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COMPARATIVE STUDY OF IONIZATION CONSTANTS AND STRUCTURAL PROPERTIES OF OXIDATIVE AND PHENOLIC ACIDS USING AM1 AND DFT METHODS

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Abstract. A theoretical study of the ionization constant (Ka) of ten oximic and phenolic acids derived from aromatic and aliphatic compounds was conducted. The factors influencing the ionization constant were investigated using two quantum mechanical methods: semi-empirical calculations (Austin AM1) and ab initio calculations (DFT), both implemented in ChemOffice 2018. AM1 and DFT are valuable tools for calculating physical properties of oximic and phenolic acids. The validity of these methods was assessed by comparing the theoretically calculated variables. These variables (quantities susceptible to change within a mathematical context) were analyzed to determine which method provided more accurate results and to establish relationships between them. The calculated ionization constants were then correlated with experimental values through simple and multiple statistical analysis. The strong correlations obtained, indicated by high R^2 values, validated the theoretical approach. Multiple statistical analysis revealed that the most influential variables for the ionization constant are the Highest Occupied Molecular Orbital (HOMO) energy, the Mulliken charge on the nitrogen atom at position 2 (MC-N2) and van der Waals interactions (Bend VDW). Other variables were excluded due to negligible or zero coefficients. These selected variables were used to establish a predictive relationship. The correlation coefficients obtained were 0.9902 for AM1 and 0.7306 for DFT. Comparison with experimental values demonstrated that the AM1 results closely matched the experimental data.

Keywords: *Oximatic and phenolic acids, aromatic and aliphatic carbon compounds, ionization constant, semi-empirical, basic.*

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1. Introduction

Oximes are organic compounds characterized by a nitrogen atom with a lone pair of electrons, double-bonded to a carbon atom that is also bonded to a hydroxyl group. This functional group, known as the oximino group, dictates the reactivity and properties of oximes, including their stereochemistry (Krylov *et al*., 2020; Albayati *et al*., 2023; Ali *et al*., 2021). Oximes exhibit diverse stereoisomerism, as illustrated in Scheme 1.

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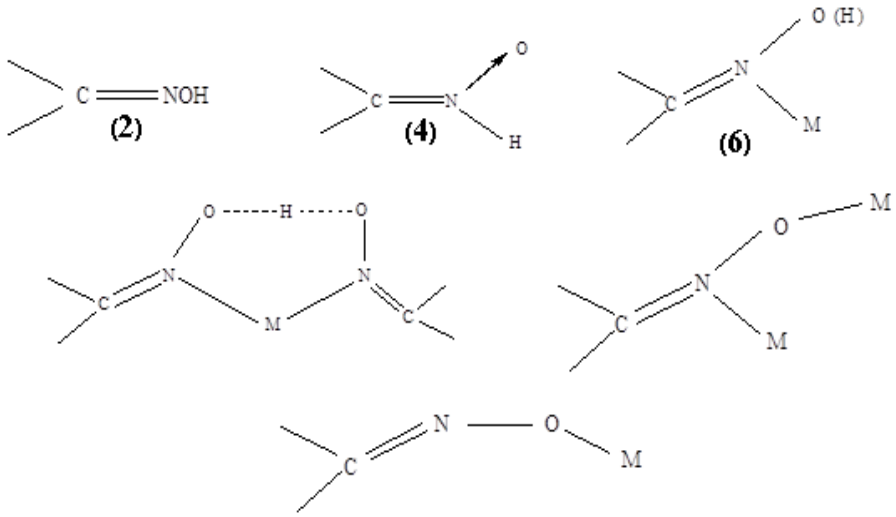


Scheme 1. The different stereoscopic of Oximes, where: M = metal ion

Oximes, sometimes referred to as conformation numbers (Hamdoon & Saleh, 2022), possess a unique characteristic: their oximino group demonstrates amphoteric behavior (Saied *et al*., 2022; Hamdoon *et al*., 2022; Ali *et al*., 2022a). This means it can act as both a weak base (due to the nitrogen atom) and a moderately strong acid (due to the hydroxyl group).

Computational chemistry has become a vital and cutting-edge area of chemistry (Dewar *et al*., 1985; Allinger *et al*., 1989). Its primary objective is to theoretically determine key properties of chemical compounds and compare these calculated values with experimental results. This allows for a deeper understanding of chemical phenomena and can aid in predicting the behavior of new or complex molecules.

Computational chemistry employs a variety of mathematical methods, which can be broadly classified into two main categories:

Molecular mechanics

It is a computational method that primarily relies on applying classical mechanics, specifically Newton's laws of motion, to atoms within a molecule. A key simplification in this approach is the neglect of electronic effects (Sheet *et al*., 2024).

Quantum mechanics

Basically, it involves the Schrödinger equation in describing molecules, taking into account the effect of the presence of electrons. (Al-Abboodi *et al.*, 2024; 2021). Quantum mechanics consists of Ab initio methods and semi-empirical methods. (Hussein *et al*., 2022; Hassan *et al*., 2023).

Molecular mechanical methods

Molecular mechanics describes the energy of molecules based on classical methods and laws adopted in this field, which can be used to calculate the potential energy of a compound, which is called field energy. Molecular mechanics methods are faster compared to quantum mechanical methods, so they are used for certain types of atoms in Calculated molecule. (Field *et al.*, 1990; Allinger *et al*., 1990).

