Original Research Article

Statistical Study of Ionization for a Number of Oximes and Schiff Bases Theoretically by Using Molecular Modeling Programs

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Abstract

In this study, the study included the calculation of fourteen ionic and aromatic compounds, which included eight oximes and six Schiff bases. The parameters of the ionization of the compounds under study were calculated at absolute temperature (293K) using molecular modeling programs. Methods that included semi-empirical calculations were AUSTEN MOMEL 1 (AM1), Hatree Fock (HF), and Density functional theory (DFT). The polarizable conductor calculation model (CPCM) was used to calculate the physical variables in the solution phase instead of the gas phase using ethanol as a solvent. The ionization constants were calculated using multiple Linear regression (MLR) analysis and using various descriptive variables selected to test their representatively of the observed variation in pK_a values These variables include a Mullikan charge on the atoms of the hydroxyl and azomethine group ($C = N$), the length of the double bond, the angles values, the value of the fixed dipole moment, DIHADRAL, the total energy and the heat of the formation temperature), molecular properties such as HOMO, LUMO, Molecular hardness, electrolyte guide and chemical potential. These values were correlated with pKa values. In this relationship, the values of pK_a were calculated theoretically. The results obtained showed that the HF method and the AM1 method were preferable to the EDP method, although all methods were able to complete this type of calculation And with a good efficiency in describing the effect of substituents on pK_a values, these results were clearly indicated by the high correlation coefficients (R^2) obtained from the regression analysis and the correlation between the practical values of pKa and those calculated theoretically.

Introduction

The method of computational chemistry is of unusual methods compared with the previous methods in its mathematical rather than practical method. In arithmetic it does not require a sample, and in principle it is not restricted in terms of material conditions, but the accuracy of the values obtained depends entirely on the model Used to perform calculations. Since its inception in the early 1970s, with the development of programs for the calculation of molecular orbits and the development of the first methods of molecular mechanics in computational chemistry, many methods have been developed to

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estimate molecular properties computationally. Many of these methods have been evaluated to determine the parameters of acid dissociation and the most accurate results available from computation, which is called *ab initio*, means that these calculations are usually oriented towards a precise mathematical solution; the equations used to describe the system are derived entirely from theoretical principles (da Silva et al., 1999). The software of physics and theoretical chemistry (Perrin et al., 1981) is defined as a science that deals with the application of theoretical and mathematical principles in solving problems. Computational chemistry is one of the branches of physical chemistry (Barlin and Perrin, 1972). The molecular modeling software is one of the most important applications of this science, and finds a number of important characteristics.

The approximation methods used to solve the Schrödinger equation for physically and chemically important systems will usually lead to complex calculations that could not be achieved solved. Quantitative theoretical calculations were disabled because of the complexities involved in solving mathematical problems. The cost was high for large calculations as well as the slow calculation speed, which could last for months to solve a relatively simple molecule and years to solve medium molecules.

Materials and methods

Theoretical calculations

The lowest molecular energy level of the compounds under study was calculated using semi-experimental AM1 methods, DFT B3LYP, bases set 3.21G and basic set calculations 6.311G (d, p) HF. The following values were calculated: lowest molecular energy, bipolar and charge and the length of the dihedral angle, the angle values (1, 2, 7 and 8, 7, 9), the higher molecular occupancy values (HOMO), and the low-molecular-activated (LUMO) orbital. HOMO and LUMO values were used to calculate some of the properties of the molecule such as Hardness (Parr and Pearson, 1983), Electronic Chemical Potential (Brouwer, 2003) and Global Electrophilicity Index (Szabo and Nostlund, 1989) and were found through the following relationships.

$$H = (E_{LUMO} - E_{HOMO}) \ldots (1)$$
$$M = (E_{HOMO} + E_{LUMO}) \ldots (2)$$
$$W = (\mu \wedge 2 / \eta) \ldots (3)$$

These values were computed by GAUSSIAN 09 and Gaussian Program Gauss View (5.0.8). The calculation of the constant ionization of the compounds under study (Table 1).

