

Original Research Article

Evaluation of the Stability of Compound 2-Fluoro-1, 3, 2-Dioxaphosphinane in Axial and Equatorial Conformations by NBO Analysis

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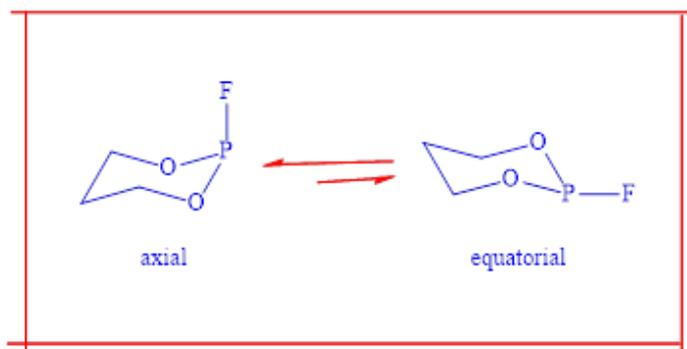
Parameter Structure

F_{ij}

ABSTRACT

Cyclohexane and hetero cyclohexane are good models for studying stereo electronics. The derivatives of 1, 3-dioxane are the good examples of ground and transition states of hyper-conjugated reactions. The structural and thermodynamic parameters for 1, 3-dioxane derivatives are investigated by MP_2 and B_3LYP methods for axial and equatorial conformations. By NBO analysis, the stabilization energy electron delocalization associated with $LP_2O \rightarrow \sigma^*P-F$ is reported in the axial conformation 13.16 and equatorial conformations 1.93, 3.45 kcal/mol for the MP_2 and B_3LYP methods, respectively. The stabilization of energy electrons delocalization in the axial conformation is higher than that of the equatorial one, indicating that the electrons delocalization transfer occurs more in the axial conformation. The studies on vibrational frequency and bond lengths P-O and P-F have also confirmed this issue. By calculating HOMO and LUMO energy, the hardness and softness, electronegativity, electron affinity energy, ionization energy, and electrophilicity index are examined.

GRAPHICAL ABSTRACT



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Introduction

The computational chemistry is a branch of chemistry which uses mathematical methods and physical concepts to justify and interpret the chemical phenomena. The main goal in this field is to obtain the optimal structures, properties of physical chemistry, and the reactivity of chemical compounds using theoretical methods. Computations are based on ab initio methods and techniques based on the experimental information. Calculations in this scientific field can be done with the computer assistance. This field of extension is used in all branches of chemistry, biochemistry, and pharmacy [1-2]. The hyper-conjugation interaction of two-electron two-orbitals is vitally important for understanding the properties and molecular reactivity. It is explicitly used in molecular mechanisms and describes covalent bonding. This reaction may be due to the equilibrium conformation of the anomeric effect, the torsional barrier of ethane, and the other molecules, as well as reactivity and selectivity [3-6]. The hyper-conjugation effect has been proposed for the intermolecular reaction of components for the base and transition states. Stereo electronics reactions involving conjugated π bonds are among the most important chemical phenomena. Reactions with hyper-conjugated δ orbitals have rarely been studied. However, Robert Maliken later pointed to the importance of the hyper conjugate stereo-electronic effect in chemistry [7]. The extracted cyclohexane and hetero cyclohexanes are two excellent models for stereo electronic studies. Recently, theoretical and experimental results obtained from 1 and 3 heterogeneous cyclohexane have indicated that fixed coupling axial protons are larger than fixed coupling equatorial protons, known as the inverse effect of Perlin [8-9]. In 2003, the structural parameters and energy of hemo-anomeric reactions $n(X) \rightarrow B-\sigma^*(C-Y)$ in 6-membered saturated hetero-cycle compounds X: O, N, S, Se and Y: H, Cl were studied by B₃LYP

computational method and NBO analysis [10-11]. Juaristi et al. showed ab initio calculations on Hexa pyridines to have weaker axial bond lengths [12]. Surveys conducted in 2010 by MO using the block-localized-wave function method proved that the electrostatic effect associated with dipole-dipole reactions results from the anomeric effect [13]. The studies illustrated that due to the presence of electron withdrawing groups such as halogens, NO₂, and CN on adjacent heteroatom, especially in the monosaccharide chair conformation, an anomeric phenomenon occurs which makes the axial conformation is more stable [14].

