

Int. J. New. Chem., 2023, Vol. 10, Issue 4, pp. 268-287.

International Journal of New Chemistry

Published online 2023 in <u>http://www.ijnc.ir/.</u> Open Access



Print ISSN: 2645-7237

Online ISSN: 2383-188x

Original Research Article

Study the efficiency of three organic pigments based on tri-azine with applicability in solar cells in order to achieve clean and renewable solar energy

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Received: 2023-10-01

Accepted: 2023-12-15

Published: 2023-12-22

ABSTRACT

With the uncontrolled increase of world population and due to the reduction of energy resources, scientists have thought about using clean and renewable energy such as wind, sun, tide, etc. to use clean and cheap energy with the aim of reducing Environmental pollution, along with increasing the productivity of photovoltaic cells, three organic dyes based on tri-azine were used. The structure of these three dyes was plotted by Gaussian software and optimized by Gaussian program, then in terms of electron excitation. Verticals were studied by DFT and TDDFT quantum methods in gas and liquid phases by SMD method. In this type of pigments, due to the presence of the pigment agent in the structure of molecules, we see the scattering of electron clouds and orbital overlap, which cause more polarization and resonance in them. The effect of polar solvent also intensifies it. As the energy gap decreases by the solvent, charge separation and bond lengths occur in the pigments. According to Homo and Lumo energy forms, λ max wavelength changes, D-CT electron transfer changes, $\Delta \pi$ charge changes and $\Delta \mu$ excitation transfer density changes, three pigment comparisons in gas and solution phases were performed and found: For the first dye, the blue or hypsochromic transfer has taken place, in the pigments, separation has occurred and the transfers are of the type $n \to \pi^*$ and are delocalized. Polyurethane,

Keywords: Solar Cell; Electronic excitation; Organic pigments; Load density; resonance

Introduction

The growth of the world's population and the industrialization of countries has led to a significant increase in energy consumption. The sun is highly regarded due to its unlimited power of infinite radiation. About 40% of solar energy is in the visible light range and about

50% is in the infrared range. The sun is a type of natural nuclear reactor that emits high-energy packages. Photons are energy packets that provide the needed energy for the exciting of electrons in semiconductor materials at the ultraviolet and visible range, as well as helping to generate electricity. These photons travel the distance between the sun and the earth (150 million kilometers) in about 5.8 minutes and are sufficient to generate annual solar energy and estimate global energy requirements. For example, photovoltaic power has consisted of only 0.5 of the energy consumption of the United States; but solar technology is evolving currently, and the cost of its process so is declining. There are various technologies to convert sunlight into consumption energy for residential and industrial units, the most common of them for residential and buildings are solar hot water technology, passive (solar design) to cool and heat the environment, and finally, solar photovoltaic technology to generate electricity. These technologies are used to improve efficiency and reduce energy costs in offices and factories. In other words, the most important type of solar energy is photovoltaic energy, and this solar system includes an electrical system consisting of solar panels [1]. The industrialization of the world and the increase of the world's population will lead to the indiscriminate use of fossil fuels such as oil, gas, etc., and due to the consumption limited of fossil fuels, these resources will be exhausted in the near future. On the other hand, the use of these resources due to their high cost and also has led to an uncontrolled increase in greenhouse gases such as carbon dioxide and methane, and all these cases will endanger human health and the ecosystem. Therefore, scientists have turned to the use of clean and renewable energy such as the sun, wind, tides, etc. These resources are easily accessible, free, and unrestricted in different ecosystems and different parts of the world with different efficiencies in most countries are usable and productive. Most countries in the world are enthusiastic to use renewable energy due to their different needs, such as industrial, domestic consumption in the fields of heating, cooling, drying, desalination, etc. Studies and surveys have shown that in some countries whose major economies are based on fossil fuels, including the GCC, electricity generation in PV compared to energy produced by fossil fuels by 2025 cheaper became more and more costeffective. Solar cells are a type of device that converts sunlight into electrical energy using a semiconductor by means of a photovoltaic effect, which is also called a photovoltaic solar cell [2, 3]. Organic material is used alone or in combination with inorganic material in the structure of exciton photovoltaic cells, which produce exciton when exposed to sunlight. These excitons are converted into holes and electrons in the electron donor and electron acceptor phase, which create an electric field and charge separation occurs. The electronic current generated in these devices is converted into electrical current by converters that can be used for various purposes [4]. Countries with economies based on hydrocarbon resources, due to greater access to resources, are facing an uncontrolled increase in energy consumption in the fields of industry, economy, science, home, etc. On the other hand, at the same time with increasing consumption of energy carriers, they will have the highest production of greenhouse gases and air pollutants. Research has shown that the GCC countries are among the top 25 countries in the world in terms of emissions and increasing greenhouse gas emissions, which in turn causes irreparable damage to ecosystem health and it will affect human health [5, 6]. Global studies have shown that areas with similar ecosystems and tropical climates, such as those in South Africa, including Morocco, are among the countries of the desert and have a tropical climate. Using renewable and clean energy in these countries has higher efficiency. Based on studies and planning by the International Energy Agency predicted that the amount of electricity generated through renewable energy sources, including photovoltaic solar cells, will increase by 16 percent by 2050 compared to similar products in the world. Today, due to the widespread need of human societies for renewable resources, the use of solar energy is not limited only to photovoltaic cells but also has other uses such as: using solar energy to heat water or oil and rotating turbines. All these cases are increasing in the direction of the industrialization of countries. Now we have to think, considering the development of the scientific industry and the widespread need of humanity for this infinite God-given blessing, what factor or factors hinder the development and progress of renewable solar energy in the world? The most important factor in the economic section is that due to the different and specific climates of each region, it needs investment by the public or private section. which unfortunately is not done efficiently and requires training the knowledge and awareness about renewable energy, especially solar energy that should be given to the investor in the field. On the other hand, due to the lack of transmission infrastructure, the electricity transmission network requires large investments in infrastructure. In order to develop and progressing in this area requires the participation of the private section and the public section. Meanwhile, governments need to take steps to make the field prosper by reducing legal restrictions and special investor protections, such as the guaranteed purchase of productive energy and cooperation with the private sector [8, 7]. In order to store excess energy of the solar energy industry, at night or for several days, it requires a type of battery or capacitors that are installed next to the panel structure. The price of these storage energy devices is expected to decrease annually as the consumption of solar panels in the world expands. Since the construction of the world's first

