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Research Article

A Comparative DFT and AM1 Study on the Ionization Constants and Electronic Properties of Schiff Base Derivatives

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About Article

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ABSTRACT

It has been studied of organic compounds was using quantum mechanics. This research included the study of factors (inductive effect and steric hindrance) that influence the structural conformations of a number of alicyclic compounds. The summary of the obtained results showed that these methods have high efficiency for this type of calculation. The variables in the developed equation were then tested to calculate the chemical shift of compounds with structures similar to those used in the study but not used in the regression analysis, which supports the accuracy of the variables selected to accomplish this study. Two methods were used for the study: AM1($R = 0.948$) and DFT ($R = 0.984$). The DFT method showed greater superiority and accuracy in calculations and a closer match with the experimental values. If the value of the correlation coefficient for the difference between the PKa practical and Pka theoretical values between the two methods is (DFT $R^2 = 0.8513$, AM1 $R^2 = 0.3808$) observe that the values of method (DFT) are higher than the values of method (AM1).

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1. INTRODUCTION

Theoretical chemistry is a broad and multifaceted branch of chemistry. It can generally be distinguished by its use of physics, mathematics, and computers to understand all aspects of chemistry, such as the properties of materials, elements, and molecules and their reactions. It is also used to simulate molecular phenomena or predict the properties of new molecules or phases of matter.

Generally, two trends can be distinguished in theoretical chemistry. The first is the use of computers to solve complex equations that govern molecular behavior, which helps in modeling or simulating molecules and their properties (Simons, 2003). Computational chemistry is a branch of chemistry that uses computer simulations to help solve chemical problems. As is well known in quantum chemistry, we can never solve the Schrödinger equation exactly and correctly for chemical systems (such as atoms and molecules) containing more than one electron. Therefore, the methods used in computational chemistry, an important extension of theoretical chemistry, aim to use efficient mathematical approximations to solve various chemical problems in order to calculate many important properties of molecules, such as total energy, dipole moments, vibrational frequencies, chemical reactivity, and other chemical and physical properties (Leach, 2001). Computational chemistry is an interdisciplinary science that combines chemistry, computer science, physics, and mathematics, ultimately enabling the development of approximate and practical theoretical solutions for understanding and studying many different chemical systems. The second approach is the development of new “analytical theories,” which involves formulating equations that describe the behavior of materials or chemical systems such as rates of chemical reactions or spectral properties methods that may use classical or quantum mechanics (Leszczynski, 1999). Quantum chemistry and statistical mechanics constitute two fundamental branches of theoretical chemistry.

There is considerable confusion in identifying areas of convergence and divergence between the fields of theoretical chemistry, computational chemistry, and molecular modeling (Ibrahim, 2021). Many researchers actually use these three terms interchangeably to refer to different aspects of their work depending on the context. Today, theoretical chemistry is closely linked to quantum mechanics and its applications in chemistry, as chemical reactions occur between small molecules that can be described by quantum phenomena. This is evident, for example, when reviewing the scientific content of theoretical chemistry conferences and specialized references in the field. Therefore, the general trend is to use the term “theoretical chemistry” as a synonym for the applications of quantum mechanics in chemistry, while the terms “computational chemistry” and “molecular modeling” are used in a broader context (Lashkaripour, 2021). This study aims to compare the experimental and theoretical results for ionization P_{ka} using different quantum mechanics methods.

1.1. Ionization constants

The ionization constant is defined as the ratio of the concentration of ionized substances of acids or bases to the concentration of unionized substances (Schwoebel, 2021).

There is a difference in bases or acids in terms of their ability to donate or accept a proton. The Bronsted-Lowry theory is one of the most important theories that provided a comprehensive description of the ionization of an acid or base (Aguilera, 2017). Accordingly, the theory defined acids as those substances that have the ability to donate a proton, while bases are substances that have the ability to accept a proton.



It can be noted that the ionization process is reversible.

$$K^c = \frac{[H^+][A^-]}{[HA]} \quad \dots(1)$$

Ionization constant in terms of concentration, which is symbolized by (K^c)

The square brackets represent the concentration of each ionic species in terms of molarity or molality. They also represent the thermodynamic ionization constant K .

This equation applies to both weak acids and bases.