Table 1. The names and structures and values of the ionization constant of the compounds.
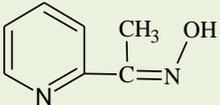
Compound	Number	Exp.pK$_a$	Compd	Number	Exp.pK$_a$
	1	12.666		8	11.688
	2	12.765		9	11.798
	3	6.94		10	12.585
	4	9.578		11	12.758
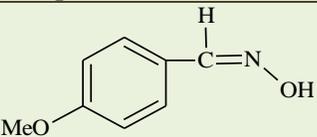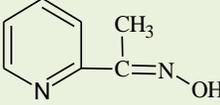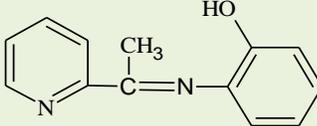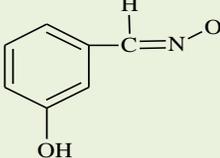
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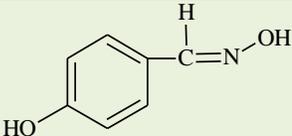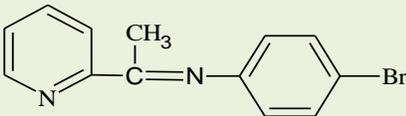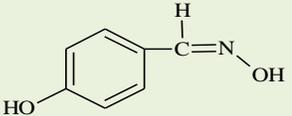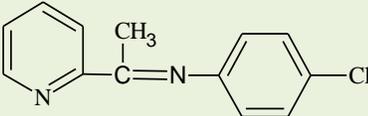
Compound	Number	Exp.pK$_a$	Compd	Number	Exp.pK$_a$
(structure: HO–C$_6$H$_4$–CH=N–OH)	5	6.398	(structure: pyridine–C(CH$_3$)=N–C$_6$H$_4$–Br)	12	2.99
(structure: HO–C$_6$H$_4$–CH=N–OH)	6	8.895	(structure: pyridine–C(CH$_3$)=N–C$_6$H$_4$–Cl)	13	3.714
(structure: MeO–C$_6$H$_4$–CH=N–OH)	7	11.919	(structure: pyridine–C(CH$_3$)=N–C$_6$H$_4$–OMe)	14	5.494

Multiple linear regression method

MLR is an advanced statistical technique that ensures the accuracy of inference to improve search results by optimizing the use of data in the creation of causal relationships between phenomena (subject of research).

Multiple linear regression is a mathematical equation that expresses the relationship between two variables and is used to estimate past values and to predict future values. It is also a regression of the dependent variable (Y) on many independent variables X1, X2, ... XK, We can predict the value of the digital pKa ionization constant based on the values of the Mullikan charge, the length of the signal and other values. Multiple linear regression is not just one method but a set of methods that can be used to determine the relationship between a continuous dependent variable and a number of independent variables that are usually continuous.

The linear equation in multiple linear regression is:

Y = a + b1X1 + b2X2 + ... + e ...... (4)

The proper and correct assessment of the correlation between variables can be inferred by Standard Deviation (SD) (Isaacs, 1969) and Correlation Coefficient (R) values. A large number of ready-made calculator programs are now available and can be used for this function in more difficult tasks such as Multiple Regression Analysis, the independent variable is not sufficient to illustrate experimental results. It is often necessary to use more than one independent variable in the correlation analysis to describe or describe a particular system. In this case, we will speak of a type of regression analysis called regression analysis die.

Number of variables (Multiple Parametric Regression Analysis) The Multivariate Linear Regression Equation of a Y Variable is a series of independent variables. After obtaining the results of the regression equation, we must show whether these transactions are statistically acceptable, which is statistically significant, noting that the morality is for each factor separately.

In order to judge the significance of regression coefficients, we use the T test and the corresponding probability level. SPSS will automatically extract the T test and the corresponding probability level.

Statistics have also been used to determine the overall morale of the model, including (R^2), (R^{-2}), (R).

Results and discussion

The compounds under study were developed in the form of a single group and the calculation of some physical variables for them and the effective sites in them and then finding the relationship between them and the values of ionization constants pKa. Ionization of ionic compounds can be affected by the charge found on the O (O) and Halogen (X) atoms. Thus, the values of pKa are determined by the effect of the compensated groups in the reaction centers represented by the R group that will affect these values through two effects: the first is the induction effect of these groups; and the second: the values of the spatial disability that these groups limit their size, and that these two effects can change the value of electronic charge on the atoms of the center of the interaction. The values of these compounds were measured at (293K) and in the above three methods as follows:

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Table 2. The values obtained theoretically in the (AM1) method.

