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Department of Physics

Determination energy gap of ZnO in sunscreen for UV protection

This Research is submitted to the College of Science / University of Salahaddin – Erbil, as Part of the Requirement for Bachelor's Degree in the Department of physics

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To…...My Mother

To…...My Father

To…...My Brothers, Sister and My Colleagues…

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Abstract

Sunscreens containing metal oxide nanoparticles appear transparent on the skin and provide excellent protection against sun burn caused by UV radiation. Zinc oxide (ZnO) is one of the most interesting metal oxides used for medicine applications to absorbed the ultraviolet (UV-rang)of sun spectrum. Different Sun screen ointment in a various medicine company made was investigated. The ZnO was deposited on glass substrate to determine the energy band gap (E_g), The UV- visible spectroscopy was used to detection the transmittance spectrum of light and the absorption coefficientfor these ointments. The results sample S1 has same value nearest to theoretical band gap (3.37 eV) of ZnO.

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Chapter one

General Introduction

1.1 Introduction

Nanotechnology is the most innovative field of 21st century. Extensive research is going on for commercializing nanoproducts throughout the world. Due to their unique properties, nanoparticles have gained considerable importance compared to bulk counterparts. Among other metal nanoparticles, zinc oxide nanoparticles are very much important due to their utilization in gas sensors, biosensors, cosmetics, drug-delivery systems, and so forth. Zinc oxide is an inorganic compound with the molecular formula ZnO. It appears as a white powder and is nearly insoluble in water. The powder ZnO is widely used as an additive in numerous materials and products including ceramics, glass, cement, rubber (e.g., car tyres), lubricants, paints, ointments, adhesives, plastics, sealants, pigments, foods (source of Zn nutrient), batteries, ferrites, and fire retardants. In the Earth crust ZnO is present as zincite mineral but mostly ZnO used for commercial purposes is produced synthetically. ZnO is often called II-VI semiconductor in materials science because zinc and oxygen belong to the 2nd and 6th groups of the periodic table. ZnO semiconductor has several unique properties such as good transparency, high electron mobility, wide band gap, and strong room temperature luminescence. These properties account for its applications in transparent electrodes in liquid crystal display and in energy-saving or heat-protecting windows and other electronic applications. Zinc oxide (wurtzite, p63m) is known as wide band gap semiconductor with band gap energy of 3.3eV at room temperature (RT). Nowadays the unique properties of nanomaterials have motivated the researchers to develop many simpler and inexpensive techniques to produce nanostructures of technologically important materials. Several metal oxide nanoparticles are produced with possible future applications. Among them zinc oxide is considered to be one of the best exploited at nanodimensions. The wide band gap and large excitonic binding energy have made zinc oxide important both for scientific and industrial applications.(Siddiqi, K.S., ur Rahman, A., Tajuddin, N. and Husen, A., 2018.)

1.2 Solar Radiation

Solar radiations are becoming increasingly appreciated because of their influence on living matter and the feasibility of its application for useful purposes. It is a perpetual source of natural energy that, along with other forms of renewable energy, has a great potential for a wide variety of applications because it is abundant and accessible. Solar radiation is rapidly gaining ground as a supplement to the nonrenewable sources of energy, which have a finite supply. The electromagnetic radiation emitted by the sun covers a very large range of wavelengths, from radiowaves through the infrared, visible and ultraviolet to X-rays and gamma rays.(Bhatia, S.C. ed., 2014.)