The importance of the ionization constant is highlighted in many sciences, most notably pharmaceutical sciences. The process of transporting drugs across membranes and the dissolution of these substances in the body depends on the acidity function, and it is essential to know the pH value of the pharmaceutical formulas. Observing drugs reveals that 95% have ionized groups, and at pH 2-12, it was found that 62.9% of drugs have the ability to ionize. The previous results indicate that 75% of drugs are weak bases and 20% are weak acids, while the remaining portion is unionized, such as alcohols and ampholytes.

In 1909, the scientist Sorenson proposed the logarithm, and with this proposal, small values were overcome (Ibrahim, 2020). The logarithm is expressed as follows:

$$p[H^+] = -\log [H^+] \quad \dots(2)$$

$$pK_a = -\log K_a \quad \dots(3)$$

2. LITERATURE REVIEW

The theoretical calculation and manipulation of the ionization constant of chemical compounds is an important method that has occupied many researchers for many years. In 1964, Paul and Grant published their work (Grant & Paul, 1964). By developing experimental additivity parameters to predict of P_{ka} atoms. These parameters were developed and refined by another group of researchers (Steroids *et al.*, 1969; Johnson *et al.*, 1970). Various types of variables, such as bond length, density, Homo, Lomo, and others, have been used by employing quantum chemistry to arrive at theoretical results.

3. METHODOLOGY

The progress achieved in the field of software and computers has prompted many researchers to use many well-known theoretical programs to complete a large number of chemical calculations. These include calculating the values of ionization constants for many acidic and basic compounds. Hameed (2021) and his group calculated the ionization constants for a group of substituted phenols by calculating the molecular charges on the atoms using quantum mechanical methods and by comparing the values obtained from semi-empirical methods and basic calculations (Abadya, 2024). Lipton and his group calculated the



pKa values for a number of substituted phenols by calculating the standard free energy values (ΔG°) according to the following equation.

$$pK_a = \Delta G^\circ / 2.303 RT \quad \dots(4)$$

AL-Taaye (2021) also calculated the ionization constant using basic calculation methods and applying the Hartree-Fock HF method and the DFT density function method. The studies included in the field of using quantum mechanical methods to calculate the values of the ionization constants of amino acids, according to our information and according to the scientific survey of the available literature, are very limited. We mention among them what (Al-Abady, 2022) did in studying the effect of electronic properties (inductive and vacuum effects) on the values of the ionization constants of the twenty known amino acids (Leach, 2001).

3.1. Mechanism of reaction

The mechanism of any reaction is expressed by a set of successive steps based on a solid scientific foundation and based on the facts specific to the chemical reaction under study, which are obtained during the measurement of the reaction rate, which together represents the overall reaction. When the reaction mechanism consists of several steps, the reaction rate depends

on the slowest of all the other steps involved in the mechanism. Therefore, it has been found in the mechanics of many reactions that the slow step represents the step determining the rate of that reaction, and the rate constant is equal to the rate constant of the aforementioned slow step. It may happen that the slow step determining the reaction rate is preceded by other fast steps (Hong, 2003), which leads to an increase in the concentration of the active intermediate compound. In order to prevent such an increase, any fast reaction preceding the slow step must be a reversible reaction. The value of the equilibrium constant for that reversible reaction is low, and the equilibrium constant for these steps is included in the rate law (Lewars, 2016).

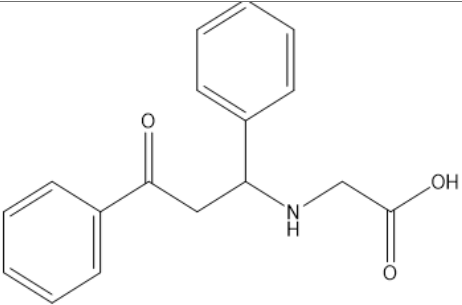
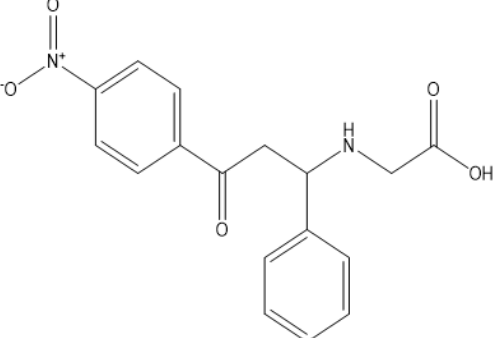
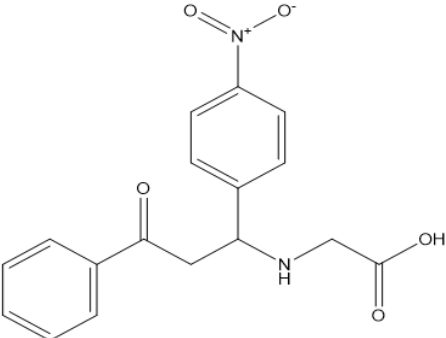
3.2. Practical part

