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Calculating stability constants for a number of aromatic Schiff bases theoretically using AM1 quasi-experimental method and DFT basic method and comparing the results

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ABSTRACT
This study includes finding the values of stability constants by theoretical methods and comparing them with the practical values of a number of Schiff bases prepared from vanillin and aniline and their substitutes in the para position using the computational chemical program (Chem Office 2011). Calculation methods can be divided into two main parts. The first part includes molecular mechanics methods (MM2), which are based in their principle of operation on Newton's laws and through which the composite can be configured for accounts. As for the second part, it includes the methods of quantum mechanics, which are divided into the methods of semi-empirical calculations of the extended structure theory, including the method (AM1), as well as the methods of basic calculations, which consist of several methods, including the (DFT) method, which is based on Schrödinger's laws. The variables that were calculated for this study included the presence of two types of variables, one of them being inductive effects such as bond energies and values of angles and charges on the atoms. The other was the energy or steric variables such as Vander Waal forces (VDW)) as well as the values of higher occupied molecular orbital (HOMO) and lower non-molecular orbital occupied (LUMO), chemical electronic potential (μ), spherical electrophilic index (W), hardness (η), and heat of formation energies (H_f). After completing the calculations by theoretical methods and extracting the results, the statistical analysis was carried out using the statistical program (SPSS version 23). And by the methods of single, binary and multiple statistics to find the relationship between the theoretically calculated variables by means of the values of the correlation coefficients (R^2). It shows the agreement of the theoretical results with the practical results.

Keywords: computational chemistry, Schiff base, stability constants.

1-Introduction
Schiff's bases are organic compounds containing azomethine group (-CH=N-). Studies[1] refer to the Schiff base molecule derived from benzaldehyde with aniline or their derivatives is an uneven molecule as the benzene ring attached to the nitrogen atom is outside the level of the rest of the molecule as Explained as follows.

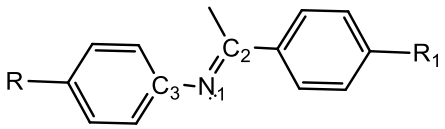

Fig.:1: The general form of the Schiff's bases

Table 1: in-situ offsets for bar- Schiff's bases

NO	Compound	logK (Exp)
1	R=P-Cl;R1=P-NO2	4
2	R1=P-NO2	4.13
3	R=P-Br	4.5
4	R=P-OH;R1=P-NO2	4.58
5	R=P-OH	4.88
6	R1=P-[-N(CH3)2]	5.6
7	R=P-Cl;R1=P-[-N(CH3)2]	5.6
8	R=P-OH;R1=P-[-N(CH3)2]	6
9	R=P-Br;R1=P-[-N(CH3)2]	6
10	R=P-CH3;R1=P-[-N(CH3)2]	6.3

Schiff bases have the ability to form hydrogen bonds between The electronic double of the azomethine group and hydroxyl compounds or solvents[2]. Studies[3] have shown that the azomethine group (-CH=N-) behaves as a donor and acquirer of electrons, which is a acceptor by the π-orbital method of the double bond, and a non-adherent double electron donor to the nitrogen atom of this group. Schiff bases prepared from aromatic aldehyde and aromatic amine are the most stable among Schiff bases and the reason for this is due to the increased stability by resonance. They have been used in industrial applications as corrosion inhibitors and in the manufacture of polymers and dyes[4,5]. Schiff's bases have also been used in medicine and pharmacy applications where they are used as antimicrobials. Anti-bacterial and anti-fungal. In addition to their use in the field of biological application[7,6] . Schiff bases have gained great importance especially in the field of pharmacology and pharmaceutical compounds[8] due to the presence of imine groups (C = N) in their structures and ease of preparation as well as prepared from a wide range of alternative amines and aromatic aldehydes This motivated many researchers and encouraged them to work in this field[9]. The ionization constant (LogK), is of importance[10] in the chemical and biochemical fields, as well as in the fields of pharmacy and other scientific fields. Since most drugs[11] include organic acids or weak bases, knowing the extent of drug molecule ionization at different pH values through ionization constant values has become necessary [12] to predict drug permeability through biological membranes and predict[13] the extent to which drug molecules are distributed in different tissues The body of the organism[14] as well as the awareness of the kinetic properties of the drug. The stability, composition, and bonding constant are a type of equilibrium constant that uses the formation of metallic complexes. The stability constant is used to measure the strength of interactions or the strength of bonding between the metal ion and the ligands that participate in the formation of complexes. In general, it is expressed by equations in the following ways.