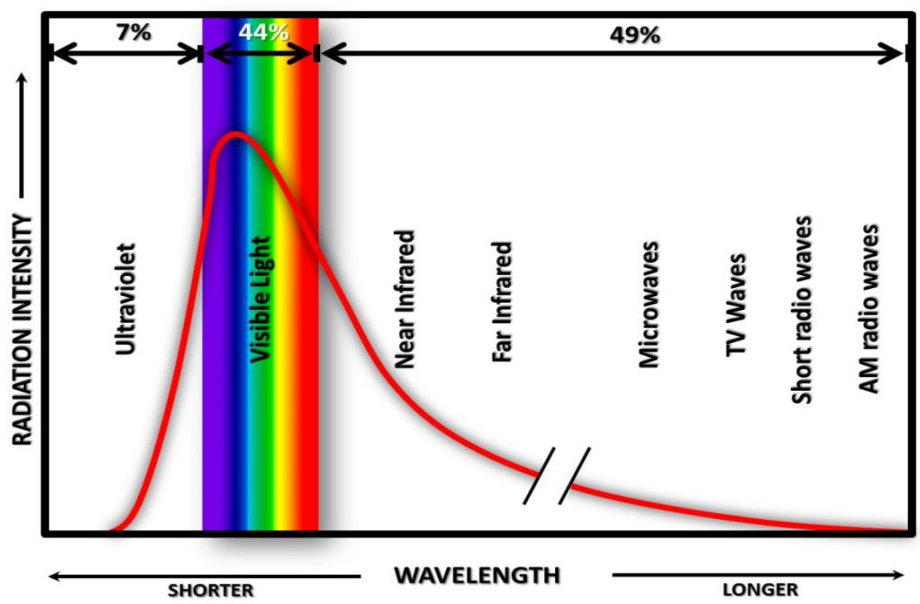

Figure 1.1 spectrum of solar radiation.

1.3 Types of UV-Spectrum

UV radiation is a simple one form of the energy coming from the sun ,The UV-spectrum wavelength is shorter than visible light, but longer than X rays, The typical range of UV-wavelength is 100-400nm.UV is invisible to human eyes. the types of UV-spectrum as showed in table 1.1, [11].

Table 0.1 Types of UV-spectrum.

Name	Abbreviation	Wavelength (nm)	Photon energy (eV, J)	UV _ rays and their effect on skin
Ultraviolet A	UVA	315–400	3.10–3.94 (0.497–0.631)	Can penetrate deep into the skin's surface, causing DNA change that can result in skin cancer.
Ultraviolet B	UVB	280–315	3.94–4.43 (0.631–0.710)	Reach skin's surface can cause surface tanning, burning and signs of aging.
Ultraviolet C	UVC	100–280	4.43–12.4 (0.710–1.987)	Not penetrate the earth's ozone layer.

1.4 Sun Screen

Sunscreens are the agents which are used to prevent the skin from the harmful ultraviolet radiation of sun. Sunscreen can be physical, chemical or natural sunscreen. The effectiveness of sunscreen agents can be measured in terms of Sun Protection Factor (SPF) (Couteau, C., Paparis, E., El-Bourry-Alami, S. and Coiffard, L.J.M., 2012.) The function of ZnO nanoparticles in sunscreens is to absorb ultraviolet radiation to reduce, eliminate and/or prevent sunburn and premature aging of the skin (Khan, A.U.H., Liu, Y., Fang, C., Naidu, R., Shon, H.K., Rogers, Z. and Dharmarajan, R., 2023.)

1.5 Zinc oxide(ZnO):

Zinc oxide (ZnO), as a material with attractive properties, has attracted great interest worldwide, particularly owing to the implementation of the synthesis of nano-sized particles. High luminescent efficiency, a wide band gap (3.36 eV), and a large exciton binding energy (60 meV) has triggered intense research on the production of nanoparticles using different synthesis methods and on their future applications ZnO nanomaterials can be used in industry as nano-optical and nano-electrical devices, in food packaging and in medicine as antimicrobial and antitumor agents. The increasing focus on nano zinc oxide resulted in the invention and development of methods of nanoparticles synthesis. (Chang, J.S., Strunk, J., Chong, M.N., Poh, P.E. and Ocon, J.D., 2020.)

1.6 Used of ZnO in medicine

Nanotechnology has witnessed tremendous advancement over the last several decades. Zinc oxide (ZnO), which can exhibit a wide variety of nanostructures, possesses unique semiconducting, optical, and piezoelectric properties hence has been investigated for a wide variety of applications. The most important features of ZnO nanomaterials are low toxicity and biodegradability. Zn2+ is an indispensable trace element for adults (~10 mg of Zn2+ per day is recommended) and it is involved in various aspects of metabolism. Chemically, the surface of ZnO is rich in -OH groups, which can be readily functionalized by various surface decorating molecules. Zinc oxide is characterized by a good biocompatibility which allows the exploitation of its antibacterial, antifungal, antiviral, and anti-cancer qualities in a therapeutic setting (Wiesmann, N., Tremel, W. and Brieger, J., 2020.)