Calculations were performed theoretically using the program Chem Office (V12, 2010)

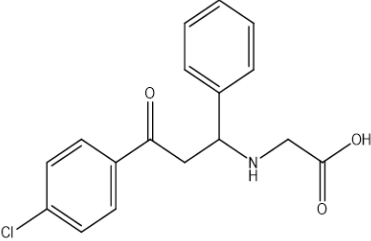
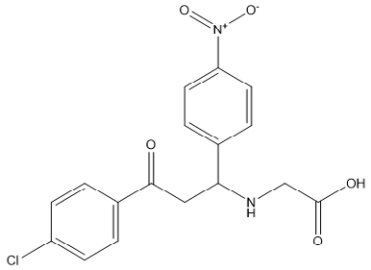
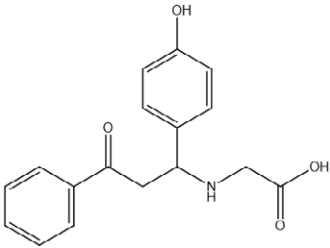
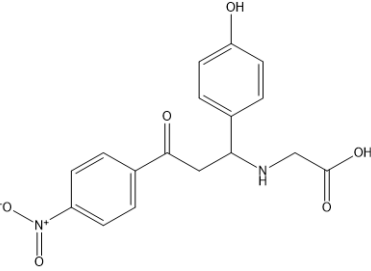
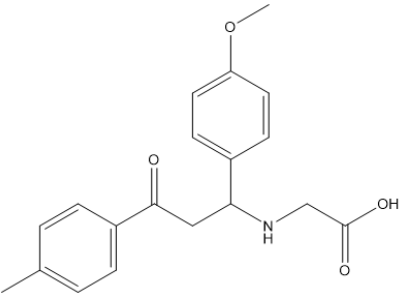
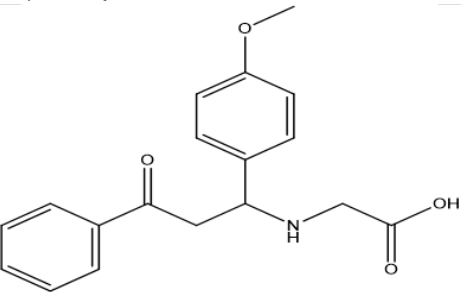
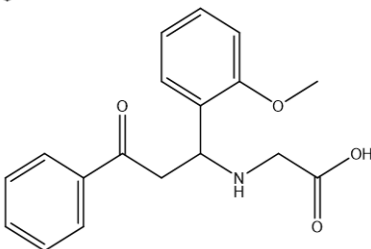
Two methods were used in the calculations: the first is the basic calculation method, and the second is the semi-empirical method AM1, DFT (16). The SPSS V21 statistical program (Venianakis, 2020) was also used to study a group of compounds mentioned below (Dewar, 1985).

The practical ionization constant of the Schiff bases under study was calculated in a 60% acidic medium.

Table 1. Compounds under study. Ionization constant was calculated at 60% pH.

NO	Name	Structure	Pka
1	2((3-oxo-1,3-diphenylpropyl) amino) acetic acid		10.4278
2	2-((3-(3-nitrophenyl)-3-oxo-1-phenylpropyl) amino) acetic acid		10.532
3	2-((4-(3-nitrophenyl)-3-oxo-3-phenylpropyl) amino) acetic acid		10.729