Compd. AM1	Charge C7	Charge CH3 or H	Charge N9	Charge O10	Charge H11	DM	Angle 127	Angle 2	Dihedral	Bond CN	H formation	ET(et)	EHOMO (et)	ELUMO (et)	η	μ	W
1	0.015	-0.258	-0.072	-0.248	0.249	3.162	111.924	109.295	4.270	1.239	8.263	4.091	-9.695	-0.700	-4.497	5.197	-3.003
2	-0.086	-0.181	-0.009	-0.256	0.255	5.835	121.083	119.414	-155.452	1.341	6.239	2.081	-9.426	-0.670	-4.378	5.048	-2.910
3	-0.082	0.132	-0.057	-0.302	0.271	0.991	119.999	120.000	0.008	1.260	3.951	0.089	-9.199	-0.494	-4.353	4.847	-2.698
4	-0.074	0.189	-0.069	-0.275	0.249	0.903	119.999	119.996	-179.998	1.260	5.174	1.330	-9.153	-0.427	-4.363	4.790	-2.629
5	-0.069	0.128	-0.075	-0.305	0.268	1.282	120.004	120.000	-0.012	1.260	3.914	0.051	-8.971	-0.376	-4.297	4.673	-2.541
6	-0.062	0.186	-0.088	-0.278	0.246	1.479	119.999	119.996	-179.998	1.260	5.134	1.288	-9.001	-0.315	-4.343	4.658	-2.498
7	-0.069	0.128	-0.074	-0.305	0.269	1.543	120.004	120.000	0.003	1.260	5.335	0.635	-8.975	-0.390	-4.292	4.682	-2.554
8	-0.063	0.186	-0.086	-0.278	0.246	1.751	120.004	119.997	180.000	1.201	6.558	1.876	-9.007	-0.328	-4.339	4.668	-2.511
9	0.046	-0.271	-0.135	-0.259	0.247	4.418	118.099	119.998	-0.002	1.260	11.364	4.794	-8.822	-1.013	-3.904	4.918	-3.097
10	0.069	-0.275	-0.153	-0.268	0.248	5.471	118.099	119.998	-0.007	1.260	11.292	4.722	-8.947	-1.072	-3.937	5.009	-3.187
11	0.049	-0.271	-0.142	-0.268	0.247	4.193	118.099	119.997	0.007	1.260	11.295	4.724	-8.701	-1.004	-3.848	4.852	-3.059
12	0.073	-0.276	-0.155	0.044	0.000	5.886	118.099	119.997	-0.003	1.260	13.035	6.860	-9.076	-1.159	-3.958	5.118	-3.309
13	0.069	-0.275	-0.152	-0.028	0.000	5.754	118.099	120.001	-0.003	1.260	13.052	6.860	-9.034	-1.131	-3.951	5.083	-3.269
14	0.050	-0.271	-0.142	-0.203	0.000	4.082	118.099	119.997	0.007	1.260	12.564	6.361	-8.707	-1.008	-3.849	4.858	-3.065

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Table 3. The values obtained theoretically in the (DFT) method.

Compd. DFT	Charge C7	Charge CH3 or H	Charge N9	Charge O10	Charge H11	DM	Angle 127	Angle 2	Dihedral	Bond CN	H formation	ET (et)
1	0.3	-0.58	-0.259	-0.484	0.426	2.0074	118.099	119.998	-0.006	1.25999	-12340.5	-12344.6
2	0.31	-0.599	-0.322	-0.43	0.38	3.2904	119.695	112.435	179.336	1.2969	-12341.8	-12346
3	0.09	0.213	-0.231	-0.472	0.413	2.4595	120	120	0	1.2936	-12879.5	-12883.2
4	0.093	0.241	-0.289	-0.442	0.395	1.1641	123.705	111.504	179.999	1.29167	-12880	-12883.8
5	0.113	0.222	-0.3	-0.45	0.385	2.319	121.48	120.791	0.009	1.28942	-12880	-12883.8
6	0.088	0.236	-0.298	-0.447	0.391	2.096	124.495	111.493	-179.993	1.29272	-12880.1	-12883.9
7	0.113	0.222	-0.3	-0.449	0.385	2.7096	121.589	120.741	-0.004	1.2895	-13943	-13947.6
8	0.087	0.235	-0.298	-0.447	0.391	3.023	117.45	111.467	-179.999	1.29257	-13943.1	-13947.7
9	0.352	-0.629	-0.705	-0.641	0.371	6.3161	116.341	125.623	0.642	1.28361	-18593.8	-18600.3
10	0.319	-0.625	-0.613	-0.619	0.381	5.3549	117.269	125.462	-5.022	1.28307	-18593.5	-18600
11	0.315	-0.625	-0.622	-0.619	0.381	5.6904	117.322	125.765	-0.5641	1.28465	-18593.5	-18600
12	0.232	-0.981	-0.599	0.182	0	8.2861	119.766	120	0	1.2936	-86245.1	-86250.9
13	0.322	-0.625	-0.612	0.055	0	7.3123	117.084	125.264	4.832	1.28301	-29004.7	-29010.9
14	0.341	-0.694	-0.603	-0.547	0	5.1574	119.766	120	0	1.2936	-19652.1	-19659.4