Molecular mechanics MM2 calculations are commonly used to calculate the energies resulting from molecular structural deformations. This method was developed by the scientist (N.L. Allinger) and his group at the University of Georgia. Molecular mechanics methods are used to calculate the vacuum energy.

Quantum mechanical methods

It is a group of physical theories that appeared in the twentieth century, to explain phenomena at the level of the atom and subatomic particles. It combined the particle property and the wave property to reveal the term wave-particle duality. Thus, it becomes responsible for the physical interpretation at the atomic level as it is applied to classical mechanics, but it does not appear. Its impact is at this level, so quantum mechanics is a generalization of classical physics because it can be applied at the atomic and ordinary levels. Calling it the term quantum mechanics is due to the importance of quantum in its structure. It is a physical term used to describe the smallest amount of energy that can be exchanged between particles and is used to refer to the specific amount of energy that is emitted intermittently and not continuously. This theory was purified in the year 1900 AD when the scientist Max Planck studied the law Distribution of black body radiation, and the scientist Schrodenker developed this theory in 1926 AD. (Streitwieser & Salzberg, 1962).

The fundamental importance of quantum mechanics in the field of chemistry in all its branches lies in giving a clear theoretical explanation of the effect of the electronic structure of complex molecules and many other properties, such as the nature of chemical allotropy, and explaining practical results such as spectroscopic measurements, polarization moments, ionization potentials, reaction methods, and chemical effectiveness. This method is concerned with the electron at The opposite of molecular mechanics methods, since the movement of the nucleus is very little (almost non-existent) compared to the rapid movement of electrons, therefore quantum mechanical methods used mathematical methods to calculate the movement of electrons and their effect in calculating many of the physical properties of molecules. (Pople & Nesbet, 1954; Sadeek *et al.*, 2023).

Quantum mechanical methods depend on the Schrodenker wave equation .It represents the most common method in use due to its simplicity in quantum chemical calculations. This equation is written in the following form:

$$\hat{H}\Psi = E\Psi \quad (1)$$

$$\hat{H} = \hat{T} + \hat{V} \quad (2)$$

Since:

$\hat{H}$ represents the Hamilton factor and gives information describing the electrons and forces in the system. It represents the sum of the two factors: kinetic energy $\hat{T}$ (Kinetic energy) and Potential energy $\hat{V}$ (Potential energy).

Ψ represents the electronic wave function or Eigen Function, which describes the state of the electron in terms of movement and location.

E is called the Eigen Value, and it represents the energy corresponding to the independent or isolated state of the electron.

The Schrodenker equation is a second-order molecular differential equation used to solve simple systems containing only two particles, such as a helium ion. As for complex systems (i.e. atoms containing more than one electron or molecules), approximate

methods were used that depend on the Schrdenker equation, and these methods include the theory of disturbance and the method of change. (Scrinzi, 2014; Nakatsuji, 2012).

Semi-empirical methods

These methods rely on experimental measurement data in calculations to find the physical properties of organic and inorganic compounds, as semi-empirical methods rely on approximating the Schrodenker equation during the calculation process, that is, replacing the values of some integrals with practical values instead of calculating them. (Dewar *et al*., 1978; Leforestier *et al*., 1991; Raoof *et al*., 2022).

The extended Hickel method can be applied to formulate valence orbitals based on orbital interactions, ionization potentials, and their experimental relevance Among.

Austin Method AM1: Austin Model

The first person to develop this method was the German scientist Michael Dewar. This method is an advanced version of the MINDO method, which is a quick method for calculating the energies and structures of organic compounds. The AM1 method is considered a semi-empirical method and is derived based on theoretical information as well as analysis of experimental data. This method has succeeded in explaining and clarifying a number of chemical phenomena that were not previously known. (Winget *et al*., 2003; Schlick, 1992; Fantacci *et al*., 2010; Banoon *et al*., 2025).

The most important information obtained from this method is the heat of formation, electronic density, atomic charges, ionization potential, bond length and angle values for the molecules containing atoms (C, H, N and O). This method uses atomic orbitals (P, S) and the central-axis repulsion function with additional Gaussian terms

Ab initio methods

(Ab initio) means basic calculations and its calculations are based on basic principles that use mathematical approximations called (Basis Sets) to calculate atomic and molecular orbitals without any guarantee of experimental results. (Saleh et al., 2024).

This method is considered one of the most accurate and best methods for calculations and approximation of real values when compared to semi-empirical methods. The only problem that these methods suffer from is that they take a lot of time in their calculations. For this reason, other alternative methods are sometimes chosen for calculations that do not It requires high accuracy, which may take less time, as in the (AM1) method. One of the basic calculation methods.

Density Functional Theory (DFT)

Density functional theory (DFT) is a widely used computational quantum mechanical modeling method in chemistry, physics, and materials science. It is used to study the electronic structure of many body systems, especially atoms, molecules, and condensed phases. DFT allows researchers to examine the electronic properties of materials and predict their behavior, such as reactivity, bonding, and stability. It is useful for studying a wide range of materials, including metals, semiconductors, and insulators, as well as biological and environmental systems. (Adekoya *et al*., 2022; Sabeeh Hasan *et al*., 2024; Ahmad *et al*., 2024).

