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Carbene compounds in solar cells: Mini-review

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Abstract
Carbene compounds have emerged as promising materials for use in solar cells due to their unique electrical and optical properties. These materials are known to have effective optical characteristics as they have effective absorption in the visible to a near-infrared region of the electromagnetic spectrum, which enables efficient conversion of light to electrical energy. Incorporating carbenes into solar cell structures can also improve the device's performance in terms of the cells' stability and power conversion efficiency. One of the main advantages of carbene compounds is that they can easily be synthesized and modified to tailor their structure and make them more suitable for solar cells. This allows intricate engineering of energy levels, absorption spectra and molecular structures so that the performance of the device is optimized. It has been reported recently that carbene compounds can achieve high power conversion efficiencies in many varieties of solar cells, such as organic photovoltaics and perovskite solar cells.

Keywords: Carbene, organic photovoltaics, perovskite solar cells, Mini-review

Introduction
Carbenes are promising materials that imply the development of w effective sensitizers to be used within solar cells. As the name suggests, solar cells or rather photovoltaic cells, are used to transform sunlight into electrical energy through the photoelectric effect [1-3]. Carbene compounds have proven to attract attention pertaining to their exceptional properties in respect to solar cells [4-6]. In order to effectively capture solar energy, they are made to have strong light-absorbing capabilities in the visible and near-infrared spectrum. In addition, their electronic structures are tunable, and this feature makes it possible to optimize their energy levels for ideal use in solar cells [7-9]. More so, some carbene compounds exhibit long excited-state lifetimes, which boost electron transfer and minimize energy loss. With this said, challenges associated with the stability of carbene compounds under prolonged exposure to light and heat still persist. The ongoing research, though, suggests remarkable opportunities for the formation of novel and efficient solar cells.

One useful aspect of carbene based sensitizers is the ability to modify their molecular structure for specific applications. This makes it possible to adjust the energy levels, absorption spectra, excited state lifetimes, and other electronic and optical features to fit the needs of different types of solar cells[9-13]. In dry and static solar cells (DSSCs), carbene based sensitizers have provided great results with power conversion efficiencies (PCEs) reaching as high as 13%. Their use in DSSCs can also increase stability and device lifetime because they form stable molecular compounds with the semiconductor material [14-16]. Carbene compounds have also been investigated for potential applications in other solar cells, such as perovskite and quantum dot solar cells. Carbene-based whole carriers in quantum dot solar cells have demonstrated enhanced stability and charge transfer mechanisms in perovskite solar cells. Carbanes are employed as ligands in quantum dot solar cells to boost the efficiency of charge transfer mechanisms [17-20]. The evolution of DSSCs was captured by Suri Babu Akula in 2017. The analysis attempted to understand the impact of long-term polymerizing of the sensitizers, which are derived from N-heterocyclic carbons. The study aimed at determining the coupling chain length of the sensitizer and its effects on electron injection efficiency, power levels, and absorption spectra of the solar cells.

The findings showed that modification of the coupling chain length resulted in the reconstruction of the absorption spectra and improved electron injection efficiency and, thus, energy conversion efficiency. N-heterocyclic carbonates with long coupling chains as sensitizers are promising for constructing efficient and cheap DSSCs [21].

