Turkish Computational and Theoretical Chemistry

Turkish Comp Theo Chem (TC&TC)

Volume(Issue): 7(2) – Year: 2023 – Pages: 20-33

e-ISSN: 2602-3237

https://doi.org/10.33435/tcandtc.1181765

Received: 29.09.2022 ***Accepted:*** 25.10.2022 *Research Article*

Theoretical Methods for coding a strand of DNA bases and nucleotides with C_2Fe^+, A DFT study

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Abstract: DNA strands are essential in a cell for growth, metabolism regulation and carrying genetic information bases to new generations, in every creatures . The function of DNA bases is a 0 and 1 system. In this theoretical research , we try to make two other 0 and 1 systems for DNA bases .In both methods, C_2Fe^+ is attached to DNA bases and nucleotides like a flag to make derivatives. In the first method NMR susceptibility and Magnetization of pristine DNA bases, nucleotides and their C_2Fe^+ varieties are determined theoretically by using Gauss view and Gaussian programs. With effect of a magnetic field (H) and NMR susceptibility of these compounds, their calculate magnetizations , certain signals can be created as a mark of DNA bases and their compounds. These resulted not only can be considered as a method to make a new 0 and 1 coding system. In the second method, by using Gauss view and Gaussian programs the theoretically UV-Visible spectrum of pristine DNA bases, nucleotides and their C_2Fe^+ varieties are determined which the spectrum absorption of the pristine compounds are in different range with the absorption range of C_2Fe^+ varieties. With a little change in spectrophotometer construction another 0 and 1 coding system can be created, again.

Keywords: DNA bases, nucleotides, C_2Fe^+, magnetic susceptibility, magnetic field , magnetization, UV-Visible spectroscopy

1. Introduction

Deoxyribonucleic acid (DNA) has been the key of inheriting the genetic information of parents to next generations in all living systems. The sequence DNA can be used to know DNA fingerprinting which has applications in, medicine, agriculture and genetic engineering. DNA strands consist of bases Adenine (A), Thymine (T), Guanine (G) and Cytosine (C) [1]. The structure of the bases is shown in figure 1 [2].

Nucleotides are the building blocks of a DNA strand and each is consisted of three parts; 1) Deoxyribose, 2) the Nitrogen base and 3) Phosphate group. The DNA bases are classified into two groups: A) Purine groups which are including Adenine and Guanine, B) Pyrimidine groups which are including Cytosine and Thymine. The DNA backbone is formed by the Phosphodiester bonds; the covalent bond between sugar and Phosphate units [3].

Two DNA strands in opposite directions, construct a helical spiral structure and the two helical chains of nucleotides are held together by Hydrogen bonds between the purine nucleic bases of one strand and pyrimidine nucleic bases of the other strand. This means, Cytosine can be connected to Guanine and Adenine with to Thymine [3].

Magnetic properties of pristine DNA and DNA-metal complexes have been investigated both in biological and non-biological researches to determine DNA properties such as replication, transcription of genetic codes, nanotechnology and other phenomena. [4].

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This theoretical research is about coding the bases and their nucleotides using two methods. In these methods both DNA bases are attached to a compound such as C_2Fe^+. C_2Fe^+ is attached like a flag to a certain base or nucleotide to creates magnetic field and certain varieties for DNA bases and nucleotides.

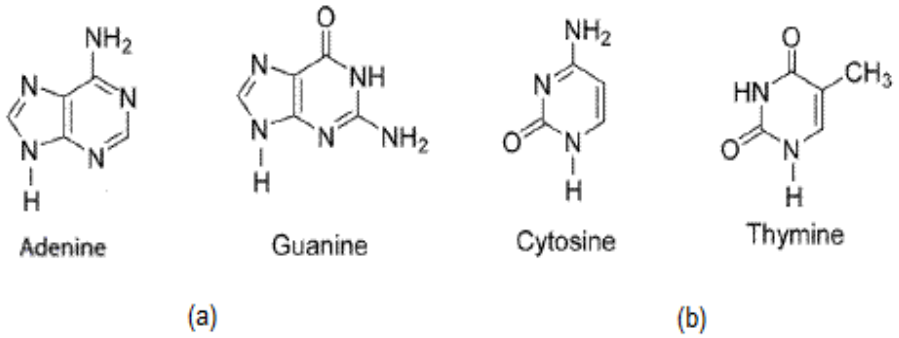


Figure 1. DNA bases (a) Purine groups: Adenine, Guanine (b) Pyrimidine groups: Cytosine, Thymine [2]

The first method used for coding is Gaussian software and Density Functional Theory (DFT) method to determine magnetic susceptibility DNA bases and nucleotides and their varieties. In the next step, the one strand of DNA which is attached to C_2Fe^+ will be through a certain magnetic field to calculate and compare the magnetization of pristine DNA bases and their attached compounds. This comparison can be used to make signals to determine certain bases on one DNA strand.

Density functional theory (DFT) calculations is one of platforms to study the interaction of the DNA bases and their interactions with other ions or compounds. [1]

The second method is using the absorption properties of DNA bases and nucleotides and their varieties in visible and ultraviolet spectrum. These absorption properties and ranges are theoretically determined by Gaussian and Gauss view software and can be detected experimentally by spectrophotometer in a lab. Using Graphene as a plate to hold DNA strand instead of a sample solution.

2. Computational Method

By using DFT functional methods (Cam-B3LYP) with SDD basis set, geometry optimizations , energy calculation and magnetic susceptibility of C_2Fe^+ and Adenine, Cytosine, Guanine and Thymine is measured. In the next step, magnetic susceptibility of theses bases attached with C_2Fe^+ are investigated. The calculations were performed in Gaussian suite of the program. Vibration frequencies were also calculated at the same level to confirm that all the stationary points correspond to true minima on the potential energy surface.

For determination of theoretical absorption ranges and peaks of these compounds in the second method Td=NSTATES=5 is used by Gaussian and Gauss view software [5].

3. Results and discussion

3.1. NMR Susceptibility of pristine DNA bases and C_2Fe^+

In the first method, Gaussian program and DFT method is used to determined theoretically NMR susceptibility and also ground state energy of Adenine, Cytosine, Thymine and Guanine. Figure 2 shows the structures and the MEPs of these bases. These calculations are also performed for C_2Fe^+ which going to be is used as an attached flag to these bases to create derivatives of these bases. The results of these calculations are listed in table 1 and table 2 and the resulted structures and MEPs are shown in figure 2. Figure 3 is the structure of C_2Fe^+ opted with (Cam-B3LYP) with SDD basis set.

