Hindawi Publishing Corporation
Journal of Chemistry
Volume 2013, Article ID 640649, 7 pages
http://dx.doi.org/10.1155/2013/640649

Research Article

Theoretical Study of the Molecular Geometries, Electronic and Thermodynamic Properties of Chlorinated Dipyrido-(3,2-a:2′,3′-c)-Phenazine

L. O. Olasunkanmi, J. Ige, and G. O. Ogunlusi

Department of Chemistry, Obafemi Awolowo University, Ile-Ife, Nigeria

Correspondence should be addressed to L. O. Olasunkanmi; loolasunkanmi@oauife.edu.ng

Received 13 December 2011; Revised 30 May 2012; Accepted 13 June 2012

Academic Editor: Antreas Afantitis

Copyright © 2013 L. O. Olasunkanmi et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Theoretical study of the molecular geometries, electronic and thermodynamic properties of dipyrido-(3,2-a:2′,3′-c)-phenazine (dppz) was carried out in the gas phase under standard conditions using PM6 Hamiltonian in semiempirical model. Effects of chlorine substituents on these properties were also investigated. The results showed that all the electronic and thermodynamic properties investigated were affected by the number and relative position of chlorine substituents. Variations in some properties are not significant for some isomeric congeners, having the same number of chlorine substituents, while a number of properties showed general variation with both the number and position of chlorine substituents. Successive addition of one chlorine atom after the other at adjacent position to the last chlorine substituent increases the total energy by 241 eV and decreases the LUMO-HOMO gap by an average value of 0.124 eV. Geometry and energy optimization show that all the molecules considered are planar.

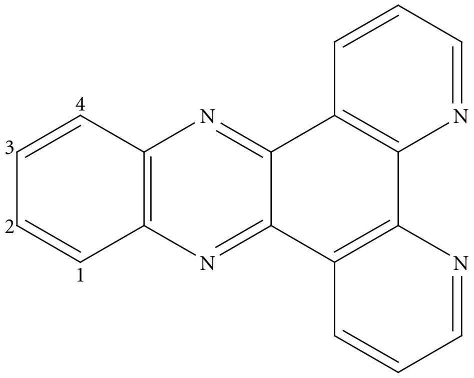
1. Introduction

Previous researches have shown that the number and position of electron-withdrawing groups like chlorine, bromine, and fluorine substituents significantly affect the structural properties and thermodynamic stabilities of heteroaromatic polycondensed rings such as phenazine and Phenoxathiin [1–3].

Dipyrido-(3,2-a:2′,3′-c)-phenazine (dppz) (Figure 1) is a derivative of phenazine with two pyridine rings on the phenazine. While the thermodynamic properties of polychlorinated phenazine (pcpz) by density functional theory calculations have been reported [1], theoretical studies on the geometries, electronic and thermodynamic properties of dppz, especially by semiempirical methods are sparse. Dppz is a polypyridine compound, and polypyridines have been severally reported [4–6] to have excellent ability to bind metal ions in solutions, and various derivatives of the ligands have been studied in order to explore their binding abilities, biological and electrochemical behavior, as well as excited state behaviour. In these reports, their metal complexes are known to bind DNA and their spectroscopic and electrochemical properties can be tuned.