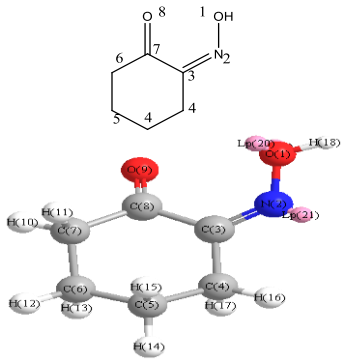
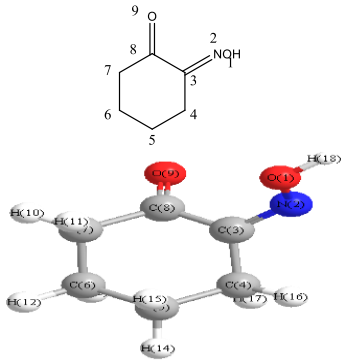
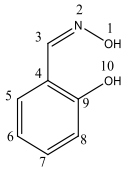
DFT calculations can aid in the development of new chemical materials and processes, drug design, and understanding environmental issues.

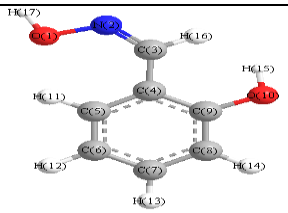
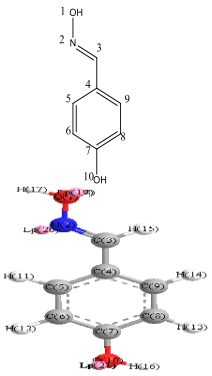
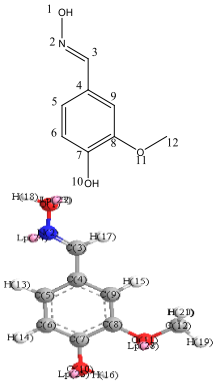
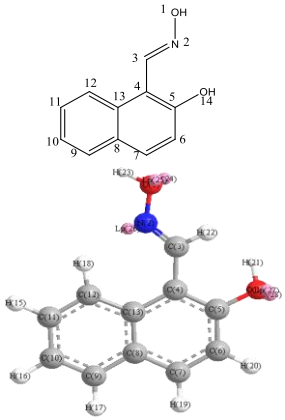
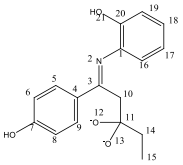
2. Results and discussion

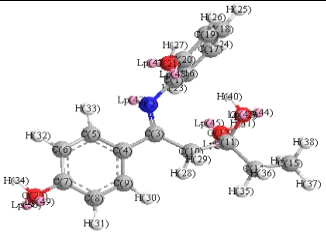
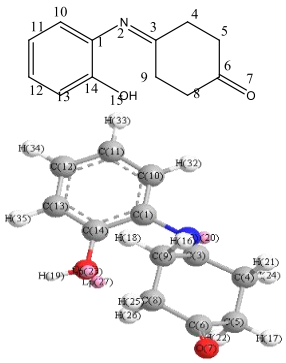
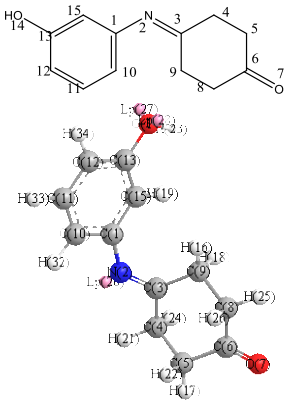
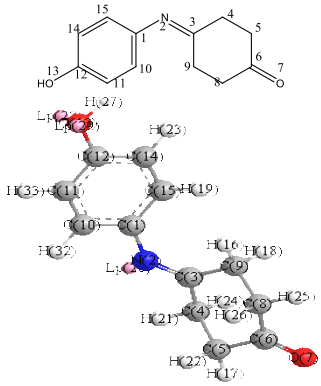
Theoretical calculations

This study includes the selection of ten materials from oxidizing and phenolic acids derived from aromatic and aliphatic compounds, whose structures and ionization constant values are shown in Table 1 (Tomboulian & Bloomquist, 1959; Schlick, 1992; Zhou *et al*., 1997; Supsana *et al*., 2001; Sunnerheim *et al.*, 2007; Kunduracı *et al.*, 2013; Alam *et al.*, 2016; Harjan *et al.*, 2024). These compounds were studied using Chem-Office 2018 and Gaussian programs. Phenolic acids are known for their significant antioxidant activity, which plays a vital role in protecting biological systems against oxidative damage. The last reference discussed on the mechanisms of antioxidant action, emphasizing their ability to neutralize free radicals, chelate metal ions and inhibit lipid peroxidation (Lawi *et al*., 2021).