3.2. NMR Susceptibility of DNA bases attached with $C2Fe^+$

Figure 4 shows the opted structure of DNA bases which are attached to C_2Fe^+ and their MEPs. NMR susceptibility and ground state energy of these derivatives are also determined with Cam-B3LYP method and SDD basis set. The results are shown in table 3. Comparison results of table 1 with table 3 indicates that NMR susceptibility of the pristine bases are negative but after connecting theses

bases with C_2Fe^+, NMR susceptibility changes to positive. Also, E total for the mentioned compounds in table 3 are more negative than compounds in table 1 which can be considered as more stability in attached bases with C_2Fe^+.

Table1. E total and NMR Susceptibility DNA bases		
Compound	E total (a.u.)	NMR susceptibility (cgs-ppm)
Adenine	-467.00	-87.52171
Cytosine	-394.68	-57.5114
Thymine	-453.86	-63.0134
Guanine	-542.21	-83.8078

Table2. E total and NMR Susceptibility C_2Fe^+		
Compound	E total (a.u.)	NMR susceptibility (cgs-ppm)
C_2Fe^+	-199.44	317.1457

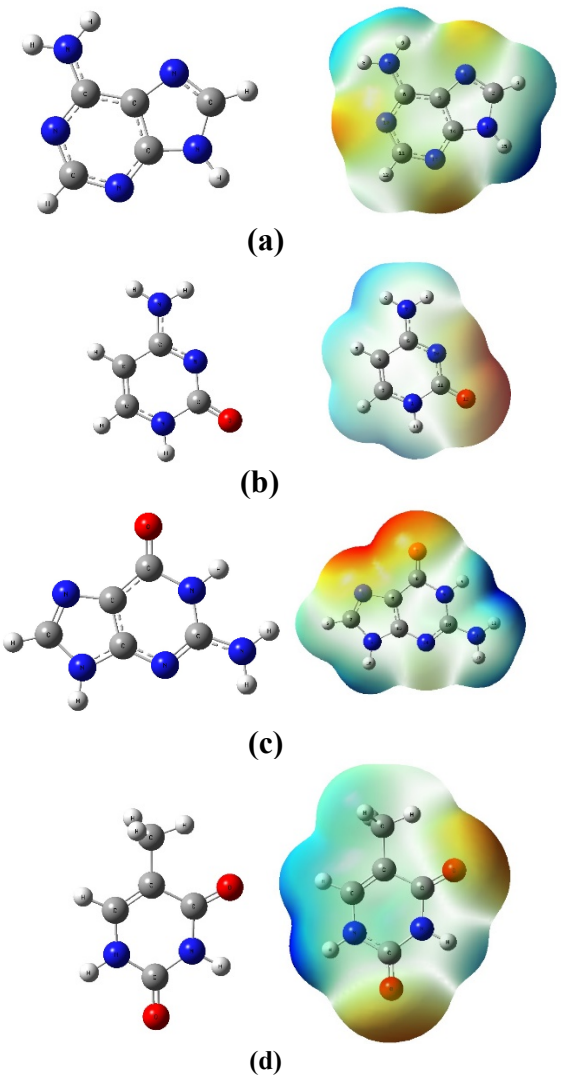


Figure 2. Structures and MEPs of (a) Adenine (b) Cytosine (c) Guanine (d) Thymine opted with Cam-B3LYP with SDD basis set

Table 3. E total and NMR susceptibility of Adenine-C_2Fe^+, Cytosine-C_2Fe^+, Thymine-C_2Fe^+, Guanine-C_2Fe^+		
Compound	E total (a.u.)	NMR susceptibility (cgs-ppm)
Adenine-C_2Fe^+	-666.62	212.8415
Cytosine-C_2Fe^+	-594.33	240.7476
Thymine-C_2Fe^+	-653.42	206.4516
Guanine-C_2Fe^+	-741.76	199.9606

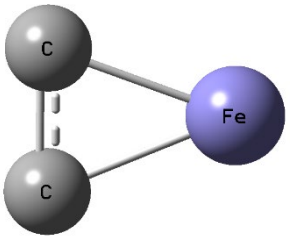


Figure 3. Structure of C_2Fe^+ opted with Cam-B3LYP with SDD basis set.

Figure 2 shows that for DNA bases, charge integrations for Adenine are more around nitrogen atoms while for Cytosine, Guanine and Thymine, charge integrations are more around oxygen atoms. After attaching C_2Fe^+ to those bases, the derivatives in figure 4 showed different kind of MEPs. C_2Fe^+ has a positive charge and its charge has been distributed around the whole molecule and has given them positive charge.

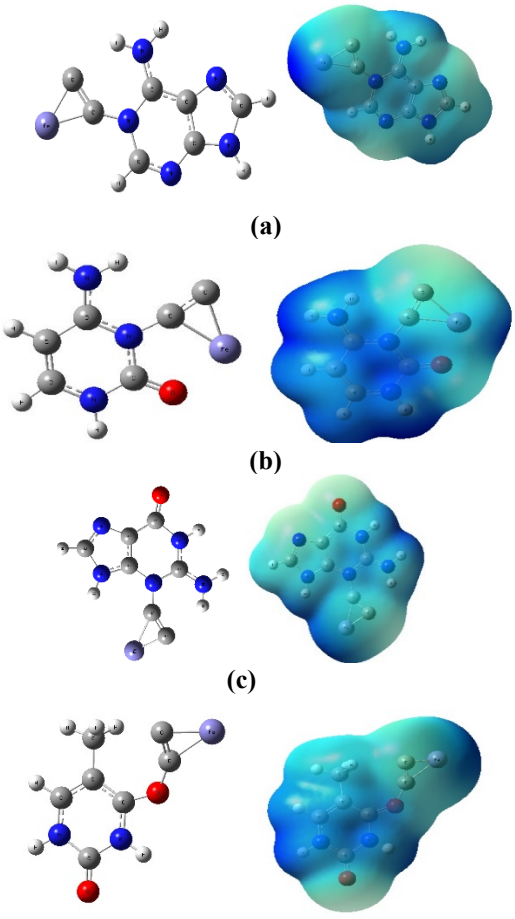


Figure 4. Structures and MEPs of (a) Adenine-C_2Fe^+ (b) Cytosine -C_2Fe^+ (c) Guanine-C_2Fe^+ (d) Thymine-C_2Fe^+ opted with (Cam-B3LYP) with SDD basis set

3.3. NMR susceptibility of pristine DNA nucleotides and their derivatives with C_2Fe^+

For further research of the C_2Fe^+ effect on DNA, NMR susceptibility and ground state energy of pristine DNA nucleotides Adenosine monophosphate, Guanosine monophosphate, cytidine monophosphate and Thymidine monophosphate are determined with using with Cam-B3LYP and SDD as basis set. Their opted structures and their MEPs are shown in figure 5. E total and NMR susceptibility of these compounds are listed in table 4.