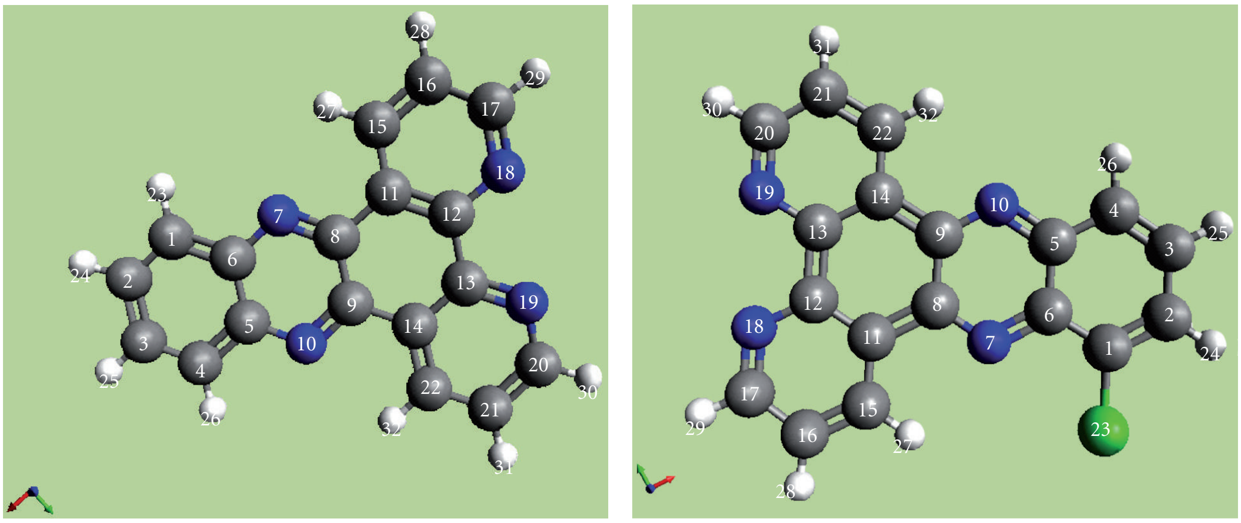
In recent researches, special attention has been given to dipyrido-(3,2-a:2′,3′-c)-phenazine, its derivatives and metal complexes partly because of the interesting characteristics of its ruthenium complexes; $[\mathrm{Ru}\ (\mathrm{bpy})^2(\mathrm{dppz})]^{2+}$ both in water and when bound to DNA [4, 7, 8]. The DNA-binding of dppz complexes of other transition metals, such as platinum, iridium, rhodium, rhenium, and chromium have also been investigated, and the chromium (III) complexes of dppz have also been studied because of their special photophysical properties [4]. Reports focusing on substituted dppzs, especially its Cr^{3+} complexes, exploring its binding interactions with DNA, its photophysical and photochemical properties and the excited state behavior of these complexes are also available in the literature [4, 5].

In view of the continuous use of dppz and its derivatives for various applications, the need for relevant information about them cannot be overemphasized. The present study



Dipyrido- (3, 2-a: 2', 3'-c)-phenazine (dppz)

(a)



(b)

(c)

Figure 1: (a) Structure of dppz showing the investigated positions of chlorine substituents. (b) Optimized structure of dppz visualized in Avogadro. (c) Optimized structure of 1-chlorodppz (1-cldppz) visualized in Avogadro.

on electronic, thermodynamic and other physical properties of dppz and its chloroderivatives will provide relevant information that will aid the study of their generation, degradation, and assessment of possible environmental risk of chlorosubstituted dppz.

The systems considered in this work are relatively large for speedy Hartree-Fock or density functional calculations. Therefore, semiempirical method was used as this will be less computationally expensive without any or serious jeopardy to the qualitative or quantitative results. PM6 Hamiltonian [9] used in this work is relatively recent and fully implemented in MOPAC 2009 [10]. PM6 method was developed based on experimental and *ab initio* data from over 9,000 compounds, while earlier semiempirical methods, MNDO, AM1, and PM3, were developed based on data from only 39, 200, and 500 compounds, respectively. Therefore, PM6 method produces more accurate heats of formation and geometries compared to the earlier semiempirical methods (AM1 and PM3), and serious errors in AM1 and PM3 have been corrected [11]. Chlorosubstituted analogous of dppz, polychloro-dppz (pcdppz) are the focus point of the present work. Future researches promise to consider other halosubstituted dppzs and possible reduction of the LUMO-HOMO energy gap of the ruthenium (II) complexes chlorosubstituted dppzs.

2. Modeling and Computational Methods

All the molecules were modeled with Avogadro 1.0.1 [12]. Molecular mechanics calculations were first performed on each molecule with the builder using Universal Force Field (UFF), which is a completely general force field [13]. The geometry at the point of convergence is fed into MOPAC 2009 as the starting geometry for Broyden-Fletcher-Goldfarb-Shanno (BFGS) geometry optimization. Electronic and energy parameters were obtained from Restricted Hartree-Fock (RHF) calculations with PM6 Hamiltonian. All the calculations were carried out in the gas phase at 298 K and 101.325 kPa.

Table 1: Entropy values used for the calculation of ΔS_f of dppz and pcdppz.

Name or formula	S^0 (J mol^{-1} K^{-1})
Dppz	506.231[a]
Graphite	5.686
Nitrogen	191.5
Hydrogen	130.6
Chlorine	223.0

[a] Data from PM6 semiempirical calculations and others from [14].