solar panel in 1980, the cost of making these devices has dropped in the amount of 10 percent annually, but as expected, solar storage devices are still expensive, and this is a serious challenge in this area. Therefore, governments and economic actors must seek a suitable solution for the development of this industry. According to the limited use of fossil fuel resources, it should be noticed that despite the problems in the solar industry, it also has advantages. These resources with their high efficiency in the future will reduce dependence on other countries and countries that export their excess solar energy to other countries will take a step towards their economic prosperity. Another advantage is the reduction of water consumption and the lack of need for it in order to generate electricity by the country, and this is consistent with this reduction of rainfall in the world. Most of the country in the world is facing drought, if the situation continues, we will soon face a water war in the world, which is a warning to humanity. Help to reduce ecosystem pollution by lack of producing greenhouse gases such as CO_2 , which have devastating and irreversible effects on human health, is another benefit of this area [9]. As mentioned before, the use of solar renewable energy without the production of harmful gases accompanied and can be utilized as a barrier against global warming and also prevent the melting of ice glaciers, floods, tornadoes, etc, and consequences of them. All of these factors are directly related to human health and the biosphere. This has prompted scientists to search for more effective and less harmful solutions to reduce pollution in order to use new energy. Therefore, they have introduced a solution called modern chemistry. In this science, research and studies are performed by considering the desired process about its interactions, and they are measured from different aspects. Among them, a method is chosen as the preferred solution that has some properties including presenting less harmful substances and pollutants into the environment, endangers the health of the biosphere less, at the same time has a better and more productive product [10]. Recently, a device has been developed that uses the air to produce drinking water without the need for chemicals, in such a way that the energy received from the sun is stored by the solar panels as cooling during the day and night. During the night, the air is converted to Drinking water. According to the above, it can be pointed to several advantages of green chemistry, including optimal water consumption, prevention of its loss by using solar energy for domestic and industrial use, high yield of chemical reactions with less consumption of raw materials, and more products. As a result, it makes this field economically viable. Computational chemistry is a branch of chemistry that, via designing molecular structures and examining related chemical reactions by computer programs. Ultimately, the achieved data examines the efficiency and effectiveness of these reactions before performing the process. This theoretical work is scientifically viable because researchers enter the practical scene of these researches with full knowledge of their usefulness, feasibility, and economic cost. Therefore, it can be said that computational chemistry is also a branch of green chemistry [11].

