to C=C in Aromatic ring.
6. 3010	3020	3020	3020	Due to C-H bonding Aromatic ring.
7. 1610	1580	1590	1590	Due to 6 membered hetero Cyclic pyrimidine ring.

Data Analysis

Table No.2 Absorption Frequencies of 2 Chloro-4-Nitro-Phenyl-Thio-Uracil-6-Phenyl-Pyrimidine and Metal Chelates of Metals



Such as Cd(II) and Mn(II)

Pure ligand	Cd(II)	Mn(II)	Inference
1. 3320 cm^{-1}	3540 cm^{-1}	3545 cm^{-1}	Due to NH bonding
2. 1640 cm^{-1}	1645 cm^{-1}	1640 cm^{-1}	Due to C-N bonding
3. 1480 cm^{-1}	1480 cm^{-1}	1485 cm^{-1}	Due to -N=OS bonding
4. 700 cm^{-1}	730 cm^{-1}	725 cm^{-1}	Due to C-Cl bonding
5. 1540 cm^{-1}	1540 cm^{-1}	1540 cm^{-1}	Due to C=C bonding in aromatic ring
6. 3060 cm^{-1}	3065 cm^{-1}	3070 cm^{-1}	Due to C-H bonding in aromatic ring
7. 1625 cm^{-1}	1625 cm^{-1}	1630 cm^{-1}	Due to 6 membered heterocyclic pyrimidine ring
8. 1410 cm^{-1}	1420 cm^{-1}	1420 cm^{-1}	Due to NO_2 bonding