$M + L \leftrightarrow ML_1$ $(K_1= [ML_1] / [M] * [L])$…....(1)

$ML_1 + L \leftrightarrow ML_2$ $(K_2= [ML_2] / [ML_1] * [L])$ …(2)

K1, K2, K3…Kn, are the equilibrium constants

$ML_2 + L \leftrightarrow ML_3$ $(K_3= [ML_3] / [ML_2] * [L])$ ....(3)

It is also called linear stability constant.

$ML_{n-1} + L \leftrightarrow ML_n$ $(K_1= [ML_n] / [ML_{n-1}] * [L])$…(4)

If the value of (α) represents the degree of dissociation of the complex (or the degree of interdependence of the complex) and (C) represents the concentration of the complex, so we can write the above equations in the following form.

$$K = \frac{C(1-\alpha)}{\alpha C \alpha C} = \frac{1-\alpha}{\alpha^2 C}$$ …….(5)

2-Theoretical methods

Chem.Office.V11 is one of the computer chemistry programs that includes the(GAUSSIAN 03) program. It is also considered one of the efficient programs in accomplishing many traditional and advanced calculations and provides the necessary means to accomplish purely theoretical research and supportive of practical research. This program includes all types of quantum mechanics. and molecular mechanics. These methods also study many effects such as inductive, electronic and resonance effects, and the study of hydrogen bonding and its effects [15] . Several factors can be calculated by quantum mechanical methods [16] of these factors are the electronic density and the total energy of the molecule. The energies of HOMO and LUMO molecular orbitals, heat of formation, charges of atoms, angle values, bond lengths, and many more effects that will be mentioned. Although there are many practical methods used to estimate (LogK) values, they are not able to display these effects. Quantum mechanics methods consist of quasi-experimental methods of extended structure theory as the AM1 method). Methods of basic calculations, it consists of several methods, including the DFT method ((All of these calculations are present within the program[17] .The term computational chemistry is used when the mathematical method is adequately developed and applied using the computer[18] . Through statistical equations and in terms of values and correlation coefficient, we can get a relationship between some chemical and structural variables such as energy of orbitals (HOMO, LUMO). In addition to studying the effects of hydrogen bonds and various steric structural effects[19] .

3-Calculation Methods

3-1-Austin Model 1(AM1):

It is considered one of the semi-experimental methods of Michael Dewar, the author of the method in 1985 AD. The AM1 method is an updated version of the (MNDO) method, which is a rapid method for determining the energy and composition of organic compounds[20] . Its working principle is based on experimental (laboratory) calculations. The most important information through which the energy of molecular orbitals is obtained, heat of formation, electronic density, charges of atoms, ionization potential, bond lengths, and angle values for molecules containing C,H,N,O atoms. This method uses atomic orbitals (P, S) and the central axis repulsion function with additional Gaussian terms[21] .

3-2-Density Functional Theory (DFT):

One of the basic calculation methods. The first to use the density function theory and develop it are the two researchers [22] (Hohenberge-Kohn) in 1964 AD. Its principle of operation is based on theoretical calculations and this theory works on finding the electronic properties of the molecule in the stable state, which we obtain by using the electronic density AM1.