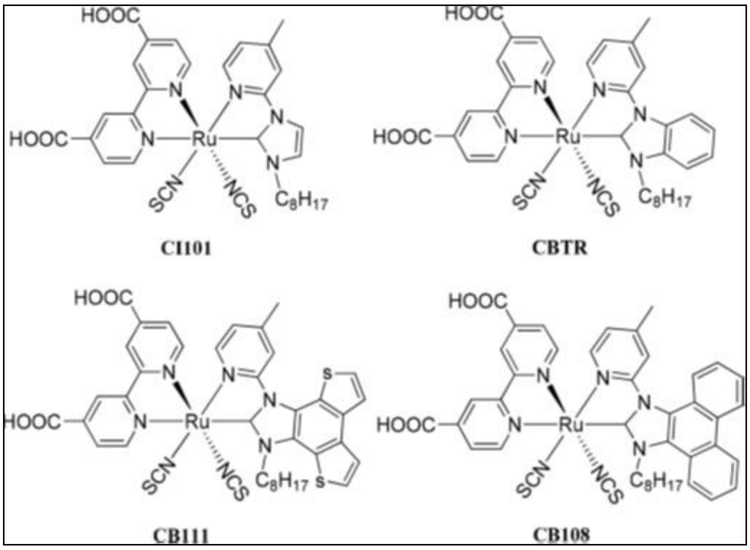
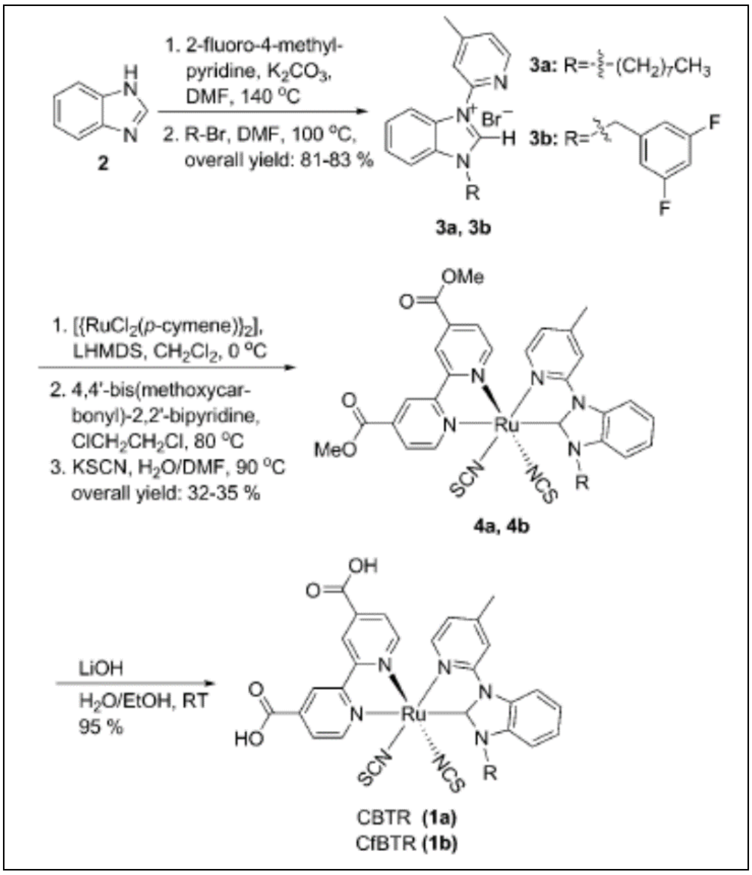


Fig 1: Molecular structures of the Ru complex sensitizers

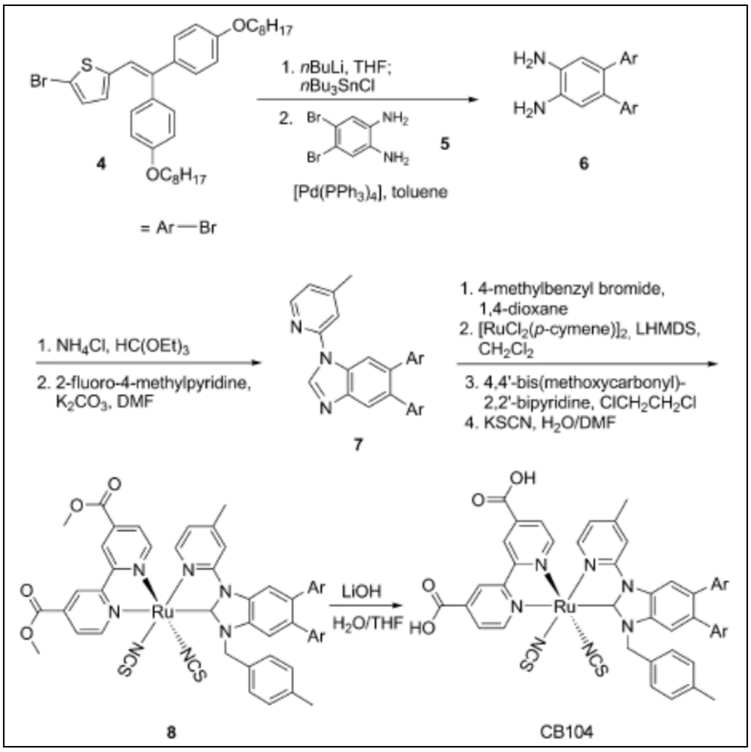
Wei Zhang-Chun Zhang worked on effective ruthenium heterocyclic carbonate/pyridine dyes in 2010 that function great in DSSCs. The work was devoted to the technology of creation of new highly efficient and stable light-harvesting Ru complexes that can absorb and convert solar light into energy. The authors furthermore concentrated on the impact of various chemical structures on the performance of the cells and the application of Solid Phase Synthesis in the sensitizer technique for the production of DSSCs. The most successful Ru sensitizers to date were the freshly created ones, achieving a power conversion efficiency of 7.4%, including those based on the ruthenium cyclic heterocyclic carbonate/pyridine. These findings indicate that the described ruthenium complexes can be effectively tuned for better performance in stable and efficient DSSCs [22]. (Scheme 1).