Table 1. Shows the names and structural formula of oxyacids and phenolic acids derived from aliphatic and aromatic carbonyl compounds and the value of the ionization constant

No.	Compound name	Structural formula	Kn
1	Cyclohexanone oxime-2-one		255.9982
2	Cyclohexanone oxime-4-one		317.8856
3	2-Hydroxy-benzaloxime		0.0039

			
4	4-hydroxy-benzaldoxime		0.0045
5	3-methoxy-4-hydroxy benzaldoxime		0.0205
6	2-Hydroxy-1-naphthyl aldoxime		0.005
7	Ethyl-3-phenyl-3-(2-hydroxy iminophenyl) propionate		71.5856

			
8	2-Hydroxy phenyl cyclohexaimino-4-one		71.2356
9	3-Hydroxy phenyl cyclohexaimino-4-one		54.1015
10	4-hydroxy phenyl cyclohexaimino-4-one		98.4318

The programs (Chem. Office) and (Gaussian) are among the important programs in theoretical calculations in chemistry, which are considered among the efficient programs in completing and completing many traditional and advanced calculations, which provide the necessary means to complete theoretical research and support scientific research. The program includes all types of quantum mechanics and molecular mechanics. Molecular mechanics methods are contained in a program called MM2 Molecular Mechanic, while

semi-empirical methods for extended structure theory (AM1) and fundamental calculation methods (DFT) are located directly within the subprogramme (GAMES). From the information obtained using the molecular mechanics method which includes the molecular mechanics program (MM2), energy minimization was performed to reach the most stable form (lowest energy) and some important information as well as some physical (Cohen *et al*., 1990; Pearlman *et al*., 1995; Honarparvar *et al*., 2014; Moore *et al*., 2018; Saleh *et al*., 2025).

In this research under study, the program (Chem. Office 2018) was used to theoretically calculate the values of ionization constants for ten compounds of oximatic and phenolic acids derived from aromatic and aliphatic compounds, as the values of Kn are obtained theoretically as in Table 2. The main reason for choosing two theories is to conduct a broad survey of most of the theories adopted in computational chemistry and choose the best of them statistically to extract Kn values and compare them with the experimental values of the selected chemical compounds to demonstrate the accuracy of these two methods in finding Kn values. These two theories were used to obtain the chemical structure with the lowest energy for the selected compounds, through which a group of factors and influences are extracted and statistical coefficients are performed on them to extract Kn values for these compounds. In this research, the basic Bubel group (3.21G) was used when performing calculations using DFT theory, while the semi-empirical theories (AM1) do not need to add basic groups.

The calculations in this research were carried out based on the following precise steps: Drawing the formula and performing the energy reduction process using the Molecular Mechanics program (MM2) to extract the values of the vacuum impedance energy. The calculations were re-performed for the lower energy compounds resulting from the previous step using the methods (AM1, DFT). Using (3-21G) as a basic set in the case of DFT theory only, this procedure was repeated for all compounds selected in this study (10 compounds). Thus, calculations were performed for each compound using two different theories. Among the values that were calculated using semi-empirical methods and basic calculation methods are the electron charge (Muliken charges) of the compounds and the values of the energies of the HOMO and LUMO orbitals. The values of hardness, the electronic chemical potential (μ) and the global electrophilicity index (W) were calculated. Also, performed a statistical treatment that included evaluating the relationship between these theoretically calculated functions and the extent of their influence on each other and the values of the practical ionization constants (Faucher-Giguere *et al*., 2009).

Calculating some physical variables

Some of the physical constants described above were calculated theoretically in two ways. The first method included semi-empirical computational methods (AM1) while the second method included basic computational methods (Ab intio) (DFT/B3LYP). The aim of choosing these two methods was to compare them and show the superiority of each method through the accuracy of the calculations and their agreement with what is known from the basics of chemistry. As a first step, the values of the physical variables of the compounds under study (bond energies) were calculated theoretically using the MM2 method

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We notice from Table 2 that there is a clear difference in the total energy values of these chemical compounds and many of these values are what control the energies and depend mainly on the value of van der Waals correlations. (1,4VDW), which range between (3.0449-7.8312 Kcal/mole) and the values of the torsion of the quadrilateral angles (Torsion), which It ranges between (2.6521-[-13.1696] Kcal/mole) and the bending energy values (Bend) for most compounds range between (1.3420-[15.6382]Kcal/mole), while the effect of stretching (Stretch) and bending - stretching (Stretch-Bend) is and slightly non-correlated Vanderwaals interferences.

Table 2. Theoretical calculations of the values of the physical variables of the vehicles using the MM2 method

NO.	Str. Kcal/mole	Bend Kcal/mole	S. B Kcal/mole	Tors. Kcal/mole	Non-1,4 VDW Kcal/mole	VDW Kcal/mole	c
1	0.2849	1.3420	0.0843	1.2902	-1.2885	4.5252	7.2381
2	0.2565	2.1119	0.0709	2.6521	-1.1259	4.5060	7.2490
3	0.3845	3.2592	0.0047	-6.6890	-0.8920	3.0449	-1.6664
4	0.1662	1.3507	-0.0148	-7.7566	-1.1050	3.2562	-5.2510
5	0.4762	4.1726	0.0027	-9.7372	-3.5836	5.8612	-4.7831
6	0.5950	2.3845	-0.0016	-13.1696	-1.6136	6.4807	-6.2679
7	1.3626	15.6382	0.2558	-1.5185	-101662	7.8312	14.1756
8	0.5678	3.6359	0.1563	2.4251	-3.4709	6.7414	10.7516
9	0.5126	5.7158	0.1747	0.3790	-1.6559	6.8652	12.6953
10	0.4487	5.2425	0.1487	0.8416	-1.7739	6.8912	12.3695

Mulliken charges were calculated, which represent the difference between the negative electronic density in the orbitals and the number of positive protons in the nucleus. As the negative value increases, the electrons in the outer orbitals increase. The charges were calculated for the nitrogen atom “N2” and carbon C3 in the compounds of oximic and phenolic acids derived from aromatic and aliphatic carbonyl compounds. Also, the orbital energy values (HOMO, LUMO) were calculated for the compounds under study using two quantum mechanical methods AM1 and DFT, Also, some functions known in the literature 30 These functions include molecule hardness (κ), electronic chemical potential (μ) and universal electrophilicity index (W). The results are shown in Tables 3 and 4.