4- Results and discussion

Theoretical calculations of the compounds were carried out according to the inductive and steric

effects after determining the effective centers of ionization, which have the most influence on the value of the logk stability constant of the compounds. It is known that there are types of charges[23] .The Millikan charge was adopted in this study and was calculated for three atoms, which are the most effective sites for calculating the stability constant, namely (C3, C2,N1). This charge is one of the most widely used charges in theoretical research [24] and it represents the difference between the negative electron density in the orbitals, and the amount of positive protons in the nucleus, as the increase in the negative charge increases the electrons in the outer orbit. We find that the electronic charge is concentrated on the N1 atom with high electrical negativity, while it decreases on the carbon atom (C2) due to its proximity to the nitrogen atom. We also note that there is a clear change in the values of the charges according to the compensated groups (R, R1) and their effect in terms of electronic withdrawal or payment. The steric effects of Schiff bases are represented in the geometric shape that these compounds can take, and the distribution of their atoms in the space controlled by various factors. As a hindrance factor, which is intended to increase the energy of the molecule and reduce its stability, and leads to an increase in the push of electrons to the obstructed atoms in the far direction to reduce the repulsion caused by these groups. As for the second effect, it is the spatial interferences with their differences, hydrogen bonds and other interferences, and the sum of these interferences can increase the stability of the molecule. Or reduce it depending on its value. The most important calculated physical and energy variables that affect the steric arrangement of the compounds under study are the length of the bonds (C=N and C-N) and the angle (C-N=C), the heat of formation (H_f), the steric retardation energy (S.E), and the Van der Waals interference energy (VDW). And energies (Bend, Dip, Strech, Torsion,). Also, the energy of HOMO and LUMO molecular orbitals [25] is related to the stability of molecules and their tendency to interact in terms of being an electrophile or a nucleophile. With some other variables that were calculated based on the values of molecular orbitals such as hardness (η), chemical potential (μ) and electrophilic index (W). The low values of (η,μ) indicate that the molecule is more effective as a nucleophile, while the high values of (η,μ) indicate that the molecule behaves as a good electrophile in its behavior.

$\eta = ½(E._{LUMO} - E._{HOMO})$ ...(6)

$\mu = ½(E._{HOMO} + E._{LUMO})$ ...(7)

$w = \frac{\mu 2}{2\eta}$ .....(8)

Table 2: Energy variables calculated theoretically for Schiff base using (MM2) method

COM.NO	$E_{Stretch}$	E_{Bend}	$E_{Torsion}$	$E_{Non\text{-}1,4\ VDW}$	$E_{1,4\ VDW}$	TE
1	0.9146	8.4005	-3.1655	2.4254	17.6974	24.4372
2	0.9063	8.2542	-3.0515	2.5568	17.2266	24.5693
3	0.8015	7.3143	-2.7864	1.3202	15.5114	22.4956
4	0.8915	8.7095	-2.9022	2.1513	15.9544	21.8653
5	0.7861	8.2631	-3.1905	0.9851	13.6407	20.5712
6	1.2282	12.1607	-4.8893	4.4891	18.4782	31.8963
7	1.25	12.4004	-5.0311	4.286	18.9257	32.4672
8	1.2645	12.9217	-4.8783	3.8827	17.1503	30.8463
9	1.2485	12.5805	-5.0981	4.1529	19.0952	32.6101
10	1.2901	12.0257	-5.3053	4.3301	19.0869	31.8203

Table 3: The values of physical and energy variables calculated theoretically for Schiff's base using AM1 method.