Function and types of solar cells

The main part of solar panels is the solar cell and they are also known as PV cells or photovoltaic cells. These cells generate electricity by absorbing sunlight. The PV name is derived from the process of converting light (photons) into electricity, and this PV effect was first used and discovered in 1954. In other words, when scientists at the Bell telephone station discovered that when silicon is exposed to the sunlight, it emits an electric charge. Sometime after the discovery, they used solar cells to the energy supply space satellites and smaller systems such as calculators and clocks. It should be noted that solar cells are derived from semiconductor materials and the main type of them is silicon crystalline. In a type of solar cell that uses organic matter, they are called organic matter-based solar cells. They are less efficient than other solar cells, but their flexibility and low expense to building them are more useful in non-industrial applications. It can be said that color sensitive solar cells, polymer solar cells, and solar cells based on liquid crystals are a variety of solar cells based on organic matter.

DSSC cells

These types of solar cells are color sensitive. Nano-dimensions have been used in contact with nanoparticles in the construction of these cells [6].



Figure 1. Structure of a color-sensitive DSSC solar cell [1]

Each part is covered with a piece of a layer containing a specific color or quantum dots that are like color. An electrolyte is used to create a channel between the pigment and the anode. Thus the pigment absorbs light and oxyton is obtained, causing photon energy packets to create the electrons for the semiconductor, then the pigment molecule is oxidized by the electrolyte. These cells have high efficiency and yield compared to the new generation cells. The three organic pigments used in this study have not been commercialized at the moment and have been discussed in terms of efficiency and productivity [1]. Methods: In this study, three organic pigments based on triazine were prepared, containing: A: -4.6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (1,4 phenylene) -2- cyano acrylic acid B: -4.6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (2,5 thiazylene) -2- cyano acrylic acid, C: -4.6 Bis (7-di ethyl amino) - (1,3,5 triazin-2-yle) - (1,4 phenylene) -2- cyano acrylic acid. Each of these pigments in terms of electron excitation and molecular structure was investigated by SMD method in two gas and liquid phases. Relevant results include information such as bond length, bond angle, and dihedral angles of the pigments in the liquid and gas phase, which are given in the relevant tables. In this project, the effects of solvents on these types of structures were evaluated using quantum study methods and electron charge density studies.

Device and method used in this project

In this project, DFT calculations for the structure of pigments were performed using Gaussian software. To determine the geometric shape of these pigments first, the structure of the pigments was drawn in Gaussian software, then by entering properties such as base series type, density factor type, the type of atoms, and the number of atoms in an input file recorded in Gaussian software. Then the calculation begins with writing a program. TD DFT calculations were performed to evaluate the vertical excitation of these pigments with density factor LC-WB97XD and base series 6-31 + + G (3df, 3pd). These calculations were down first in the gas phase and then in the solution phase by the SMD method. Using the TD DFT method, the maximum wavelength for all three pigments was calculated in both liquid and gas phases.

In this project, DFT calculations for the structure of pigments were performed using Gaussian software. The data related to the structural parameters of these calculations are given in the tables of the next section.

Structural specifications of three tri-azine pigments:



A: -4,6 Bis(7-di ethanol amino)- (1,3,5 triazin-2-yle)-(1,4 phenylene)-2- cyano acrylic acid



B: -4,6 Bis(7-di ethanol amino)- (1,3,5 triazin-2-yle)-(2,5 thiazylene)-2- cyano acrylic acid



C: -4,6 Bis(7-di ethyle amino)- (1,3,5 triazin-2-yle)-(1,4 phenylene)-2- cyano acrylic acid

Structure	Amount	Structure	Amount	Structure	Amount
O39-H40	0.95 (Å)	C18-C20	1.48 (Å)	C12-C14-C17	114.94 (°)
C34-H37	1.09 (Å)	C20-O22	1.32 (Å)	C14-C17-C18	137.01 (°)
C34-C23	1.51 (Á)	C34-O39-H40	109.29 (°)	H37-C34-C33-N26	169.43 (°)
C33-N26	1.45 (Á)	H37-C34-H38	108.3 (°)	C17-C18-C24≡N25	3.03 (°)
N ₂₆ -C ₄	1.34 (Å)	H36-C33-C34	108.67 (°)	C3-C7-C9-C12	179.67 (°)
C3-C7	1.48 (Á)	N ₂₆ -C ₄ -N ₅	118.06 (°)	C14-C17-C18-C20	0.44 (*)
C ₂₄ ≡N ₂₅	1.15 (Å)	N5-C4-N6	124.23 (°)	N2-C3-C7-C8	4.74 (°)
N43-C1	1.34 (Á)	N2-C3-N6	124.23 (°)	N6-C3-C7-C9	5.69 (°)
N ₂₆ -C ₄	1.33 (Å)	C8-C7-C9	119 (°)	C10-C14-C17-C18	0.85 (°)
C18-C24	1.43 (Á)	C7-C9-C12	119.89 (°)	O21=C20-O22-H23	0.34 (°)