4	2-((3-(4-chlorophenyl)-3-oxo-1-phenylpropyl) amino)acetic acid	10.131
		
5	2-((3-(4-chlorophenyl)-1-(oxopropyl)amino)acetic acid	9.986
		
6	2-((1-(4-hydroxyphenyl)-3-oxo-3-phenylpropyl) amino)acetic acid	10.297
		
7	2-((1-(4-hydroxyphenyl)-3-(4-nitrophenyl)-3-oxopropyl) amino)acetic acid	9.826
		
8	2-((1-(2-methoxyphenyl)-3-oxo-3-(p-tolyl) propyl) amino)acetic acid	9.036
		
9	2-((1-(4-methoxyphenyl)-3-oxo-3-phenylpropyl) amino)acetic acid	10.167
		
10	2-((1-(2-methoxyphenyl)-3-oxo-3-phenylpropyl) amino)acetic acid	10.021
		



4. RESULTS AND DISCUSSION

In this study, theoretical calculations were performed for some of the physical variables of the compounds under study (HOMO, LUMO, μ , η , and W) to calculate the ionization constants of the compounds, to obtain the best relationship between the variables and the ionization constants (pK_a). It was observed that the values of the electronic charges in the active centers have an effect on the ionization of these compounds. Therefore, the values of pK_a can be determined through the effect of the substituent groups on the reaction centers through the effect of (induction, resonance, and vacuum effects) (Szabo, 1989). Two methods from quantum mechanics were chosen. The first method, called (AM1) (Austin Model), is a semi-empirical calculation method. Another basic calculation method used is the Density Functional Theory method. After reviewing Table (4), Since the HOMO value of compound 10 is greater than that of compound 7, this means that the HOMO electrons in compound 10 are more easily removed. Therefore, compound 10 is a stronger nucleophile and has a greater tendency to donate a pair of electrons in reactions. Conclusion from HOMO: Compound 10 exhibits higher nucleophile properties than compound 7. we observe that compound 10 is the most reactive. Compound 10 exhibits high reactivity due to its high malleability (its general

elemental composition) and high nuclear strength (its ability to form electrons). In contrast, compound 7 is characterized by strong stability resulting from its high rigidity. We observe the results in Table (5). Compound 7 is the more reactive compound compared to compound 10. Its low hardness contributes to the ease of reactions in general, while its high HOMO energy indicates that it is a strong nucleophile. Compound 10 is the most stable and least reactive compound due to its greater hardness. This large change in direction (Flip) between the AM1 and DFT methods suggests that the reactivity may be highly dependent on electron-bonding or solvent effects, which are better handled by the DFT methods than by the AM1 methods.

4.1. Quantum mechanical methods

During our study of quantum methods, we calculated a number of physical variables, including those represented by (Total Energy, Density, Angle, etc.) for a group of compounds under study. We also calculated some energy variables (HOMO, LUMO, η , M , W). This process was accomplished using two quantum mechanical methods: one based on fundamental calculations (DFT) and the other based on semi-empirical calculations (AM1). The following results were obtained, as shown in the following tables.

Table 2. Values of physical variables with energy for the compounds under study using the AM1 method

Stretch	Bend	S/B	Torsion	non-VDW	VDW	T.E	Dip-Di	N
1.2873	3.9213	0.199	-13.13	-2.1243	16.952	2.0147	-3.051	-0.29536
1.2835	5.0098	0.2025	-12.216	-2.1249	19.0326	3.5602	0.1481	-0.29727
1.3541	4.7885	0.2205	-12.079	-0.8704	19.5856	-2.1574	-3.1336	-0.2971
1.2035	4.3625	0.2041	-12.666	-4.0441	17.2308	5.8141	-0.4772	-0.2898
1.2814	5.1176	0.2169	-12.054	-2.7427	19.7775	-1.8785	0.1526	-0.2913
1.295	4.6581	0.1738	-13.12	-2.6437	15.664	2.9234	-3.1036	-0.2967
1.387	5.3546	0.1801	-13.045	-1.5359	18.1592	1.6766	-6.8801	-0.29766
1.6175	6.5968	0.2542	-13.838	-1.9747	20.31	9.7734	-3.192	-0.29428
1.5765	6.4097	0.257	-13.118	-1.7507	19.6652	9.9457	-3.0943	-0.29784
1.6575	5.3421	0.2632	-12.43	-1.8621	18.2763	1.8742	-3.1263	-0.28725

Table 3. Values of physical variables with energy values for the compounds under study using the DFT method