EHOMO (et)	ELUMO (et)	η	μ	W
-6.13671	-1.27812	-2.4293	3.707417	-2.82899
-6.42135	-1.45799	-2.48168	3.939666	-3.12711
-6.22461	-1.13281	-2.5459	3.678709	-2.65778
-6.15386	-1.32601	-2.41392	3.739935	-2.89717
-5.86106	-1.08356	-2.38875	3.472311	-2.52369
-5.97916	-1.07213	-2.45352	3.525645	-2.53313
-5.83249	-1.10342	-2.36453	3.467957	-2.54315
-5.94134	-1.08138	-2.42998	3.511359	-2.53699
-5.7631	-1.9331	-1.915	3.8481	-3.86628
-5.85943	-1.69554	-2.08194	3.777487	-3.42694
-5.54133	-1.64112	-1.9501	3.591225	-3.30672
-5.11738	-1.73418	-1.69275	3.428121	-3.47127
-6.0744	-1.78371	-2.14681	3.93174	-3.60035
-6.40747	-1.73119	-2.33974	4.07211	-3.54358

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Table 4. The values obtained theoretically in the HF method.

Compd HF	Charge C7	Charge CH3 or H	Charge N9	Charge O10	Charge H11	DM	Angle 127	Angle 2	Dihedral	Bond CN	H forma-tion	ET(et)
1	0.103	-0.168	-0.181	-0.406	0.293	3.7103	116.819	121.678	0.001	1.25757	-12337.2	-12341.5
2	0.08	-0.247	-0.149	-0.413	0.335	7.0197	121.083	119.414	-155.452	1.34078	-12335.6	-12339.8
3	0.249	0.113	-0.187	-0.395	0.295	0.6221	121.537	120.347	0	1.25094	-12877.5	-12881.5
4	0.242	0.137	-0.153	-0.461	0.338	1.9503	119.999	119.996	-179.998	1.26003	-12875.2	-12879.2
5	0.255	0.108	-0.203	-0.401	0.292	1.8999	122.524	119.965	-0.005	1.252	-12877.5	-12881.6
6	0.216	0.131	-0.211	-0.411	0.131	1.9519	126.119	112.245	-180	1.25688	-12877.4	-12881.5
7	0.253	0.108	-0.282	-0.401	0.292	2.4112	122.709	11.943	0	1.25201	-13938.6	-13943.5
8	0.214	0.13	-0.211	-0.411	0.299	2.5026	126.203	112.225	179.999	1.25697	-13938.5	-13943.4
9	0.189	-0.241	-0.422	-0.494	0.289	4.8281	117.054	125.966	-1.574	1.25419	-18583.5	-18590.3
10	0.173	-0.247	-0.416	-0.482	0.29	6.0395	117.16	125.983	0.496	1.25405	-18583.6	-18590.4
11	0.169	-0.257	-0.422	-0.489	0.287	4.3311	117.309	126.453	2.181	1.2549	-18583.5	-18590.4
12	0.175	-0.25	-0.417	-0.068	0	7.1535	117.159	125.974	1.161	1.25479	-86528.1	-86534.5
13	0.173	-0.18	-0.465	-0.131	0	4.8226	116.499	126.368	-1.483	1.25666	-29034.4	-29040.8
14	0.107	-0.227	-0.367	-0.468	0	5.2822	118.099	119.997	0.007	1.26	-19641.4	-19649.1

EHOMO(et)	ELUMO(et)	η	μ	W
-9.13732	2.321949	-5.72963	3.407684	-1.01336
-8.69187	1.91541	-5.30364	3.388227	-1.08228
-8.71962	2.34399	-5.53181	3.187816	-0.91852
-8.41621	2.341813	-5.37901	3.0372	-0.85746
-8.43036	2.71216	-5.57126	2.859102	-0.73363
-8.54057	2.709439	-5.625	2.915565	-0.7556
-8.36669	2.673248	-5.51997	2.846721	-0.73405
-8.47662	2.677874	-5.57725	2.899375	-0.75363
-8.3637	2.301812	-5.33275	3.030942	-0.86134
-8.50383	2.406304	-5.45507	3.048765	-0.85196
-8.15254	2.390794	-5.27166	2.880871	-0.78717
-8.66384	2.31569	-5.49352	3.176243	-0.91822
-8.71064	2.17664	-5.44736	3.269234	-0.98102
-7.58545	1.415809	-4.50371	3.086929	-1.05792