Scheme 1: Synthesis of the N-heterocyclic carbene-pyridine-based Ru sensitizers

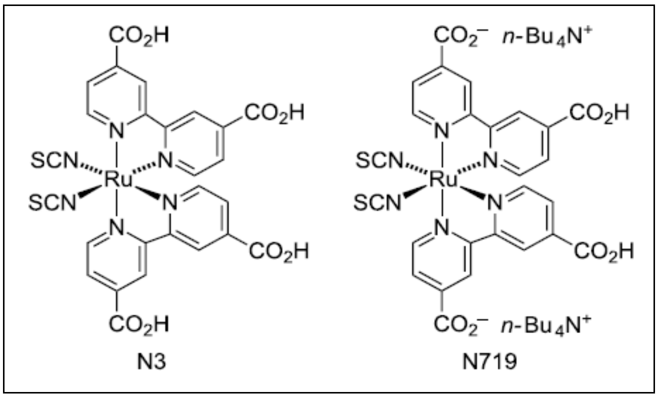
CBTR (1a) and CfBTR (1b)

In her 2013 study, Shih-Yu Hu focused on a highly conjugated ruthenium sensitizer based on supported ruthenium benzimidazole carbene, regarding ruthenium ion pairing in DSSCs. The study's goal was to create and synthesize a novel ruthenium compound and examine how it affected solar cell performance. Light-harvesting efficiency, photovoltaic performance, DSSCs performance, and stability were all examined using the recently created sensor. The findings revealed that the carbon-based ruthenimidazole benzimidazole carboxylate akylation showed high light-harvesting efficiency and outstanding stability on prolonged illumination. With this sensor, the power conversion efficiency of the solar cells was achieved at 8.36%, indicating its feasibility for the development of more stable and efficient dye-sensitized solar cells. The research indicates that highly conjugated benzimidazole carbon based ruthenium sensitizers are winning candidates for future developments of dye-sensitized solar cells [23] (Scheme 2).



Scheme 2: Synthetic route for sensitizer CB104. LHMDS=lithium hexamethyldisilazide

In 2018, Maria Karpacheva studied the efficiency of NHC-type iron (II) dye sensitizers in modification of electrolyte in dye solar cells. The aim of the investigation was to establish how efficient are NHC type iron (II) dye sensitizers in DSSCs. The light-harvesting efficiency, photovoltaic performance, and stability of the cells with diverse compositions of the electrolyte were analyzed.The findings revealed that the performance of solar cells varies with each electrolyte and some electrolytes have higher energy conversion efficiency than others. Performance optimization by aligning the redox potential of the electrolyte with the power level of the sensitizer was also shown in the study. The research confirms that for iron (II) sensitive NHC designers solar cells, careful selection of the electrolyte is fundamental for high performance output [24] (Scheme 3).



Scheme 3: Structures of the ruthenium dyes (N3) and N719

In 2011, Huey-Seo Chen conducted research on ruthenium carbonate-based photosensitizers. The aim of this research was to design and synthesize new ruthenium complexes with NHC ligands and study their effect on the performance of integrated carbon-carbon photocatalyst cells. The new photosensitizers were used and the researchers examined the photovoltaic performance, light harvesting efficacy, and cell stability. The results obtained show that carbonate-based ruthenium photosensitizers are distinguished by high light harvesting efficiencies and excellent stability during prolonged illumination. They can play a role in future development of reliable efficient DSSCs because the power conversion efficiencies of solar cells using these are up to 7.5 percent. It is clear from the research that developments in dye sensitive solar cells can benefit from carbene ruthenium-based photosensitizers [25].

In 2016 Mariachiara Pastore explored the link between photovoltaic efficiency and interfacial charge separation in iron II carbenes sensitive solar cells (Figure 2). Design and synthesis of novel iron-based sensitizers with carbene ligands and their impact on dye-sensitized solar cells' photovoltaic efficiency were the main objectives of the work. The research's maximum energy conversion efficiency of over 8.5 percent demonstrated that the direct sensitized solar cells' solutions to the challenge of increasing efficiency and power reliability were effective. More work went into testing and optimizing cell stability, their photovoltaic performance as well as interfacial charge separated kinetics through the sensitizers that were designed and generated during the study. Thanks to the robustness exhibited by the carbene tethered iron-based sensors, it was possible to achieve efficacious interfacial charge separation which led to a much greater photovoltaic performance than anticipated [26].

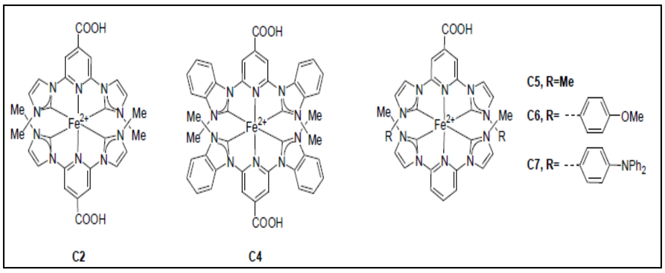


Fig 2: Chemical structures of the investigated iron complexes

As illustrated in Figure 3, Ejasui Gela was doing research in 2016 on heterogeneous Ru(II) complexes for usage in dye-sensitized solar cells by applying benzimidazole-phenylene carbene ligands. The performance of dye-sensitized solar cells was investigated by designing and synthesizing novel ruthenium-based sensitizers with carbene ligands. Along with the examination of the newly synthesized sensitizers and their electro-physical properties, efforts were made to improve the design of the efficient desensitized solar cells. According to the findings, heterogeneous Ru(II) complexes based on benzimidazole-phenylcarbinol ligands exhibit enhanced light absorption and quicker charge transfer at the interface between the TiO2 layer and the sensitizers. With the use of this sensitizer, a solar cell's power conversion efficiency was 7.6%. This suggests the possibility of developing dye-sensitized solar cells that are more dependable and effective. According to a study that was presented, the heterocyclic Ru(II) complex seems to improve dye-sensitized solar cells' long-term performance [27].