In order to determine the standard Gibbs free energy of formation (ΔG_f), (1) was designed for the formation of dppz ($C_{18}H_{10}N_4$) from its elements in their standard states:

$$18C_{(\text{graphite})} + 5H_2 + 2N_2 \longrightarrow C_{18}H_{10}N_4. \quad (1)$$

It then follows that

$$\Delta H_r = \Delta H_{f(C_{18}H_{10}N_4)} - 18\Delta H_{f(\text{graphite})} - 5\Delta H_{f(H_2)} - 2\Delta H_{f(N_2)}. \quad (2)$$

Also,

$$\Delta S_r = S_{(C_{18}H_{10}N_4)} - 18S_{(\text{graphite})} - 5S_{(H_2)} - 2S_{(N_2)} \quad (3)$$

Equation (2) gives $\Delta H_r = \Delta H_{f(C_{18}H_{10}N_4)}$, since every other parameter is equal to zero. The data in Table 1 are used to implement (3). Therefore, the standard free energy (ΔG_f) for the formation of dppz (1) could be expressed as

$$\Delta G_f = \Delta H_f - T\Delta S_r. \quad (4)$$

For the chlorosubstituted analogous, reaction (5) gives a general scheme for the formation of a particular chlorinated dppz from its element in its standard state:

$$18C + \left(5 - \frac{n}{2}\right)H_2 + 2N_2 + \frac{n}{2}Cl_2 \longrightarrow C_{18}H_{(5-n/2)}N_4Cl_{n/2}, \quad (5)$$

where n is the number of chlorine atoms on the polychloro-dppz (pcdppz), that is, $n = 1, 2, 3, 4$. Then the entropy change for the formation of pcdppz in (5) is generally expressed as

$$\Delta S_{f(\text{pcdppz})} = S_{(\text{pcdppz})} - 18S_{(\text{graphite})} - \left(5 - \frac{n}{2}\right)S_{(\text{hydrogen})} - 2S_{(\text{nitrogen})} - \frac{n}{2}S_{(\text{chlorine})} \quad (6)$$

$\Delta G_{f(\text{pcdppz})}$ is calculated by (7):

$$\Delta G_{f(\text{pcdppz})} = \Delta H_{f(\text{pcdppz})} - T\Delta S_{f(\text{pcdppz})}. \quad (7)$$

The data used for the implementation of (6) are contained in Table 1.

3. Results and Discussions

3.1. Geometric Parameters. For dppz and all the chlorine-substituted analogues, the geometric parameters were obtained after geometry optimization. In order to investigate the effect of chlorine substituents on dppz, the geometries of polychlorodipyrido-(3,2-a:2′,3′-c)-phenazines (pcdppz) were compared with that of the unsubstituted dppz. The effects of the positions of chlorine substituents on the geometries were investigated by comparing the geometries of the various pcdppzs. Tables 2(a), 2(b), 2(c), and 2(d) show some of the selected bond lengths, bond angles, dihedral angles, and symmetry point groups, respectively for the optimized structures. From these results, it could be established that some kind of weak (Cl⋯H) interactions occur between a chlorine atom and the hydrogen atom on the adjacent carbon, causing a slight increase in the corresponding Cl–C bond length. For example, the chlorine atom in 2-Cldppz is flanked by two hydrogen atoms, one at each side (one on C1 and one on C3); therefore, Cl24–C2 is slightly longer than Cl23–C1. The same effect is reflected in the bond lengths Cl25–C3 and Cl23–C1 for 1,3-Cldppz, the former being longer. Another kind of weak interaction was found to occur between the lone pair of electrons on the nitrogen atoms in the phenazine ring and the chlorine atoms in positions 1 and 4 for the molecules that possess such chlorine atoms (1-, 1,2-, 1,3-, 1,2,3-, 1,2,4-, and 1,2,3,4-), and also between two adjacent chlorine atoms in molecules like 1,2-, 2,3-, 1,2,3-, 1,2,4-, and 1,2,3,4-polychloro-dppzs. These are reflected in the slight difference observed in the common bond lengths that are supposedly equal if all other conditions were constant. Slight variations in assumed similar bond angles also confirmed the presence of these weak interactions.

The dihedral angles in all the optimized structures were repeatedly 0°, 180°, and 360°. These values together with the symmetry point groups of the optimized structures of the molecules suggest that all the molecules are planar.

3.2. Electronic Properties. Table 3 shows the calculated electronic properties of the molecules. The total energy (TE), which is the sum of electronic energy and core-core repulsion decreases with increasing number of chlorine substituents. In terms of electronic stability, it could be inferred that 1,2,3,4-tetrachlorodipyrido-(3,2-a:2′,3′-c)-phenazine is the most stable of all the species considered. There was no significant difference in the total energies among isomers of the same congener. The energy band gap (LUMO-HOMO) was also found to decrease with increasing number of chlorine substituents. Ionization potentials (IP) and dipole moments of the optimized structures did not follow a regular pattern. The dipole moment was found to depend more on the positions of the chlorine substituents than the number of chlorine atoms. This is expected as dipole moment is a Euclidean vector. Overall, polarity cancelled out for many of the chlorine atoms, more so that the molecules have been established to be essentially planar.