In this work, the transfer of electrons delocalization from electron donor orbitals LP (O), LP (F), and LP (P) to the electron acceptor orbitals σ^* P-F, σ^* P-O, and σ^* C-O is investigated. The effect of anomeric applied on the O-P, P-F, and C-O bond lengths is studied. The thermodynamic parameters such as Gibbs free energy (G), enthalpy (H), corrected electronic energy (E₀), and zero-point energy (ZPE) are investigated by the computational method MP₂ with basis set 3-21G and B₃LYP with basis set Aug-cc-pv-dz for compound 2-fluoro-1, 3, 2-dioxaphosphinane with both axial and equatorial conformations. The global hardness and softness, ionization energy, electron affinity energy, and electrophilicity index are evaluated. The stability energy (E₂) is dependent on the electrons delocalization LP O \rightarrow σ^* , LP F \rightarrow σ^* , and LP P \rightarrow σ^* , and the overlap of electron donor and electron acceptor orbitals (Fij) is calculated.

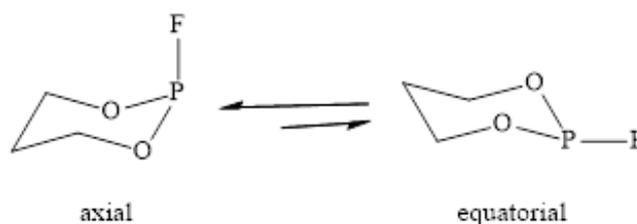


Figure1. Exchange of axial and equatorial conformations in compound 2-fluoro-1, 3, 2-dioxaphosphinane

Calculation method

The molecular mechanics calculations are used to optimize the structure of compound 2-fluoro-1,3,2-dioxaphosphinane with axial and equatorial conformations. Calculations are performed using Gaussian (09) software [15] and different computational levels of the second-order Moller-plesset perturbation theory (MP₂) with base set 3-21G [16] and Becke-3-Lee-Yang-Parr density functional theory (B₃LYP) with base set Aug-cc-pv-dz [17]. By natural bond orbital (NBO) analysis, all bonding orbital and stability energy dependent on the electrons delocalization LP O→σ*P-F, LP P→σ*C-O, and LP F→σ*P-O are calculated.

Thermodynamic parameter

Table 1 indicates the corrected electronic energy (sum of electronic and zero-point energy) and enthalpy (sum of electronic and thermal enthalpies), Gibbs free energy (sum of electronic and thermal free energy), and zero-point energy for the compound 2-fluoro-1,3,2-dioxaphosphinane with axial and equatorial conformations using the MP₂/3-21G and B₃LYP/Aug-cc-pv-dz computational methods. Thermodynamic studies have shown that axial conformation is more stable than the equatorial one.

Table 1. E₀, H, G, and ZPE parameters (Hartree) in 298 k and 1 atm for axial and equatorial conformations of compound 2-fluoro-1,3,2-dioxaphosphinane

	E ₀		H		G		ZPE	
	ax	eq	ax	eq	Ax	eq	ax	eq
MP ₂ /3-21G	-	-	-	-	-703.916	-	0.1004	0.0993
B ₃ LYP/Aug-cc-pv-dz	703.885	703.866	703.878	703.858	-709.632	703.898	0.0970	0.0965

Parameter structure

The bond lengths r O-P, r P-F, and r C-O of the compound 2-fluoro-1,3,2-dioxaphosphinane with axial and equatorial conformations by the computational method MP₂/3-21G and B₃LYP/Aug-cc-pv-dz are given in Table 2. Calculations show that bond lengths P-F and C-O

in the axial conformation are longer than in the equatorial one. The bond length of the O-P in the axial conformation is shorter than in the equatorial one. The results obtained from the calculations indicate that transfer of electrons delocalization LP O→σ*P-F and LP P→σ*C-O takes place in a more axial position.