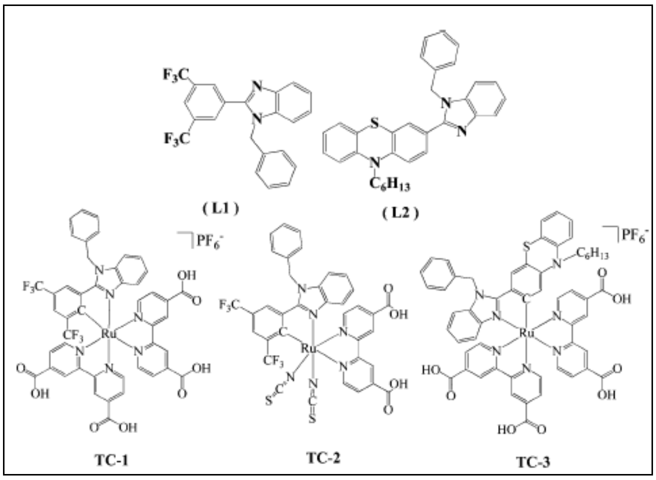
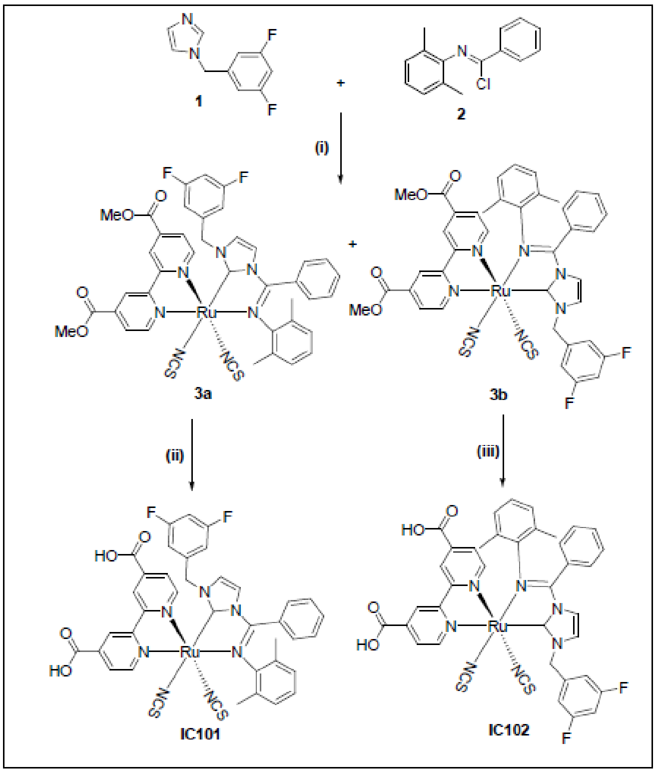


Fig 3: Molecular structure of the ligands and Ru complexes

Research undertaken on imine-carbene based Ruthenium complexes with regards to the isomeric mixtures and their impact on photovoltaic performance indicates that there is considerable scope for developing better and more stable DSSCs. Different isomeric mixtures of iminecarbene based Ruthenium compounds showed better photovoltaic performance as compared to single isomes, possibly due to greater coverage and absorption by the spectra of the isomeric mixture. Different substituents on the carbene bonds were also studied and it was found that some substituents had drastic effects on the photovoltaic performance of the assembled ruthenium complexes. The results suggest that indeed more work on the iminecarbene based Ruthenium complexes can be undertaken in regards to the field of DSSCs. This field is however still open and requires more research to be done on the impact of different isomeric mixtures and other materials on the performance of these multiplexed systems to find optimal design configurations for efficiency and stability in real world applications.



