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Original Research Article

NMR Susceptibility and Magnetization of DNA Bases, Nucleotides and Their Derivatives with C_2Fe^+, A DFT Study

Leila Hojatkashani[1*], Amir Ali Omidi[2]

[1]Department of Chemistry, College of Basic Sciences, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University. Tehran. Iran
[2]Department of General Biology, College of Biological Sciences, Tehran North Branch, Islamic Azad University. Tehran. Iran

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***Corresponding author:** Leila Hojatkashani
Department of Chemistry, College of Basic Sciences, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University. Tehran. Iran

Abstract

DNA strands and their bases are in the cells in every creature. They essential for growth, metabolism regulation and carrying genetic information bases to new generations. The bases of DNA are working with 0 and 1 system. In this theoretical research, first, by using Gaussian program, NMR susceptibility of DNA bases and their C_2Fe^+ attached varieties are determined. In the next step, with effect of magnetic field (H) and NMR susceptibility of these compounds, their resulted Magnetization (M) is calculated. These resulted magnetizations not only can be considered as a method to make a new (0) and (1) system for DNA bases but also can be used as creating certain signals to mark of DNA bases and their compounds which are attached to C_2Fe^+.

Keywords: DNA bases, nucleotides**,** C_2Fe^+, magnetic susceptibility, magnetic field, magnetization.

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 and their interaction which is caused by Hydrogen bond are 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: 1- Purine groups which are including Adenine and Guanine, 2- 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 Thymine. As it has been shown in the Figure 1, Cytosine and Guanine base are connected together by three Hydrogen bonds, including two N-H...O type and one N-H...N interactions, but Adenine-Thymine base pair can form two Hydrogen bonds which are typical N-H...O and N-H...N interactions [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 phenomen [4].

This theoretical research is about using Gaussian software and Density Functional Theory (DFT) method to determine magnetic susceptibility of DNA bases and their varietives which are DNA bases attached to a compound such as C_2Fe^+. C_2Fe^+ is attached like a flag to a certain base to create magnetic field. In the next step, the one strand of DNA which is attached with some 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 are one of platforms to study the interaction of the DNA bases and their interactions with other ions or compounds [5].

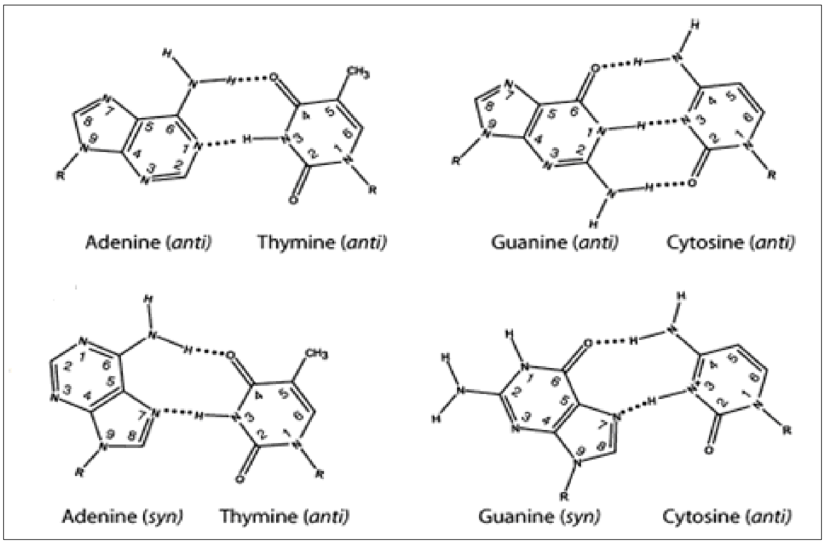


Figure 1: DNA bases and their interaction [2]

2. COMPUTIONAL METHODS

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.