Table 2. The computed structural parameters bond lengths (Å) compound 2-fluoro-1,3,2-dioxaphosphinane with axial and equatorial conformations

	r O-P		r P-F		r C-O	
	ax	eq	ax	eq	ax	eq
MP ₂ /3-21G	1.6958	1.7140	1.6777	1.6462	1.4959	1.4846
B ₃ LYP/Aug-cc-pv-dz	1.6615	1.6803	1.6788	1.6393	1.4497	1.4455

Vibrational frequencies

Vibration frequency calculations with MP₂ and B₃LYP methods for compound 2-fluoro-1,3,2-dioxaphosphinane are investigated with Gaussview 6.0 software [18]. Although resonance and hybridization factors alter the experimental

and calculated frequency values, these studies provide fruitful information. In Table 3, the infrared spectroscopy calculations related to the stretching vibrations frequency of P-O (ν₁), P-F (ν₂), and C-O (ν₃) with MP₂/3-21G and B₃LYP/Aug-cc-pv-dz methods for 2-fluoro-1,3,2-

dioxaphosphinane compound are depicted. Based on Equation 1 and recent studies, the frequency increases by enhancing bond strength and constant force, so the transfer of electrons delocalization occurs more often [19].

$$\nu = 1/2\pi c\sqrt{k/M} \quad \text{Eq.1}$$

The stretching vibrations of P-F in the MP₂/3-21G and B₃LYP/Aug-cc-pv-dz method for compound 2-fluoro-1, 3, 2-dioxaphosphinane in the axial conformation are less than that of the equatorial conformation, which means axial conformation

has a lower force constant. These results confirm the increase in P-F bond length. The stretching vibrations of P-O in axial conformation are higher than equatorial one, demonstrating greater constant force in axial conformation than in equatorial one. These results confirm reductions in the P-O bond length. From the obtained vibrations frequency, it can be concluded that transfers of electrons delocalization LPO → σ*P-F have occurred more frequently.

Table 3. Calculative stretching vibrations frequency for P-O, P-F, and C-O (cm⁻¹)

	ν ₁		ν ₂		ν ₃	
	ax	eq	ax	eq	ax	eq
MP ₂ /3-21G	728.72	726.57	807.00	897.11	1097.25	1095.19
B ₃ LYP/Aug-cc-pv-dz	722.06	721.65	703.36	806.52	1077.31	1079.44

Anomeric effect and energy stabilization

Transfers of electrons delocalization from single electron pairs (LP O, LP F, and LP P) to anti-bonding orbitals (δ*F-P, δ*C-O, and δ*O-P) are investigated. The stabilization energy is associated with the electrons delocalization and the different energy between the electron donor and acceptor orbitals, and further the overlap of the electron donor and acceptor orbitals are presented in Tables 4 and 5 for compound 2-fluoro-1, 3, 2-dioxaphosphinane with the MP₂/3-21G and B₃LYP/Aug-cc-pv-dz methods, respectively. The relationship between the stabilization energy and overlap of the donor and acceptor orbitals [20] is observed according to Equation 2.

$$E_2 = \Delta E_{ij} = q_i \frac{F^2(i, j)}{\epsilon_j - \epsilon_i} \quad \text{Eq.2}$$

According to Tables 4 and 5, the stabilization energy associated with electrons delocalization and the overlap of the electron donor and acceptor orbital by computational levels MP₂ and B₃LYP demonstrate that the proper orientation for the orbital overlap of delocalization of the

electrons LP₂ O → σ*P-F and LP₁ P → σ*C-O occurs in axial conformation and the proper orientation for the orbitals overlap of electron delocalization LP₁ O → σ*P-F, LP₂ F → σ*P-O, and LP₃F → σ*P-O occurs in equatorial conformation. This can be verified with stabilization energy. Stabilization energy associated with electron delocalization LP O → δ*F-P by the MP₂ and B₃LYP methods is reported to be higher in the axial conformation than the stability energy of the other transitions. The overlapped orbitals LPO and δ*F-P in the axial conformation with the computational methods for the compound 2-fluoro-1, 3, 2-dioxaphosphinane indicates that the electron transitions occur in a more appropriate direction and that LP O → δ*F-P does more. The orientations, the overlap of the electron donor and acceptor orbitals, and the vibrational frequencies as well as bond lengths further confirm this issue. The total stability energy (ΣE) dependent on the delocalization of the electrons in the axial and equatorial conformations is calculated by MP₂, and B₃LYP shows more stability and transitions in the axial conformation than in the other position.