A plot of total energies (Figure 2) for dppz, 1-, 1,2-, 1,2,3- and 1,2,3,4-polychloro-dppzs showed a linear correlation

Table 2: (a), (b) and (c) Selected bond lengths of the optimized structures, (d) Symmetry point groups (Schoenflies notation) of the optimized structures.

(a)

Bond length (Å)	Dppz	1-	2-	1,2-	1,3-	1,4-	2,3-	1,2,3-	1,2,4-	1,2,3,4-
C2–C1	1.3685	1.3709	1.3688	1.3756	1.3711	1.3725	1.3690	1.3762	1.3772	1.3767
C3–C2	1.4322	1.4292	1.4304	1.4292	1.4275	1.4257	1.4344	1.4328	1.4259	1.4308
C5–C4	1.4356	1.4341	1.4372	—	1.4323	1.4360	1.4348	1.4333	1.4377	1.4369
C6–C5	1.4333	1.4339	1.4334	1.4334	—	1.4341	1.4334	—	1.4338	1.4333
H23–C1	1.0914	—	1.0927	—	—	—	1.0941	—	—	—
H24–C2	1.0908	1.0917	—	—	1.0935	1.0928	—	—	—	—
N7–C6	1.3803	1.3781	1.3811	—	—	1.3789	1.3805	—	1.3794	1.3786
H27–C15	1.0953	1.0962	1.0955	1.0962	1.0960	1.0962	1.0954	1.0961	1.0963	1.0962
Cl23–C1	—	1.7128	—	1.7017	1.7094	1.7104	—	1.7004	1.7002	1.6993
Cl24–C2	—	—	1.7221	1.7119	—	—	1.7109	1.7023	1.7103	1.7023
Cl25–C3	—	—	—	—	1.7198	—	1.7108	1.7106	—	1.7023
Cl26–C4	—	—	—	—	—	1.7104	—	—	1.7079	1.6993

(b)

Bond Angles/°	Dppz	1-	2-	1,2-	1,3-	1,4-	2,3-	1,2,3-	1,2,4-	1,2,3,4-
C8–N7–C6	118.23	118.17	118.24	118.20	118.21	118.32	118.25	118.23	118.36	118.36
H23–C1–C2	122.34	—	122.81	—	—	—	122.34	—	—	—
H24–C2–C1	120.70	120.99	—	—	121.50	120.93	—	—	—	—
H27–C15–C11	119.47	119.49	119.50	119.51	119.52	119.51	119.53	119.53	119.53	119.54
C5–C4–C3	119.46	119.62	119.74	119.81	118.48	120.88	118.88	118.98	120.91	119.85
C4–C3–C2	121.09	121.27	119.76	120.31	122.94	120.40	121.34	121.75	119.63	120.81
C3–C2–C1	121.08	120.11	122.93	121.72	119.05	120.39	121.34	120.35	121.82	120.81
C6–C5–C4	119.46	119.84	119.66	119.95	120.03	118.73	119.78	120.08	118.89	119.33
Cl23–C1–C2	—	120.32	—	121.20	120.21	120.30	—	120.82	121.11	120.80
Cl24–C2–C1	—	—		120.30	—	—	120.41	120.90	120.27	120.76
Cl25–C3–C2	—	—	—	—	117.33	—	118.26	117.93	—	118.43
Cl26–C4–C3	—	—	—	—	—	120.30	—	—	120.23	120.80

(c)

Dihedral Angles/°	Dppz	1-	2-
C4–C3–C2–C1	360.00	0.00	360.00
C6–C5–C4–C3	0.00	360.00	0.00
N7–C6–C5–C4	179.99	180.01	179.99
N10–C9–C8–N7	359.99	0.00	359.99
H23–C1–C2–C3	180.00	—	180.00
Cl23–C1–C2–C3	—	180.00	—

(d)

Molecule	Dppz	1-	2-	1,2-	1,3-	1,4-	2,3-	1,2,3-	1,2,4-	1,2,3,4-
Symmetry point group	C_{2v}	C_s	C_s	C_s	C_s	C_{2v}	C_{2v}	C_s	C_s	C_{2v}

with the number of chlorine atoms in consecutive adjacent positions. This implies that the total energy decreases (i.e., electronic stability increases) by a constant value of about 241 eV for every one chlorine atom substituted at the adjacent position to the last chlorine substituent. Similar correlation was found for the energy gaps of the chlorosubstituted dppzs (Figure 3) in which successive chlorine substituent is added at the position adjacent to the last chlorine substituent. For these sets of species, LUMO-HOMO gap decreases by an average value of 0.124 eV each time a chlorine atom is put on the ring at a position adjacent to the last substituted chlorine atom.