Table 1.Structural parameter calculations {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (1,4phenylene) -2- cyano acrylic acid} in gas phase

Table 2.Structural parameter calculations {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (2,5thiazylene) -2- cyano acrylic acid} in gas phase

C3-N5 1.35 C43-C44 1.38 C47-C48 1.35	(Å) C48-C50 (Å) N6-C3-N	1.48 (Å) I5 116.68 (°)	O ₅₁ =C ₅₀ -O ₅₂ -H ₅₃ C ₄₄ -C ₄₇ -C ₄₈ -C ₅₀	179.96 (°)
C43-C44 1.38 C47-C48 1.35	(Å) N ₆ -C ₃ -N	Is 116.68 (°)	C44-C47-C48-C50	170.07 (8)
C47-C48 1.35			10 TO 10	1/9.97()
	(A) N5-C40-	C ₄₁ 116.64 (°)	C44-C47-C48-C54	0.019 (°)
C ₅₄ ≡N ₅₅ 1.15	(Å) C41-S42-	N ₄₆ 27.23 (°)	N2-C40-C41-S42	5.79 (°)
N ₂₃ -C ₁ 1.34	(Á) S42-C44-	C47 128.01 (°)	N5-C40-C41-N46	5.39 (°)
N ₆ -C ₃ 1.34	(Å) C14-O19	·H ₂₀ 109.34 (°)	S42-C44-C47-C48	0.27 (°)
C48-C54 1.42	(Á) C13-N6-	C ₃ 120.04 (°)		10000

Table 3.Structural parameter calculations {-4,6 Bis (7-di ethyle amino) - (1,3,5 triazin-2-yle) - (1,4phenylene) -2- cyano acrylic acid} in gas phase

Structure	Amount	Structure	Amount	Structure	Amount
C34-C33	1.51 (Å)	C33-N26-C4	115.3 (°)	C ₁₇ -C ₁₈ -C ₂₄ ≡N ₂₅	0.17 (°)
C14-C17	1.41 (Á)	N26-C4-N6	111.43 (°)	C14-C17-C18-C20	0.059 (°)
C ₂₄ ≡N ₂₅	1.15 (Å)	C4-N6-C3	113.12 (°)	C3-C7-C9-C12	179.74 (°)
C18-C20	1.46 (Á)	C3-C7-C9	121.7 (°)	N2-C3-C7-C8	0.025 (°)
C18-C24	1.43 (Å)	C9-C12-C14	122.43 (°)	N6-C3-C7-C9	0.48 (°)
N39-C1	1.35 (Á)	H37-C34-H49-H38	118.2 (*)	C10-C14-C17-C18	0.16 (°)
N26-C4	1.49 (Å)	O21=C20-O22-H23	179.98 (*)		0.3895

Structure	Amount	Structure	Amount	Structure	Amount
C3-C7	1.48 (Å)	N ₂₆ -C ₄	1.34 (Å)	C9-C12-C14	120.51 (°)
C14-C17	1.46 (Á)	H40-O39-C34	108.35 (°)	C ₁₈ -C ₂₄ ≡N ₂₅	179.62 (°)
C17-C18	1.34 (Å)	C34-C33-N26	114.26 (°)	O ₂₁ =C ₂₀ -O ₂₂ -H ₂₃	179.63 (°)
C ₂₄ ≡N ₂₅	1.15 (Å)	C33-N26-C4	119.64 (°)	C17-C18-C24≡N25	44.72 (°)
C20-C18	1.49 (Á)	N26-C4-N6	117.6 (°)	N2-C3-C7-C8	12.98 (°)
C18-C24	1.43 (Á)	C3-N2-N6	27.28 (°)	N6-C3-C7-C9	13.27 (°)
N43-C1	1.34 (Å)	C7-C9-C3	30.81 (°)	C10-C14-C17-C18	38.75 (°)
	56650		Califier		1022.45

Table 4.Structural parameter calculations {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (1,4 phenylene) -2- cyano acrylic acid} in solution phase.

Table 5.Structural parameter calculations {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (2,5 thiazylene) -2- cyano acrylic acid} in solution phase.