Scheme 4: Synthesis ruthenium complexes, (i) 1. RT, THF; 2. Ag_2O, DCM, RT; 3. $[RuCl_2(p\text{-cymene})]_2$, DCM, RT; 4. dimethyl2,2-′ bipyridine-4,4'-dicarboxylate, DCE, 80 °C; 5. KNCS, H_2O/DMF = 1/9, 90 °C. (ii) THF/H_2O, 0.5 M NaOH(aq), RT; (iii) DMF, 0.5 M LiOH(aq), RT

For usage in dye-sensitized solar cells, Yogesh S. Tengar concentrated on imine-carbene-based ruthenium complexes in 2020. Additionally, he examined how the complex's performance was affected by the isomeric mixture. They demonstrated that the isomeric mixtures of these complexes produced greater photophysical performance than the single isomeric complexes as a result of the greater spectra of absorption the mixture produced. Furthermore, the researchers analyzed the influence of substituent groups on the carbene bonds, and some substituents were found to have very strong effects on the photovoltaic performance of the ruthenium complexes. The researchers believed and stated that imine-carbene-based ruthenium complexes are promising compounds that can be used to develop more efficient and stable DSSCs. Nevertheless, these complexes require further exploration to enhance their design for practical use[28]. (Scheme 4).

The study showed that charge transport and light absorption in the solar cell nanostructure were enhanced by the imine-carbene-based ruthenium complexes when blended in an isomeric mixture. The blend of isomers also outperformed the single isomers in terms of efficiency because of the broader absorption bandwidth.

The importance of isomeric blends of imine-carbonate-based Ru complexes as dye sensitizers in DSSCs is underlined in this publication and demonstrates means by which the photovoltaic performance can be improved by such means.

Further exploration in this field can lead to the development of better and cheaper solar energy systems, which is very important for the renewable energy industry.

Important prospects in renewable energy were outlined by Linde Lenya's 2021 study on DSSCs made using Fe-NHC photosensitizers, which showed optimum push-pull rod-like action. This indicates that Fe-NHC photosensitizers can be used to increase the dye-sensitized solar cells' efficiency [29].

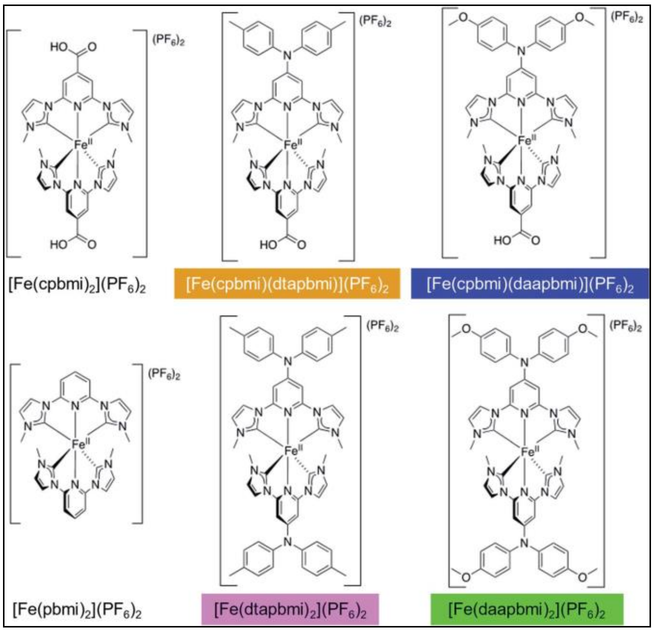


Fig 4: Every complex mentioned in this paper. The hues represent the color scheme that is employed constantly throughout this essay

The quantitative findings of the research depict that the iron N-ring heterocyclic carbonate photosensitizers with a rod like push-pull action can greatly enhance the photovoltaic light absorption and charge transport within a solar cell. The research also suggests that these photosensitizers are better in terms of energy levels and molar extinction coefficients than other type of sensitizers. The report demonstrates the primary possibility of employing Fe NHC photosensitizers which axial symmetry with improved rod like push-pull action can be used in DSSCs. More research in this direction should make it possible to find more efficient and cheaper solar energy technologies, which should be beneficial for the renewable energy industry. This study demonstrates the potential of Fe N-heterocyclic carbene push-pull photosensitizers to significantly impact the efficiency of DSSCs, and indicates where the research may go in the future.

In 2014, Ruby Srivastava did a theoretical study on the developing use of Ru (II) n-heterocyclic carbene complexes as potential candidates for dye-sensitized solar cells. The purpose of the study was to determine whether it would be possible to incorporate these complexes as different types of dyes in DSSCs. The research simulated the absorption spectra and the electronic structures of the complexes using computer modeling techniques. The findings indicated that there is notable similarity between the photo absorption characteristics of the ruthenium (II) NHC Complexes and those of the conventional dyes used in DSSCs. Additionally, the study determined that these complexes are capable of demonstrating high stability and efficiency in DSSCs. With all of this in mind, the research strongly advocates that ruthenium (II) N-Heterocyclic Carbene Complexes have promising prospects when compared to the classic dyes usually preferred in DSSCs [30].

In this regard, the investigation into the use of ruthenium (II) n-heterocyclic carbonate complex of ruthenium (II) as dyes broadens the scope of DSSCs.

