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Optical and Spectral Properties of Aqueous Magnesium Chloride Solution: An Experimental Study

This spectroscopic study presents absorption and fluorescence spectra of $MgCl_2$ to provide valuable insights into the electronic structure, energy levels, and interaction of 10^{-3} M $MgCl_2$ solution with light as an absorption peak was recorded at 255 nm. The $MgCl_2$ solution can be commonly used for dust control, ice control and road stabilization. In addition, it has a wide range of applications such as serving as a fertilizer, a mineral supplement for animals, a wastewater treatment agent, a component of artificial seawater, and a material for textiles, paper and cement. It can also be found in many pharmaceutical, topical or skin-related applications, and the understanding of its absorption for UV radiation could contribute to the development of UV-blocking materials or environmental sensors in the future.

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1. Introduction

Magnesium chloride is a highly soluble white crystalline solid that absorbs moisture from the air, often to the point of dissolution in water, to give an aqueous form, called aqueous magnesium chloride solution [1]. It has a linear structure containing four pairs of electrons and one pair of electrons around the central magnesium atom [2]. Magnesium chloride, $MgCl_2$, has 16 valence electrons in its valence shell, eight of which are bonded electrons [3]. It is an important industrial chemical compound [4]. Also, it is a versatile compound known for its interesting optical properties, especially when dissolved in water. Understanding the optical behavior of this solution is essential for basic scientific research and practical applications in various fields including chemistry, biology and environmental science. It is used in the production of magnesium [5]. In addition, magnesium chloride is one of the substances used in some medications and nutritional supplements that help treat or prevent low blood magnesium levels [6,7]. It is also used in the manufacture of wound disinfectants and the removal of suspended particles in water and sewage treatment plants [8,9]. It is also used in sugar beet processing, preventing soil erosion, processing of cotton and woolen fabrics, de-icing agent, keeping drilling tools cool, and in manufacture of paper and ceramic materials [10]. The optical properties of $MgCl_2$ using UV-visible and fluorescence spectroscopy can provide valuable information about its electronic structure, purity, and chemical environment [11,12]. This knowledge has diverse applications in materials science, analytical chemistry, biology, environmental monitoring, and various industries [13]. Fluorescence spectroscopy provides valuable insights into the electronic structure and interactions within the solution, while UV absorption measurements offer detailed information about the energy levels and electronic transitions of the species present [14]. The unique structure of $MgCl_2$ solution, where each Mg^{2+} ion is surrounded by water molecules and Cl^{2-} ions, influences its optical properties significantly. The presence of water molecules as ligands can modify the electronic environment around the Mg^{2+} ion, affecting its interaction with light and thus altering its absorption and emission spectra [15]. By systematically exploring these optical properties, this study aims to elucidate the underlying mechanisms governing the behavior of magnesium chloride solutions in different solvent environments. Such insights are crucial for advancing our understanding of solution behavior and for potentially guiding the development of novel optical materials or chemical, and physics sensors [16].

In this study, the experimental methods employed to measure fluorescence and UV absorption spectra of $MgCl_2$ solution were presented, followed by the analysis and interpretation of the obtained data. The results contribute to the broader understanding of how molecular structure impacts optical properties in aqueous solutions, thereby bridging fundamental research with practical applications, and its' potential future applications span across energy storage, construction, healthcare, and environmental sectors pending further research and development.

2. Experimental Part

An $MgCl_2$ solution was prepared in 99.99% pure dioxin concentration, with $1x10^{-3}$ M. The optical properties and constants of $MgCl_2$ solution were determined and studied using SHIMADZU UV-3101PC UV-VIS-NIR spectrophotometer. Specifically, chloride ions can absorb UV light in the 200-250 nm range due to electronic transitions, while the visible light is not significantly absorbed by the magnesium ion.

3. Results and Discussion

The optical constants of the $MgCl_2$ solution were determined by studying its absorption spectrum in the wavelength range of 200-900 nm. An absorption peak was recorded at 255 nm as shown in Fig. (1) while no absorption activity was observed in the wavelength range > 255 nm. The reflectance can be determined according to the law of conservation of energy [1]:

$$R = 1 - A - T \qquad (1)$$

From Fig. (2), it is clearly shown that the reflectance curve reaches its maximum value of 0.057 nm at 210 nm and then it gradually decreases to its second maximum at 250 nm (0.039).