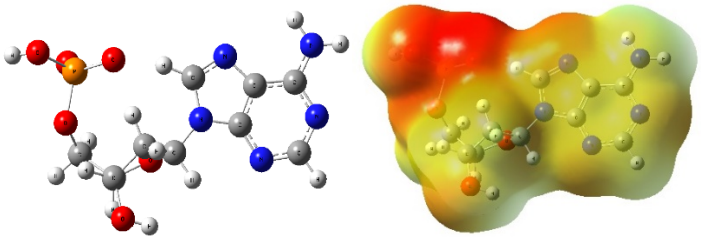
The procedure of theoretical determining NMR susceptibility is repeated again with these nucleotides attached with C_2Fe^+. The resulted structures their MEPs are also shown in figure 6. Their E total and NMR susceptibilities are listed in table 5. The effect of C_2Fe^+ on NMR susceptibility of pristine nucleotides and their derivatives with C_2Fe^+ can be seen by comparing results of table 4 and 5, which C_2Fe^+ can change the negative NMR susceptibility of the nucleotides to positive. Also, E total for the C_2Fe^+-derivatives in table 5 are more negative than the pristine DNA nucleotides in table 4 which can be considered as more stability in the resulted compounds with C_2Fe^+. Also by comparing MEPs in figures 5 and 6, the charge integration in the pristine DNA nucleotides are around phosphate group in figure 5. For the derivatives resulted of attaching C2Fe$^+$ the nucleotides shown in figure 6, not only there are charge integration and negative charges around phosphate groups but also positive charge distributions can be seen which caused by C_2Fe^+.

Table 4. E total and NMR Susceptibility of DNA Nucleotides

Compound	E total (a.u.)	NMR Susceptibility (cgs-ppm)
Adenosine monophosphate	-1454.77	-202.6909
Guanosine monophosphate	-1529.98	-198.8191
Cytidine monophosphate	-1382.45	-173.1896
Thymidine monophosphate	-1441.64	-178.5998

Table5. E total and NMR susceptibility of DNA Nucleotides attached with C_2Fe^+

Compound	E total (a.u)	NMR Susceptibility (cgs-ppm)
Adenosine monophosphate-C_2Fe^+	-1654.48	97.0661
Cytosinid monophosphate-C_2Fe^+	-1582.22	123.2543
Thyminidine monophosphate-C_2Fe^+	-1641.32	91.3340
Guanosine monophosphate-C_2Fe^+	-1729.59	214.3579



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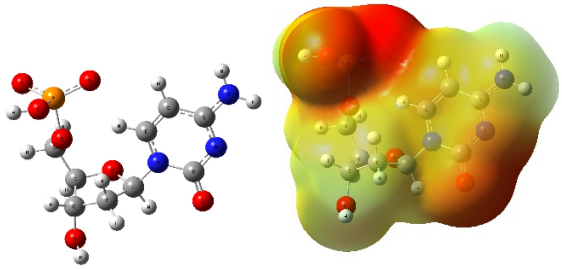

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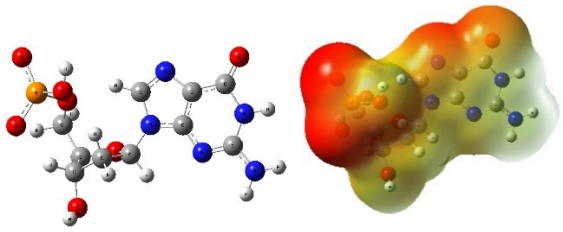

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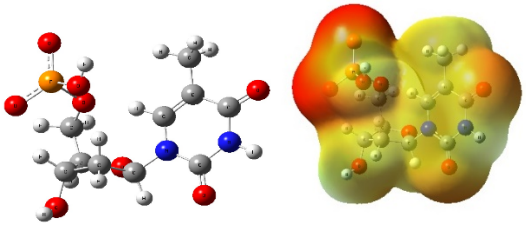
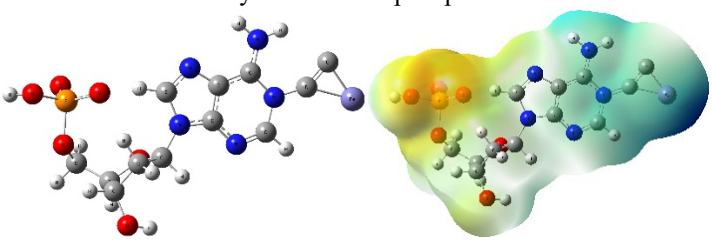


(d)

Fig.5: Structure of DNA nucleotides and their MEPs opted with Cam-B3LYP method and SDD as basis set. (a) Adenosine monophosphate, (b) Cytidine monophosphate, (c) Guanosine monophosphate , and (d) Thymidine monophosphate



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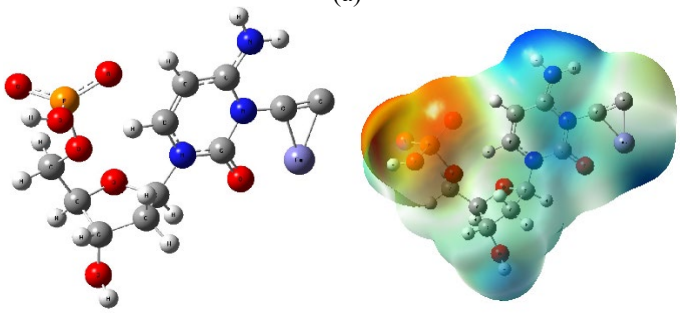

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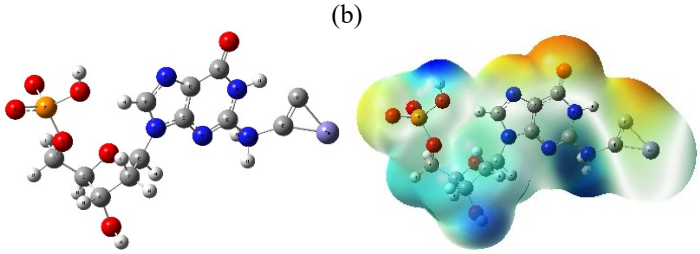