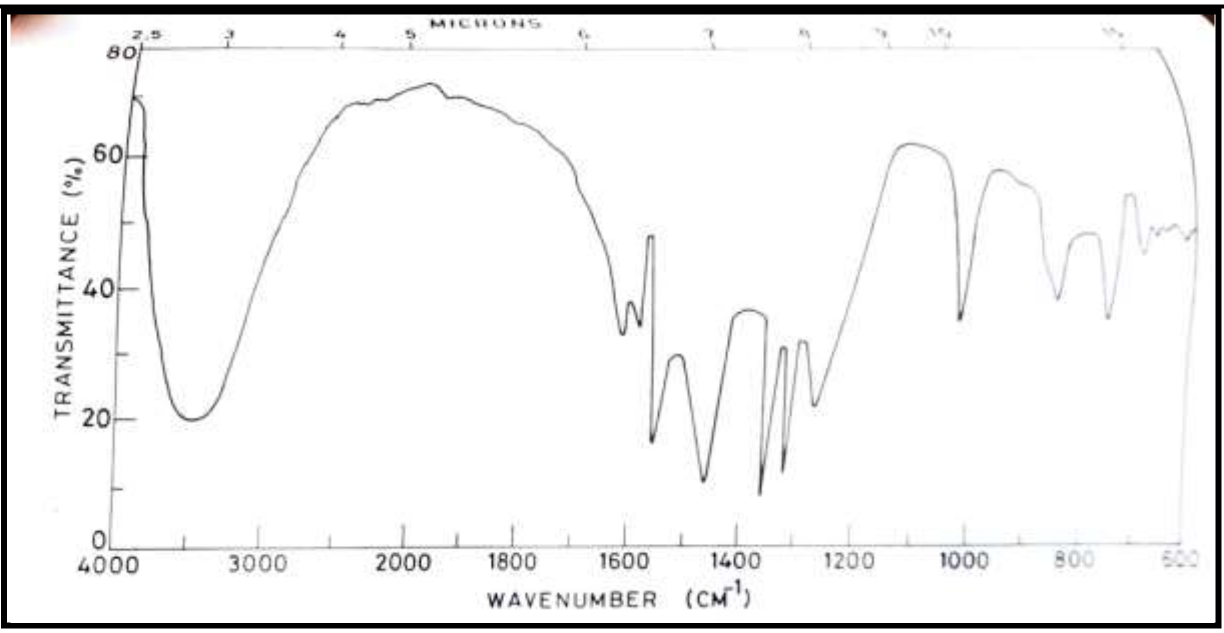


Figure 1 IR spectrum of Cd(II) CNpTUpP

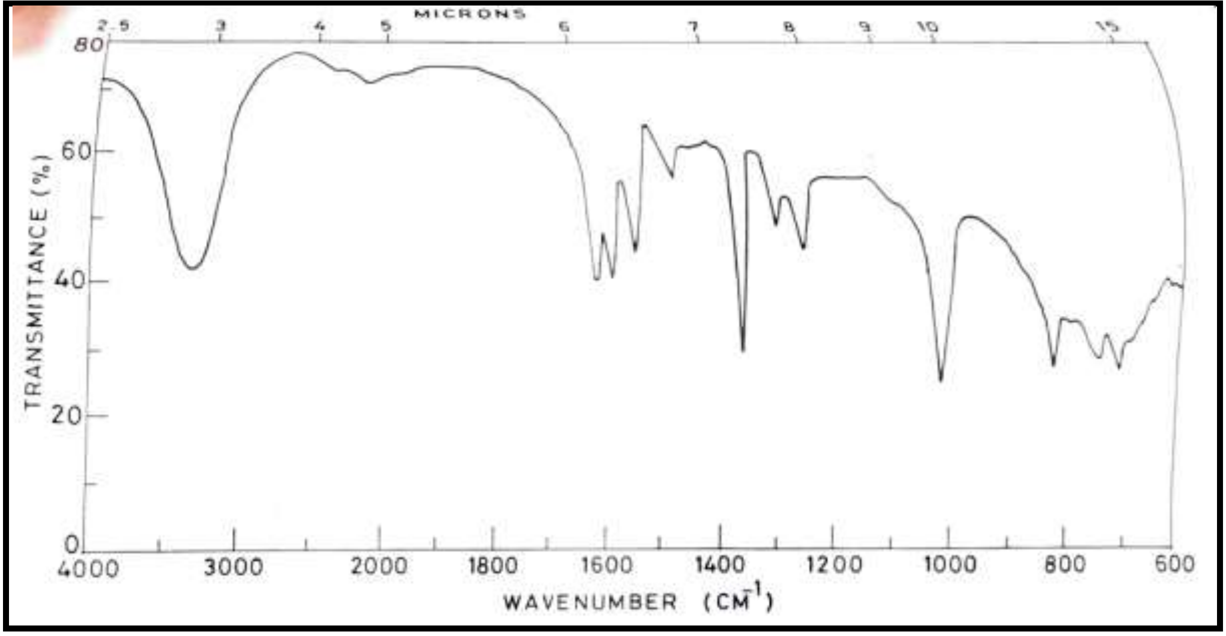


Figure 2 IR spectrum of Mn(II) CNpTUpP

METAL CHELATES OF METALS SUCH AS Cu(II), Cd(II), Ni(II) Co(II) and Mn(II):-

A Gouy In order to determine the magnetic susceptibilities of the metal chelates, a magnetic balance was utilised. The composition ML2 corresponds to the metal chelates that contain the aforementioned elements.

Where M Cu(II), Cd(II), Ni(II) Co(II) and Mn(II)