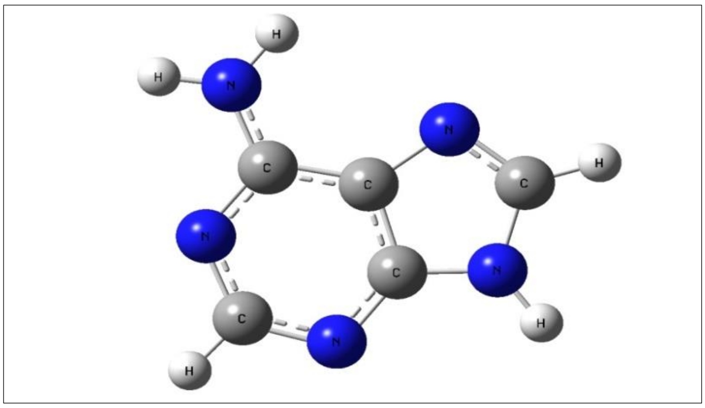
3. RESULTS AND DISCUSSION

3.1. NMR Susceptibility of Pristine DNA Bases and C_2Fe^+

In the first step of this research, DFT method is used to determined NMR susceptibility and also ground state energy of Adenine, Cytosine, Thymine and Guanine (Figure 2). This calculations are also performed for C_2Fe^+ (Figure 3) which going to be is used as an attached flag to this bases to create derivatives of these bases. The results of these calculations are listed in Table 1 and Table 2.

Table 1: 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



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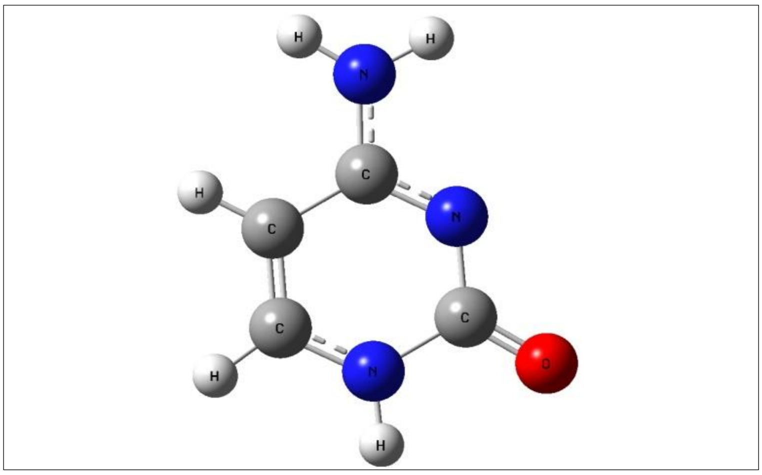

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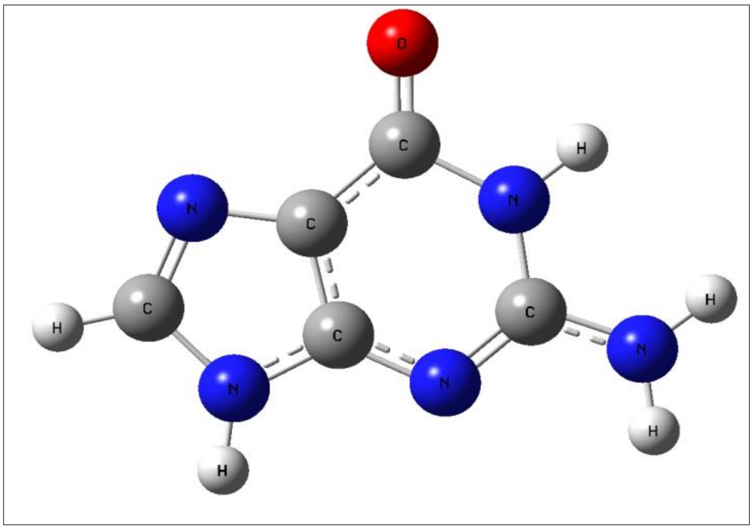