The absorption coefficient (α) was calculated from the following equation:

$$\alpha = 2.303\ A/t \qquad (2)$$

where A is the absorbance, and t is the sample thickness

The extinction coefficient (k_0) can be determined from the following equation:

$$k_o = \frac{\alpha\lambda}{4\pi} \qquad (3)$$

where λ is the wavelength of the incident radiation

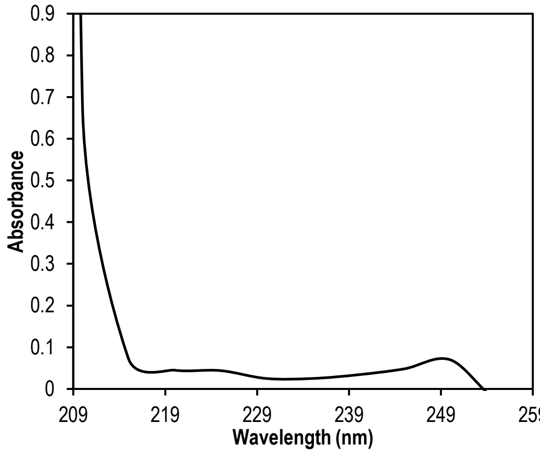

Fig. (1) Absorption spectrum of $MgCl_2$ solution with concentration of 10^{-3} M

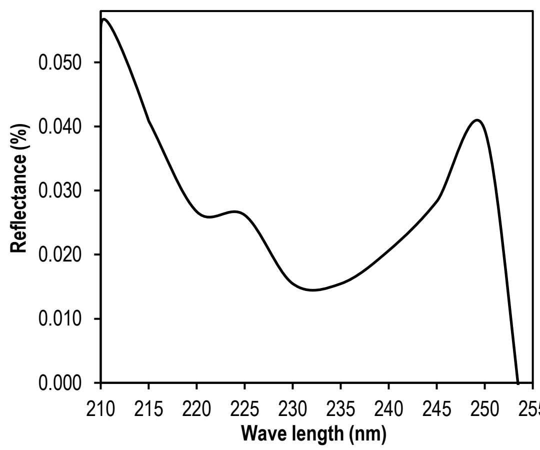

Fig. (2) Reflectance as a function for $MgCl_2$ solution with concentration of 10^{-3} M

From Fig. (3), it was clear that the extinction coefficient (k_0) is maximized at 205 nm and the relationship between the extinction coefficient and wavelength for $MgCl_2$ in UV region depends on the specific electronic transitions and energy levels involved in the molecule's absorption spectrum. So, it represents a measure of how strongly a substance absorbs light at a particular wavelength.

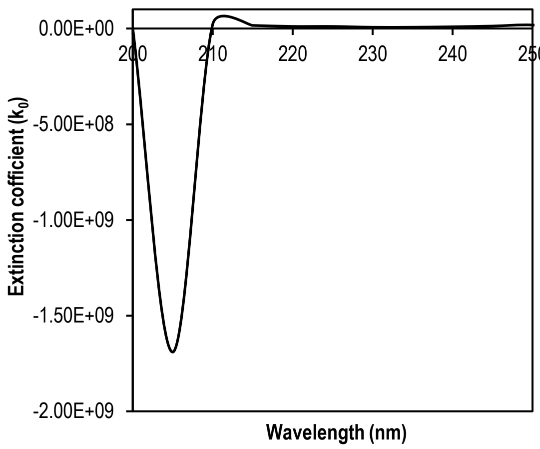

Fig. (3) Relationship between extinction coefficient and wavelength for $MgCl_2$ solution with concentration of 10^{-3} M

The refractive index of the sample is related to the reflectance and extinction coefficient as shown below:

$$n_0 = \Big[\Big(\frac{1+R}{1-R}\Big)^2 - \big({k_0}^2 + 1\big)\Big]^{1l2} + \Big(\frac{1+R}{1-R}\Big)\Big] \qquad (4)$$

Figure (4) shows the variation in the refractive index as a function of the wavelength. It can be seen that the refractive index shows the same behavior as the reflectance according to Eq. (4).