Structure	Amount	Structure	Amount	Structure	Amount
O19-C14	1.42 (Å)	N23-C1	1.34 (Å)	C41-N46-C43	110.26 (°)
C14-C13	1.51 (Á)	N ₆ -C ₃	1.34 (Á)	C44-C47-C48	129.85 (*)
C40-C41	1.48 (Á)	C50=O51	1.2 (Á)	C47-C48-C50	122.52 (*)
C41-S42	1.71 (Á)	C54≡N55	1.15 (Á)	N2=C40-C41-S42	1.79 (°)
C41-N46	1.3 (Å)	C7-N6-C3	121.35 (°)	N5=C40-C41=N46	1.26 (°)
C48-C54	1.42 (Á)	N5-C40-C41	117.03 (°)	S42-C44-C47=C48	0.23 (°)
C48-C50	1.48 (Å)	C41-S42-C44	89.12 (°)	C43-C44-C47=C48	179.61 (°)

Table 6.Structural parameter calculations {-4,6 Bis (7-di ethyle amino) - (1,3,5 triazin-2-yle) - (1,4phenylene) -2- cyano acrylic acid} in solution phase.

Structure	Amount	Structure	Amount	Structure	Amount
C28-C27	1.52 (Å)	N26-C4	1.34 (Å)	C14-C17-C18	129.68 (°)
C27-N26	1.46 (Á)	C18-C20	1.49 (Á)	C10-C14-C17-C18	34.67 (°)
C3-C7	1.49 (Å)	C18-C24	1.43 (Å)	N2-C3-C7-C8	2.89 (°)
C14-C17	1.46 (Á)	C33-N26-C4	120.37 (°)	N6-C3-C7-C8	176.5 (°)
C20-O21	1.2 (Å)	N6-C3-N2	126.15 (°)		0.4297
C ₂₄ ≡N ₂₅	1.15 (Á)	C3-C7-C9	120.48 (°)		
N39-C1	1.34 (Å)		187/45118		

Studying the structure of three pigments by Gause View software, the results were obtained in two phases gas and solution phase, which has shown in the above tables. In the structure of the pigments, due to the presence of the pigmenting agent (triazine), which is located between the electron donor and electron acceptor groups, it causes more orbital overlap and more diffusion of electron clouds. These cases lead to resonance and polarization in the molecule. Changes the bond lengths occur in the gas phase. The changes in bond lengths in the solution phase are slightly greater than in the gas phase, which can be explained by the effect of the solvent. Acetonitrile was used as the solvent, which is highly polar and has a high dielectric constant. The larger the dielectric constant, the greater the polarity of the solvent. Due to the dipoledipole interactions, the structures have a significant order and form complexes with the help of their single electron pair in the pigments. In the solution phase, with the increasing polarity of the solvent, the orbital interactions within the pigments are intensified, which causes the charge to separate in the molecules. The study of the HOMO energy forms of the soluble and gaseous phases shows the greater scattering of electron clouds in the soluble phase, which is directly related to the increase in density changes in the soluble phase. Due to the change of dihedral angles values for the pigments, the molecule moves out of the plate or flat state in the solution phase more than the gas phase. Then the orbital pressure in the pigments and their local polarization increase.

Table 7.Calculation of molecular parameters of {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) -
(1,4 phenylene) -2- cyano acrylic acid} in the gas phase.

Transition electric	λmax(nm)	Singlet A	Oscillator strength
Homo-2, Lumo $n \rightarrow \pi^*$	306.67	0.672	1.15
Homo-4, Lumo+2 $n \rightarrow \pi^*$	186.71	0.515	0.577
Homo-1, Lumo+2 $n \rightarrow \pi^*$	213.53	0.409	0.249

Table 8.Calculation of molecule parameters {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) -
(1,4 phenylene) -2- cyano acrylic acid} in solution phase.

Transition electric	λmax(nm)	Singlet A	Oscillator strength
Homo-2, Lumo $n \rightarrow \pi^*$	305.03	0.68	0.95
Homo-3, Lumo+2 $n \rightarrow \pi^*$	189.4	0.388	0.565
Homo-1, Lumo+11 $n \rightarrow \pi^*$	215.14	0.352	0.364

Table 9.Calculation of molecular parameters of {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle) - (2,5 thiazylene) -2- cyano acrylic acid} in the gas phase.

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Transition electric	λmax(nm)	Singlet A	Oscillator strength
Homo-2, Lumo $n \rightarrow \pi^*$	319.51	0.685	0.797
Homo-1, Lumo+4 $n \rightarrow \pi^*$	212.11	0.280	0.371
Homo-13, Lumo $n \rightarrow \pi^*$	207.01	0.394	0.168

Table 10.Calculation of molecular parameters of {-4,6 Bis (7-di ethanol amino) - (1,3,5 triazin-2-yle)- (2,5 thiazylene) -2-cyano acrylic acid} in solution phase.