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An example of this is compound number one, which is illustrated as follows:
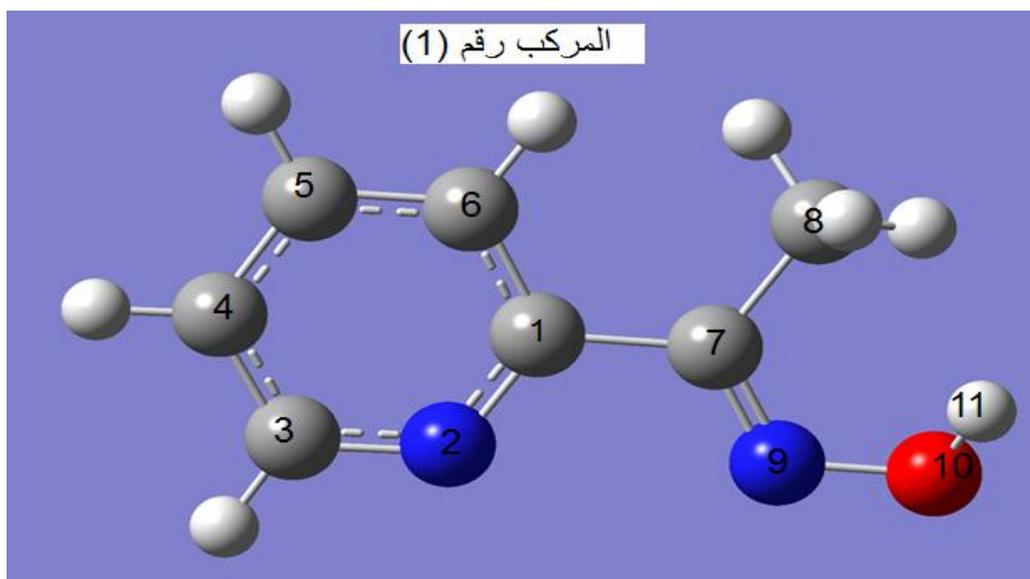
These variables have been included and chosen for accuracy and validity and therefore rely on them in statistical analysis, so that the correct statistical analysis must have the basic conditions is to obtain a correlation coefficient strong and close to one and be a match between practical and theoretical values and that the values are consistent with the chemical principles and principles For each effect, the relationship between each variable was then determined with the constants and then the variables were added sequentially in the input and deletion method to determine the sensitivity of these variables and their applicability to calculate the pKa ionization constant is given below. In considering the above tables, it may be noted that:

Table 5. Correlation coefficient values between variables calculated by AM1 method at (K293)

	charge7C	charge CH3	chargeN9	chargeO10	chargeH11	angle127	angle 2	dihadral	duble CN	DM	EHOMO	ELUMO	hardness	potential	electrophilicity	Hformation	ET ev
charge7C	1	-.864**	-.886**	.624*	-.631*	-.556*	-.088	.289	-.144	.741**	.337	-.933**	.836**	.603*	-.901**	.963**	.943**
charge CH3	-.864**	1	.656*	-.526	.510	.563*	.243	-.128	-.251	-.898**	-.059	.934**	-.683**	-.805**	.951**	-.877**	-.879**
chargeN9	-.886**	.656*	1	-.540*	.588*	.331	-.156	-.059	.070	-.532	-.537*	.813**	-.864**	-.348	.737**	-.813**	-.769**
chargeO10	.624*	-.526	-.540*	1	-.873**	-.215	.051	.093	.029	.642*	.006	-.659*	.462	.594*	-.693**	.688**	.752**
chargeH11	-.631*	.510	.588*	-.873**	1	.169	-.139	-.131	.017	-.549*	-.235	.644*	-.579*	-.415	.628*	-.723**	-.780**
angle127	-.556*	.563*	.331	-.215	.169	1	.863**	-.236	.318	-.254	.375	.401	-.070	-.636*	.487	-.429	-.499
angle 2	-.088	.243	-.156	.051	-.139	.863**	1	-.064	.173	.006	.725**	-.020	.417	-.508	.120	.018	-.088
dihadral	.289	-.128	-.059	.093	-.131	-.236	-.064	1	-.675**	.041	.227	-.157	.235	-.022	-.120	.269	.212
duble CN	-.144	-.251	.070	.029	.017	.318	.173	-.675**	1	.411	-.196	-.160	.003	.288	-.197	-.048	-.034
DM	.741**	-.898**	-.532	.642*	-.549*	-.254	.006	.041	.411	1	.046	-.878**	.637*	.764**	-.900**	.819**	.820**
EHOMO	.337	-.059	-.537*	.006	-.235	.375	.725**	.227	-.196	.046	1	-.267	.742**	-.484	-.076	.363	.234
ELUMO	-.933**	.934**	.813**	-.659*	.644*	.401	-.020	-.157	-.160	-.878**	-.267	1	-.844**	-.714**	.981**	-.950**	-.930**
hardness	.836**	-.683**	-.864**	.462	-.579*	-.070	.417	.235	.003	.637*	.742**	-.844**	1	.227	-.725**	.863**	.777**
potential	.603*	-.805**	-.348	.594*	-.415	-.636*	-.508	-.022	.288	.764**	-.484	-.714**	.227	1	-.835**	.599*	.674**
electrophilicity	-.901**	.951**	.737**	-.693**	.628*	.487	.120	-.120	-.197	-.900**	-.076	.981**	-.725**	-.835**	1	-.913**	-.918**
Hformation	.963**	-.877**	-.813**	.688**	-.723**	-.429	.018	.269	-.048	.819**	.363	-.950**	.863**	.599*	-.913**	1	.984**
ET ev	.943**	-.879**	-.769**	.752**	-.780**	-.499	-.088	.212	-.034	.820**	.234	-.930**	.777**	.674**	-.918**	.984**	1