As with most studies, this one also has a major weakness it is based on a theoretical model and not an experimental design. Accordingly, their results do not accurately depict the properties of ruthenium (II) NHC complex in practice. Moreover, the findings of this study were restricted to the particulars of the complexes in the investigation, and subsequent studies are needed to evaluate the scope of other carbine complexes for application in DSSCs. N-heterocyclic iron (II) carbene (NHC) dyes can be possibly used in dye sensitized solar cells (DSSCs) and Karpacheva Maria researched on this problem in 2019 (Picture 5). The study investigated the problem of selecting the proper electrolyte for DSSCs as it determines the redox potential of the dye and the efficiency of electron injection [31].

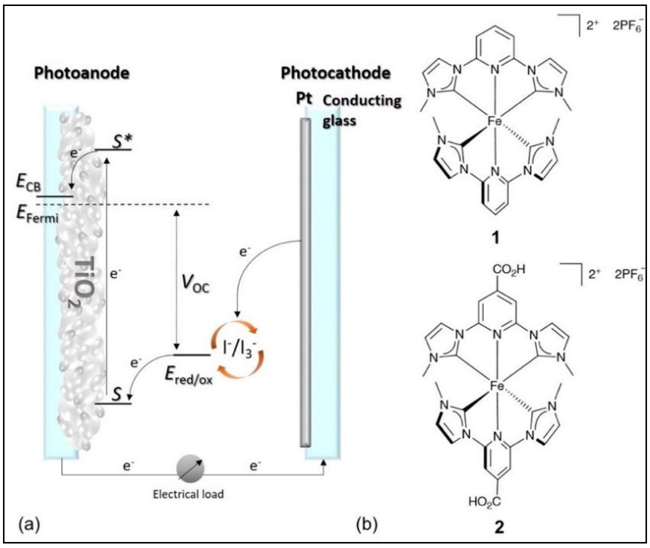


Fig 5: Investigation of (DSSCs) using (NHC) iron (II) dyes

At last, the study was able to elaborate on the merits that N-heterocyclic carbene Fe (II) pigments offer in comparison to conventional pigments based on ruthenium, such as their good absorption within the visible spectrum and small toxicity. With NHC Fe (II) dyes used in semiconductor DSSCs co-sensitizers and other stabilising groups that improve the attachment of dye to the surface of the semiconductor are taken into consideration for improvement of the overall performance. Maria Karpacheva spoke on this issue.

The research determined that there is potential utilization of NHC Fe (II) dyes on dry and static semiconductor DSSCs and there exists the capability to enhance these dyes through modification of the electrolyte. But still the study have stated that more investigation is required to comprehend the mechanisms of operation of the Fe(II) NHC pigments for the DSSCs and optimization approaches for their performance in these devices. The research gives an overview on the prospects of the NHC iron (II) pigments used in DSSCs and indicate the demand of more investigations in this area. In 2022, Jain Nimisha studied the introduction of ruthenium complexes, which include heterocyclic bicyclic NHC donors, for use in sensitization of TiO2 in Dye Sensitized Solar Cells (DSSCs) (Figure 6). The study's objective was to assess what impact the heterocyclic bicylic carbocarbene bond would have on the photophysical and electrochemical dynamics of the ruthenium composites and their performance in dye-sensitized solar cells [32].

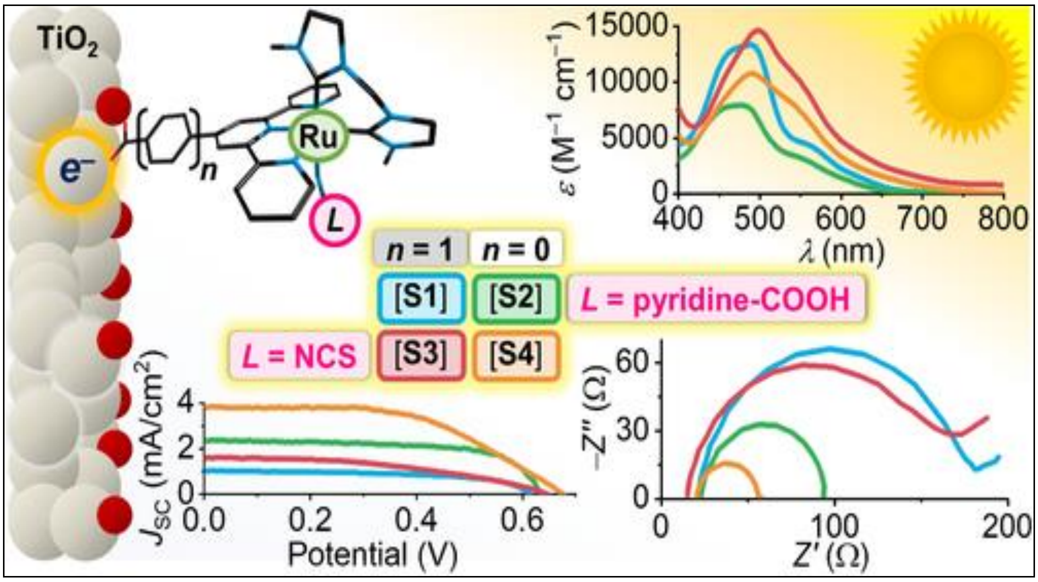


Fig 6: Investigation of the effect of the bis- *NHC* complexes in DSSCs

Different ruthenium complexes containing DSSC donors and a broad range of their functionality were synthesized and their photophysical and electrochemical properties were studied. The complexes were then integrated into DSSCs as sensitizers and their performance was measured.