Stretch	Bend	S/B	Torsion	non-VDW	VDW	T.E	Dip-Di	N
1.2873	3.9213	0.199	-13.13	-2.1243	16.952	4.0547	-3.051	-0.29536
1.2852	3.9179	0.1987	-13.129	-2.1268	16.9585	4.0551	-3.0497	-0.58961
1.2831	5.0071	0.2024	-12.209	-2.1155	19.0337	3.5613	0.1498	-0.59744
1.3529	4.7869	0.2205	-12.082	-0.865	19.5867	-2.1573	-5.293	-0.59246
1.2019	4.3626	0.2036	-12.67	-4.0401	17.2318	5.8146	-0.478	-0.57844
1.2764	5.1277	0.1728	-13.128	-2.6421	15.687	2.8791	-3.1041	-0.5823
1.253	4.6612	0.1891	-13.042	-1.587	18.1561	1.6987	-6.8762	-0.5864
1.347	5.3531	0.2536	-13.834	-1.9751	20.3983	9.7198	-3.1521	-0.59432
1.6132	6.5847	0.252	-13.286	-1.7582	19.6543	9.9321	-3.0952	-0.59832
1.5455	6.4081	0.2641	-12.41	-1.8686	18.3218	1.8931	-3.1293	-0.58613
1.6543	5.3432	0.1961	-13.117	-2.1272	16.8543	4.0631	-3.0463	-0.58532



(T.E) Total Energy kcal/mol
(S\B) Stretch-Bend

4.2. Energy function variables calculated using AM1 and DFT

This study relied on energy variables that represent the stability of different molecules through interactions and spatial changes. These variables, obtained through calculations, include the steric hindrance energy and the orbital energies (HOMO and LUMO), which were used to calculate some known variables related to the stability of molecules and their propensity to react, whether as electrophiles or nucleophiles. Other variables that were calculated include hardness (η), chemical potential (μ), and electron affinity index (W). Low values of (η, μ) indicate that the molecule is more effective as a nucleophile, while high values of (η, μ) indicate that the molecule is in the form of an electrophile that behaves well (Allinger, 1989). The energy variables shown above were calculated using the two methods of quantum mechanics, and each method was done separately, as shown in Tables (1, 2).

Table 4. The theoretically calculated energy variables values for Schiff bases using the (AM1) method.

Comp	HOMO Ev	LUMO Ev	W Ev	μ ev	η Ev
1	0.0704	-0.0702	0.0350	-0.14061	0.00017
2	0.0027	-0.0013	0.0003	-0.00395	0.0014
3	0.0705	-0.0703	0.0350	-0.1408	0.00023
4	0.0686	-0.0608	0.0270	-0.12937	0.00774
5	-0.0655	0.0734	-0.0411	0.13893	0.0079
6	0.0706	-0.0705	0.0352	-0.14118	0.00011
7	1.5707	-1.5698	0.7845	-3.14047	0.00084
8	0.0677	-0.0645	0.0307	-0.13215	0.00321
9	0.0731	-0.0729	0.0363	-0.145976	0.00023
10	0.0703	-0.0689	0.0338	-0.139254	0.0014

(η) Hardness (μ) Electronic Chemical Potential (w) Global Electrophilicity Index

Table 5. The theoretically calculated energy variables values for Schiff bases using the DFT method.

Comp	HOMO Ev	LUMO Ev	W Ev	μ ev	η Ev
1	-0.0370	0.0170	0.00332	-0.07739	0.0404
2	-0.0660	0.0313	0.00359	-0.13564	0.0696
3	-0.0629	0.0290	0.00525	-0.13105	0.0682
4	-0.0683	0.0299	0.00983	-0.14642	0.0781
5	-0.0619	0.0268	0.0096	-0.13337	0.0715

6	-0.0649	0.0284	0.00917	-0.13892	0.0740
7	-0.0595	0.0258	0.00912	-0.12819	0.0687
8	-0.0610	0.0277	0.00612	-0.12817	0.0671
9	-0.0667	0.0323	0.0021	-0.13552	0.0688
10	-0.0272	0.0031	0.092	-0.14647	0.1192
11	-0.0370	0.0170	0.00332	-0.07739	0.0404

4.3. Multiple statistical analysis

Multiple statistical analysis was conducted to determine the best value for the correlation coefficient and to identify the variables that could have an impact on the chemical displacement value. The best values obtained were as follows:

Table 6. Results of the regression analysis of carbon compounds using the AM1 method

LUMO	-44.440
T.E	-2.458
SB	-.056
Constant	10.995
R	0.948
S.E	1.396

Table 7. Results of regression analysis of carbon compounds using DFT method.