Table 3. Theoretical energy values calculated for the compounds using the AM1 method

NO.	HOMO	LUMO	Ŋ	μ	W	MC-"N2"	MC-C3
1	-0.3713	0.0081	0.1897	-0.1816	-0.086922	-0.0183	-0.1397
2	-0.3828	0.0285	0.20565	-0.17715	-0.076299	-0.0550	-0.0860
3	-0.3339	-0.0079	0.163	-0.1709	-0.089591	-0.0591	-0.0841
4	-0.3292	-0.0042	0.1625	-0.1667	-0.08550	-0.0626	-0.0891
5	-0.3208	-0.0050	0.1579	-0.1629	-0.084029	-0.0597	-0.0905
6	-0.3162	-0.0235	0.14635	-0.16985	-0.098561	-0.0351	-0.1136
7	-0.3218	-0.0021	0.15985	-0.16195	-0.090078	-0.1738	0.1140
8	-0.3352	-0.0033	0.16595	-0.16925	-0.08630	-0.1416	-0.0073
9	-0.3367	-0.0218	0.15745	-0.17925	-0.102034	-0.1727	0.0214
10	-0.3263	-0.0041	0.1611	-0.1652	-0.08470	-0.0417	-0.1501

Table 4. Theoretical energy values calculated for the compounds using the DFT method

NO.	HOMO	LUMO	Ŋ	μ	W	MC-"N2"	MC-C3
1	-0.2213	-0.0331	0.0941	-0.1272	-0.08597	-0.282837	0.265873
2	-0.2316	-0.0104	0.1106	-0.121	-0.06618	-0.301534	0.329644
3	-0.2163	-0.0312	0.09255	-0.12375	-0.08273	-0.271534	0.100136
4	-0.2062	-0.0204	0.0929	-0.1133	-0.06908	-0.286432	0.125017
5	-0.1944	-0.0184	0.088	-0.1064	-0.06432	-0.288039	0.127230
6	-0.2035	-0.0457	0.0789	-0.1246	-0.09838	-0.375681	0.182971
7	-0.1904	-0.0232	0.0836	-0.1068	-0.06821	-0.656844	0.367733
8	-0.2096	-0.0297	0.08995	-0.11965	-0.07957	-0.657008	0.357219
9	-0.2075	-0.0256	0.09095	-0.11655	-0.07467	-0.588910	0.334657
10	-0.1988	-0.0209	0.08895	-0.10985	-0.06783	-0.600066	-0.443160

When observing the values of the energy functions in the tables for compounds, we find that the value of the HOMO energy in the AM1 method increases in the compounds and is the lowest possible in Compound No.2, while in the DFT method, it is close, while the value of LUMO is as high as possible for the same compound compared to other compounds whose values are lower. Variably with the change in locations of the compensators on the ring. The increase in the value of the HOMO and the decrease in the value of the LUMO means an increase in the difference in energy between the two molecular levels and thus an increase in the energy required for electronic transfer (excitation energy). The rest of the variables will be close and different. The purpose of calculating these variables is to apply them in simple regression analysis to obtain values that affect the values of the ionization constant. Therefore, statistical processing of these calculations was followed to evaluate the mutual relationship between each of the calculated variables and their effect on the values of the ionization constant as a dependent factor.

Statistical analysis can be deceptive and misleading at times and gives results by chance. Therefore, to adopt its results, three basic conditions must be provided, the first of which is to obtain strong correlation coefficient values close to one and the second is to have a good match between the practical and theoretical values (low S.D.). Finally, the nature of the effect of the variables must be compatible with the chemical foundations and principles of each effect. The relationship between each of the variables with each other and with the two methods used for the compounds under study was found using simple and multiple regression analysis (Rocha *et al*., 2006; Deml *et al*., 2016; ul Qamar *et al*., 2025), in addition to the ionization constant values and the results were listed in Tables 5 and 6.

3. Statistical Analysis

The (SPSS 2018) program was used to conduct the multivariate correlation analysis and by using the successive input method of variables to find the best linear relationship through which the best result and the best equation can be reached to calculate the values of the constants theoretically and compare them with the practical values. After completing the simple regression analysis (Pilling & Robertson, 2003) between the energy functions calculated theoretically from the two methods as non-dependent variables and the ionization constant as a dependent variable, the functions that most affect ionization are determined through the values of the correlation coefficients (R2), the values of the coefficients of the variables (a1) and the experimental error and then entering the functions into Equation No.3 shown in the introduction and calculating the values of the theoretical ionization constants. Finally, the multiple regression analysis was conducted using the mathematical Equation No.4 mentioned in the introduction to determine the relationship between the adopted functions with each other and the extent of their impact on the values of Kn obtained from the literature (Wang, 2016).