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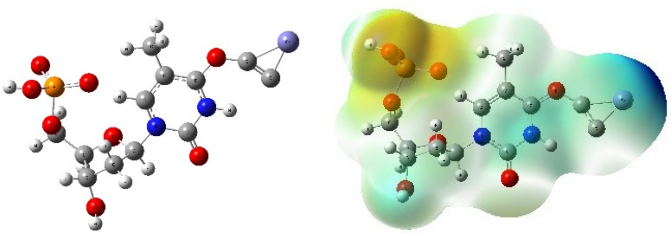


(d)

Fig.6: Structure of DNA nucleotides and and their MEPs opted with Cam-B3LYP method and SDD as basis set. (a) Adenosine monophosphate-C_2Fe^+, (b) Cytidine monophosphate-C_2Fe^+, (c) Guanosine monophosphate-C_2Fe^+, and (d) Thymidine monophosphate-C_2Fe^+

3.4. Magnetization and Magnetic Susceptibility of DNA bases, nucleotides and their derivatives

Magnetization $(\vec{M})$ is related to magnetic susceptibility (χ_m) and magnetic field intensity which can be written as formula 1:

$$\vec{M} = \chi_m \vec{H} \qquad (1)$$

The formula 1 indicate that $\vec{M}$ and $\vec{H}$ are vector quantities but χ_m is a scalar quantity. If $\chi_m \langle 0$, there is diamagnetic response and if we have $\chi_m \rangle 0$, the response is paramagnetic [6].

Magnetic susceptibility (χ_m) refers to the magnetic ability of a material when placed in a magnetic field and a material's (χ_m) is dependent on its molecular constituents, spins, motions of nuclei and their electrons. (χ_m) can be positive or negative, reflecting whether magnetization aligns with the field (paramagnetic), or opposes it (diamagnetism). Paramagnetic phenomena generally originate from field-induced alignment of unpaired electron spins, whereas diamagnetism is associated with field-induced alteration of electron orbits. [7]

In these research χ_m is used in the unit of 10^{-6} cm^3/mol or 1 cgs-ppm, defined per mole of molecules [8]. The calculation in formula 2 shows conversion 10^{-6} cm^3/mol to $m^3/molecule$. NMR susceptibility in table 6 and 7 is calculated as $m^3/molecule$ so the resulted Magnetization can be obtain as $A.m^2/molecule$. If a certain magnetic field is considered such as H=1 A/m, by using formula 1 and 2, the calculated magnetization for each DNA bases, nucleotides and their attached derivatives with C_2Fe^+ will be the values which are shown in the table 6 and 7.

$$1 cgs/ppm = 10^{-6}\left(\frac{cm}{mol}^3\right)\left(\frac{1m^3}{10^6 cm^3}\right)\left(\frac{mol}{6.02\times10^{23} molecule}\right) = 0.166\times10^{-35} m^3/molecule$$

Table6. Magnetization and NMR susceptibility of Adenine, Cytosine, Thymine, Guanine, and their derivatives with C_2Fe^+

Name	**NMR susceptibility** (m^3/molecule)	Magnetization ($A.m^2$/molecule)
Adenine	-14.52×10^{-35}	-14.52×10^{-35}
Cytosine	-9.54×10^{-35}	-9.54×10^{-35}
Thymine	-10.45×10^{-35}	-10.45×10^{-35}
Guanine	-13.91×10^{-35}	-13.91×10^{-35}
Adenine-C_2Fe^+	35.33×10^{-35}	35.33×10^{-35}
Cytosine- C_2Fe^+	39.96×10^{-35}	39.96×10^{-35}
Thymine- C_2Fe^+	34.27×10^{-35}	34.27×10^{-35}
Guanine-C_2Fe^+	33.193×10^{-35}	33.193×10^{-35}

Table7. Magnetization and NMR susceptibility of Adenosine monophosphate, Cytidine monophosphate, Guanosine monophosphate, Thymidine monophosphate and their derivatives with C_2Fe^+

Name	**NMR susceptibility** (m^3/molecule)	Magnetization ($A.m^2$/molecule)
Adenosine monophosphate	-33.66×10^{-35}	-33.66×10^{-35}
Guanosine monophosphate	-32.89×10^{-35}	-32.89×10^{-35}
Cytidine monophosphate	-28.73×10^{-35}	-28.73×10^{-35}

Thymidine monophosphate	-29.56×10^{-35}	-29.56×10^{-35}
Adenosine monophosphate - C_2Fe^+	16.11×10^{-35}	16.11×10^{-35}
Cytidine monophosphate - C_2Fe^+	20.47×10^{-35}	20.47×10^{-35}
Thymidine monophosphate - C_2Fe^+	15.17×10^{-35}	15.17×10^{-35}
Guanosine monophosphate - C_2Fe^+	35.60×10^{-35}	35.60×10^{-35}

The results of tables 6 and 7 indicates that the value of calculated NMR susceptibility of DNA bases and the DNA nucleotides are negative or they have $\chi\langle 0$ which means they have diamagnetic response to a magnetic field. When they all these compounds are attached with C_2Fe^+, value NMR susceptibility of all of them will change to positive value or it can be said that they have $\chi\rangle 0$ and their response to a magnetic field is paramagnetic. The Magnetization results also show negative value for **DNA** bases and **DNA** nucleotides and positive value for their compounds which are attached to C_2Fe^+. These results show the effect of C_2Fe^+ which can change these compounds to paramagnetic ones.

This theoretical research and the results can help us to determine DNA bases , nucleotides or even to create a new way in saving information in one strand of DNA . The pristine bases, nucleotides which are diamagnetic with negative **NMR susceptibility** and magnetization values can be considered as 0 and their derivatives with C_2Fe^+ with paramagnetic response and positive **NMR susceptibility** and magnetization values can be considered as 1. To detect the magnetization of these derivatives with C_2Fe^+ (positive magnetization) , a suggested method is converting magnetization to current electricity signals. In this suggested method, a strand of DNA which some of bases are attached to C_2Fe^+ is crossing a certain magnetic field and a metal ring like copper. Magnetization for each molecule changes to a electric current signal for each molecule and the ring can convert the Magnetization the pristine compound or the derivatives with C_2Fe^+ to a electric current that can be detected as a signal. The pristine bases or nucleotides with negative magnetization cannot make that signal in that metal ring which we consider it as 0. Figure 7a and 7b show the produced signals of the pristine bases, their derivatives in a DNA strand in a magnetic field and converting it to current with the help of the metal ring. For detecting better signals, an amplifier can be used which is shown in both figure 7a and 7b.