3.3. *Energy and Thermodynamic Properties of the Molecules.*

Table 4 shows the calculated values of the thermodynamic data (H°, S°, G°, C_p, ΔH_f, ΔS_f, ΔG_f, and ΔG_R), where ΔG_R is the relative standard Gibbs free energy of formation

Table 3: Electronic properties of the optimized structures.

Molecule	TE (eV)	HOMO (eV)	LUMO (eV)	Energy gap (eV)	IP	Dipole moment
Dppz	−3055.53	−9.42	−1.654	7.766	9.42	3.45
MCldppz						
1-Cl	−3296.48	−9.433	−1.804	7.629	9.43	3.04
2-Cl	−3296.58	−9.464	−1.846	7.618	9.46	1.78
DCldppz						
1,2-	−3537.38	−9.447	−1.952	7.495	9.45	2.08
1,3-	−3537.51	−9.509	−1.982	7.527	9.51	1.16
1,4-	−3537.41	−9.378	−1.946	7.432	9.38	2.21
2,3-	−3537.46	−9.533	−1.987	7.546	9.53	0.43
Tri-Cldppz						
1,2,3-	−3778.25	−9.579	−2.089	7.49	9.58	0.78
1,2,4-	−3778.29	−9.412	−2.085	7.327	9.41	1.01
Tetra-Cldppz						
1,2,3,4-	−4019.03	−9.461	−2.188	7.273	9.46	0.06

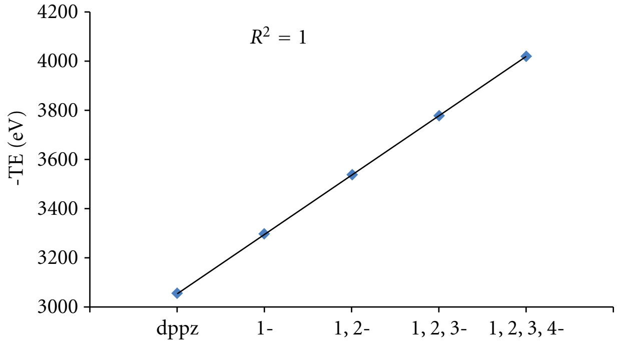


Figure 2: The plot of total energies (−TE) (eV) for dppz, and 1-, 1,2-, 1,2,3-, and 1,2,3,4-chlorosubstituted dppzs.

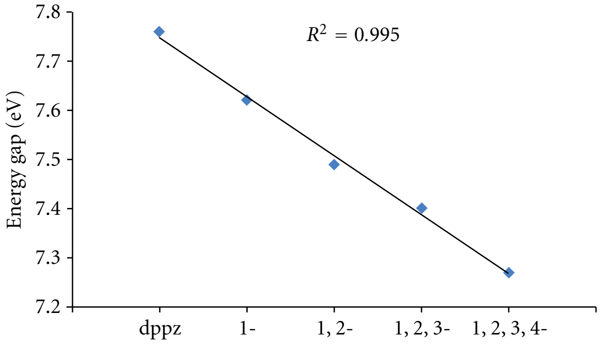


Figure 3: The plot of energy gap (LUMO-HOMO) (eV) for dppz, and 1-, 1,2-, 1,2,3-, and 1,2,3,4-chlorosubstituted dppzs.