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Table 6. Results of the statistical analysis of the relationship between the values of pKa and the variables calculated by(AM1) at (293 K)

Model	R	R Square	Adjusted R Square	Std. Error of the estimate	F	Sig.
1	0.997[a]	0.995	0.966	0.6601793	34.156	0.029[a]

Coefficients		B
1	(Constant)	-76.240
	charge6C	-53.005
	charge CH3	114.979
	chargeN9	-51.929
	chargeO10	-22.167
	chargeH11	75.306
	angle 2	-2.846
	dihadral	.069
	duble CN	392.027
	DM	2.237
	EHOMO	13.590
	ET ev	7.777

COMPUTE PKA=-76.240+-53.005 *charge6C+114.979*chargeCH3+51.929*chargeN9 +-22.167*chargeO10 +75.306*chargeH11 +-2.846*angle2 +.069*dihadral +392.027*dubleCN +2.237*DM +13.590* EHOMO +7.777*ETev.

Table 7. Correlation coefficient values between variables calculated by (HF) method at (K293)

HF 293	charge7C	charge CH3	chargeN9	chargeO10	chargeH11	angle127	angle 2	dihadral	duble CN	DM	EHOMO	ELUMO	hardness	potential	electrophilicity	Hformation	ET ev
charge7C	1	.787**	.163	-.015	.238	.493	-.366	.084	-.578*	-.748**	.016	.726**	-.423	-.682**	.804**	.100	.100
charge CH3	.787**	1	.656*	-.145	.314	.812**	-.404	-.058	-.284	-.898**	-.086	.609*	-.414	-.482	.599*	.388	.388
chargeN9	.163	.656*	1	-.310	.548*	.644*	-.139	-.326	.349	-.553*	-.330	.227	-.330	.091	.042	.491	.491
chargeO10	-.015	-.145	-.310	1	-.667**	-.201	.070	.109	-.063	.303	-.380	.004	-.233	.348	-.207	-.788**	-.788**
chargeH11	.238	.314	.548*	-.667**	1	.269	-.173	-.046	.204	-.371	-.242	.416	-.388	-.164	.323	.623*	.623*
angle127	.493	.812**	.644*	-.201	.269	1	-.368	-.036	.074	-.610*	.003	.518	-.306	-.481	.539*	.371	.371
angle 2	-.366	-.404	-.139	.070	-.173	-.368	1	-.058	.095	.289	-.098	-.317	.130	.381	-.384	-.171	-.171
dihadral	.084	-.058	-.326	.109	-.046	-.036	-.058	1	-.431	-.013	.078	.140	-.038	-.199	.194	-.131	-.131
duble CN	-.578*	-.284	.349	-.063	.204	.074	.095	-.431	1	.455	-.144	-.403	.155	.500	-.529	.132	.132
DM	-.748**	-.898**	-.553*	.303	-.371	-.610*	.289	-.013	.455	1	.064	-.553*	.366	.451	-.558*	-.538*	-.538*
EHOMO	.016	-.086	-.330	-.380	-.242	.003	-.098	.078	-.144	.064	1	-.407	.839**	-.542*	.112	.090	.090
ELUMO	.726**	.609*	.227	.004	.416	.518	-.317	.140	-.403	-.553*	-.407	1	-.838**	-.547*	.861**	.101	.101
hardness	-.423	-.414	-.330	-.233	-.388	-.306	.130	-.038	.155	.366	.839**	-.838**	1	.002	-.445	-.002	-.003
potential	-.682**	-.482	.091	.348	-.164	-.481	.381	-.199	.500	.451	-.542*	-.547*	.002	1	-.895**	-.178	-.178
electrophilicity	.804**	.599*	.042	-.207	.323	.539*	-.384	.194	-.529	-.558*	.112	.861**	-.445	-.895**	1	.148	.148
Hformation	.100	.388	.491	-.788**	.623*	.371	-.171	-.131	.132	-.538*	.090	.101	-.002	-.178	.148	1	1.000**
ET ev	.100	.388	.491	-.788**	.623*	.371	-.171	-.131	.132	-.538*	.090	.101	-.003	-.178	.148	1.000**	1

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Table 8. Results of the statistical analysis of the relationship between the values of pKa and the variables calculated by (HF) at (293 K).