Magnetization is a vector unit and for a molecule can be expresses as A.m^2. The origin is the magnetic moments or spin of the electrons in a certain atom of a compound. Magnetization can be responsible for electric currents. Electric current is a scalar unit and is expresses as A(Ampere). For each positive magnetization resulted by attached bases or attached nucleotide there will be an electric current as signal which is expressed in Ampere. This method is completely theoretical way to distinguish DNA bases in one strand.

3.5. Absorption spectrum of DNA bases, nucleotides and their derivatives

The second method for coding DNA bases, nucleotides and their derivatives with C_2Fe^+, is determination of their absorption peak and wavelength theoretically with using Gaussian and Gauss view software. With this two software, the theoretical UV-visible absorption, maximum peak in absorptions and wavelength range of their maximum absorption can be determined. Figure (8) is about UV-visible spectrum of DNA bases and their derivatives with C_2Fe^+ while Figure (9) shows UV-visible spectrum of nucleotides and their derivatives with C_2Fe^+.

The resulted maximum absorptions and the ranges of those absorptions are gathered in tables 8 and 9. These two table shows the range of theoretically spectrums resulted by Gaussian and Gauss view software of DNA bases nd, nucleotides are almost 140 -210 nm which belong to ultraviolet region while the resulted range spectrums of their derivatives have shifted to almost 350-750nm that is visible region. Also tables 8 and 9 show that pristine DNA basses and nucleotides have high epsilons in ultraviolet region but their derivatives have very much lower epsilons, so we can decide that C_2Fe^+ has the ability to reduces absorption of DNA basses and nucleotides.

To coding a strand of DNA with or without C_2Fe^+ with their UV-visible, The Authors of this paper suggest to make chances in spectroscopy method:

UV-visible spectroscopy is a technique for qualitative and quantitative determination that

measures the absorbance of emitted light through a sample or detects the transmitted light out of a sample. UV wavelength ranges from 100nm to 380nm and the visible spectrum is 400 nm up to 800 nm but most of the spectrophotometers have can operate in wavelength range between 200nm and 1100 nm. In UV-visible spectrophotometers a light source is passing through a sample and the sample based on its electronic structure absorbs certain wavelength ranges that a detector on the opposite side records absorbed and also transmitted light. Typically, graphs of the data have the baseline at the bottom with the peaks pointing upward and they report wavelength in nanometers (nm) on the x-axis and absorbance (A) on the y-axis (no units) [9].

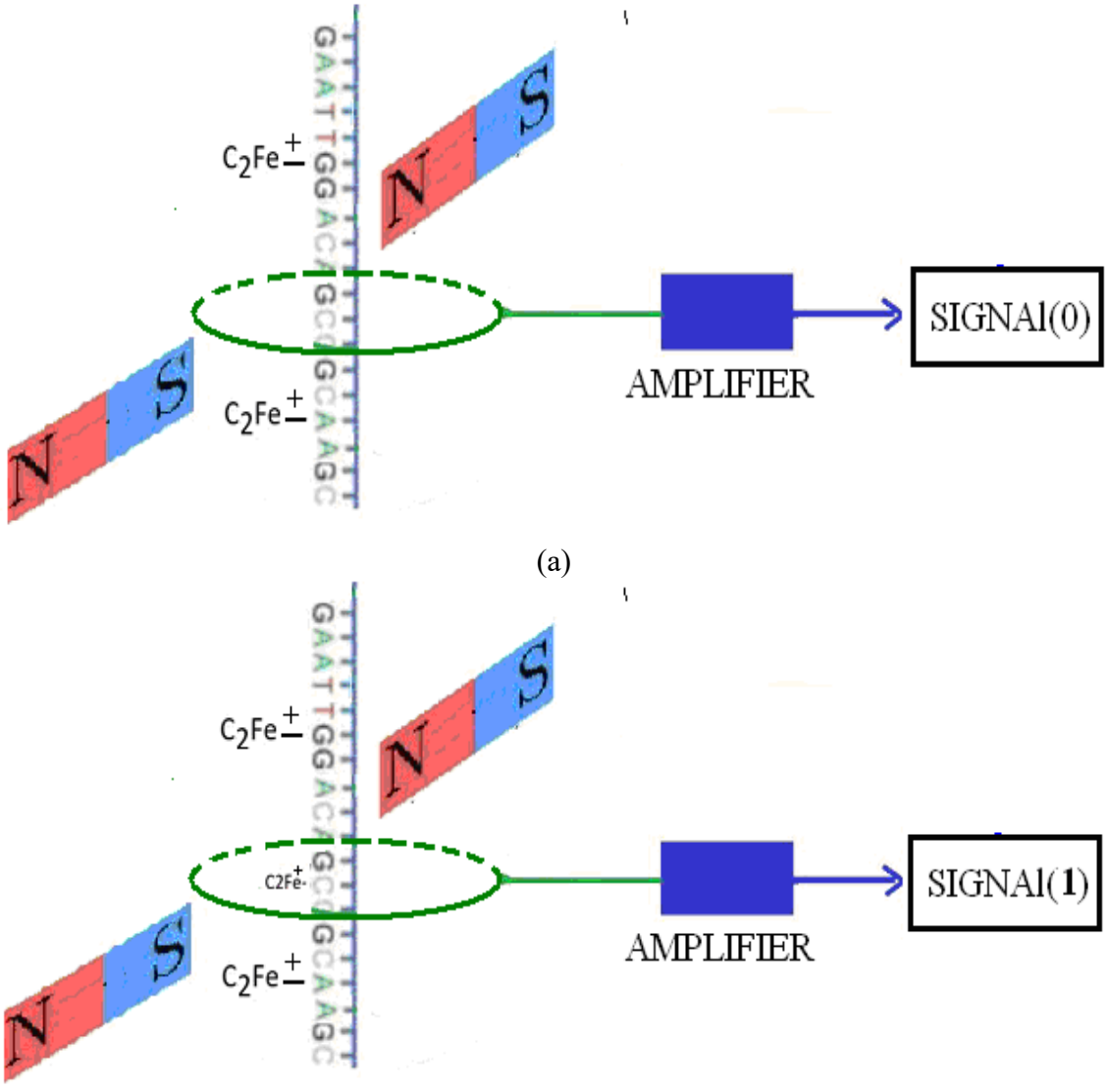


Fig7. The signals of (a) pristine bases and (b) their derivatives with C_2Fe^+ of a strand of DNA in a magnetic field.