Variables	Values of the coefficients of a
T.E	-0.121
Bend	-0.320
VDW	0.134
Constant	9.8795
R	0.984
S.E	1.41

4.4. Calculation of chemical shift values in theory

The chemical shift values for carbon are obtained using this method by referring to the table above. We note the best value.

4.5. Calculation of Ionization Constant values using the AM1 method

The chemical shift values for carbon are calculated using this method by referring to Table (7). We note that the best value obtained for the correlation coefficient was ($R = 0.948$). The variables for this value are used to arrive at the theoretical shift (Dinur, 1991).

We then use the following equation to obtain the theoretical chemical shift values for the compounds under study.

$$Pka = 10.995 + (-44.440 * LUMO) + (-0.056 * T.E) + (-2.458 * S.B) \dots (5)$$



Table 8. Calculation of PKa values using the AM1 method

(Constant)					10.995
LUMO					-44.440
S.B					-2.458
T.E					-.056
LUMO	S/B	T.E	Kcal	Pka Exp	Res
0.0002	0.199	2.0147	10.2728	10.4278	-0.04165
0.0014	0.2025	3.5602	10.23702	10.532	-0.29498
0.00023	0.2205	-2.1574	10.56246	10.729	-0.16654
0.00774	0.2041	5.8141	9.8261	10.131	-0.3049
0.0079	0.2169	-1.8785	10.21496	9.986	0.228958
0.00011	0.1738	2.9234	10.40026	10.297	0.103264
0.00084	0.1801	1.6766	10.42162	9.826	0.595616
0.00321	0.2542	9.7734	9.684291	9.036	0.648291
0.00023	0.257	9.9457	9.800268	10.167	-0.36673
0.0014	0.2632	1.6742	10.19263	10.021	0.171627

4.6. Calculating Ionization Constant Values Using the DFT Method

The chemical shift of carbon is calculated using this method by referring to Table (7). We note that the best value obtained for the correlation coefficient was (R=0.984). The variables in this value are used to arrive at the theoretical shift.

We then use the following equation to obtain the theoretical chemical shift values for the compounds under study (Mayo, 1990):

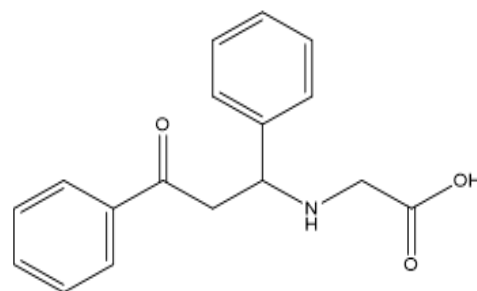
$$Pka = 10.995 + (-44.440 * LUMO) + (-0.056 * T.E) + (-2.458 * S.B) \quad \dots (6)$$

Table (9): Practical and theoretically calculated chemical shift values and the difference between them for linear compounds using the DFT method.

Table 9. Calculation of PKa values using the AM1 method

Constant					9.880
T.E					-.121
Bend					-.320
VDW					.134
T.E	Bend	VDW	Kcal	Pka Exp	Res
4.0551	3.9179	16.9585	10.41158	10.4278	-0.01622
3.5613	5.0071	19.0337	10.40086	10.532	-0.13114
-2.1573	4.7869	19.5867	11.23592	10.729	0.506923
5.8146	4.3626	17.2318	10.09343	10.131	-0.03757
2.8791	5.1277	15.687	9.995309	9.986	0.009309
1.6987	4.6612	18.1561	10.61869	10.297	0.321686
9.7198	5.3531	20.3983	9.729829	9.826	-0.09617
9.9321	6.5847	19.6543	9.209811	9.036	0.173811
1.8931	6.4081	18.3218	10.05788	10.167	-0.10912
4.0631	5.3432	16.85431	9.940062	10.021	-0.08094

After observing the results we obtained in Table (9 and 8), it becomes clear to us that there are values, some of which are very close to the practical ones for some compounds, and others are different, and there is a difference between the theoretical and practical values for the compounds. This phenomenon can be observed in all the methods that were studied for the compounds under study, and the reason for that is due to the difference in the basic principle of work of each method from the other (Amein, 2021). When observing the results in the two tables above for the compound.