Table 5. Linear relationship resulting from simple regression analysis linking the experimental values of the ionization constants of the compounds under study with the theoretically calculated variables using the AM1 method for these compounds

Var	Kn	HOMO	LUMO	ŋ	μ	W	MC-"N2"	MC-C3	Str.	Bend	S.B	Tors.	Non-1,4VDW	VDW	TE
Kn	1														
HOMO	0.857	1													
LUMO	0.685	0.636	1												
ŋ	0.871	0.936	0.854	1											
μ	0.374	0.584	0.049	0.332	1										
W	0.272	0.238	0.772	0.458	0.023	1									
MC-"N2"	0.050	0.066	0.070	0.075	0.018	0.150	1								
MC-C3	0.032	0.055	0.025	0.046	0.044	0.099	0.892	1							
Str.	0.050	0.205	0.057	0.150	0.228	0.097	0.418	0.614	1						
Bend	0.026	0.144	0.016	0.086	0.228	0.040	0.478	0.648	0.885	1					
S. B	0.050	0.0	0.001	0.0	0.001	0.025	0.544	0.488	0.471	0.577	1				
Tors.	0.494	0.383	0.289	0.381	0.181	0.095	0.110	0.052	0.001	0.026	0.486	1			
Non-1,4VDW	0.019	0.128	0.0	0.055	0.311	0.002	0.388	0.613	0.878	0.859	0.428	0.008	1		
VDW	0.012	0.164	0.113	0.158	0.088	0.134	0.321	0.262	0.529	0.428	0.540	0.044	0.383	1	
TE	0.207	0.073	0.050	0.071	0.039	0.0	0.333	0.242	0.177	0.288	0.883	0.784	0.160	0.323	1

Table 6. Linear relationship resulting from simple regression analysis linking the experimental values of the ionization constants of the compounds under study with the theoretically calculated variables using the DFT method for these compounds

Var	Kn	HOMO	LUMO	ŋ	μ	W	MC-N2	MC-C3	Str.	Bend	S.B	Tors.	Non-1,4VDW	VDW	TE
Kn	1														
HOMO	0.490	1													
LUMO	0.126	0.009	1												
ŋ	0.544	0.660	0.433	1											
μ	0.124	0.591	0.318	0.063	1										
W	0.018	0.040	0.906	0.165	0.605	1									
MC-"N2"	0.015	0.225	0.0	0.135	0.147	0.020	1								

MC-C3	0.038	0.076	0.008	0.024	0.081	0.028	0.0	1							
Str.	0.050	0.402	0.016	0.307	0.197	0.003	0.420	0.064	1						
Bend	0.026	0.387	0.020	0.150	0.368	0.109	0.428	0.021	0.885	1					
S.B	0.050	0.074	0.026	0.013	0.108	0.070	0.771	0.027	0.471	0.577	1				
Tors.	0.494	0.153	0.169	0.288	0.004	0.106	0.226	0.014	0.001	0.026	0.486	1			
Non-1,4VDW	0.019	0.388	0.012	0.165	0.346	0.087	0.310	0.086	0.878	0.859	0.428	0.008	1		
VDW	0.012	0.376	0.012	0.278	0.194	0.004	0.701	0.0	0.529	0.428	0.540	0.044	0.383	1	
TE	0.207	0.0	0.070	0.025	0.027	0.084	0.591	0.006	0.177	0.288	0.883	0.784	0.160	0.323	1

The two tables show the nature of the good relationship between the ionization constant and some variables and these relationships differ in their values depending on the method used. After that, we moved to the next stage, which is conducting the process of binary, triple and quadruple regression analysis to reach the final relationships. Through a separate statistical analysis of the theoretically calculated variables and charges with the ionization constants, the following can be observed: The comparison between the two methods showed good agreement and when looking at the general correlation, we find that the highest correlation was between the ionization constants as a dependent variable and the hardness (Ƞ), as it gives the value of the correlation coefficient. (R2) was high with the AM1 method (0.871) and the DFT method was (0.544), followed by the correlation between the ionization constant and HOMO for the two methods. When looking at the correlation value between the ionization constants with other theoretical values, we find that the correlation is acceptable with some variables, while the correlation results were. The rest of the variables are somewhat weak, so they were excluded and not relied upon.

Two- and three-way statistical analysis was performed, the results of which are listed in Table 7 to (10) for the AM1 and DFT methods, between the ionization constants as a dependent variable and the variables that gave acceptable results in the individual analysis. The results showed a noticeable improvement, which indicates the presence of an influence by these variables on Ionization constants: It was found that the most common binary and ternary variables affecting the ionization constant were HOMO (the first variable), MC-"N2", Bend, LUMO, MC-C3, S.B and Tors. Non-1,4VDW and Vander Waals correlation interferences (as a second and third variable) respectively, gave relatively high R2 correlation coefficient values ranging between (0.88 - 0.969) in the AM1 method and (0.707 - 0.891) in the DFT method.

