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The Electronic Properties and Reactivity of 4 (4-Substituted phenyl) -1,2,5- Selenadiazole Derivatives

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ABSTRACT

This study presents a theoretical investigation of 4-(4-substituted phenyl) -1,2,5- selenadiazole derivatives, focusing on the impact of para-substituents on their electronic properties and reactivity. Semi-empirical PM3 and density functional theory (DFT) methods (B3LYP/3-21G) were employed for molecular geometry optimization and electronic structure analysis. Key findings include significant substituent effects on HOMO-LUMO energy gaps, proton affinities, and reactivity indices. Electron-donating groups, particularly NMe2, notably enhanced molecular softness and reduced energy gaps, indicating increased chemical reactivity. Proton affinity calculations revealed systematic trends for electron-donating groups, while electron-withdrawing groups showed less consistent behavior. These insights provide a foundation for the potential application of these derivatives in catalysis, materials science, and drug development, highlighting the utility of computational methods in predicting structure-property relationships.

1. Introduction

Organoselenium rings containing nitrogen are an essential category of heterocyclic compounds. They have attracted continuous interest recently due to their valuable biological and medical applications, such as antioxidant and anticancer agents [1-6]. The five-member ring selenium compounds with two nitrogen atoms like 1,2,3-; 1,2,4-; 1,3,4 and 1,2,5-selenadiazole are investigated as antifungal and antibacterial agents [7]. In 2017, Yanxin et al. [8] studied the effect of 5-selenadiazole derivatives as effective inhibitors of Dex-induced osteoblast apoptosis. They found that the protective effect was correlated with their lipophilicity, cellular uptake and antioxidant activities. In 2017, Haoqiang et al. [9] found that the Selenadiazole derivatives inhibit the Angiogenesis of human breast tumour growth by suppressing the VEGFR2-mediated ERK and AKT signalling pathway. In 2024, Yanchao and his team [10] Investigated the effect of Selenium derivatives in promoting the immunogenic radiotherapy against cervical cancer metastasis through evoking P53 activation. Furthermore, these types of heterocyclic compounds have significant applications in light-emitting diodes and conducting materials chemistry [11]. Protonation reactions of nitrogen bases are very important in biochemistry. Many medicinal drugs, such as anesthetics,

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antiarrhythmic, neuroleptics, and antihistaminic, contain a nitrogen atom or amino group that can react quickly with a proton ion to form a cation [12]. These potent molecules may be found in positively charged and uncharged forms at a range of physiological pH. Many theoretical approaches based on density functional theory have been carried out to study the properties of potent molecules and their chemical reactivity. These studies gave helpful explanation about using them as suggested drugs [13, 14]. Reactivity indices such as; electrophilicity [15], chemical potential [16], hardness [17, 18], softness [19], and nucleophilicity [20] are effective parameters to predicate behavior of organic molecules in chemical reactions.

In this work, a series of 4-(4-substituted phenyl)-1,2,5-selenadiazole molecules have been investigated theoretically by performing semi empirical and DFT methods. The proton affinity, reactivity indices and spatial distribution and positions of the (HOMO) and the (LUMO) are obtained.

2. Method of calculations

Quantum mechanical calculations of this work have been done using hyperchem program 7.5 [21]. The geometry of the 4-(4-Substituted phenyl)-1,2,5-selenadiazole molecules were optimized by carrying out the semi empirical molecular orbital theory at the PM3 level [22], using the restricted Hartree–Fock (RHF) procedure [23]. The Polak–Ribier algorithm [24] was used for the optimization, with the termination condition being a root mean square (RMS) of <0.001 kcal/mol. Further, Geometry optimization was done by performing the B3LYP/3-21G theory method [25-27] to study their structural and electronic properties. The proton affinity of a base B from the ab initio calculations was determined as the negative ΔEp value of the exothermic reaction:

$$B(g) + H+(g) = BH+ (g)$$

i.e. the difference between the energies of the neutral and protonated species

$$\Delta E_p = E_B - E_{BH}^{+} \qquad (1)$$

The semi empirical quantum-chemical AM1 method allows the calculation of the standard formation enthalpies $\Delta Hf°.298$ [22]. The proton affinity of base PA(B) can be computed by the equation:

$$PA(B) = \Delta H°f.T\ (H^{+}, g) + \Delta H°f.T\ (B , g) - \Delta H°f.T(BH^{+}, g) \qquad (2)$$

$\Delta H°f.T$ represents the heat of formation of the species stated between parenthesis.

For $\Delta H°f.T$ (H+, g) the experimental value 1537. 1 KJ mol^{-1} is used [23].

The ab initio calculations were carried out using the GAUSSIAN 80 program [24] and the AM1 calculations were conducted using AMPAC.