$LH = C_{17}H_{13}N_4SCl$

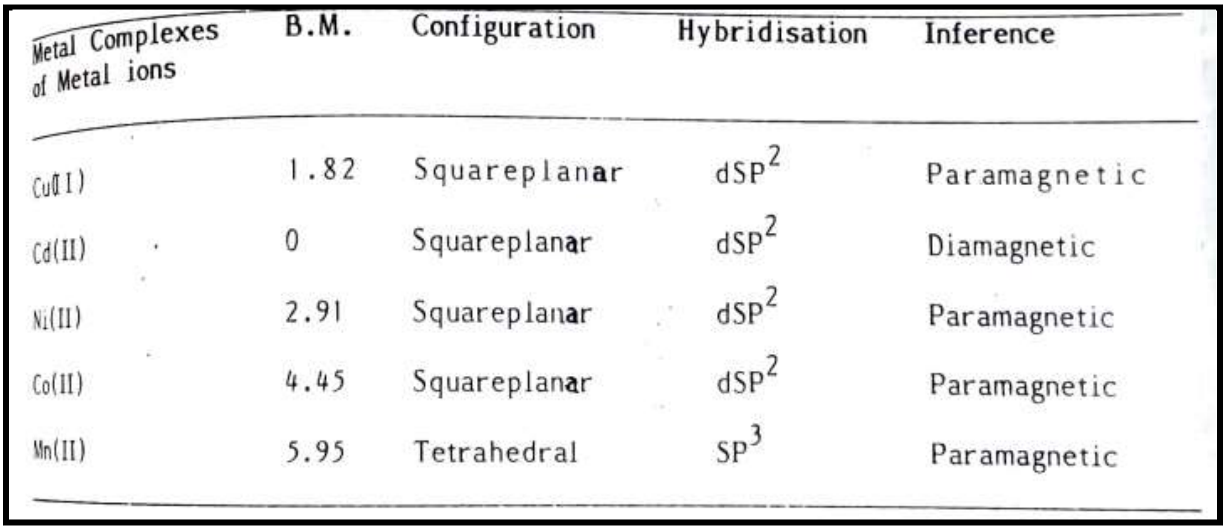
$C_{17}H_{12}N_4SClBr$

$C_{17}H_{12}O_2N_5SCl$

The magnetic moments that are possessed by the copper complexes fall somewhere in the region of 1.8-1.9 B.M. On the basis of the electronic spectra, it is anticipated that the Cu(II) complex has either a planar or tetragonally distored octahedral configuration. It is more likely that the complex has a planar configuration. It was discovered that the Cu(II) complexes have one unpaired electron, making them paramagnetic.

It has been discovered that Cd(II) complexes are diamagnetic because they do not contain any unpaired electrons. Their configuration is square and planar, and they have. It has been determined that magnetic moments are zero. hybridization with dSp2 It was discovered that the magnetic moments of Ni(II) complexes lie in the range of (2.9-3.4) B.M., which are more or less comparable to those of the metal ion. Ni(II) complexes were found to have two electrons that were not linked up. It was discovered that dSp2 hybridization produces a paramagnetic state in Co(II) complexes. It was discovered that Mn(II) complexes that have a tetrahedral structure and Sp hybridization are magnetic in a paramagnetic state.

The magnetic moments of each of the metal complexes described above may be found in the tables that follow: The magnetic moments of metal complexes containing the ligand CpTUPP, including those containing the metals Cu(II), Cd(II), Ni(II), Co(II), and Mn(II), are listed in Table No. 3.



Metal Complexes of Metal ions	B.M.	Configuration	Hybridisation	Inference
Cu(II)	1.82	Squareplanar	dSP^2	Paramagnetic
Cd(II)	0	Squareplanar	dSP^2	Diamagnetic
Ni(II)	2.91	Squareplanar	dSP^2	Paramagnetic
Co(II)	4.45	Squareplanar	dSP^2	Paramagnetic
Mn(II)	5.95	Tetrahedral	SP^3	Paramagnetic

Table No. 3 presents the magnetic moments of metal complexes containing the ligand CbpTUPP, such as Cu(II), Cd(II), Ni(II), Co(II), and Mn(II).

Conclusion

The analysis of the absorption at and the position of the maxima provides us with helpful information that enables the identification of typical functional groups found in organic compounds. Molecules that contain double or triple bonds have stable excited states that, when stimulated, give rise to spectra in the near ultraviolet range. As a result, the presence of such a spectrum assists us in detecting and determining the presence of unsaturation. Molecules that are saturated with hydrocarbons, alcohols, ethers, and other substances are see-through in the near ultraviolet. Compounds with only a single multiple bond, such as acetone, acetic acid, and others, have absorbance intensities that are extremely low and are thus not nearly acceptable for identification. When there are two or more double bonds (or triple bonds) in a molecule that are separated by two or more single bonds, the absorbance is nearly additive. On the other hand, if two multiple bonds are separated from one other by a single bond, which is the case with conjugated bonds, a very high absorbance is the consequence.

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