Table 7. Results of the statistical analysis of the binary correlation between the physical variables measured using the AM1 method and the ionization constants of the compounds under study

Var	Constant B	coefficient X_1	coefficient X_2	R^2	S. E
K & H L	-1160.342	-3716.324	1895.985	0.879	44.333
K & H MC-N2	-1513.890	-4736.836	-30.667	0.857	48.168
K & H MC-C3	-1517.320	-4764.863	56.199	0.859	47.941
K & H Str	-1738.663	-5285.231	83.577	0.905	39.216
K & H Bend	-1676.106	-5145.754	5.965	0.900	40.420
K & H S. B	-1527.209	-4713.323	269.551	0.906	39.029
K & H Tors.	-1267.109	-4051.453	4.157	0.885	43.327
K & H Non	-1663.522	-5117.684	-8.866	0.900	40.409
K & H VDW	-1843.815	-5367.039	21.391	0.940	31.153
K & H TE	-1415.664	-4411.690	3.010	0.902	39.877
K & L MC-N2	110.176	6368.604	9.365	0.685	71.520

K & L MC-C3	105.021	6318.883	-67.396	0.688	71.257
K & L Str.	114.017	6327.497	-9.405	0.686	71.440
K & L Bend	115.995	6323.650	-1.504	0.689	71.170
K & L S. B	88.106	6329.130	240.031	0.724	66.942
K & L Tors.	126.519	4876.590	7.153	0.779	59.929
K & L Non	122.539	6360.909	4.935	0.701	69.787
K&L VDW	39.773	6864.758	12.747	0.717	67.864
K & L TE	89.713	5887.893	3.870	0.762	62.230
K & Ƞ MC-N2	-934.379	6084.616	-67.233	0.872	45.607
K & Ƞ MC-C3	-921.985	6055.206	31.579	0.871	45.715
K & Ƞ Str.	-1013.772	6427.200	54.817	0.893	41.668
K & Ƞ Bend	-972.745	6258.117	3.324	0.885	43.235
K & Ƞ S. B	-937.732	6002.905	255.241	0.915	37.152
K & Ƞ Tors.	-769.501	5205.847	4.048	0.897	40.905
K & Ƞ Non	-949.167	6151.710	-3.412	0.878	44.578
K & Ƞ VDW	-1167.514	6813.315	20.890	0.951	28.242
K & Ƞ TE	-868.968	5641.030	3.043	0.917	36.685

After completing the quadratic statistical analysis, the variables that affect the ionization constants of the compounds under study were the energy interactions HOMO, MC-N2, Bend and VDW. The remaining variables were deleted because their coefficient values were small or close to zero as shown in the binary and ternary analysis Tables 7, 8, 9 and 10. Only the values of these four variables were selected to obtain a mathematical relationship through which the ionization constants of the compounds under study can be calculated, which are difficult to calculate their ionization constants accurately in practice. The results of the quadratic statistical analysis of the selected variables and the two methods are listed and illustrated in Table 11 and Figure 1. It is noted from the table that the values of the correlation coefficients R2 in the AM1 method are good (0.9902), while in the DFT method, they are average (0.730). Through these results, the conclusion of the mathematical relationship shown below (Equation 3) was reached to calculate the values of the ionization constants of the compounds under study and compare them with the results obtained practically and listed in Table 12.

Table 8. Results of the statistical analysis of the binary correlation between the physical variables measured using the DFT method and the ionization constants of the compounds under study

Var	Constant B	coefficient X_1	coefficient X_2	R^2	S. E
K & H L	-1082.834	-6044.755	3376.101	0.574	83.250
K & H MC-N2	-1534.839	-7434.216	-175.794	0.546	85.970
K & H MC-C3	-1221.056	-6288.965	0.744	0.490	91.076
K & H Str	-1720.548	-8388.432	124.662	0.571	83.535
K & H Bend	-1797.461	-8801.956	12.024	0.613	79.288
K & H S. B	-1498.284	-7391.759	544.937	0.676	72.588
K & H Tors.	-819.965	-4511.111	9.986	0.707	68.989
K & H Non	-1840.700	-9018.422	-19.552	0.652	77.061
K & H VDW	-2000.732	-9107.137	34.594	0.652	75.194
K & H TE	-1245.227	-6268.243	6.151	0.693	70.622
K & L MC-N2	226.486	4095.539	78.091	0.140	118.262
K & L MC-C3	180.864	4350.812	106.309	0.177	115.681
K & L Str.	217.467	3848.105	-61.381	0.158	117.009
K & L Bend	228.290	4468.849	-5.752	0.171	116.1109
K & L S.B	166.715	3796.643	208.615	0.155	117.255

K & L Tors.	152.030	919.159	13.213	0.499	90.236
K & L Non	218.597	4346.811	7.221	0.158	117.035
K & L VDW	219.066	4024.109	-5.013	0.131	118.861
K & L TE	137.958	2926.952	5.302	0.266	109.223
K & Ƞ MC-N2	-951.556	10878.759	-111.335	0.569	83.748
K & Ƞ MC-C3	-817.396	9859.499	37.862	0.550	85.524
K & Ƞ Str.	-1055.684	12046.264	90.601	0.593	81.321
K & Ƞ Bend	-915.115	10810.292	3.961	0.562	84.359
K & Ƞ S.B	-902.936	10505.918	377.668	0.639	76.592
K & Ƞ Tors.	-513.033	6881.442	8.502	0.676	72.560
K & Ƞ Non	-944.500	11100.479	-7.771	0.575	83.130
K & Ƞ VDW	-1222.957	12784.620	26.042	0.650	75.400
K & Ƞ TE	-780.082	9280.819	4.728	0.661	74.255

Table 9. Results of the statistical analysis of the three-way correlation between the physical variables measured by the AM1 method and the ionization constants of the compounds under study