Model	R	R Square	Adjusted R Square	Std. Error of the estimate	F	Sig.
1	0.998[a]	0.997	0.979	0.5111011	57.109	0.017[a]

Coefficients		B
1	(Constant)	-50.892
	charge7C	-101.204
	chargeN9	-43.455
	chargeO10	-18.900
	chargeH11	28.943
	angle 2	-.017
	dihedral	-.006
	double CN	21.258
	ELUMO	4.724
	potential	5.626
	H formation	-8.933E-5
	charge CH3	35.518

COMPUTE PKA = -50.892+-101.204*charge7C +43.455*chargeN9 +-18.900*chargeO10 + 28.943*chargeH11 +-.017*angle2 +-.006*dihedral +21.258*double CN +4.724*ELUMO + 5.626*potential +-8.933E-5*H formation +35.518*chargeCH3.

Table 9. Correlation coefficient values between variables calculated by (DFT) method at (K293).

DFT 923	charge7C	charge CH3	chargeN9	chargeO10	chargeH11	angle127	angle 2	dihadral	duble CN	DM	EHOMO	ELUMO	hardness	potential	electrophilicity	Hformation	ET ev
charge7C	1	-.913**	-.758**	-.030	-.395	-.691**	.600*	.279	-.394	.660*	-.002	-.860**	.520	.666**	-.859**	-.172	-.172
charge CH3	-.913**	1	.767**	-.267	.566*	.616*	-.527	-.244	.290	-.796**	-.253	.869**	-.694**	-.459	.856**	.539*	.539*
chargeN9	-.758**	.767**	1	-.129	.572*	.592*	-.689**	-.012	.054	-.902**	-.416	.934**	-.842**	-.373	.921**	.447	.447
chargeO10	-.030	-.267	-.129	1	-.694**	.041	-.015	.023	.137	.480	.366	-.178	.349	-.168	-.164	-.780**	-.780**
chargeH11	-.395	.566*	.572*	-.694**	1	.161	-.255	-.015	-.178	-.721**	-.158	.582*	-.456	-.321	.580*	.674**	.674**
angle127	-.691**	.616*	.592*	.041	.161	1	-.630*	.080	.420	-.604*	-.164	.597*	-.472	-.323	.595*	.109	.109
angle 2	.600*	-.527	-.689**	-.015	-.255	-.630*	1	.025	-.420	.629*	.363	-.606*	.609*	.163	-.589*	-.184	-.184
dihadral	.279	-.244	-.012	.023	-.015	.080	.025	1	.049	-.038	-.267	-.281	-.007	.442	-.283	.009	.009
duble CN	-.394	.290	.054	.137	-.178	.420	-.420	.049	1	.017	-.024	.118	-.087	-.070	.107	-.150	-.150
DM	.660*	-.796**	-.902**	.480	-.721**	-.604*	.629*	-.038	.017	1	.537*	-.855**	.874**	.211	-.839**	-.707**	-.707**
EHOMO	-.002	-.253	-.416	.366	-.158	-.164	.363	-.267	-.024	.537*	1	-.238	.808**	-.659*	-.189	-.703**	-.703**
ELUMO	-.860**	.869**	.934**	-.178	.582*	.597*	-.606*	-.281	.118	-.855**	-.238	1	-.764**	-.573*	.997**	.441	.441
hardness	.520	-.694**	-.842**	.349	-.456	-.472	.609*	-.007	-.087	.874**	.808**	-.764**	1	-.090	-.730**	-.734**	-.734**
potential	.666**	-.459	-.373	-.168	-.321	-.323	.163	.442	-.070	.211	-.659*	-.573*	-.090	1	-.613*	.249	.249
electrophilicity	-.859**	.856**	.921**	-.164	.580*	.595*	-.589*	-.283	.107	-.839**	-.189	.997**	-.730**	-.613*	1	.414	.414
Hformation	-.172	.539*	.447	-.780**	.674**	.109	-.184	.009	-.150	-.707**	-.703**	.441	-.734**	.249	.414	1	1.000**
ET ev	-.172	.539*	.447	-.780**	.674**	.109	-.184	.009	-.150	-.707**	-.703**	.441	-.734**	.249	.414	1.000**	1

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Table 10. Results of the statistical analysis of the relationship between the values of pKa and the variables calculated by (DFT) at (293 K).