Nowadays double beam UV-visible spectrophotometers are used widely for their simplicity of application. The operation of this instrument is shown in figure 10 which the tungsten lamp emits visible light while the D2 lamp generates ultraviolet light. The electromagnetic radiation is directed to a monochromator that chooses the wavelengths to the sample [9].

To detect which the mentioned compounds has absorption in ultraviolet range or visible light range, It is suggested that instead of using cuvettes and solutions for the reference and samples, a very thin layer of Graphene selected as the reference and also as a nano platform for holding the sample. The chosen number of Carbons of the platform is variant and it is depended to the experimental research [10].

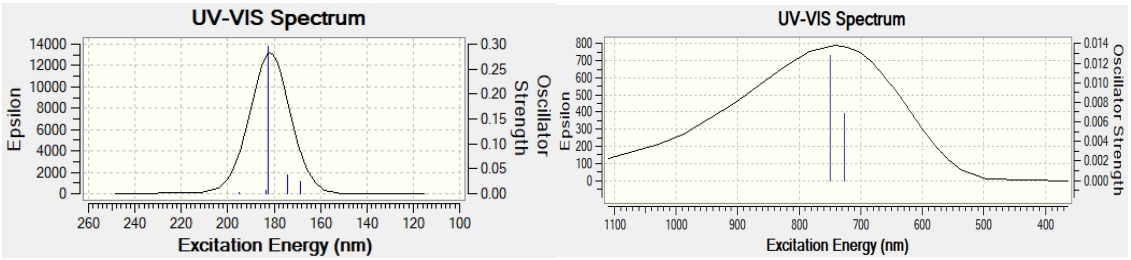
By moving the sample up and down, If resulted absorption range of a DNA bases or nucleotide happens in Ultraviolet range so it is the pristine form and it can be considered as code 0. On the other hand, if the absorption happens in visible spectrum the compound is DNA bases or nucleotide attached to C_2Fe^+ and can be considered as code 1 which is showed in figure 11. It is a new version on coding a DNA strand based on UV-visible absorptions.

Table8. Maximum Absorption Wavelengths of Adenine, Cytosine, Thymine, Guanine, and their derivatives with C_2Fe^+

Name	MaximumAbsorption Wavelengths (nm)	Epsilon
Adenine	182.35	14000
Cytosine	148.36	40000
Thymine	172.87	18000
Guanine	161.62	15000
Adenine-C_2Fe^+	749.28	800
Cytosine- C_2Fe^+	845.41	500
Thymine- C_2Fe^+	766.55	300
Guanine-C_2Fe^+	733.74	800

Table 9. Maximum Absorption Wavelengths and Epsilon of Adenosine monophosphate, Cytidine monophosphate, Guanosine monophosphate, Thymidine monophosphate and their derivatives with C_2Fe^+

Name	Maximum Absorption Wavelengths (nm)	Epsilon
Adenosine monophosphate	183.37	15000
Guanosine monophosphate	200.17	12000
Cytidine monophosphate	203.83	6500
Thymidine monophosphate	176.39	22500
Adenosine monophosphate - C_2Fe^+	757.29	350
Cytidine monophosphate - C_2Fe^+	774.66	350
Thymidine monophosphate - C_2Fe^+	758.09	325
Guanosine monophosphate - C_2Fe^+	751.67	45



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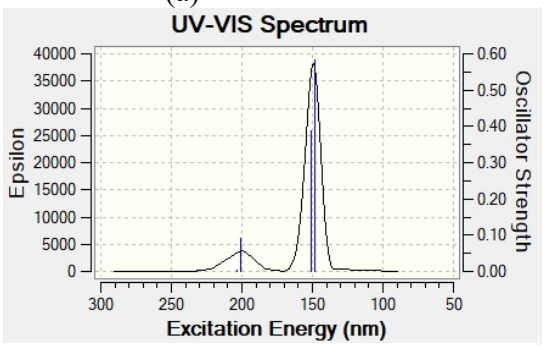

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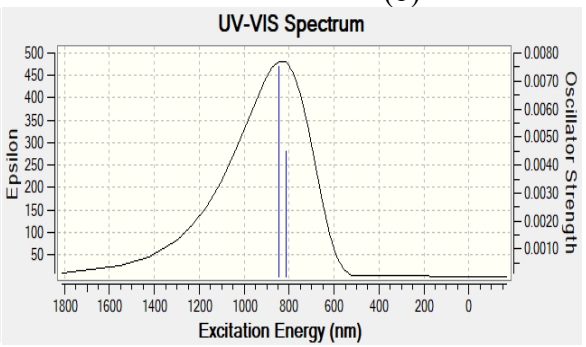