Table 4. The calculated second-order stability energy (E_2 : kcal/mol⁻¹), ΣE (kcal/mol⁻¹), off-diagonal elements (F_{ij} : Hartree), orbital energy differences ($\Delta\epsilon$: Hartree) axial, and equatorial conformation of compound 2-fluoro- 1, 3, 2-dioxaphosphinane

MP ₂ /3-21G	Axial			Equatorial		
	E_2	ϵ_i-j	F_{ij}	E_2	ϵ_i-j	F_{ij}
LP ₁ O→ δ^* F-P	1.21	1.07	0.033	8.52	1.10	0.087
LP ₂ O→ δ^* F-P	13.16	0.71	0.087	1.93	0.75	0.034
LP ₁ P→ δ^* C-O	3.24	1.02	0.052	1.43	1.04	0.035
LP ₂ F→ δ^* O-P	6.05	0.88	0.066	7.02	0.87	0.071
LP ₃ F→ δ^* O-P	8.35	0.88	0.077	9.78	0.86	0.083
ΣE		32.01			28.68	

Table 5. The calculated second-order stability energy (E_2 : kcal/mol⁻¹), ΣE (kcal/mol⁻¹), off-diagonal elements (F_{ij} : Hartree), orbital energy differences ($\Delta\epsilon$: Hartree) axial, and equatorial conformations of compound 2-fluoro-1, 3, 2- dioxaphosphinane

B ₃ LYP/Aug-cc-pv-dz	Axial			Equatorial		
	E_2	ϵ_i-j	F_{ij}	E_2	ϵ_i-j	F_{ij}
LP ₁ O→ δ^* F-P	0.60	1.07	0.033	4.84	0.73	0.053
LP ₂ O→ δ^* F-P	13.16	0.71	0.087	3.45	0.43	0.035
LP ₁ P→ δ^* C-O	4.58	0.69	0.050	1.97	0.71	0.033
LP ₂ F→ δ^* O-P	3.51	0.58	0.041	4.07	0.57	0.043
LP ₃ F→ δ^* O-P	4.85	0.57	0.047	5.36	0.57	0.049
ΣE		26.70			19.69	

Occupancy orbital

The results obtained from the NBO, population of the electron donor orbitals (LP O, LP P, and LP F) and the electron acceptor orbitals (δ^* F-P, δ^* C-O, and δ^* O-P) illustrate a compound 2-fluoro-1, 3, 2-dioxaphosphinane of axial and equatorial conformations by B₃LYP/Aug-cc-pv-dz and

MP₂/3-21G methods. Table 6 demonstrates that the electron donor orbital population is larger than the electron acceptor orbital one. The electrons migrate from electron donor orbitals (Higher electron density) to the electron acceptor orbitals (Low electron density).

Table 6. Orbital occupancy (e) for axial and equatorial conformations of compound 2- fluoro- 1, 3, 2- dioxaphosphinane

Electron donor and acceptor orbital	MP ₂ /3-21G		B ₃ LYP/Aug-cc-pv-dz	
	ax	eq	ax	eq
LP ₁ O	1.97062	1.96455	1.95893	1.95548
LP ₂ O	1.91956	1.94264	1.89364	1.91761
LP ₁ P	1.98734	1.99393	1.97205	1.98552
LP ₂ F	1.96847	1.96953	1.96508	1.96541
LP ₃ F	1.95722	1.95159	1.95704	1.9469
δ^* F-P	0.09951	0.06312	0.12887	0.07097
δ^* C-O	0.02265	0.01811	0.03158	0.02508
δ^* O-P	0.08511	0.08213	0.08559	0.08375