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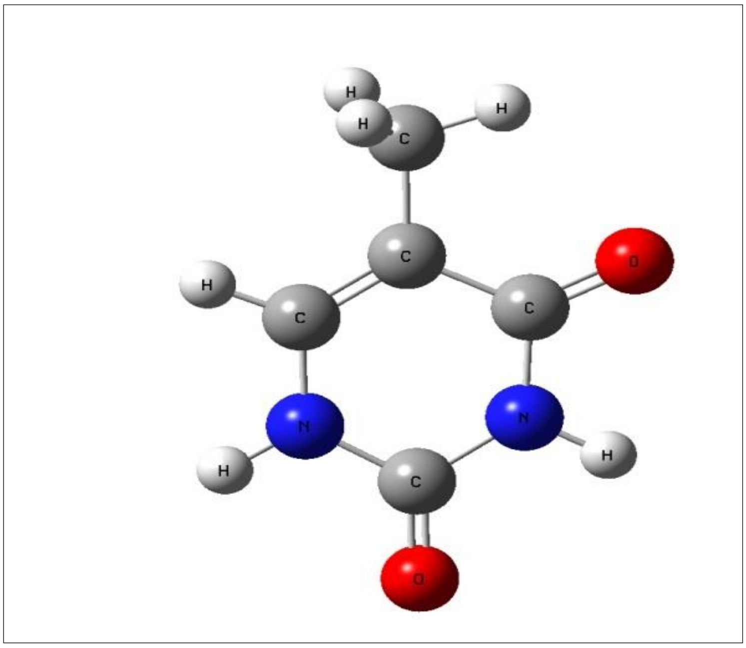

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Figure 2: Structure of (a) Adenine (b) Cytosine (c) Guanine (d) Thymine opted with(Cam-B3LYP) with SDD basis set

Table 2: E Total and NMR Susceptibility C_2Fe^+

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

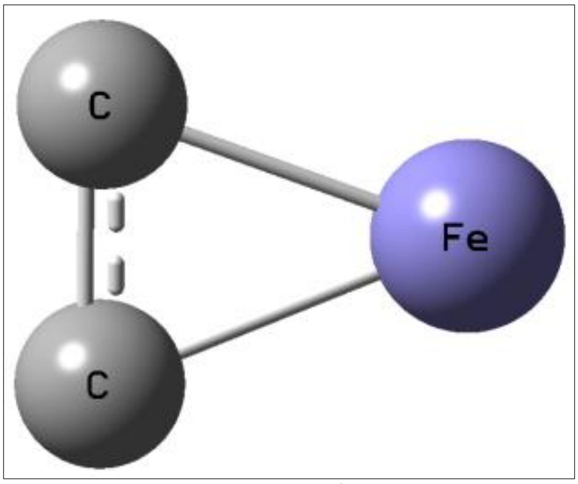
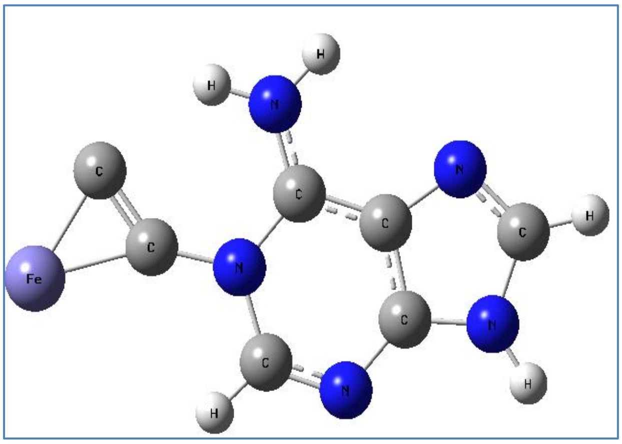


Figure 3: Structure of C_2Fe^+ opted with (Cam-B3LYP) with SDD basis set

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^+. 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^+.