We note that there is a convergence between the experimental and theoretical results, as well as between the two methods (AM1 and DFT). It can be observed that the compound above has the lowest possible energy value for gaining an electron in the outer orbital due to the influence of the substituent groups. To obtain the best methods, chemical displacement values for the atoms under study were obtained by comparing the values we would obtain theoretically for each method studied with the experimental results using the regression correlation coefficient.

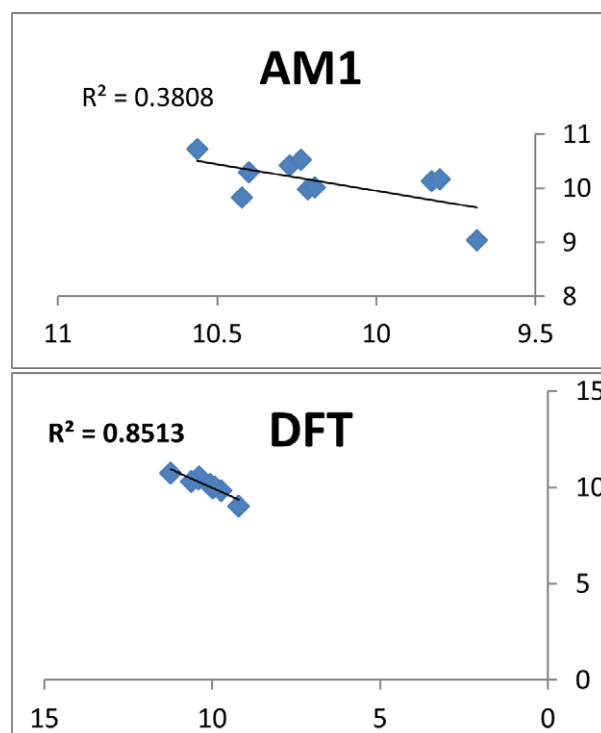


Figure 1. The relationship between the practical and theoretical ionization constant in quantum mechanics methods.



In the results we obtained, there was a convergence between the experimental and theoretical results of the two methods. However, to choose the best method, the correlation coefficient between the theoretical and experimental Pka values was calculated for both methods. As shown in Figure 1, we observe that the higher value was obtained in the DFT method. This study is consistent with a previous study conducted (Al-Taaye, 2021).

5. CONCLUSION

The aim of this study was to investigate a group of base compounds using quantum chemistry. The study employed two methods: one semi-experimental (AM1) and the other fundamental (DFT). This study relied on values obtained after the synthesis of the chemical compounds. Then the same vehicle was studied theoretically in computing. It obtained good results, showing a degree of agreement between the methodological values. The harmonic correlation values in the DFT method were $R = 0.984$, while in the AM1 method, $R = 0.948$, which is a fairly good result. However, the DFT results were more acceptable, as the difference between the methodological and theoretical values of the ion constant was closer.