Transition electric	λmax(nm)	Singlet A	Oscillator strength
Homo-2, Lumo $n \rightarrow \pi^*$	329.72	0.672	0.855
Homo , Lumo+4 $n \rightarrow \pi^*$	213.96	0.335	0.575
Homo-1, Lumo+4 $n \rightarrow \pi^*$	206.82	0.356	0.238

Table 11.Calculation of molecular parameters of {-4,6 Bis (7-di ethyle amino) - (1,3,5 triazin-2-yle) -(1,4 phenylene) -2- cyano acrylic acid} in the gas phase.

	1		
Transition electric	$\lambda max(nm)$	Singlet A	Oscillator strength
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Homo-2, Lumo	308.68	0.66	1.146
1101110 2 , 2u 110	200.00	0.00	111.10
n→π*			
Homo-4, Lumo+5	185.69	0.337	0.524
*			
n→π ⁺			
Homo Lumo+3	208 52	0.383	0.273
Homo, Lumo 15	200.52	0.505	0.275
n→π*			

Table 12.Calculation of molecule parameters {-4,6 Bis (7-di ethyle amino) - (1,3,5 triazin-2-yle) - (1,4 phenylene) -2- cyano acrylic acid} in solution phase.

Transition electric	λmax(nm)	Singlet A	Oscillator strength
Homo-2, Lumo	309.25	0.679	0.99
n→π*			
Homo-4, Lumo+3	189	0.427	0.513
n→π*			
Homo, Lumo+3	210.71	0.304	0.499
n→π*			

Table 13. Relevant D-CT parameters in the gas phase

Gas parameter	Α	В	С
D-CT (Å)	1.44	1.75	0.734
$\Delta \mu_{excitation}$ (Debye)	1.01	0.25	2.18

Table 14. D-CT parameters in solution phase

Solution parameter	Α	В	С
D-CT (Å)	0.72	2.03	1.07
$\Delta \mu$ excitation(Debye)	2.66	0.31	3.81

Placing the pigmenting agent as a π bridge between the electron donor and acceptor arm has resulted in better and more orbital overlaps and interactions. Orbital overlap is directly related to molecular conjugation. The energy level of electron transitions is reduced by a highly polarized solvent with a high dielectric constant and is accompanied by an increase in electron motions in the pigments, which leads to an increase in electron transitions with low energy. With increasing the distance of electron transfer, charge separation occurs in the molecule. It should be noted that along with the increase in electronic transfers, there is also an increase in the density of electronic transfers. In the first pigment, which contains the electron donor group of diethanolamino (Å), CT-D decreases in the solution phase compared to the gas phase. No charge separation occurs as a result of these electrons, as well as transfers are localized. However, the pigment that includes the electron donor group of diethylamino and the pigment including the thiazome functional group, the CT-D (Å) increased in the solution phase compared to the gas phase which was due to the solvent effect and high polarity because of the solvent (acetonitrile). Acetonitrile also has a high dielectric constant that helps to charge separation in the molecules and makes the mobility of the molecules easier. As well as it has reduced the energy gap so that transfers are done with less energy. The distance length is increased and the charge is separated. As a result, the transfers will be of charge transfer or delocalization type. According to the HOMO and LUMO energy forms, most of the scattering of electron clouds is due to an orbital interaction with the solvent. With charge separation, it has occurred an increase in CT-D (Å) transitions, $\Delta \pi$ charge changes, $\Delta \mu$ excitation, and density changes. Comparison of two pigments including the electron donor groups of diethylamino and diethanolamino so that both pigments have the same electron acceptor group has shown that the higher electron donor power of diethylamino than the diethanolamino caused more charge induction occurs in the pigment. So in the pigment, which contains the electron donor group of diethylamino, charge separation occurs. By comparing the pigment containing the benzene electron acceptor group and the pigment containing the thiazome electron acceptor group with the same electron-donating group, both have diathanolamino amino acid. More and easier load separation occurs. In pigments, when light is absorbed by the pigmenting agent, their structures change which leads to changes in the values of λ max and the intensity of light absorption. This effect is called bathochromic, which makes the pigment appear more colorful (The color shifts from blue to red). This effect is also called red transfer. If the location changes of λ max are towards shorter wavelengths, it is also called aqueous or