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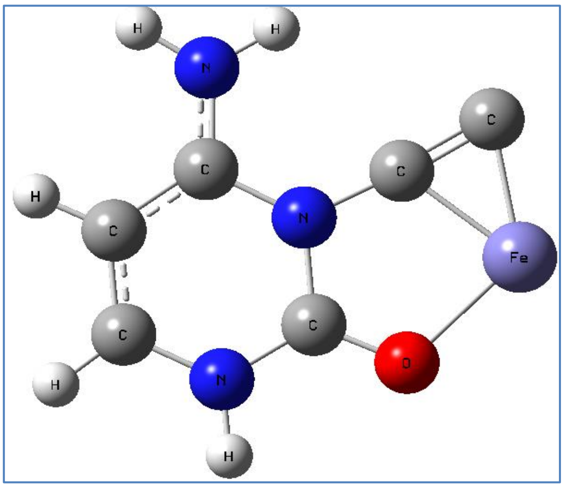

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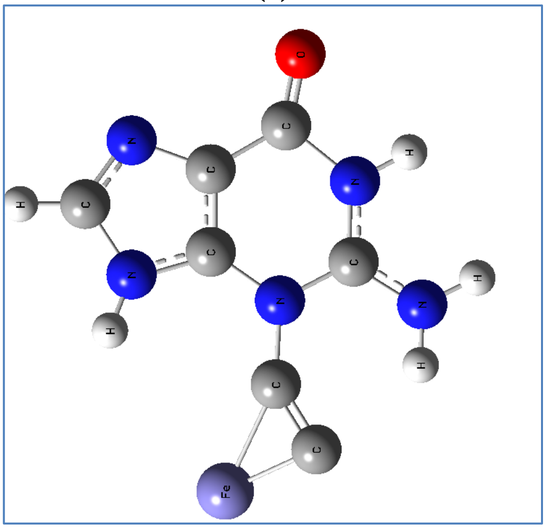

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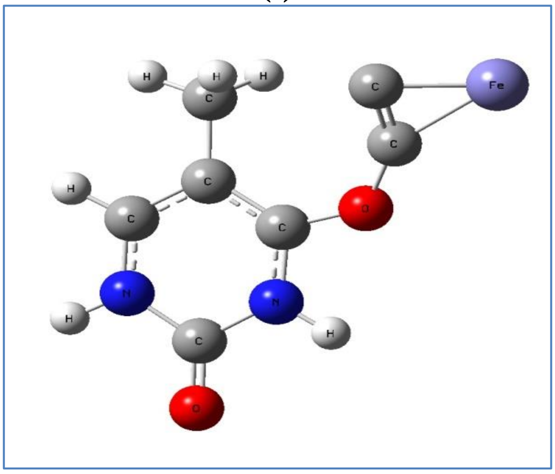

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Figure 4: Structure of (a) Adenine-C_2Fe^+ (b) Cytosine -C_2Fe^+ (c) Guanine-C_2Fe^+ (d) Thymine-C_2Fe^+ opted with(Cam-B3LYP) with SDD basis set

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

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 are shown in (Figure 5). E total and NMR susceptibility of these compounds are listed in (Table 4).

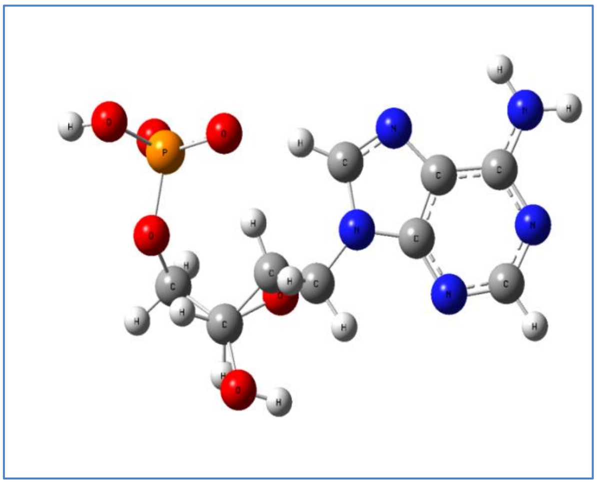
The procedure of theoretical determining NMR susceptibility is repeated again with these nucleotides attached with C_2Fe^+. The resulted structures are shown in (Figure 6) and their E total and NMR susceptibility are listed in (Table 5). The effect of C_2Fe^+ on NMR susceptibility of pristine nucleotides and their derivatives with C_2Fe^+ can be seen by comparing results of (Tables 4 & 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^+.