COM.NO	Charge(Coulomb)			Bond Length(Å)		Angle	H_f	TE
	N1	C2	C3	C=N	C-N	C2N1C3		
1	-0.13	-0.0118	-0.0244	1.28	1.409	127	72.101	-118
2	-0.126	-0.0179	-0.0286	1.279	1.41	126.2	78.952	-104
3	-0.155	0.011	0.0033	1.281	1.408	126.82	78.399	-86.76
4	-0.131	-0.02	-0.059	1.278	1.471	129.9	34.8	-116
5	-0.157	0.0019	-0.044	1.279	1.405	129.77	30.9	-86
6	-0.177	0.0243	-0.0009	1.281	1.405	129.6	83.137	-93
7	-0.178	0.0296	0.003	1.281	1.404	129.2	76.217	-107
8	-0.168	0.0161	-0.0374	1.281	1.405	129	87.4	-106
9	-0.181	0.0335	0.0163	1.281	1.404	129.3	38.69	-105
10	-0.174	0.0213	-0.0071	1.281	1.404	129.1	115.6	-99
-	HOMO(ev)	LUMO(ev)	Ƞ (ev)	μ (ev)	ω (ev)			
1	-0.345	-0.059	0.143	-0.202	0.143			
2	-0.345	-0.055	0.145	-0.2	0.138			
3	-0.334	-0.015	0.16	-0.175	0.096			
4	-0.332	-0.056	0.138	-0.194	0.136			
5	-0.321	-0.011	0.155	-0.166	0.088			
6	-0.301	-0.009	0.146	-0.154	0.082			
7	-0.306	-0.012	0.147	-0.159	0.086			
8	-0.288	-0.015	-0.007	-0.004	0.214			
9	-0.298	-0.024	-0.012	-0.006	0.106			
10	-0.29	-0.014	-0.007	-0.004	0.136			

Table 4: Energy variables calculated theoretically for Schiff base using (DFT) method

COM. N0	Charge(Coulomb)			Bond Length(Å)		Angle	TE
	N1	C2	C3	C=N	C—N	C2N1C3	
1	-0.568	0.113	0.194	1.28	1.411	129.5	-1213.91
2	-0.562	0.108	0.191	1.28	1.413	129.1	-756.57
3	-0.569	0.104	0.194	1.281	1.41	128.3	-3114.39
4	-0.584	0.104	0.195	1.284	1.41	131.2	-831.34
5	-0.593	0.103	0.197	1.284	1.412	130.9	-628.08
6	-0.59	0.101	0.202	1.285	1.41	128.7	-686.47
7	-0.595	0.103	0.206	1.286	1.406	129.3	-1143.8
8	-0.609	0.101	0.205	1.286	1.409	131.3	-761.42
9	-0.633	0.113	0.216	1.289	1.404	133.7	-3247.53
10	-0.619	0.142	0.207	1.29	1.417	123.1	-725.56
COMP NO.		**HOMO(ev)**	**LUMO(ev)**	**Ƞ (ev)**	**μ (ev)**	**ω (ev)**	
1		-0.228	-0.113	0.058	-0.17	0.251	
2		-0.22	-0.107	0.057	-0.164	0.236	
3		-0.207	-0.057	0.075	-0.132	0.117	
4		-0.21	-0.104	0.053	-0.157	0.234	
5		-0.194	-0.049	0.072	-0.122	0.102	
6		-0.183	-0.033	0.075	-0.108	0.078	
7		-0.191	-0.043	0.074	-0.117	0.092	
8		-0.163	-0.031	0.066	-0.097	0.071	
9		-0.172	-0.04	0.066	-0.106	0.085	
10		-0.172	-0.032	0.07	-0.102	0.074	

Tables (4,3,2) above show the values of physical and energy variables with some properties and characteristics of the compounds that were obtained in the theoretical study. Table No. (2) represents the structural energies values obtained by the molecular mechanics method, in which the compound is in the lowest energy And more stable. Tables (3.4) represent the values of physical and energy variables that were obtained by quantum mechanics methods. The (AM1) method from the quasi-experimental methods (DFT) is one of the basic methods of calculations. Through these values, the theoretical stability constants (logK) values for Schiff bases can be calculated through statistical operations and the values of the correlation coefficient (R^2).