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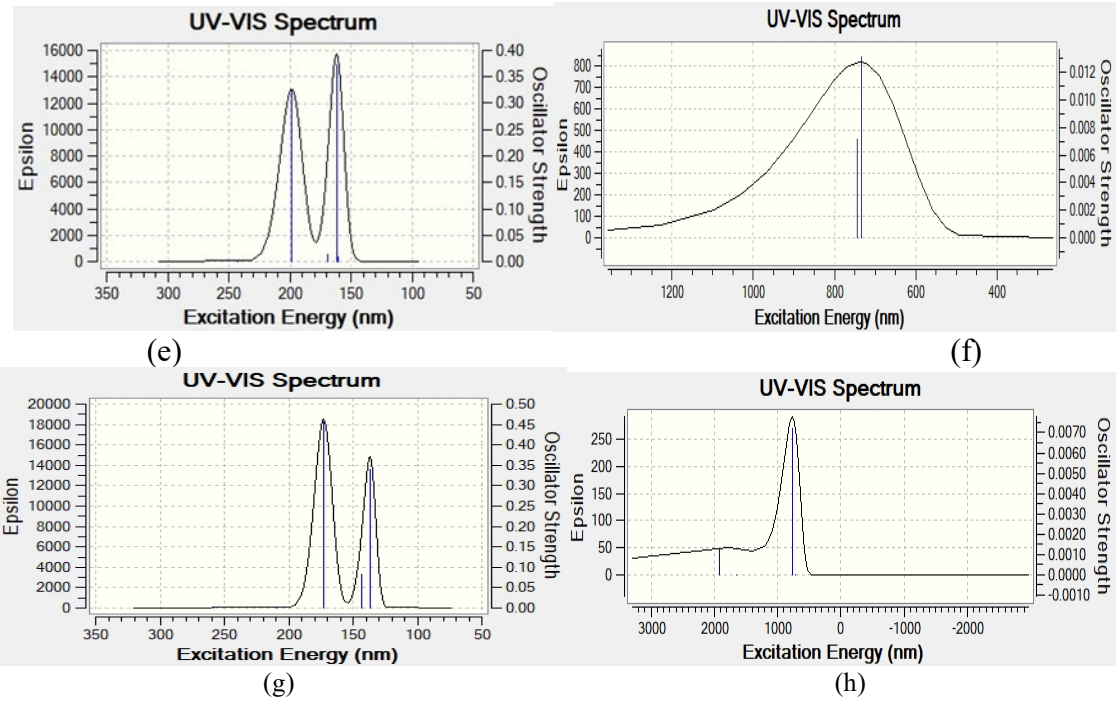
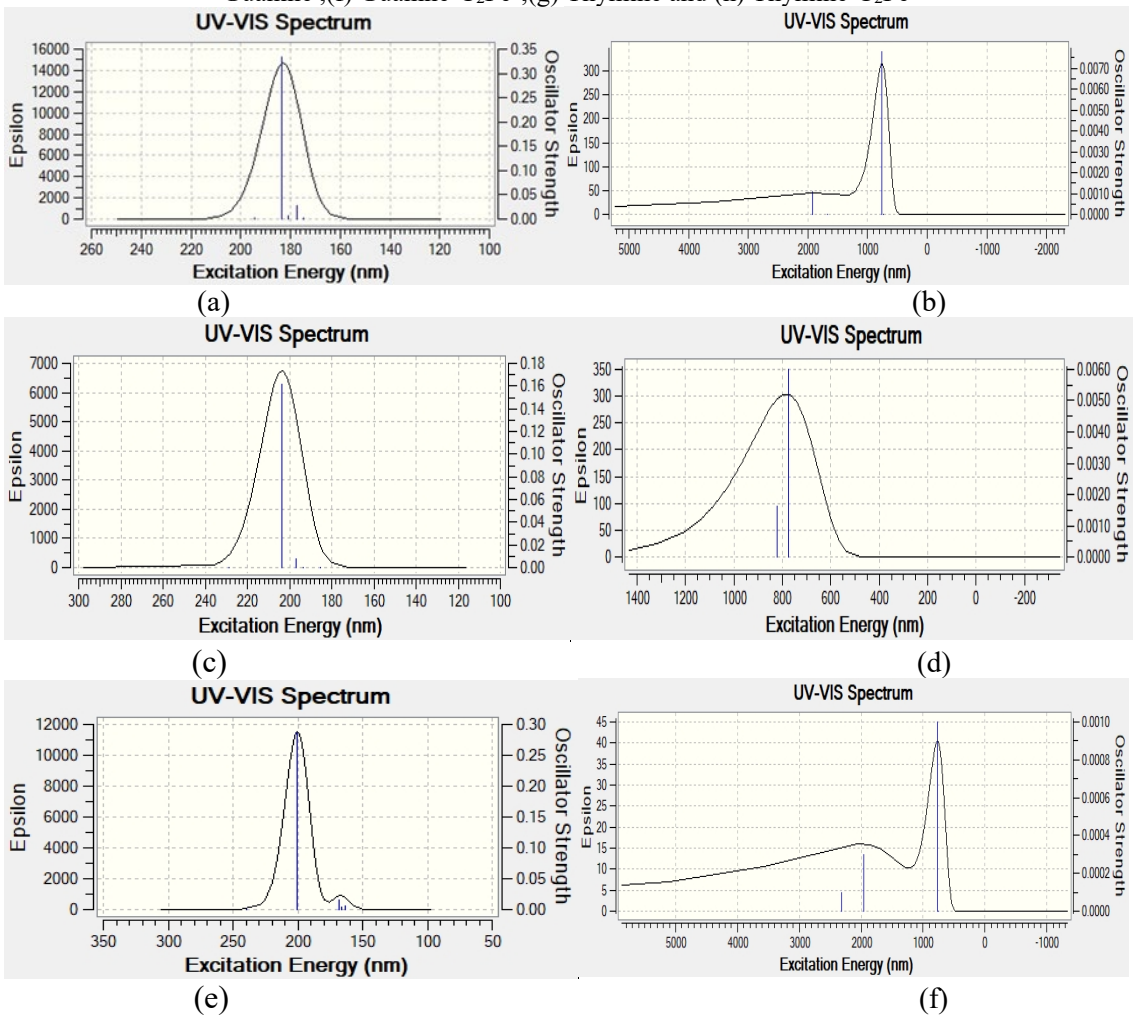
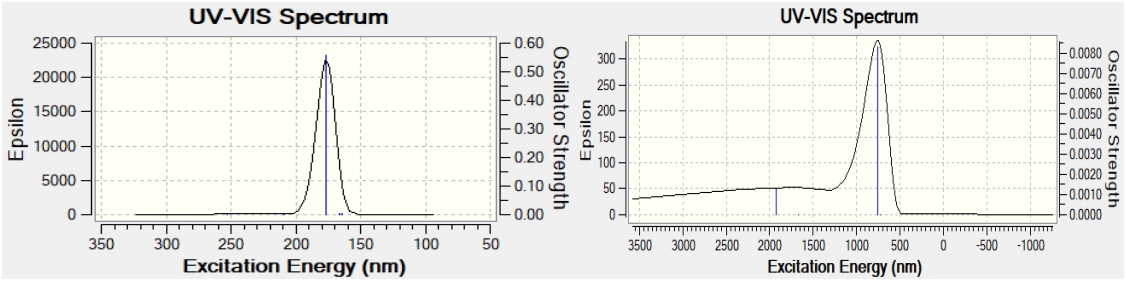


Fig 8. Absorption spectrum of (a)Adenine, (b)Adenine-C_2Fe^+, (c) Cytosine ,(d) Cytosine- C_2Fe^+, (e) Guanine ,(f) Guanine-C_2Fe^+,(g) Thymine and (h) Thymine-C_2Fe^+





(g) (h)

Figure 9. Absorption spectrum of (a) Adenosine monophosphate, (b) Adenosine monophosphate-C_2Fe^+, (c) Cytidine monophosphate, (d) Cytidine monophosphate-C_2Fe^+, (e) Guanosine monophosphate, (f) Guanosine monophosphate-C_2Fe^+, (g) Thymidine monophosphate and (h) Thymidine monophosphate-C_2Fe^+