Table 4: E Total and NMR Susceptibility of DNA Nucleotides

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

Table 5: E Total and NMR susceptibility of DNA Nucleotides attached with C_2Fe^+

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



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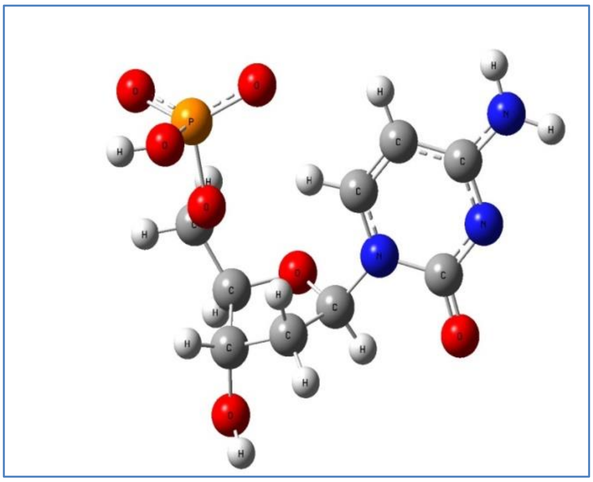

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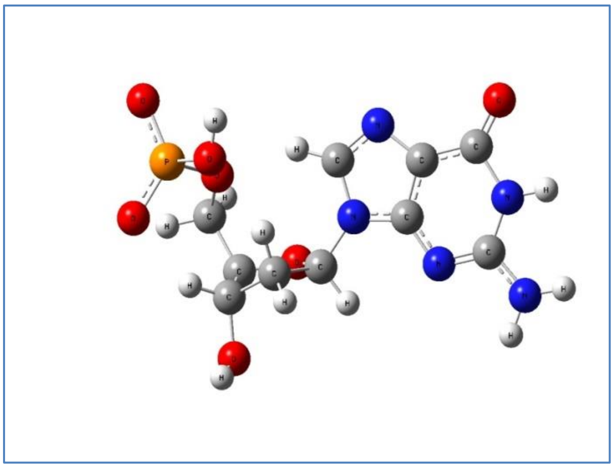

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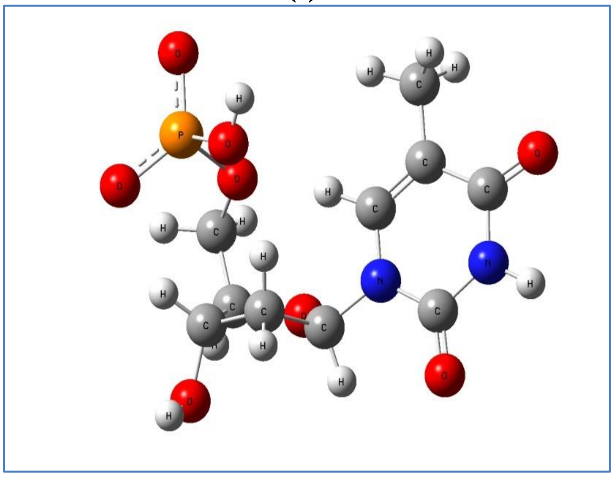

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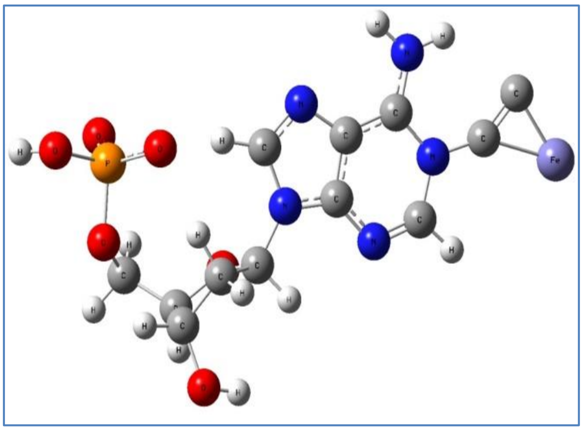
Figure 5: Opted structure of DNA nucleotides with (Cam-B3LYP) method and SDD as basis set. (a) Adenosine monophosphate, (b) Cytidine monophosphate, (c) Guanosine monophosphate , and (d) Thymidine monophosphate