Table 5: values of the correlation coefficient for the one-way statistics of the theoretical variables computed using the AM1 method and the practical value of the stability constant.

Variables	logK	H	L	Ƞ	μ	H_f	M-N1	M-C2	BL-C=N	A- C=N-C	Stretch	Bend	Torsion
logK	1												
H	0.97	1											
L	0.5	0.54	1										
Ƞ	0.57	0.53	0.064	1									
μ	0.75	0.71	0.227	0.943	1								
H_f	0.01	0.00	0.003	0.003	0.004	1							
M-N1	0.79	0.8	0.773	0.257	0.46	0.074	1						
M-C2	0.7	0.68	0.684	0.242	0.426	0.176	0.96	1					
BL- C=N	0.41	0.41	0.444	0.207	0.333	0.337	0.612	0.745	1				
A- C=N-C	0.4	0.43	0.223	0.083	0.143	0.178	0.318	0.176	0	1			
Stretch	0.77	0.76	0.209	0.483	0.552	0.118	0.587	0.579	0.468	0.186	1		
Bend	0.82	0.84	0.274	0.471	0.566	0.045	0.658	0.616	0.411	0.306	0.958	1	
Torsion	0.87	0.85	0.352	0.472	0.593	0.105	0.745	0.716	0.513	0.254	0.953	0.953	1

H=HOMO; L=LUMO; M= Mullikan Charge; H_F=Heat of formation; BL=Bond Length; A=Angle

Table 6: values of the correlation coefficient for the one-way statistics of the theoretical variables computed using the DFT method and the practical value of the stability constant.

Vareable	logK	H	L	BL-C=N	BL-C-N	M-C2	M-N1	M-C3	Stretch	Bend	Torsion	Non- VDW	VDW
logK	1												
H	0.931	1											
L	0.774	0.824	1										
BL- C=N	0.891	0.771	0.56	1									
BL- C-N	0.235	0.299	0.294	0.207	1								
M-C2	0.112	0.036	0.012	0.218	0.012	1							
M-N1	0.823	0.79	0.529	0.912	0.139	0.142	1						
M-C3	0.769	0.681	0.533	0.776	0.091	0.058	0.867	1					
Stretch	0.776	0.613	0.441	0.623	0.056	0.095	0.548	0.679	1				
Bend	0.826	0.714	0.521	0.664	0.087	0.03	0.63	0.752	0.958	1			
Torsion	0.87	0.712	0.599	0.724	0.079	0.11	0.653	0.771	0.953	0.949	1		
Non- VDW	0.594	0.413	0.28	0.469	0.028	0.084	0.377	0.549	0.949	0.863	0.856	1	
VDW	0.285	0.124	0.067	0.249	0.007	0.188	0.19	0.38	0.692	0.531	0.579	0.826	1

H=HOMO; L=LUMO; M= Mullikan Charge; H_F=Heat of formation; BL=Bond Length; A=Angle

Table 7: values of correlation coefficients for binary statistics for theoretical methods

AM1 method				**DFT method**			
log K	R^2	S. E	Constant	log K	R^2	S. E	Constant
HOMO,C3	0.981	0.13	16.68				
HOMO,H_f	0.982	0.129	16.741	Torsion, HOMO	0.981	0.133	8.44
HOMO,1,4 VDW	0.981	0.132	15.96	Length(C=N), HOMO	0.973	0.158	-121.18
HOMO,N1	0.978	0.142	15.715	1,4 VDW, HOMO	0.975	0.15	9.92
HOMO,C2	0.979	0.139	16.166	HOMO,N1	0.943	0.227	5.75
HOMO,Length(C=N)	0.977	0.145	7.635	C2, HOMO	0.956	0.2	10.9
HOMO,Angle(C=N-C)	0.977	0.144	19.168	C3, HOMO	0.952	0.208	5.34
HOMO,Stretch	0.978	0.14	15.824	Stretch, HOMO	0.973	0.158	9.06
HOMO, Torsion	0.980	.1360	14.995	Angle(C=N-C),HOMO	0.949	0.214	17.48
				Bend, HOMO	0.963	0.184	9
				TE , HOMO	0.930	0.250	12.321