Var	Constant B	coefficient X_1	coefficient X_2	coefficient X_3	R^2	S. E
K & H L VDW	-1488.321	-4329.789	1982.359	21.657	0.964	25.987
K & H MC-N2 S. B	-1326.163	-4208.291	742.930	612.674	0.963	26.366
K & H MC-N2 VDW	-1842.722	-5334.471	375.966	28.660	0.966	25.493
K & Ƞ MC-N2 VDW	-1165.166	6753.310	313.522	26.848	0.969	24.413
K & Ƞ MC-C3 VDW	-1206.650	6800.292	-204.446	25.985	0.967	24.942
K & Ƞ Non-VDW	-1186.808	6825.415	5.334	26.515	0.962	26.913

Table 10. Results of the statistical analysis of the three-way correlation between the physical variables measured by the DFT method and the ionization constants of the compounds under study

Var	Constant B	coefficient X_1	coefficient X_2	coefficient X_3	R^2	S.E
K & H VDW L	-1887.309	-8974.183	3683.708	36.288	0.752	68.621
K & H MC-N2 S. B	-991.428	-5668.036	496.464	1287.845	0.773	65.640
K & H MC-N2 VDW	-2040.993	-9243.452	157.370	48.829	0.669	79.201
K & Ƞ MC-N2 VDW	-1285.567	13262.776	226.086	46.843	0.685	77.306
K & Ƞ MC-C3 VDW	-1212.382	12656.362	19.030	25.645	0.652	81.256
K & Ƞ Non-VDW	-1223.251	1298.830	-0.379	25.683	0.650	81.435

$$Y = -1871.467 - 5476.432 * HOMO + 584.906 * MC - N2 + 6.169 * Bend + 23.356 * VDW \quad (3)$$

The findings of this study provide insights into the ionization properties of phenolic acids that may be used in different applications (Kumar & Goel, 2019; Zeb, 2020; Falih *et al*., 2021; Al-Jubori *et al*., 2024). Recent advancements in antimicrobial research have demonstrated the efficacy of nanoparticles functionalized with phenolic compounds exploiting the ionization potential properties in disrupting bacteria and biofilms (Ahmed *et al*., 2018; Al-Saady *et al*., 2022; Ali *et al*., 2022b). Further exploration of these interactions highlights the importance of extending computational studies to practical applications.

Table 11. Results of the statistical analysis of the four-way correlation between the physical variables measured by the AM1 and DFT methods and the ionization constants of the compounds under study

No.	Var	Cont. B	coefficient X_1	coefficient X_2	coefficient X_3	coefficient X_4	R^2	SE
1	K & H MC-N2 Bend VDW	-1871.467	-5476.432	584.906	6.169	23.356	0.9902	16.925
2	K & H MC-N2 Bend VDW	-2294.809	-10509.274	256.243	9.935	46.797	0.7306	78.317

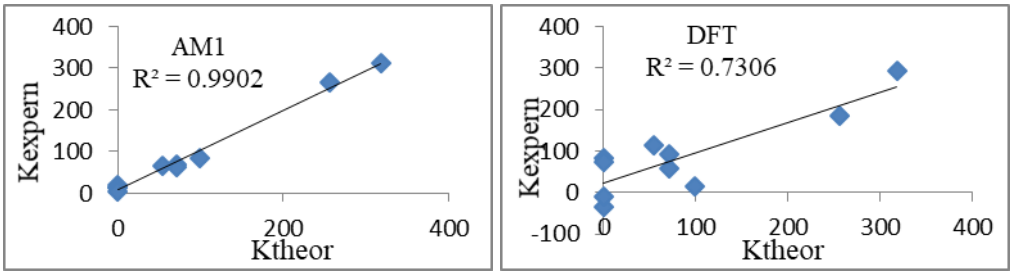

Figure 1. The graphical relationship between the ionization constants of acids, practical and theoretically calculated by AM1 and DFT methods

Table 12. Values of ionization constants calculated theoretically by the two methods and values of the correlation coefficient between the practical and theoretical values for

K_n (experimental)	Theoretical			
	AM1	DFT	The difference between the Ka Exp - Ka (AM1)	The difference between the Ka Exp - Ka (DFT)
255.9982	265.1978	183.5169	-9.1996	42.4813
317.8856	311.0118	293.7219	6.8738	24.1666
0.0039	13.76839	83.64062	-13.76449	-83.63672
0.0045	20.8564	-35.3933	-20.8519	35.3978
0.0205	13.08845	-9.87275	-13.06795	9.89325
0.005	5.723807	74.52996	-5.718807	-74.52496
71.5856	68.56972	59.68728	3.01588	11.89832
71.2356	61.29232	91.18109	9.94328	-19.94549
54.1015	67.03877	113.0185	-12.93727	-58.917
98.4318	84.39403	15.24368	14.03777	83.18812
R^2	0.9902	0.7306		

4. Conclusions

The theoretical results obtained from simple and multiple regression analysis explained the nature of the relationship between the various functions and the ionization constant. These analyses highlighted the influence of key variables in determining the ionization behavior of oximic and phenolic acids, offering a deeper understanding of their chemical properties. A significant finding of this study is the large correspondence between the theoretically calculated values of the ionization constant and the practical values in the AM1 method, whose theoretical results were closer to the practical than the DFT method, underscoring its robustness and reliability for accurate modeling of ionization processes in molecular systems.

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