Figure 1.2 uses zinc oxide in medicine

1.7 UV-VIS spectroscopy

UV-VIS spectroscopy is considered as the most important spectrophotometric technique that is most widely used for the analysis of variety of compounds. This technique works on the basis of themeasurement of interaction of electromagnetic radiations (EMR) with matter at particular wavelength. For proper working of UV-VIS spectroscopy and to get accurate results, it is very important to understand the components of UV-VIS spectroscopy and their individual role in the proper functioning of UV-VIS spectrophotometer. In UV-VIS spectroscopy, absorption of light is the basic phenomenon as showed in figure 1.3 (Förster, H., 2004.)

Figure 1.3 UV-VIS spectroscopy

1.8 Energy Band Gap

A band gap is the distance between the valence band of electrons and the conduction band. Essentially, the band gap represents the minimum energy that is required to excite an electron up to a state in the conduction band to the lower energy level is the valence band, and thus if a gap exists between this level and the higher energy conduction band. Energy band gap is usually referred to the energy difference between the conduction band and the valence band, An electron residing in the valence band cannot jump to the conduction band until and unless it is provided the amount of energy needed for the electron to cross the energy barrier between the aforementioned bands, which is just the band gap energy. The size and existence of this band gap allows one to visualize the difference between conductors, semiconductors, and insulators. These distances can be seen in diagrams known as band diagrams, as shown in Figure 1.4.

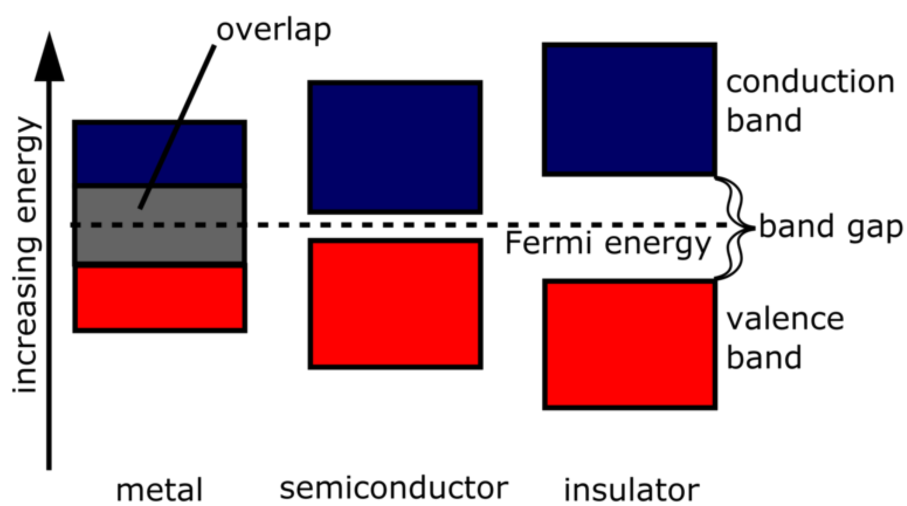

Figure 0.4 Bandgap diagrams.

The expression of Beer-Lambert law is:

$$\mathbf{A = \log (I_0/I) = \epsilon cl} \qquad \mathbf{(1)}$$

Where,
C = molar concentration of solute (M)
L = length of sample (cm)
ϵ = molar absorption coefficient (1/M*cm)
Absorption coefficient (α) was calculated by using the following equation:

$$\mathbf{I = Io \exp (-\alpha x)} \qquad \mathbf{(2)}$$

Hence
A = 2.303/x

$$\mathbf{\log (I/Io) = (2.303/x)\ A} \qquad \mathbf{(3)}$$

where I_0= incident intensity, I= transmitted intensity, A= absorbance
alpha = absorption co efficient, t = Thickness of the material
In the energy level the photon is incident by its energy direct band gap obtained and the absorption coefficient is given by

$$\mathbf{\alpha h\upsilon = C\ (h\upsilon - E_g\ )1/2} \qquad \mathbf{(4)}$$

Where, C is Constant, α is the absorption coefficient

hν (eV) = 1240 / λ(nm)]