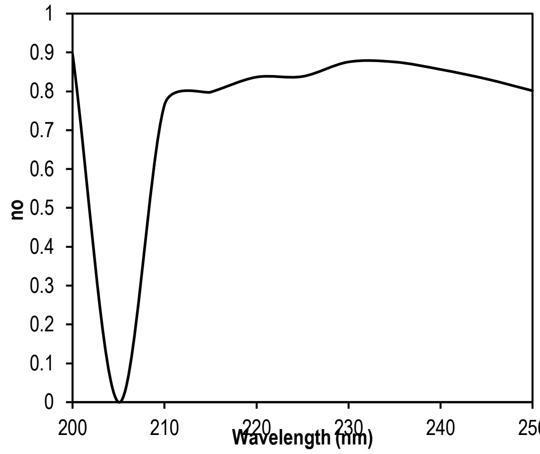

Fig. (4) Relationship between the refractive index (n_o) and the wavelength

The real (ε_r) and imaginary (ε_i) parts of the dielectric constant are determined as [6]:

$$\varepsilon_r = {n_o}^2 - k_o \qquad (5)$$

$$\varepsilon_i = 2n_o\, k_o \qquad (6)$$

Figures (5) and (6) show the variation of real and imaginary parts of dielectric constant with photon energy ($h\nu$) to describe the ability of the material ($MgCl_2$) to store and release the energy, where its maximum value equals 0.25 when photon energy is

(4.509), while the imaginary part (ε_i) of the dielectric constant maximum value (2.254) at the same value of photon energy.

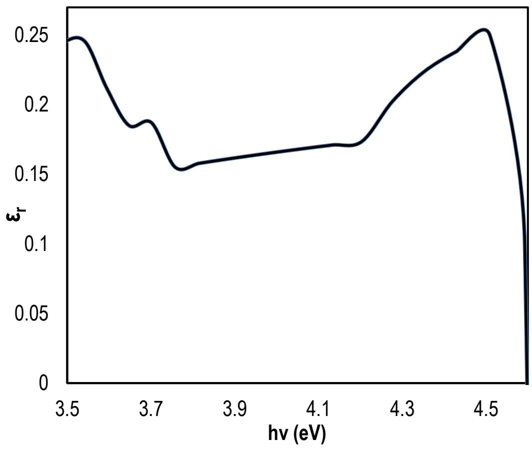

Fig. (5) Relationship between the real part of dielectric constant (ε_r) and the photon energy (hv)

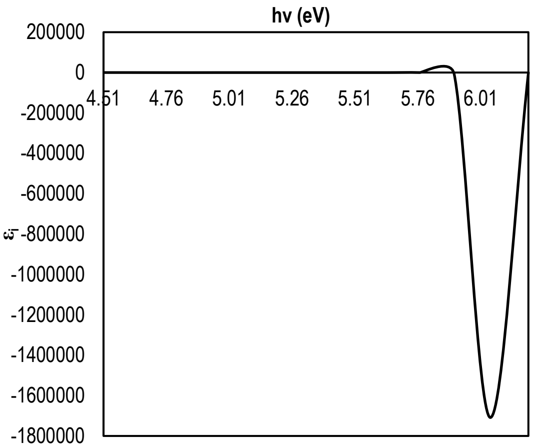

Fig. (6) Relationship between the imaginary Part of the dielectric constant (ε_i) and the photon energy (hv)

The real part of the dielectric constant of the $MgCl_2$ solution is relatively small, which may be attributed due to the concentration of ions in the solution and the interaction between ions and solvent molecules. The imaginary part (εi) accounts for the energy loss due to the dissipation of energy in the material. For $MgCl_2$ solution, the presence of mobile ions (Mg^{+2} and Cl^{-}) can conduct energy, thereby significantly affecting the imaginary part of dielectric constant. Therefore, a high ε_i value indicates that the solution has a significant ability to dissipate energy as heat. The fact that the real part of the dielectric constant in a solution of $MgCl_2$ is smaller than the imaginary part indicates that the solution is more capable of dissipating energy (ε_i) than storing it (ε_r). This behavior is typical for electrolytes and solutions containing mobile ions, enabling remarkable conductivity and energy dissipation. It is important to consider this behavior when analyzing the dielectric properties of $MgCl_2$ solutions, especially in applications where energy loss and conductivity are critical factors.