Table 8: values of correlation coefficients for triangular statistics for theoretical methods

AM1 method				**DFT method**			
Constant	*199.3*			Constant	-77.43		
C3	*6.933*			HOMO	17.79		
HOMO	*39.26*			Torsion	-0.238		
Length (C=N)	*-141.9*			Length C=N	66.24		
log K	R^2	S. E	Constant	log K	R^2	S. E	Constant
N1, H_f, HOMO	*0.982*	*0.139*	*16.959*	Length C=N , Torsion, HOMO	0.995	0.076	-77.432
N1, C3, HOMO	*0.983*	*0.135*	*18.697*	Length C-N, HOM, Torsion	0.983	0.135	-7.435
C2, C3, HOMO	*0.984*	*0.131*	*18.364*	N2, Torsion, HOMO	0.984	0.132	5.126
Length (C=N), HOMO, C3	*0.989*	*0.11*	*199.33*	C2, HOMO, Torsion	0.988	0.112	8.139
Stretch, C3, HOMO	*0.982*	*0.139*	*16.311*	Dipole, HOMO, Torsion	0.985	0.126	8.176
Torsion, C3, HOMO	*0.982*	*0.139*	*15.964*	Bend, HOMO, Torsion	0.984	0.13	8.869

5-Statistical analysis

It was conducted using the program (SPSS) and represents the amount of correlation strength or the relationship between the values of the variables calculated by the theoretical methods with the values of the stability constants (LogK) calculated by practical methods in terms of the values of the correlation coefficient in order to know the most variables affecting the stability of the compound and through which the values of the theoretical stability constants are calculated . The calculations were carried out in three stages: the simple statistic, the binary statistic, and the multiple (triple) statistic, as shown in the tables (5 to 10) above. It was found that one of the most influential physical variables on stability is the effect of the bond length of the imine group (C = N), which represents the center of activity for the compounds, and the effect of the charge on the carbon atom (C3) had a significant impact on stability. With regard to the energy effects, the most important effect on stability was the higher occupied air orbital (HOMO), and the effect of the torsion energy (Torsion) also had a significant effect on the stability, which is expected to be caused by the fact that the aromatic rings of the compounds are not at the same level.

6-Calculate the values of the stability constants LogK theoretically:

The values of the stability constants were calculated using the theoretical methods and for both methods through an arithmetic equation linking the variables with the highest value of (R^2) with the lowest value of (S.E) for the multiple statistic.

Method (AM1) Variables (Length C=N, HOMO, C3)

The equation LogK=199.327+(HOMO*39.263)+(C3*6.933)+(Length C=N*-141.888)

Table 9: values of the theoretical stability constants by (AM1) method

COM .NO	Constant	199.327		
	C3	6.933		
	HOMO	39.263		
	Length C=N	-141.888		
	HOMO	C3	Length C=N	Log K (The)
1	-0.345	-0.024	1.28	4.015
2	-0.345	-0.029	1.279	4.104
3	-0.334	0.003	1.281	4.462
4	-0.332	-0.059	1.278	4.546
5	-0.321	-0.044	1.279	4.952
6	-0.3	-0.001	1.281	5.799
7	-0.306	0.003	1.281	5.587
8	-0.288	-0.037	1.281	5.998
9	-0.298	0.016	1.281	5.989
10	-0.29	-0.007	1.281	6.145

Method (DFT) Variables (Torsion , HOMO, Length C=N)

The equation LogK= -77.43236+ (17.79446*HOMO)+(-0.2383254*Torsion)+(66.23773*Length C=N)