UV-visible Spectroscopy is used for identify the energy band gap values of the materials the transmitting radiation. In an energy level a photon is absorbed in its orbit, when an electron is jumps from lower energy level to higher energy level, where the optical band gap energies be determined. Conducting materials are having energy bands and classified in to two types band gap (1) Direct band gap (2) Indirect band gap, This two type band gap involves in the interaction with an electron in the valence band showed in figure 1.5, However, direct band gap involves a vertical transition of electrons from the valence band to the conduction band, If the momentum of the lowest energy state in the conduction band and the highest energy state of the valence band of a material are the same, the material has a direct band gap. If they are not the same, then the material has an indirect band gap. For materials with a direct band gap, valence electrons can be directly excited into the conduction band by a photon whose energy is larger than the band gap, In contrast, for materials with an indirect band gap, a photon and phonon must both be involved in a transition from the valence band top to the conduction band bottom. Therefore, direct band gap materials tend to have stronger light emission and absorption properties [18].

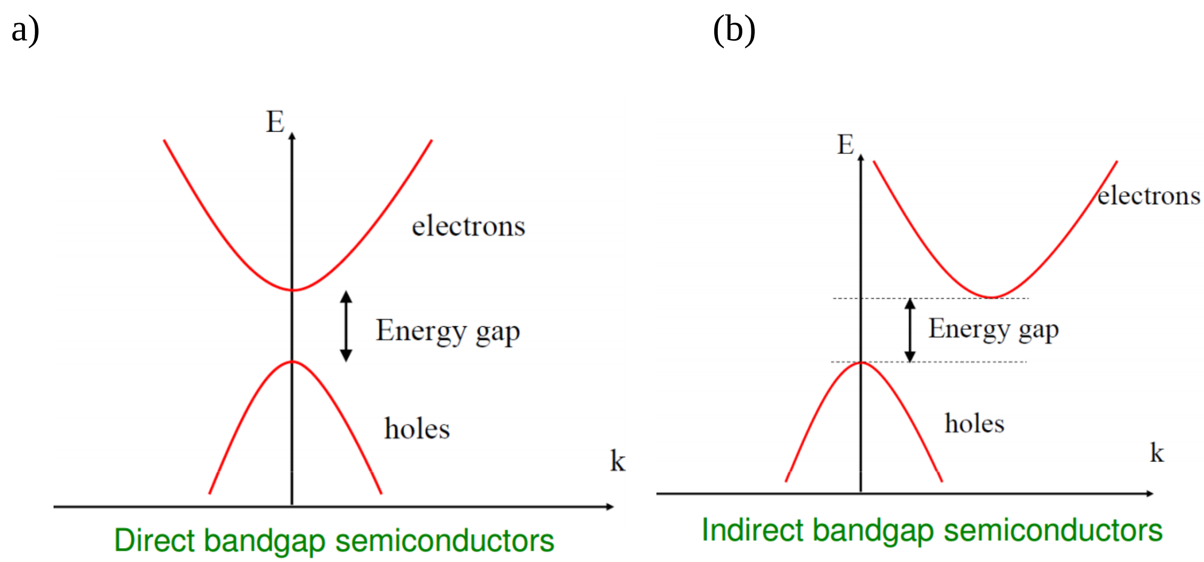

Figure0.5 a) Direct band and b) Indirect band semiconductors.

Chapter Two

Results and Discussion

2.1 Preparation Samples

• Many sample of sun protect ointments manufactured in different companies were purchase from pharmacy in Erbil.

• In our research, ZnO thin film was deposited on the glass substrate.

• Ultraviolet-visible (UV-Vis) spectroscopy is one of the most popular analytical techniques because it is very versatile and able to detect nearly every molecule. With UV-Vis spectroscopy, the UV-Vis light is passed through a sample and the transmittance of light by a sample is measured, finally energy band gap (E_g) for each sample was be determined.