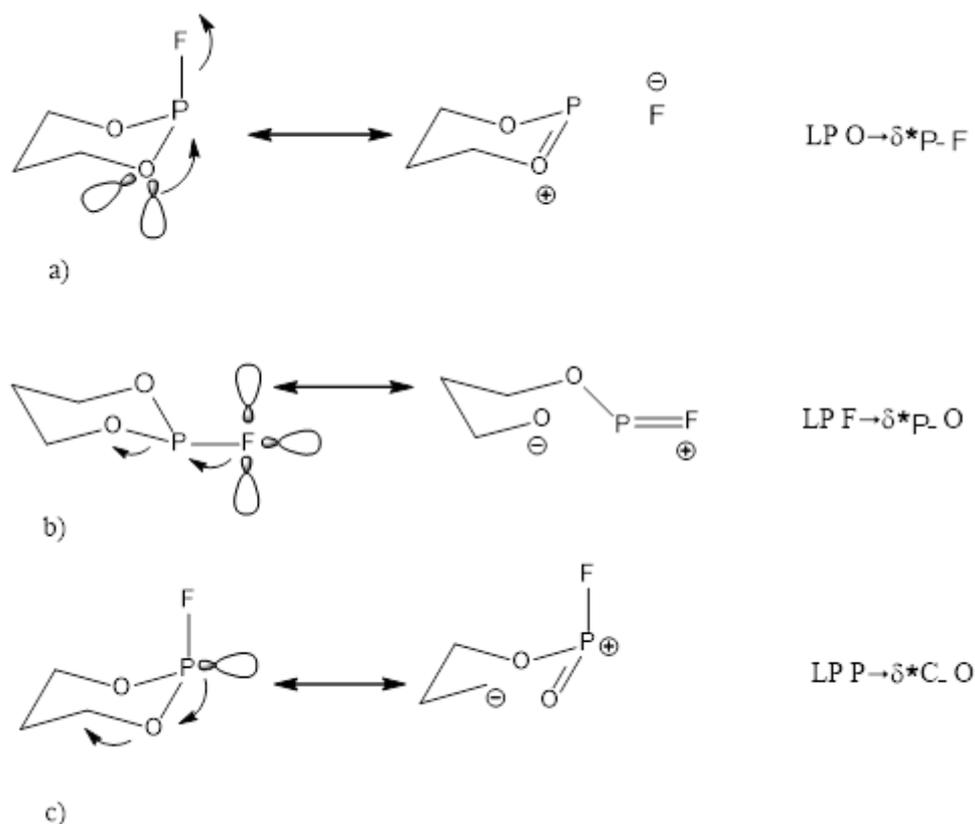


Figure 2. a) Optimal orientation of overlap electron donor orbital LPO and electron acceptor orbital δ^*P-F . b) Optimal orientation of overlap electron donor orbital LPF and electron acceptor orbital δ^*P-O . c) Optimal orientation of overlap electron donor orbital LPP and electron acceptor orbital δ^*C-O

Reactivity parameters

Energy HOMO refers to the ability to donate an electron from an electron donor orbital to an electron acceptor orbital. Energy LUMO refers to the ability to receive an electron from an electron acceptor orbital. The energy of the highest level of the occupied molecular orbitals (ϵ_{HOMO}) and the energy of the lowest level of the unoccupied molecular orbitals (ϵ_{LUMO}) are given in Table 7. The relationship between the hardness of chemical compounds and energies HOMO and LUMO is described by Equation 3:

$$\eta = 0.5(\epsilon_{LUMO} - \epsilon_{HOMO}) \quad \text{Eq.3}$$

The difference between HOMO and LUMO is another important aspect of molecular activity. With increasing HOMO and LUMO gap, the stability of chemical compounds becomes greater [21-22]. The required energy to remove an

electron from a neutral atom is called ionization energy. The amount of released energy to receive an electron and convert it into a negative ion is known as the electron affinity energy. The hardness relationship of chemical compounds with ionization energy and electron affinity energy is obtained according to Equation 4.