Table 10: values of the theoretical stability constants by (DFT) method

COM .NO	Constant	-77.43236		
	HOMO	17.79446		
	Torsion	-0.2383254		
	Length (C=N)	66.23773		
	HOMO	Length (C=N)	Torsion	logK (The)
1	-0.2283	1.28	-3.1655	4.044
2	-0.2203	1.28	-3.0515	4.159
3	-0.2069	1.281	-2.7864	4.401
4	-0.21	1.284	-2.9022	4.572
5	-0.1939	1.284	-3.1905	4.927
6	-0.1833	1.285	-4.8893	5.587
7	-0.1906	1.286	-5.0311	5.557
8	-0.1627	1.286	-4.8783	6.017
9	-0.1718	1.289	-5.0981	6.106
10	-0.1718	1.29	-5.3053	6.222

Table 11: The difference between the values of practical and theoretical stability constants

COM.NO	AM1			DFT		
	logK\Calcu.	logK\Theo.	ΔlogK	logK\Calcu.	logK\Theo.	ΔlogK
1	4	4.015	-0.015	4	4.044	-0.044
2	4.13	4.104	0.026	4.13	4.159	-0.029
3	4.5	4.462	0.038	4.5	4.401	0.099
4	4.58	4.546	0.034	4.58	4.572	0.008
5	4.88	4.952	-0.072	4.88	4.927	-0.047
6	5.6	5.799	-0.199	5.6	5.587	0.013
7	5.6	5.587	0.013	5.6	5.557	0.043
8	6	5.998	0.002	6	6.017	-0.017
9	6	5.989	0.011	6	6.106	-0.106
10	6.3	6.145	0.155	6.3	6.222	0.078

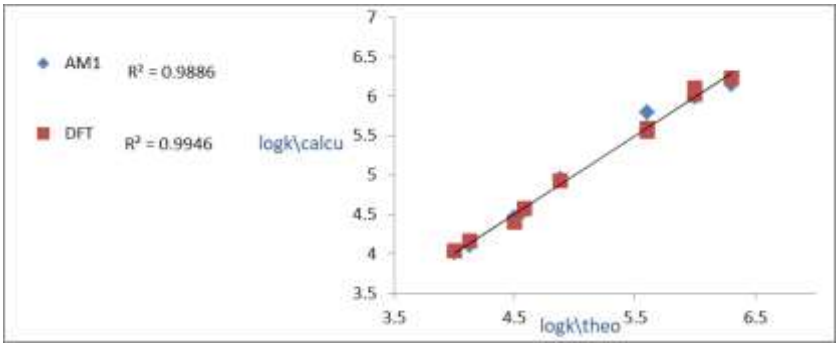

Diagram 1: shows the relationship between the values of practical and theoretical stability constants and the values of the correlation coefficients for both methods graphically

The graph shows the difference between the values of stability constants calculated by practical and theoretical methods with the values of the correlation coefficients for each method. We can notice that both methods gave excellent results with a very small difference for almost all compounds with correlation coefficient (R^2 = 0.9886) for (AM1) method. Also, the value of the coefficient of Correlation (R^2=0.9946) for the (DFT) method. The values of (R^2) indicate that the values obtained using the (DFT) method were better than the (AM1) method, and they are closer to the practical values.

The components of Schiff bases that were studied and the values of their stability constants were found by theoretical methods within the current study and within the literature, it was found that the values of their stability constants increase according to their sequence in the tables from compound No. 1 to compound No. 10. There are several reasons that affected the stability values of the compounds, including the inductive effects, the effect of rosones, and the stereostructural effects.