According to the results, the bond of dihydroxy hydrogen-N-carbon greatly affected the photophysical and electrochemical properties of the Ru complexes. The complexes were characterized by strong light absorption from the solution in the visible region and good stability in the solution. The DSSCs utilizing ruthenium complexes as the sensitives showed good photovoltaic performance, high short-circuit current density, and good fill factor. The study concludes that the incorporation of DBH donor-bearing ruthenium complexes into TiO2 sensitization of DSSCs is a step forward towards improving the efficiency of these devices. The study reveals the possibility of applying dihydrogen dihydroxide ligands and gives useful information for designing new sensitizers for DSSCs.

The study made by Mary Angelina in 2022 on the application of ruthenium (II) complexes in DSSCs is another very interesting and prospective study area (Figure 6). The study presents these complexes as potential ones that would improve the efficiency of DSSCs because they could be used as the sensors which converts light into electrical energy [33].

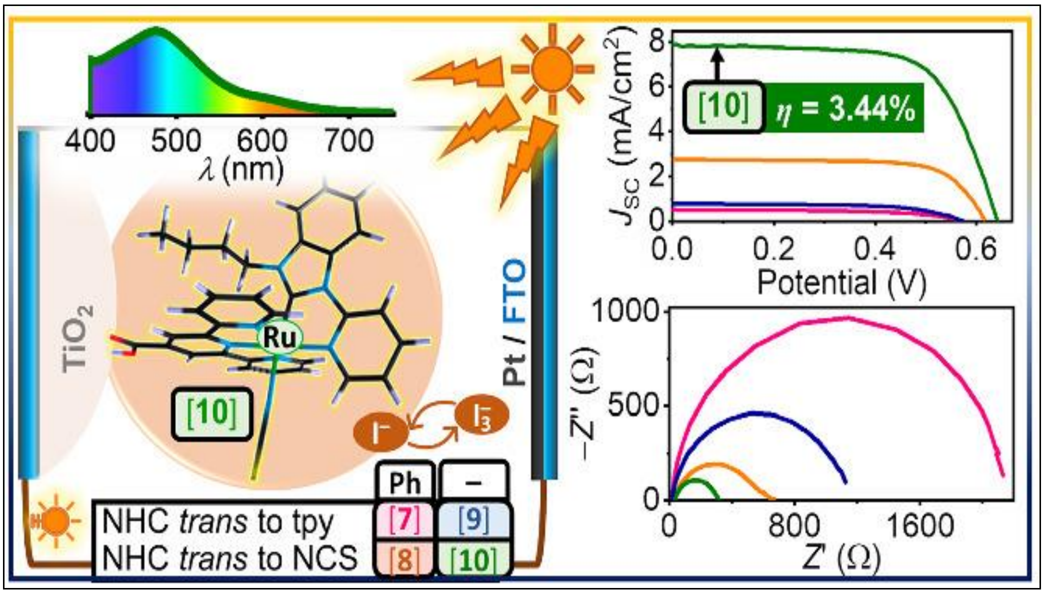


Fig 7: Enhancement of the efficiency of DSSCs by Ruthenium (II) complexes

The conclusions drawed from the research state that these complexes have a number of benefits compared to other sensitizers such as high molar extinction coefficients and more suitable energy levels. This means that DSSCs and new and improved solar technologies can be more productive. To sum up, the results of this work are quite informative regarding the use of C=N based cyclic heteroic carbon donor molecules containing ruthenium (II) dyads in DSSCs. Further studies in this regard can aid in the development of advanced cost-efficient solar technologies.

Linnea Lind began her 2020 project to learn more about the photophysics and photochemistry of iron carbene complexes for photocatalysis and solar energy conversion. The studies revealed that these complexes possess unique characteristics which enable them to be used for many applications such as efficient electron transport, long life excited states, and strong light absorption [34].