computed as the difference between ΔG_f of the reference molecule and ΔG_f of the most thermodynamically stable isomer in that congener. The results obtained from this study revealed that all the chlorosubstituted dppzs are thermodynamically more stable than unsubstituted dppz, with the tetrasubstituted molecule being the most stable of all the species considered. This is reflected in the calculated values of the heats of formation (ΔH_f) and the standard Gibbs free energies (ΔG_f). For the monosubstituted congeners, 2-chlorodppz was found to be more stable than 1-chlorodppz. This could be attributed to the closeness of the chlorine atom in position 1 to the nitrogen atom in the phenazine ring. A kind of interaction has already been established between these atoms from the geometry properties results. For the disubstituted congeners, 1,3-dichlorodppz was found to be the most stable. Ordinarily, one would have expected 1,4-dichlorodppz to be the most stable as the chlorine atoms are much more far apart in this isomer than other dichloro isomers, thus reducing any form of Cl⋯Cl steric repulsion. However, relative instability of 1,4-isomer could still be as a result of the repulsive interaction between the neighboring electronegative chlorine and the lone pair of electron on the nitrogen atoms. 1,2-isomer suffers from both Cl⋯Cl repulsion and Cl⋯N repulsion, while 2,3-isomer suffers from only Cl⋯Cl repulsion, thereby more stable than the former. 1,3-isomer does not suffer from any of the interactions, thereby making it the most stable isomer. 1,2,4-isomer was found to be the most stable isomer for the trisubstituted isomers. ΔG_R values show the relative stability among congeners at a glance. ΔG_R was zeroed for the most stable isomer in a family. There is a linear correlation between the ΔH_f values for the molecules with successive substitution of chlorine atom adjacent to the last added chlorine (Figure 4), and also between their ΔG_f values (Figure 5).

4. Conclusion

Semiempirical quantum chemical calculations of the molecular geometry, electronic and thermodynamic properties of dppz and its chlorosubstituted derivatives have been carried out by PM6 Hamiltonian in MOPAC 2009. Calculations reveal that all the molecules are essentially planar. Presence of some weak interactions between chlorine atoms and hydrogen atoms on the adjacent carbon, and also between the lone pair of electrons on the ring nitrogen atoms and neighboring chlorine atoms was established in some molecules.

TABLE 4: Thermodynamic parameters by PM6 calculations.

Molecule	ΔH_f (kJ/mol)	H^0 (kJ/mol)	S^0 (J/mol·K)	C_p (J/mol·K)	G^0(kJ/mol)	ΔS_f(J/mol·K)	ΔG_f(kJ/mol)	ΔG_R(kJ/mol)
Dppz	575.03	41.69	506.23	267.17	−109.17	−632.12	763.40	—
MCldppz								
1-Cl	546.74	44.92	540.83	282.23	−116.24	−643.72	738.57	9.65
2-Cl	537.15	44.90	541.04	282.27	−116.33	−643.51	728.92	0.00
DCldppz								
1,2-	523.93	48.34	570.81	297.48	−121.77	−659.94	720.59	12.65
1,3-	511.15	48.25	570.40	297.42	−121.72	−660.35	707.94	0.00
1,4-	520.55	48.29	565.05	297.41	−120.10	−665.70	718.93	11.00
2,3-	515.67	48.32	565.30	297.56	−120.14	−665.45	713.97	6.04
Tri-Cldppz								
1,2,3-	503.09	51.75	600.10	312.80	−127.08	−676.85	704.79	3.64
1,2,4-	499.39	51.71	599.89	312.64	−127.05	−677.06	701.15	0.00
Tetra-Cldppz								
1,2,3,4-	491.71	55.27	624.15	328.13	−130.73	−699.00	700.01	—

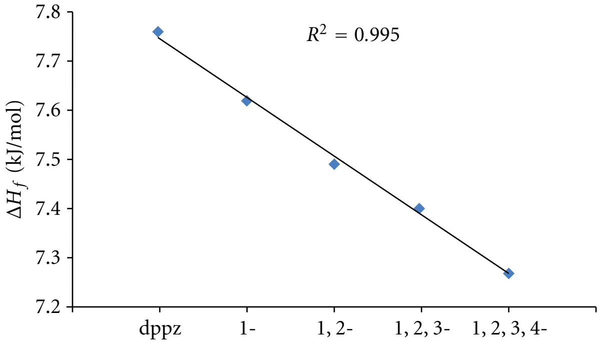


FIGURE 4: The plot of ΔH_f for dppz, and 1-, 1,2-, 1,2,3-, and 1,2,3,4-chlorosubstituted dppzs.

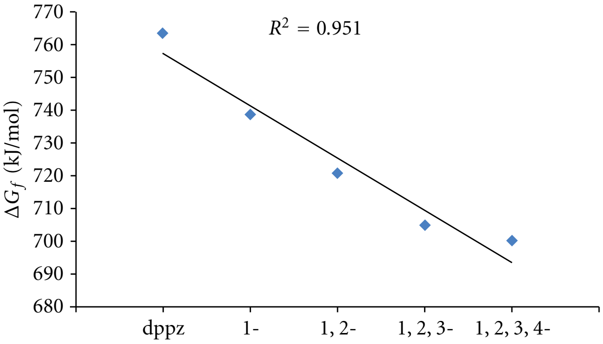


FIGURE 5: The plot of ΔG_f for dppz, and 1-, 1,2-, 1,2,3-, and 1,2,3,4-chlorosubstituted dppzs.