It is known to us that there are several types of charges [26] .The Millikan charge was adopted in this study. This is because this charge is one of the most widely used charges in theoretical research [27] and represents the difference between the negative electronic density in orbitals, and the amount of positive protons in the nucleus, as With an increase in the negative charge, the electrons in the outer orbit increase. The Millikan charges were calculated for the ionic compounds of three atoms, which are (C3, C2,N1), which can be the most effective sites for calculating the stability constant by computational programming. The electronic charge is concentrated on the N1 atom with high electrical negativity, while it decreases on the carbon atom (C2) due to its proximity to the nitrogen atom, according to the compensated groups (R, R1) and their inductive and resonant effects in terms of electronic drag or electronic push. It was observed that there is a clear increase in the charge on the imine nitrogen (N1) atom of the compound (10) due to the presence of the like group (-CH3) that drives electrons and this is also reinforced by its presence in the para site, where this site is characterized by an inductive and resonant effect, which had the highest share From the stability. Also, the compensated groups in the para-site of benzylidene have an effect on the stability and this is evident in the compounds (6 to 10) containing azomethine group N(CH3)2 in the para-site that share the phenomenon of resonance because they contain unshared electron pairs that contribute to the charge diffusion. The steric effects also have an effect. The extent of its effect can be seen when comparing compound (3) with (5). We note that the two compounds have the same structural formula, and the difference between them is the type of compensator that represents the bromine atom (Br) on compound No. (3) and represents the hydroxide group (OH) of the compound. No. (5) and that both compensators are on the same site (in the bar site of the phenylalanine ring), but there is a clear difference in the values of energies in general and for all methods such as total energy, kinetic energy, potential energy and van der Waals energy. There is also a difference in the values of stability, lengths of bonds and the value of the angle for a group azomethane. One of the

main reasons for these differences is the effect of steric obstruction in addition to the inductive effect represented by the large size of the bromine atom which causes a steric obstruction effect compared to the small size of the (OH) group.

With regard to energy functions and their impact on the stability of compounds, it is the energy of the molecular orbital HOMO and LUMO, which were used in calculating some[28] known variables that have to do with the stability of molecules and their tendency to interact in terms of being electrophiles or nucleophiles. With some other variables that were calculated based on equations (8,7,6), such as hardness (η), chemical potential (μ) and electrophilic index (W). The low values of (η,μ) indicate that the molecule is more effective as a nucleophile, while the high values of (η,μ) indicate that the molecule behaves as a good electrophile in its behavior. The values of (HOMO) energies were high for compounds compensated with driving groups such as compound No. (1) compared to compounds compensated with driving groups such as compound No. (10), meaning that compounds compensated with driving groups behave as nucleophiles. We can also note that compounds (10,9,8) have In general, the methods have the lowest values for the energy differences. Thus, the proximity of the energy distance (excitation or transfer energy) facilitates the transfer of electrons between them from HOMO orbitals to LUMO orbitals, and therefore behaves like a nucleophilic, and what confirms this is the low values of the hardness values (η) and the chemical potential) μ) Also, the compensated groups have an effect, whether they are pulling or pushing electrons, as the driving groups work to reduce (reduce) the energy distance through the process of concentrating the negative charge on the active group in the part, and thus the behavior of the molecule is the behavior of a nucleophile as the compensated group (CH3) in the site Para to compound No. (10) and that the pulling groups increase the efficiency of searching for electrons, because they increase the density of the positive charge on the active group. There are also many influences on the stability of compounds (values of stability constants), such as the effect of the interfacial or implicit hydrogen bond, which is expected to occur in compounds No. (4) and (5).

Conclusion: There is a large congruence in the values of stability constants calculated by practical and theoretical methods, which indicates the importance of theoretical chemistry.The best methods were (DFT) method for basic calculations, followed by (AM1) method for quasi-experimental calculations. The (DFT) method, despite being completely dependent on software calculations without resorting to experiment, gave the most accurate results.All variables start with the same importance, then some of them are excluded, and some others come to the attention and gradually.Theoretical chemistry can do things that practical chemistry cannot do, such as our vision of compounds, the shape of their atoms, their spatial distribution, the shape of orbitals, and charge density.We can shorten the time, effort and cost when using computational chemistry.

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