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate	F	Sig.
1	0.988[a]	0.976	0.691	1.9776005	3.424	0.401[a]

Coefficients		B
1	(Constant)	1298.882
	Charge7C	-62.106
	ChargeN9	-21.615
	ChargeO10	-44.068
	ChargeH11	18.937
	Angle127	1.547
	Angle 2	-1.568
	Dihedral	0.075
	DM	15.362
	Potential	-111.888
	Double CN	-1076.885
	H formation	5.607E-5
	EHOMO	-72.439

COMPUTE PKA = 1298.882+-62.106*charge7C +-21.615*chargeN9 +-44.068*chargeO10 +18.937*chargeH11 +1.547*angle127 +-1.568*angle2 +.075*dihedral +15.362*DM + -111.888*potential +-1076.885*double CN +5.607E-5*H formation +-72.439*EHOMO.

Therefore, the values of the static constant values were calculated theoretically and compared with the values of the constant ionization process through the linear equation obtained as follows:

Table 11. The practical values, theoretical values and the amount of difference in each of the methods used.

Com No.	pKa practical	pKa AM1	ΔpKa	pKa DFT	ΔpKa	pKa HF	ΔpKa
1	12.666	12.666	0.000	12.790	-0.124	12.644	0.023
2	12.765	12.765	0.000	12.652	0.113	12.833	-0.068
3	6.940	6.940	0.000	7.690	-0.750	6.756	0.184
4	9.578	9.578	0.000	9.851	-0.273	9.753	-0.175
5	6.398	6.398	0.000	6.405	-0.007	6.612	-0.214
6	8.895	8.895	0.000	9.247	-0.352	8.873	0.022
7	11.919	11.919	0.000	10.879	1.040	11.925	-0.006
8	11.688	11.688	0.000	11.652	0.036	11.599	0.089

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Com No.	pKa practical	pKa AM1	ΔpKa	pKa DFT	ΔpKa	pKa HF	ΔpKa
9	11.798	11.798	0.000	11.185	0.613	11.575	0.223
10	12.585	12.585	0.000	12.424	0.161	13.101	-0.516
11	12.758	12.758	0.000	14.058	-1.300	12.439	0.319
12	2.990	2.990	0.000	3.047	-0.057	2.988	0.002
13	3.714	3.714	0.000	3.926	-0.212	3.733	-0.019
14	5.494	5.494	0.000	5.559	-0.065	5.565	-0.071

In considering the tables, it may be noted that

1. By studying the effect of charges in all studied amines, which represents the sensitivity of the theoretical method adopted, it was found that the AM1 and HF methods give more accurate results and correspond to the previous literature (Najim, 2010) and studies in this field.

2. The success of the study of the temporal order of all imines and the three theoretical methods used when compared with previous empirical studies (Toma Al-Bakzo, 2012).

3. The calculated energy variables were theoretically calculated using the three methods, and at the five thermal degrees of all imines, which represent the stability of molecules through interference and spatial changes (HOMO, LUMO, hardness, chemical electron voltage, and electrolyte guide). In the literature (Chipman, 2002; Ebead et al., 2010) related to the stability of molecules and their tendency in terms of electrophilic or nucleophile, and it was found that the values vary according to the location of the compensators and their size and spatial structure. The small values of the variable (W) The reaction of nucleoclophyl (which has the ability to give electrons), as has been demonstrated in previous studies (Al-Tayar, 2004).

4. The variables in the third paragraph were introduced in the three theoretical methods and linked with each other and with pKa values and their validity and accuracy in the statistical analysis of all the imines under study and at different temperature grades. We obtained a good match between the practical and theoretical values as well as the good correlation values close to one.

5. The values of the coefficients of the variables B (beta) Coefficients of the variables (C7, N9, O10, H11, CH3 or H were varied in sequence and this indicates that the variables have a clear effect in the values of pKa and this corresponds to what was observed in the literature (Hollingeworth et al., 2002). These variables represent the center of the interaction for the ionization constants. This indicates the validity of the selection of the variables used in this study. The standard error (SE) for the relationship between the values of the ionization constants and the variables calculated theoretically in the regression analysis and for all the compounds and the three methods was little and within acceptable ranges of experimental errors, The correlation coefficient values of the variables used For the pKa of the compounds under study in the multiple regression analysis was close to one. This indicates the importance of using these variables in calculating the value of pKa and comparing them with the practical values. Although the nature of these variables is different and different, most of them include the values of the interaction center as well as other values on the correlation coefficient in the regression analysis. The significant value (sig.) was significant (0.05), and the value of (F) was also high, meaning that the choice of values in the calculations was got.

Conflict of interest statement

Authors declare that they have no conflict of interest.

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