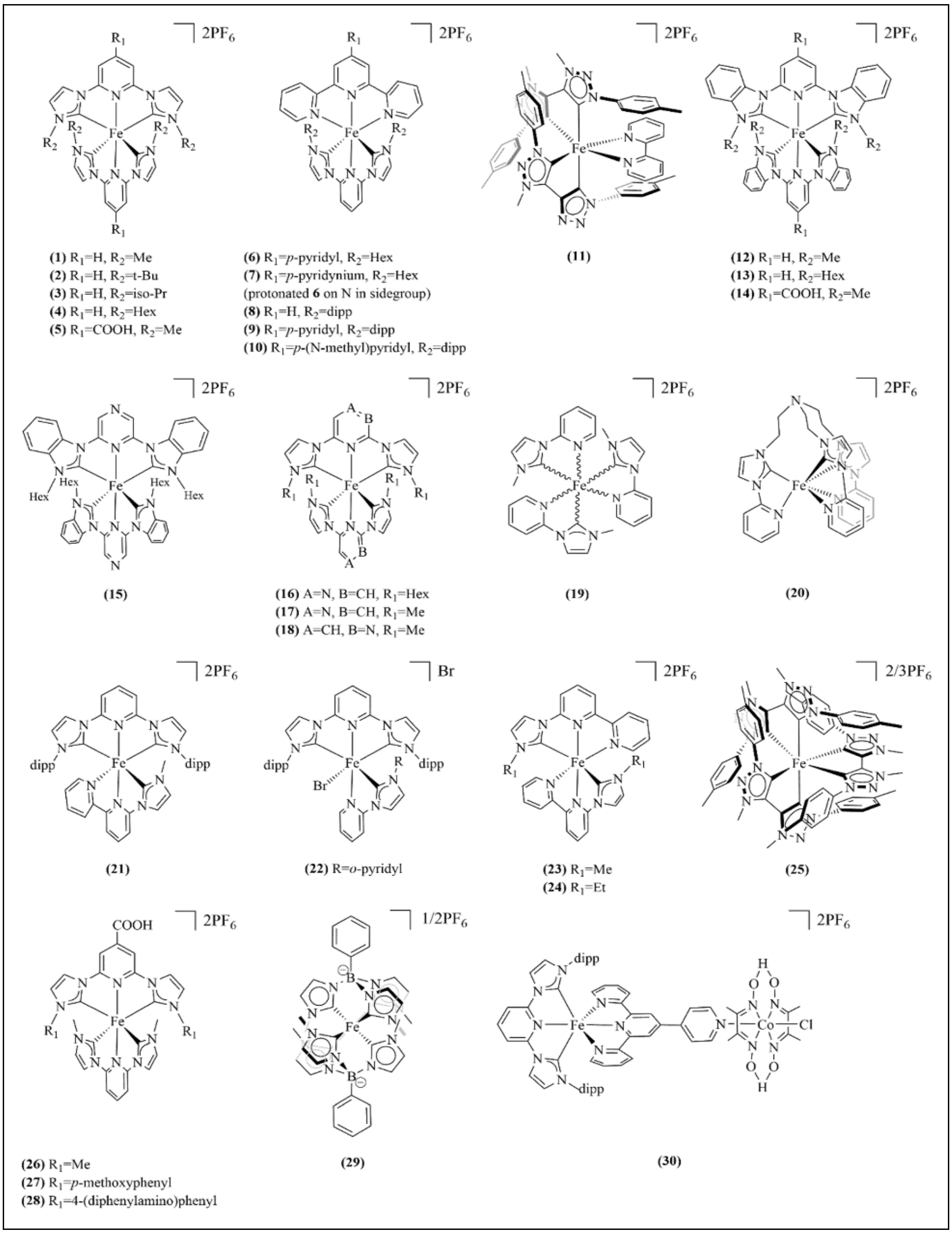


Fig 8: Investigation of (DSSCs) using (NHC) and some transition complexes

Based on the study, the performance of iron carbene complexes in solar energy conversion can also be influenced by other factors such as the electronic structure and bonding environment of the complex. Therefore, this study contributes toward th e understanding of these fundamental processes by offering deeper examination of the possibilities of iron carbene complex systems as sensitizers in solar energy conversion and other related systems.

All in all, the work is a huge step forward in the advancement of sustainable and hardworking solar energy techniques. Additional works pertaining to this topic may include the improvement of NHC iron carbene complexes for solar energy transformation and other applications, which could significantly address the issues of sustainable energy generation.

Conclusion

According to certain research, carbene chemicals may find use in Dye Sensitized Solar Cells (DSSCs), among other kinds of solar cells. Carbene chemicals, for instance, are known to convert light into energy in a variety of solar cell types, making them potential sensitizers. The ingredients used feature high molar extinction coefficients, which suggests low molar extinction coefficient means lower light transmission. DNA strands efficiently inject electrons into the supporting material; efficiently transferring electrons from the excited-state sensitizer molecule to the electrode. This signifies the system will be able to produce more electricity from sunlight than traditional devices. In perovskite solar cells, researchers have also investigated the use of carbene compounds as whole carriers boron-doped. These compounds assist in lowering recombination and boosting charge transport abilities without negatively impacting the overall effectiveness of the device. In organic solar cells, eye-catching carbene compounds are actively studied as great electron acceptors. Compared to other compounds, they are more soluble and easier to process, which facilitates their implementation into an organic solar cell device

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