LUMO-HOMO energy gap decreases with increasing number of chlorine substituents. Ionization potential and dipole moment do not follow a simple pattern as they both depend on the positions of chlorine atoms more than the number of chlorine atoms on the ring. Total electronic energy increases in a regular pattern with a constant value of 241 eV, while LUMO-HOMO energy gap decreases with an average value of 0.124 eV, for every single addition of chlorine atom at adjacent position to the last chlorine substituent. Thermodynamic stability increases generally, with increasing number of chlorine atoms, but varies with the position of chlorine atoms among isomeric structures. All the chlorosubstituted dppzs are thermodynamically more stable than unsubstituted dppz, with tetrachloro-dppz being the most stable of all the nine molecules. To the best of our knowledge, there has not been any experimental or theoretical work on the properties of the systems reported in this work. Our results may, therefore, provide a reference for further work in this regard. We hope to employ other theories in predicting these properties for comparison purpose and to consider the effects of other halogens in future researches.

References

[1] H. Yu, H. Liu, Z. Wang, and L. Wang, "DFT calculation on 76 polychlorophenazines: their thermodynamic function and implication of Cl substituted position," *International Journal of Chemical Engineering*, vol. 2008, Article ID 938645, 6 pages, 2008.

[2] C. Wang, Z. Fang, H. Liu, and S. Xu, "Thermodynamic properties and relative stability of polybrominated phenoxathiins by density funtional theory," *International Journal of Physical Science*, vol. 3, no. 10, pp. 250–256, 2008.

[3] I. A. Gad El-karim, "Quantum mechanical study of substituted phenoxathiin: a study of the structure of fluorinated phenoxathiins," *Journal of Molecular Structure*, vol. 945, no. 1–3, pp. 17–22, 2010.

[4] S. Vasudevan, J. A. Smith, M. Wojdyla et al., "Substituted dipyridophenazine complexes of Cr(III): synthesis, enantiomeric resolution and binding interactions with calf thymus DNA," *Dalton Transactions*, vol. 39, no. 16, pp. 3990–3998, 2010.

[5] M. Wojdyla, J. A. Smith, S. Vasudevan, S. J. Quinn, and J. M. Kelly, "Excited state behaviour of substituted dipyridophenazine Cr(III) complexes in the presence of nucleic acids," *Photochemical & Photobiological Sciences*, vol. 9, no. 9, pp. 1196–1202, 2010.

[6] N. Raman, R. Jeyamurugan, B. Rajkapoor, and L. Mitu, "Novel, biologically imperative, highly versatile and planar systems: synthesis, characterization, electrochemical behavior, DNA binding and cleavage properties of substituted β-diketimine copper(II) and zinc(II) complexes with dipyrido(3,2-a:2$'$,3$'$-c)phenazine ligand," *Journal of the Iranian Chemical Society*, vol. 7, no. 4, pp. 917–933, 2010.

[7] I. Ortmans, B. Elias, J. M. Kelly, C. Moucheron, and A. K. Mesmaeker, "$[\mathrm{Ru(TAP)_2(dppz)}]^{2+}$: a DNA intercalating complex, which luminesces strongly in water and undergoes photo-induced proton-coupled electron transfer with guanosine-5$'$-monophosphate," *Dalton Transactions*, pp. 668–676, 2004.

[8] B. Elias, C. Creely, G. W. Doorley et al., "Photooxidation of guanine by a ruthenium dipyridophenazine complex intercalated in a double-stranded polynucleotide monitored directly by picosecond visible and infrared transient absorption spectroscopy," *Chemistry*, vol. 14, no. 1, pp. 369–375, 2008.

[9] J. J. P. Stewart, "Optimization of parameters for semiempirical methods V: modification of NDDO approximations and application to 70 elements," *Journal of Molecular Modeling*, vol. 13, no. 12, pp. 1173–1213, 2007.

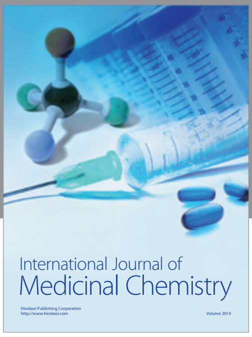
[10] J. J. P. Stewart, Stewart Computational Chemistry, MOPAC2009, Version 10.341W, http://OpenMOPAC.net.