$$\eta = I - A / 2 \quad \text{Eq.4}$$

The ionization energy and the electron affinity energy are calculated according to the equation: $-\epsilon_{HOMO} = IP$ and $-\epsilon_{LUMO} = EA$. Softness is another parameter for measuring the ability and activity of a molecule which follows the $S = 1/\eta$ equation. Electronegativity refers to the ability of an atom to attract shared electrons in a covalent bond. The higher the electronegativity value, the more strongly that element attracts the shared electrons. Electronegativity determines the Lewis

acid and base properties of a molecule. A molecule with a larger χ acts like a lewis acid, and the one with a smaller χ acts as a lewis base [23]. The electrophilicity index introduced by Parr measures the electron acceptor tendency to obtain an additional electronic charge from the environment [24]. Equation 5 shows the relationship between electronegativity and

ionization energy and electron affinity energy, and equation 6 further depicts the relationship between hardness, electrophilicity index, and electronegativity.

$$\chi = I + A/2 \quad \text{Eq.5}$$

$$\omega = \chi^2/2\eta \quad \text{Eq.6}$$

Table 7. The computed energies of HOMO (ϵ_{HOMO}), LUMO (ϵ_{LUMO}), global hardness (η), softness (S), electronegativity (χ) and electrophilicity index (ω), softness (S), and potation chemical (μ) in (a. u.) parameters for the (axial) and (equatorial) of compound 2- Fluoro- 1, 3, 2- dioxaphosphinane

Method Conformation	MP ₂ /3-21G		B ₃ LYP/Aug-cc-pv-dz	
	Axial	Equatorial	Axial	Equatorial
ϵ_{HOMO}	-0.4190	-0.3909	-0.3001	-0.2689
ϵ_{LUMO}	0.1670	0.1558	-0.0182	-0.0278
Gap _{HOMO-LUMO}	0.5860	0.5466	0.3184	0.2968
IP	0.4190	0.3909	0.3001	0.2689
EA	-0.1670	-0.1558	0.0182	0.0278
η	0.2930	0.2733	0.1592	0.1484
S	1.7064	1.8294	3.1407	3.3692
χ	-0.1260	-0.1175	-0.1591	-0.1483
μ	0.1260	0.1175	0.1591	0.1483
ω	0.0270	0.0252	0.0795	0.0741

Dipole moment

In general, a molecule with a smaller dipole moment has a lower energy level in the gas phase, so the molecule's stability is higher [25-26]. Studies show that the dipole moment with the method MP₂/3-21G for compound 2- fluoro- 1, 3, 2-dioxaphosphinane with the axial and equatorial conformations is 6.0943, 6.5319, and with the method B₃LYP/Aug-cc-pv-dz for the axial and equatorial conformations is 5.2993 and 5.8335, respectively. Studies on the dipole moment showed that the axial conformation is more stable than the equatorial one.

Conclusion

This research evaluated the structural and thermodynamic parameters as well as chemical reactivity such as global hardness, global softness, electronegativity, and electrophilicity index for compound 2- fluoro- 1, 3, 2-dioxaphosphinane that were performed with

axial and equatorial conformations with MP₂ and B₃LYP computational levels. Studies have demonstrated that the axial conformation is more stable than the equatorial one. Calculations of stability energy dependent on electrons delocalization LP O \rightarrow σ^* P-F, LP P \rightarrow σ^* C-O, LP F \rightarrow σ^* P-O, bond lengths, and vibrational frequencies P-O, P-F and C-O showed that due to the constant force, more LP O \rightarrow σ^* P-F electron transfers took place, which is corresponded to the anomeric effect. The studies of the dipole moment in the gas phase with computational methods MP₂/3-21G and B₃LYP/Aug-cc-pv-dz for the compound 2- fluoro- 1, 3, 2-dioxaphosphinane demonstrated that the axial conformation is more stable than the equatorial one. These results are directly related to the stability energy and reactivity parameters such as hardness. Stretching vibrations and short and long of P-O, P-F, and C-O bonds more than usual confirm the effect of

anomeric and hyper-conjugation interactions in the compound.

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