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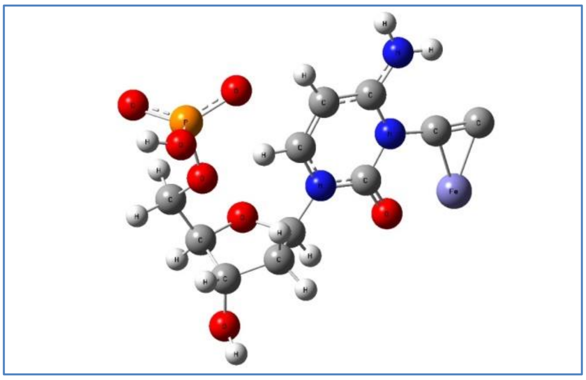

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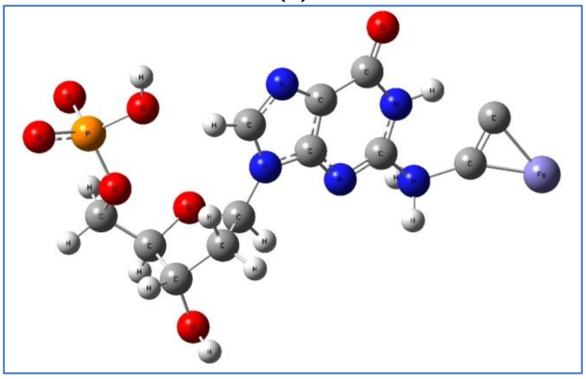

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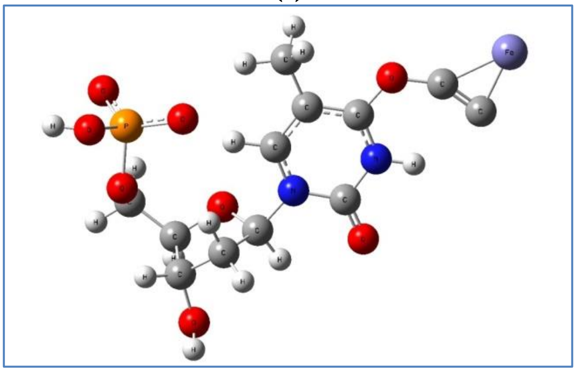

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Figure 6: Opted structure of DNA nucleotides with (Cam-B3LYP) method and SDD as basis set. (a) Adenosine monophosphate-C_2Fe^+, (b) Cytidine monophosphate-C_2Fe^+, (c) Guanosine monophosphate-C_2Fe^+ , and (d) Thymidine monophosphate-C_2Fe^+

Figures (4) shows us that C_2Fe^+ likes to attach to Nitrogen atoms in Adenine and Guanine bases but prefers to attach to Oxygen atoms in Cytosine and Thymine bases. But in (Figure 6), in nucleotides, C_2Fe^+ likes to attach to Nitrogen atoms in Adenosine, Cytidine and Guanosine but prefers to attach to Oxygen atom in Thymidine.

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) indicates that $\vec{M}$ and $\vec{H}$ is 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 (paramagnetism), or opposes it (diamagnetism). Paramagnetism fenomena generally originates 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 of 10^{-6} cm^3/mol to m^3/molecule. NMR susceptibility in (Table 6 & 7) is calculated as m^3/molecule so the resulted Magnetization can be obtained 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 & 7).

$$1cgs/ppm = 10^{-6}\left(\frac{cm^3}{mol}\right)\left(\frac{1m^3}{10^6 cm^3}\right)\left(\frac{mol}{6.02\times10^{23} molecule}\right) = 0.166\times10^{-35} m^3/molecule \quad \textbf{(2)}$$