hypsochromic transition. When the pigmenting agent is placed in the structure of the molecule, between the electron donor and acceptor's arms, it increases the overlap and the orbital and resonance interactions. As a result of this overlap, the pigment's ability to absorb light increases. Therefore, these pigments are highly efficient and are used as sensors in solar cells. λ max increase in the solution phase compared to the gaseous phase, which is due to the effect of the solvent. The acetonitrile solvent is highly polar and has a large dielectric constant that increases the orbital overlap and reduces the HOMO to LUMO energy gap. As a result, electron transitions will require less energy, and we have an absorption with λ max wavelength for pigments. In the first pigment, the λ max wavelength (nm) of the solution phase is reduced than the gaseous phase. Blue or hypsochromic transitions have taken place. For the other two pigments, the λ max wavelength (nm) of the solution phase is incremental to red or bathochromic transitions. Due to the energy forms and the effect of the solvent in order to reduce the energy gap of the transitions, as a result, the conjugation of the molecule will be accompanied by an increase in the orbital overlap, and by reducing the energy gap, the level of transitions $\pi \rightarrow \pi^*$ decreases. Hence the probable transitions $n \rightarrow \pi^*$ occur.

Table 15. Calculation of molecul	e parameters -4,6 Bis(7-di ethanol amino)- (1,3,5 triazin-2-yle)-(1,4
	phenylene)-2- cyano acrylic acid

nor	Elements	Gas	Solution
Group e dor	N26	0.8	0.8
	N43	0.78	0.801
Group e receiver	C28	-0.25	0.37
	O21	-0.8	-0.79
	O22	-1.03	-0.56
	H23	0.44	0.48
	C24	-0.4	-0.36
	N25	0.22	0.14
	Δπ Load changes	-1.56	

lor	Elements	Gas	Solution
Group e dor	N6 N23	0.72 0.81	0.77 0.85
Group e receiver	$\begin{array}{c} C_{50} \\ O_{51} \\ O_{52} \\ H_{53} \\ C_{54} \\ N_{55} \end{array}$	1.4 -0.8 -0.55 0.39 -0.15 0.18	1.46 -0.9 -0.6 0.42 -0.2 0.1
	Δπ Load changes	-1.94	-2.02

Table 16.Calculation of molecule parameters -4,6 Bis(7-di ethanol amino)- (1,3,5 triazin-2-yle)-(2,5 thiazylene)-2- cyano acrylic acid

Table 17.Calculation of molecule parameters -4,6 Bis(7-di ethyle amino)- (1,3,5 triazin-2-yle)-(1,4phenylene)-2- cyano acrylic acid

or	Elements	Gas	Solution
don			
b e	N ₂₆	0.63	0.65
irou	N39	0.62	0.65
0	57		
'er	C_{20}	1.22	1.5
eiv	O_{21}	-0.78	-0.8
rec	O_{22}	-0.59	-0.56
e	H_{23}	0.44	0.5
Ino	C ₂₄	-0.36	-0.35
Gr	N ₂₅	0.21	0.14
$\Delta \pi$		-2.35	-2.55
	Load changes		

Due to the value of the charge change, which indicates the charge transfer from the donor part of the molecule to the acceptor part, the charge separation in the molecules occurred under the influence of overlap and resonance. In the first pigment, the values of charge changes in the solution phase compared to the gas phase are decreased. Also the distance of electron transitions related to the solution phase than the gas phase is decreased, so the electronic transfers are localized and no charge separation is performed. For the second and third pigments, the values of charge changes and the distance of electron transitions in the solution phase have increased compared to the gas phase. The charge separation is due to the solvent effect. Due to the high polarity and dielectric constant of the solvent, the reduction of the transitions energy level occur, which increases the electronic transitions with low energy.

As a result, charge separation, increasing the values of the charge changes, and the electronic transfers distance is appeared. It is of delocalization type. In triazine-based organic dyes, electron transfer depends on the configuration of the molecule and the substitutions on it. In these pigments, due to the existence of orbital overlap and resonance, the polarization of the molecules is higher. The solvent also intensifies this polarization with its high dielectric property, which caused the charge separation in the molecules. Increasing the electron-donr and electron-affinity properties of pigments with positive and negative induction properties also cause easier separation of charge in them.

In pigment A, separation of positive and negative phases is less common (Å) CT-D transitions of soluble phase to gas are less, so we do not have separation. The transitions are $n \rightarrow \pi *$ and are localized. But in pigments B and C, separation of positive and negative phases occurred more and (Å) CT-D transitions of soluble phase to gas are more. As a result, we have a charge separation and the transfers are of type $n \rightarrow \pi *$ and are delocalized.

Discussion and conclusion

According to the obtained computational parameters, the three organic triazine desired pigments due to the presence of the pigment reagent (triazine) in their structure, which is located between the electron donor and electron acceptor groups. This have increased the orbital overlap and further diffusion of electron clouds.