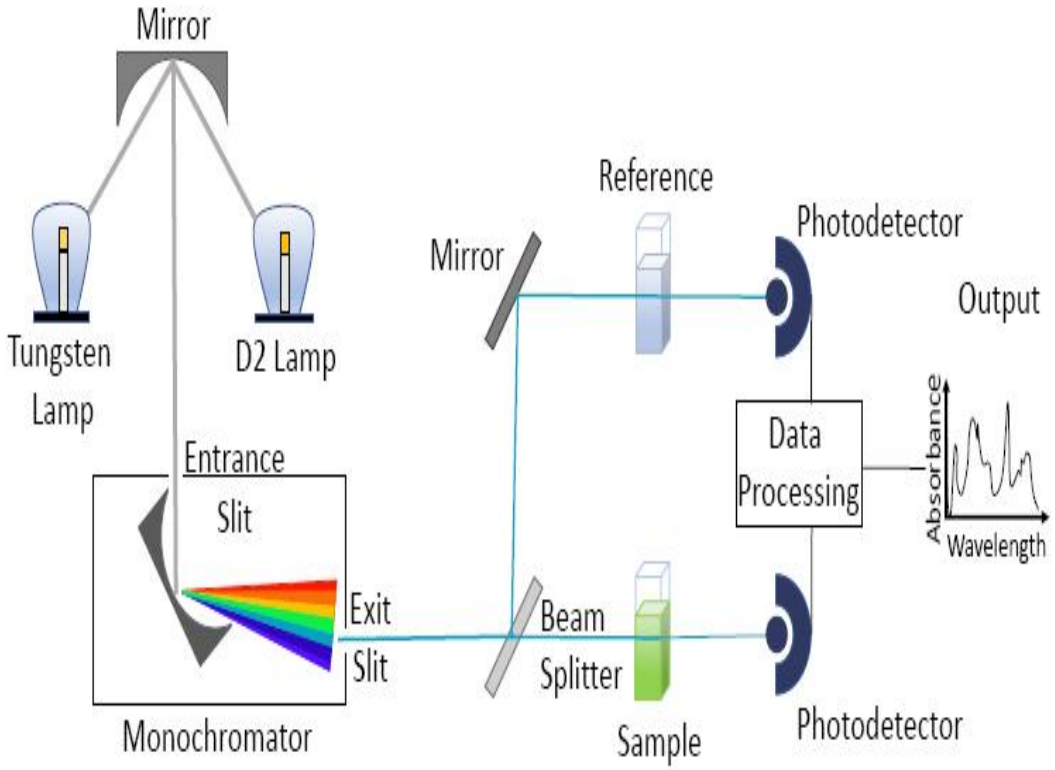


Fig10. UV-vis spectrophotometer schematic for a double beam instrument [9]

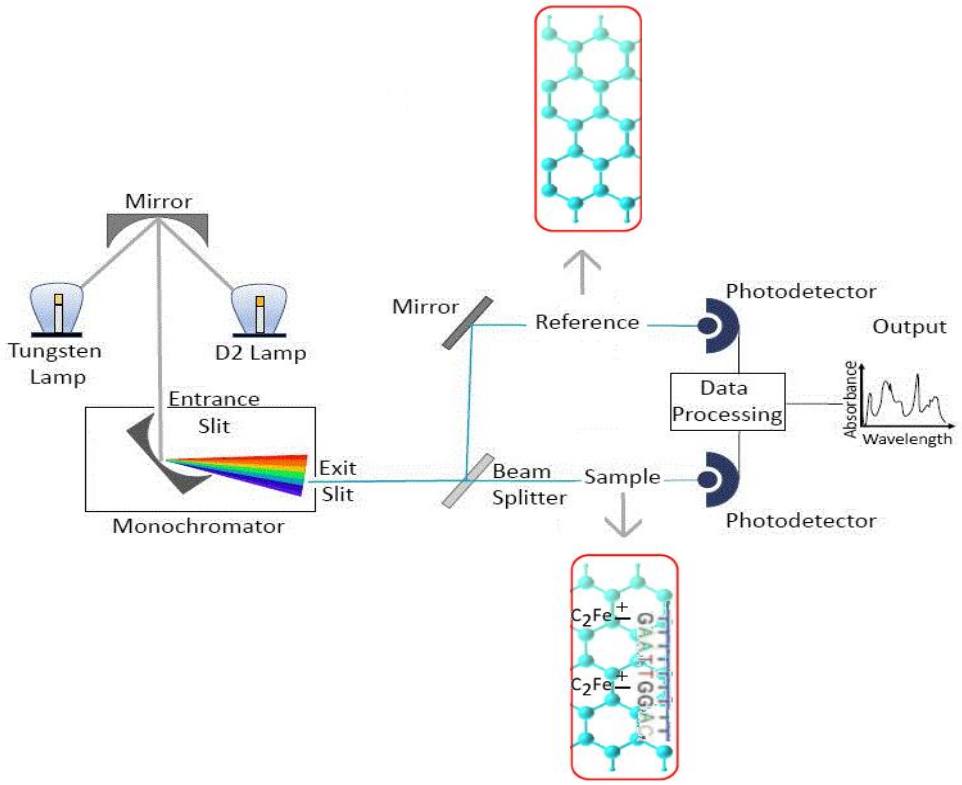


Figure 11. Suggested Changes on UV-vis spectrophotometer for a double beam instrument for detecting pristine bases, nucleotides and their derivatives of one strand of DNA [10]

4. Conclusions

The setting pattern of bases in one strand DNA in general is (0) and (1). If C_2Fe^+ attaches to those DNA bases or nucleotides causes changes in their NMR susceptibilities, Magnetizations, absorption properties and charge distributions. The value of their NMR susceptibilities and absorption properties can be calculated theoretically by Gauss view and Gaussian software and with using them we can create a new version of (0) and (1) coding that can make marking a specific DNA base or store and save information in one strand DNA. In the first mentioned method in this research, by converting resulted Magnetizations to electric current signals a new code (new 1 and 0) that a new marking in one strand DNA can be created. while the second mentioned method a new pattern for (0) and (1) system can be concluded by absorption ranges of DNA bases, nucleotides and their derivatives. The results and methods in this research are all theoretical, but can help to study properties of DNA and creating new methods for next generation.

ACKNOWLEDGEMENT

Special thanks to, Islamic Azad University, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch and Tehran North Branch for supporting this work. Also special thanks to Professor Farokh Hodjatkashani of Islamic Azad University Tehran South Branch for his guidance and help.

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