REFERENCES

- Aguilera, A. (2017). *Computational study of nuclear magnetic shielding constants* [Doctoral dissertation, University of Girona].
- Al-Abady, R., Altaiea, F., & Al-Hyali, A. (2022). Determination Of Thermodynamic Functions from the pKa Values of a Number of Schiff bases by Employing the DFT Method: Theoretical Study. *Diyala Journal for Pure Science*, 18(2), 65–86.
- Al-Abady, R. E. T. G., Altaie, F., & Al-Hyali, E. (2021). Correlation Study for the Determination of Pka of A Number of Schiff Bases Derived from N-Formyl Pyridine Using Quantum Mechanical Methods. *Egyptian Journal of Chemistry*, 64(1), 375–386.
- Al-Taaye, D. (2021). *Development of a new set of additivity parameters for the calculation of N-13 chemical shifts* [Master's thesis, Tikrit University].
- Allinger, N. L., Yuh, Y. H., & Lii, J. H. (1989). Molecular mechanics. The MM3 force field for hydrocarbons. *Journal of the American Chemical Society*, 111(23), 8551–8566.
- Ameen, M. G., Najim, Z. A., & Ahmed, N. G. (2021). Influence of different of ethanol percentages on the acidity of Aza Michael compounds. *Samarra Journal of Pure and Applied Science*, 3(4), 1–25.
- Dewar, M. J., Zoebisch, E. G., Healy, E. F., & Stewart, J. J. (1985). Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. *Journal of the American Chemical Society*, 107(13), 3902–3909.
- Dinur, U., & Hagler, A. T. (1991). New Approaches to Empirical Force fields. In K. B. Lipkowitz & D. B. Boyd (Eds.), *Reviews in Computational Chemistry* (Vol. 2, pp. 99–164). VCH Publishers.
- Dorsett, H., & White, A. (2000). *Overview of molecular modeling and Ab-initio molecular orbital methods suitable for use with energetic materials* (DSTO Aeronautical and Maritime Research Laboratory Report). Commonwealth of Australia.
- Grant, D. M., & Paul, E. G. (1964). Carbon-13 magnetic resonance. II. Chemical shift data for the alkanes. *Journal of the American Chemical Society*, 86(15), 2984–2990.
- Hameed, D. N., Hameed, F. M., & AL-Healy, E. (2021). Development of New Variables for the Calculation of Chemical Shift For Nucleus Nitrogen-15 Using Quantum Mechanics Methods (AM1 Method and DFT Method). *J. AL-utroha*, 2(2), 57–83.
- Hong, C. (2003). Application of ChemOffice in Chemistry. *Journal of Sichuan Institute of Light Industry and Chemical Technology*, 4, 17.
- Ibrahim, A. A., Younis, A. A., Sulliman, E. K., Ibrahim, M. Z., & Yaareb, Z. A. (2020). *Study The Effect of Factors on the Rate Constant (K) for Some Substituted Benzyl-amine Using Theoretical Calculations*. IMDCSDSP.
- Ibrahim, A. S., Ibrahim, M. Z., Sulliman, E. K., Daoood, S. A., & Ismael, G. G. (2021). Comparison Study of HOMO-LUMO Energy Gaps for Tautomerism of Triazoles in Different Solvents Using Theoretical Calculations. *Journal of Pure Sciences*, 1, 38–43.
- Johnson, L. F., Heatley, F., & Bovey, F. A. (1970). Polymer Nuclear Magnetic Resonance Spectroscopy. XIX. Carbon-13 Resonance Observations of Stereochemical Configuration. *Macromolecules*, 3(2), 175–177.
- Lashkaripour, A. (2021). Introduction to Quantum Chemistry: The Schrödinger Equation. In *Introduction to Quantum Chemistry: The Schrödinger Equation* (7th ed., Chapter 1). Pearson Education.
- Leach, A. (2001). *Molecular Modelling Principles and Applications* (2nd ed.). Pearson Education England.
- Leszczynski, J. (1999). *Computational Molecular Biology*. Jackson State University.
- Lewars, E. (2016). *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*. Springer.
- Mayo, S. L., Olafson, B. D., & Goddard, W. A. (1990). DREIDING: a generic force field for molecular simulations. *Journal of Physical chemistry*, 94(26), 8897–8909.
- Philipsborn, W., & Muller, R. (1986). *Angew. Chem. Int. Ed. Engl.*, 25, 383.



- Reich, H. J., Jautelat, M., Messe, M. T., Weigert, F. J., & Roberts, J. D. (1969). Nuclear magnetic resonance spectroscopy. Carbon-13 spectra of steroids. *Journal of the American chemical society*, 91(26), 7445-7454.
- Schwoebel, S. D., Höhlich, D., Mehner, T., & Lampke, T. (2021). Stabilization of the Computation of Stability Constants and Species Distributions from Titration Curves. *Computation*, 9(5), 55.
- Simons, J. (2003). *An Introduction to Theoretical Chemistry*. Cambridge University Press.
- Szabo, A., & Ostlund, N. (1996). *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*. Dover Publication Inc.
- Venianakis, T., Oikonomaki, C., Siskos, M., Varras, P., Primikyri, A., Alexandri, A., & Gerothanassis, I. P. (2020). DFT Calculations of ¹H and ¹³C-NMR Chemical Shifts of Geometric Isomers of Conjugated Linoleic Acid (18:2 ω-7) and Model Compounds in Solution. *Molecules*, 25(16), 36-60.