These factors lead to resonance and polarization in molecules and change the bond lengths in the gas phase. The bond lengths changes in the solution phase are slightly greater than in the gas phase, which can be explained by the solvent effect. Acetonitrile solvent has high polarity and dielectric constant (the higher dielectric constant, the higher polarity of the solvent). In the solution phase, when the polarity of the solvent increas the orbital interactions within the pigments are intensified, which causes the charge to separate in the molecules. Comparison of HOMO energy forms related to the soluble and gaseous phases shows that more electron cloud scattering occurs in the soluble phase, which is directly related to the increase in density changes in the soluble phase.

Due to the alteration of the dihedral angles values related to the pigments, the molecule in the solution phase than the gas phase deviates from the plane or flat state. it leads to an increase in orbital pressure in the pigments and causes local polarization in them.

The energy level of electron transfer is reduced by a highly polarized solvent with a high dielectric constant. Electron motions in the pigments increase, which leads to an enhancement in electron transfer with low energy. In the first pigment containing the electron donor group of diethanolamine (Å), CT-D in the soluble phase is reduced compared to the gaseous phase. which can be concluded that no charge separation occurs and finally these electron transitions are localized. The pigments containing the electron donor group diethylamino and the pigment-containing the thiazole unit, because CT-D (Å) increases in the solution phase compared to the gas phase, the solvent effect is highlighted and since the solvent (acetonitrile) has more polarity.

It also has a high dielectric constant, helps to separate the charge in the molecules, and makes the molecules move more easily. These factors have reduce energy gaps and require little energy to make transfers. The length of the route will be increased, the cargo will be separated and the transfers will be charge transfer or delocalized. Observing the HOMO and LUMO energy forms, the scattering of most electron clouds is evident due to the orbital interaction with the solvent. Charge separation leads to an increase in CT D (Å) values of transitions, $\Delta \pi$ charge changes and $\Delta \mu$ excitation density changes. They have the same electron acceptor group. It is concluded that the greater electron donor power of diethylamino than diethanolamine induces more charge in the pigment.

Therefore, charge separation occurs in the pigment containing the diethylamino electron donor group. By comparing the pigments containing the benzene and the thiazome electron acceptor group with the same electron donor group, both have the amino-amino diethanol element. The more negatives, the more and easier the separation of the load occurs. When the pigmenting agent is placed in the structure of the molecule, between the electron donor and acceptor arm, it will be increased the overlap and the interactions of orbital and resonance. As a result of this overlap, the ability of the pigment to absorb light will be shown an increase. Therefore, these pigments are highly efficient and are used as sensors in solar cells.

Since the λ max of the soluble phase increases in comparison with the gaseous phase. The effect of the solvent is significant. The acetonitrile solvent has high polarity and high dielectric

constant, which has increased the orbital overlap and reduced the HOMO to LUMO energy gap.

As a result, electron transitions will require less energy, and we have a max wavelength absorption for pigments. In the first pigment, the λ max (nm) wavelength of the soluble phase to the gaseous phase is decreasing. Blue or hypochromic shifts have taken place. Investigation of energy forms and the effect of solvent indicate the reduction in the energy gap of transitions as a result of molecular conjugation will be accompanied by an increase in the orbital overlap. As the energy gap decreases, the energy levels of the transfers $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ decrease and the probable transitions will be $n \rightarrow \pi^*$.

Due to the value of charge changes that indicate the charge transfer from the donor part of the molecule to the acceptor part. The charge separation in the molecules occurred under the influence of the overlap and resonance factor. In the first pigment, the values of charge changes in the solution phase compared to the gas phase are decreased, and also the distance of electron transitions related to the solution phase than the gas phase is decreased. So the electronic transfers are localized and no charge separation is performed.

For the second and third pigments, the values of charge changes and the distance of electron transitions in the solution phase have increased compared to the gas phase. The charge separation is due to the solvent effect. In triazine-based organic pigments, electron transfer depends on the configuration of the molecule and the substitutions on it. In these pigments, due to the existence of orbital overlap and resonance, the polarization of the molecules is higher and the solvent also intensifies this polarization with its high dielectric property. Which caused the charge separation in the molecules. Increasing the electron-donr and electron-affinity properties of pigments with positive and negative induction properties also cause easier separation of charge in them.



Figure 2. HOMO and LUMO energy in the gas phase



Figure 3. HOMO and LUMO energy in the solution phase

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How to Cite This Article

Robabeh Mousavi, Amirnaser Shamkhali, Mohammadreza Zammanlo, Rahmat Imani, "Study the efficiency of three organic pigments based on tri-azine with applicability in solar cells in order to achieve clean and renewable solar energy" International Journal of New Chemistry., 10 (4) 268-287 (2023). DOI: 10.22034/ijnc.2023.1988848.1325.