Figure 0.1 **UV-Vis spectroscopy device.**

2.2 Absorption of Sun Protect

The instrument used in UV-spectroscopy is called a UV/Vis spectrophotometer are devices that are used to measure the spectra of samples. Typically, they measure the electromagnetic radiation intensity as a function of the wavelength. spectrophotometer measures ultraviolet light that from transmitted through a sample, the radiation measures the intensity of light after passing through a sample (I), and compares it to the intensity of light before it passes through the sample (Io). The ratio I/Io is called the transmittance, and is usually expressed as a percentage (%T). The absorbance, A, is based on the transmittance: A = -log (T). Figure 3 shows the absorption of light from the sun protect ointment samples S1, S2, S3, S4, S5 and S6. The graph indicated that the samples (S1-S2) and (S3-S5) approximately the same absorption from rang wave length 100 to 400 nm (UV range) higher than sample S4 and S6.

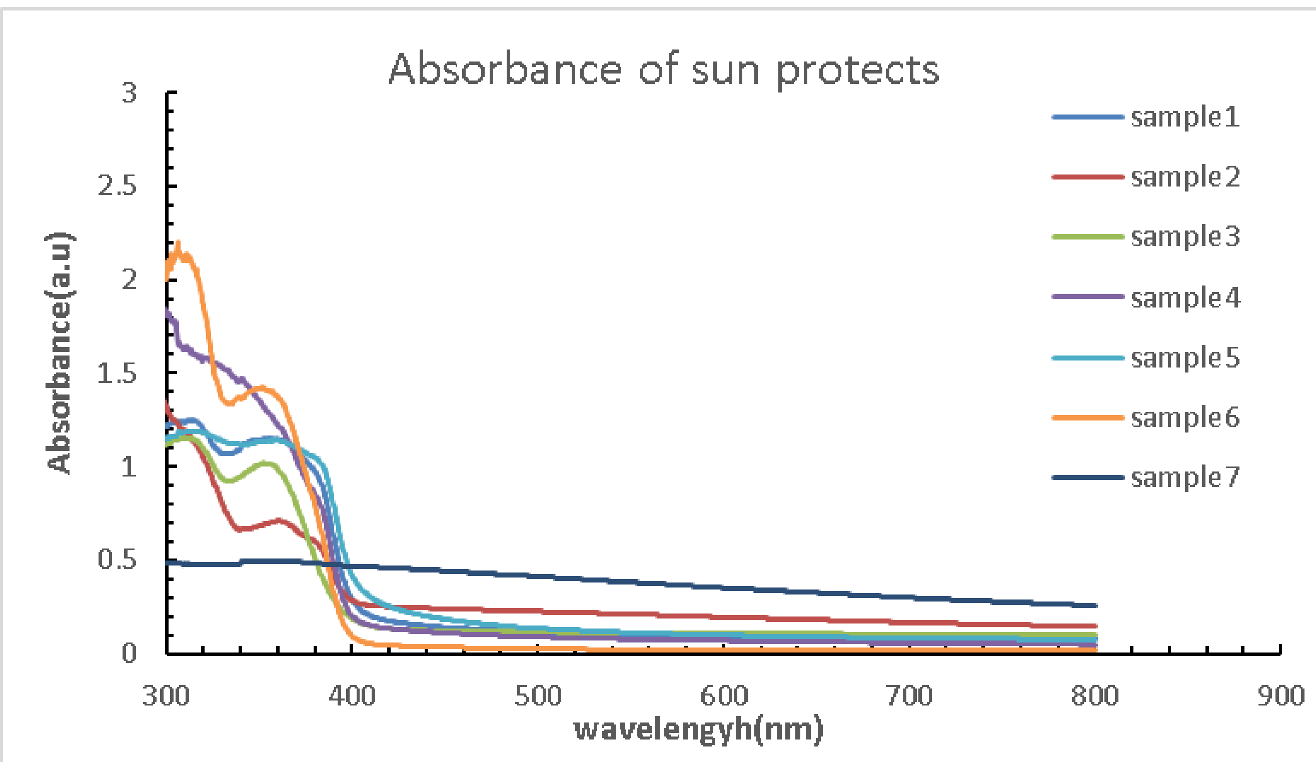

Figure 0.2 The absorbance of sun protects

2.3 Energy Band Gap (E_g) of Sun Protects

Figure 2.2 shows the graph of thin film samples S1, S2, S3, S4 and S5 deposited on glass substrate. The found energy band gaps are presented in table 2.1, The high differences energy gap was observed of S2, S3, S4, S5, and S6 owing to excites of ZnO in sun protect and material ointments contributed to absorption of light. The appears of small peaks in S2 and S3 refers to excites of 50% castor oil in samples. The sample S3 has (3.22 Ev) value nearest to a theoretical band gap (3.37 eV) of ZnO. Actually, considered it is the best sun protects ointments to protect the skin from the UV spectrum of sun light.