Table 6: Magnetization and NMR susceptibility of Adenine, Cytosine, Thymine, Guanine, and their derivatives with C_2Fe^+

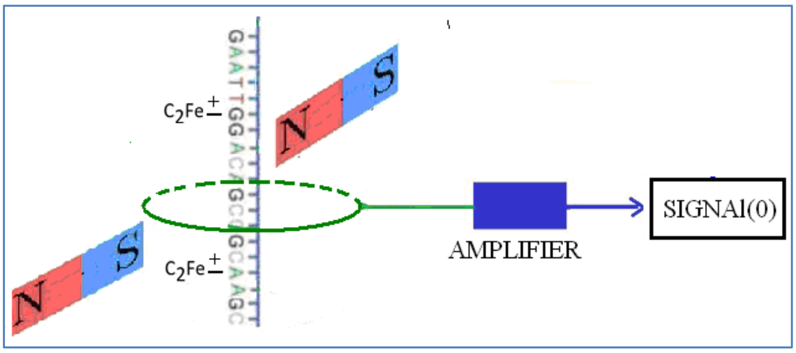
Name	NMR susceptibility(m^3/molecule)	Magnetization ($A.m^2$/molecule)
Adenine	-14.52×10^{-35}	-14.52×10^{-35}
Cytosine	-9.54×10^{-35}	-9.54×10^{-35}
Thymine	-10.45×10^{-35}	-10.45×10^{-35}
Guanine	-13.91×10^{-35}	-13.91×10^{-35}
Adenine-C_2Fe^+	35.33×10^{-35}	35.33×10^{-35}
Cytosine- C_2Fe^+	39.96×10^{-35}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

Table 7: 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}
Guanosinemonophosphate- C_2Fe^+	35.60×10^{-35}	35.60×10^{-35}

The results of (Tables 6 & 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^+, the resulted 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 show also the same conclusion which shows 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 diamagnetic compounds to paramagnetic ones.

This theoretical research and the results can help us to determine certain DNA bases , nucleotides or even to create a new way in saving information in one strand of DNA . The pristine DNA bases and nucleotides which are diamagnetic and have 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 of paramagnetic 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 and their derivatives in a DNA strand in a magnetic field and converting it to current with the help of the metal ring. For fortification these signals to get better detecting, an amplifier can be used which is shown in both (Figure 7a & 7b).



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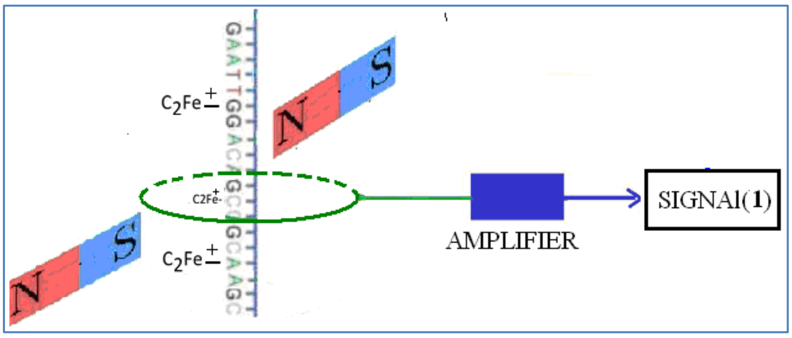

(b)

Figure 7: The signals of (a) pristine bases and (b) their derivatives with C_2Fe^+ of a strand of DNA in a magnetic field

Magnetization is a vector unit and for a molecule can be expresses as A.m^2/molecule. Its 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 a attached bases or attached nucleotide there will be a electric current as signal which is expressed in Ampere. This method is completely theoretical way to distinguish DNA bases in one strand.

4. CONCLUSION

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 susceptibility and Magnetization. The value of their NMR susceptibility can be calculated by Gaussian software and also their response to a magnetic field can be concluded which is the resulted Magnetization. By converting resulted Magnetization to electric current signals a new code (new 1 and 0) or a new marking in one strand DNA can be created .The results and methods in this research are all theoretical, but can help to study properties of DNA.

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