By studying the fluorescence spectrum of $MgCl_2$ solution within a wide range of wavelengths (250-520nm) when the solution is excited with a 400nm radiation. The maximum wavelength corresponding to the highest intensity of the fluorescence spectrum (λ_{maxflu}) was 429nm at the highest width of the aperture. This peak was shifted towards longer wavelengths (redshift) – specifically at 433nm – when the aperture width was decreased, then the apex position became at 405nm for the smallest aperture width. This corresponds to a decrease in the relative intensity of fluorescence, as shown in Fig. (7).

The following equation was used to calculate the quantitative efficiency of the studied particles in an approximate manner and with a water solvent

$$q_{FM} = \frac{Area\ under\ the\ curve\ of\ the\ fluorescence}{Area\ under\ the\ curve\ of the\ relative\ absorption} \qquad (7)$$

Table (1) shows the effect of changing the aperture width on the fluorescence spectrum of $MgCl_2$ solution with concentration of 10^{-3} M. The fluorescence quantum yield was roughly estimated by calculating the area under the curves of the fluorescence spectrum and the relative absorption spectrum using Eq. (7) and MATLAB 6.5 software. The solution was diluted to reduce the internal quenching processes competing the fluorescence emission from the electronic state S10.

Table (1) Effect of changing the aperture width on fluorescence and quantum yield

Width slit (nm)	Relative Intensity (a.u.)	$\lambda_{max(flu)}$ (nm)	Bandwidth Δλ (nm)	q_{FM}
1.5x1.5	23.300	407	151	0.24
1.5x1.3	23.056	406	51	0.25
3x1.5	137.720	409	54	0.95
3x3	515.015	425	20	0.96

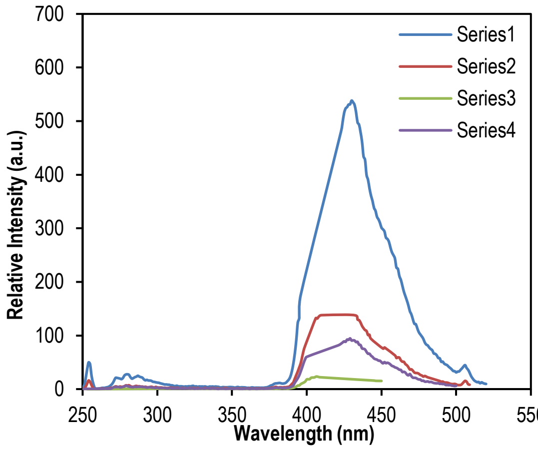

Fig. (7) Fluorescence spectra of 10^{-3} M $MgCl_2$ solution

Table (1) shows the experimental values of the fluorescence intensity and quantum yield that were calculated throughout the difference in the aperture width of the device for $MgCl_2$ solutions.

4. Conclusion

The absorption of aqueous $MgCl_2$ solution within the UV region was studied and attributed to the electronic interaction and transitions of Mg^{2+} ions, just like most metal ions. This absorption promotes electrons to higher energy levels. These transitions can occur together, contributing to shaping the absorption spectrum in complex ways. The extinction coefficient in the UV region is influenced by several factors; mainly electronic transitions, energy levels, molecular structure, overlapping, or complex electronic transitions. The real part of dielectric constant behaves the same way as the refractive index, while the imaginary part of dielectric constant behaves the same way as the extinction coefficient. This is because the real part is related to reflection and the interaction of the material with the electric field, while the imaginary part is related to absorption processes.

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