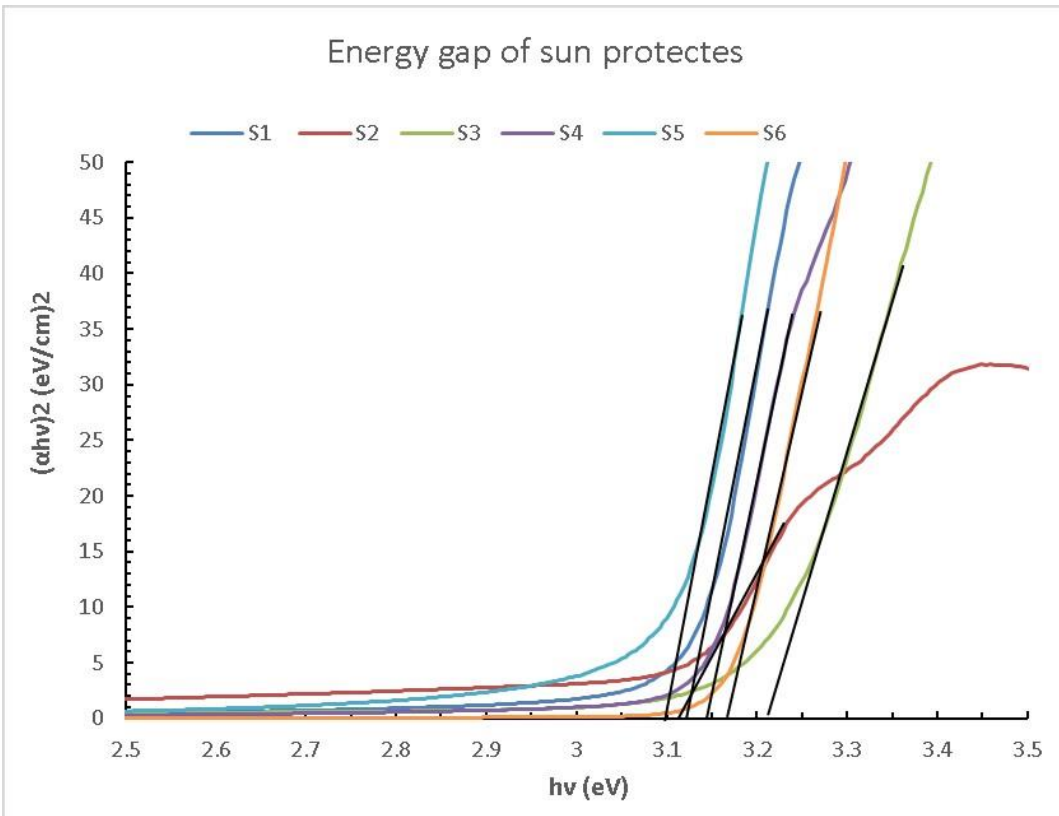

Figure 0.3 The energy gap (E_g) for various sun protects

Table 0.1 The energy bandgap of different sun protects ointment.

Sun protect	S1	S2	S3	S4	S5	S6	theoritical
Energy gap (eV)	3.12	3.11	3.22	2.15	3.1	3.17	3.37

Chapter Three

Conclusions and Reference

3.1 Conclusions

In this research we investigated that:

1. Zinc oxide nanoparticles (ZnO) have long been utilized as UV-protective sunscreen components due to their high durability and lower skin irritation.

2. Zinc oxide (ZnO) is an important versatile and technologically semiconducting material which is widely used in medication.

3. ZnO is one of the most promising wide band semiconductors for short wavelength medication applications also has high stability, good optical characteristics, it is an important material for manufacturing sun protect ointments.

4. Its easy growth with high purity makes it a low-cost material as high-quality substrate and its easily etched property makes it possible to be made as medical applications.

5. It has a good energy gap (3.37 eV) to the hazard partial UV rang from the sun light which is reached to our earth.

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