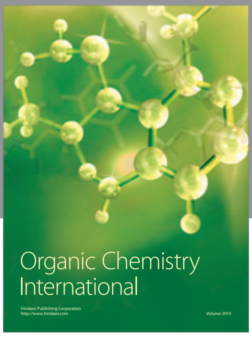
[11] J. J. P. Stewart, "MOPAC2009 Brochure: The Next Generation Quantum Chemistry Tool for Property Prediction," Stewart Computational Chemistry, MOPAC2009-DS-DG1, 1, 2008.

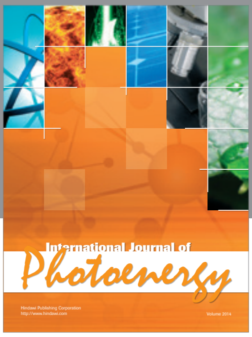
[12] Avogadro: an open-source molecular builder and visualization tool, Version 1.0.1, http://avogadro.openmolecules.net/.

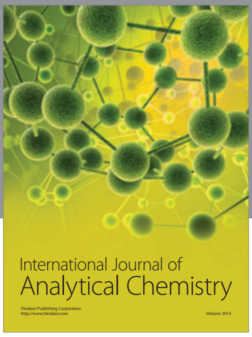
[13] C. J. Cramer, *Essentials of Computational Chemistry Theories and Models*, John Wiley & Sons, New York, NY, USA, 2nd edition, 2004.

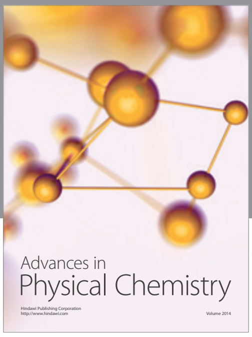
[14] D. D. Ebbing and M. S. Wrighton, *General Chemistry*, Houghton-Mifflin Company, Boston, Mass, USA, 1987.

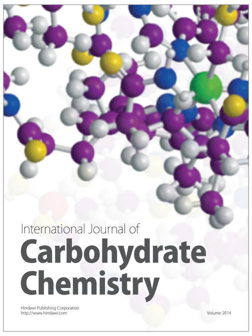

International Journal of
Medicinal Chemistry


Organic Chemistry
International


International Journal of
Photoenergy


International Journal of
Analytical Chemistry

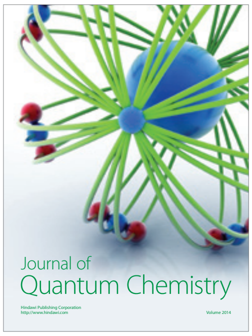

Advances in
Physical Chemistry

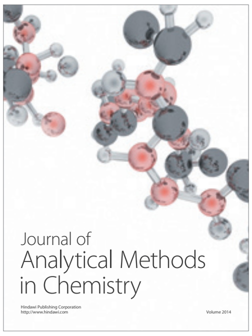

International Journal of
Carbohydrate
Chemistry

The Scientific
World Journal

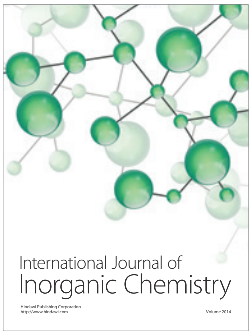
Hindawi

Submit your manuscripts at
http://www.hindawi.com

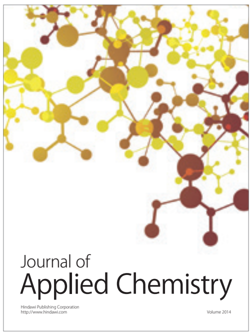

Journal of
Quantum Chemistry

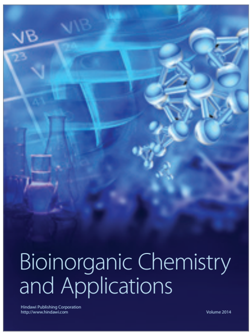

Journal of
Analytical Methods
in Chemistry

Journal of
Spectroscopy

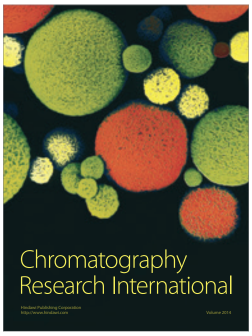

International Journal of
Inorganic Chemistry

International Journal of
Electrochemistry


Journal of
Applied Chemistry


Bioinorganic Chemistry
and Applications

Journal of
Theoretical Chemistry


Chromatography
Research International

Journal of
Catalysts

Journal of
Chemistry

International Journal of
Spectroscopy