It is well known that global reactivity indices defined within conceptual DFT is a powerful tool to explain reactivity and molecular properties. Consequently, we have calculated global hardness (η), electronic chemical potential (μ), electronegativity (χ), global softness (S), nucleophilicity index (N), and electrophilicity index (ω) for all compounds by following formulas [28]:

$$\eta\ (eV) = \frac{(\varepsilon_{LUMO} - \varepsilon_{HOMO})}{2}$$

$$\mu\ (eV) = -\frac{(\varepsilon_{LUMO} + \varepsilon_{HOMO})}{2}$$

$$\chi\ (eV) = -\mu$$

$$S\ (eV) = \frac{1}{2\eta}$$

$$N\ (eV) = \varepsilon_{HOMO} - \varepsilon_{HOMO(Tetracyanoethelyene)}$$

$$\omega\ (eV) = \frac{\mu^2}{2\eta}$$

3. Results and discussion

Scheme 1 depicts the chemical structure of 4-(4-substituted phenyl)-1,2,3-selenadiazole derivatives. The para substitution on the phenyl group with electron-donating and electron-withdrawing groups allowed for an investigation into how structural variations influence electronic properties. These properties were analyzed using PM3 and B3LYP/3-21G calculations, as summarized in Table 1, which includes data on HOMO, LUMO, energy gaps (ΔE), binding energy, heat of formation, partial charges, and proton affinities.

Substituents exerted slight but consistent effects on HOMO and LUMO energies. The NMe2 group caused a significant reduction in the energy band gap, with decreases of 0.953 eV (PM3) and 0.960 eV (DFT), highlighting the influence of strong electron-donating groups. Selenium atoms displayed positive partial charges (PM3:

0.203 to 0.756; DFT: 0.708 to 0.756), while nitrogen atoms (N2 and N5) exhibited negative charges (e.g., for N2, PM3:

-0.162 to -0.186; DFT: -0.689 to -0.703).

These variations in charge distribution suggest that substituent effects subtly alter the electronic environment of the selenadiazole ring.

Proton affinities (PA) of the nitrogen atoms varied, with N2 consistently displaying higher basicity than N5. This difference arises from variations in steric and electronic environments. Electron-donating substituents significantly increased PA, following the order:

NMe2 > NH2 > OCH3 > CF3 > H.

However, electron-withdrawing groups exhibited less systematic trends, with PM3 predicting slight decreases and DFT showing marginal increases in PA. To our knowledge, this study provides the first theoretical PA values for selenadiazole rings, offering comparative insights into PM3 and DFT methodologies. The higher PA values predicted by DFT underscore its sensitivity to electronic substituent effects, particularly for electron-donating groups.

Table 2 summarizes reactivity indices derived from electronic properties, including ionization potential (IP), electron affinity (EA), chemical potential (μ), electronegativity (χ), chemical hardness (η), and softness (S). These parameters elucidate the reactivity profiles of the studied derivatives.

The chemical potential μ, an indicator of electron-donating ability, follows the order:

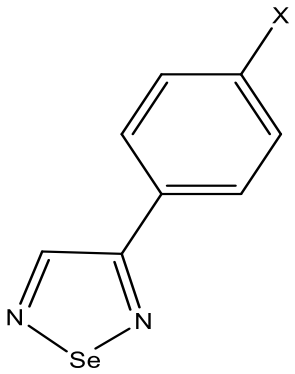
NMe2 > NH2 > OCH3 > OH > H > CH3 > Ph > I > F > Br > Cl > CF3 > CN > NO2, while the opposite trend is observed for electronegativity χ. Chemical hardness η, which reflects resistance to electron density changes, decreases in the order:

H > CF3 > CH3 > F > Cl > CN > Br > NO2 > OH > OCH3 > I > NH2 > Ph > NMe2. Conversely, chemical softness S ranks the derivatives as:

NMe2 > Ph > NH2 > I > OCH3 > OH > NO2 > Br > CN > Cl > F > CH3 > CF3 > H. These findings highlight how substituent electronic effects influence the stability and reactivity of the derivatives.

The electrophilicity index (ω), calculated as $\omega = \mu^2/2\eta$, measures the stabilization energy upon electron acquisition. The derivatives rank as:

NO2 > CN > CF3 > Ph > Cl > I > Br > F > CH3 > H > OH > OCH3 > NH2 > NMe2, reflecting the interplay between μ and η. These trends provide insight into the electrophilic potential of the molecules, reinforcing the complementary nature of the computational methods employed.



X= NMe_2; NH_2; OMe;OH; Me; CF_3; H; Ph; Cl; Br; I; CN; NO_2

Scheme 1: The general structure of 4-4-Substituted phenyl)-1,2,5-selenadiazole molecules.

Table 1. The calculated highest occupied and the lowest unoccupied molecular orbital energies (HOMO and LUMO respectively) of 1,2,5-selenadiazole derivatives.

	3-21G	**-5.794**	**-1.874**	**3.92**	**-1780905.3**		**0.777**	**-0.7**	**-0.622**	**210.4**	**199.71**
F	PM3	-9.513	-1.385	8.128	-1931.23	-4.41	0.227	-0.181	-0.164	186.31	180.77
	3-21G	-6.308	-1.593	4.715	-1822372.6		0.733	-0.696	-0.627	227.66	223.86
Cl	PM3	-9.336	-1.346	7.99	-1904.53	32.38	0.224	-0.18	-0.165	188.22	182.03
	3-21G	-6.385	-1.72	4.665	-2047432.1		0.737	-0.694	-0.627	224.96	221.93
Br	PM3	-9.533	-1.381	8.152	-1887.65	47.01	0.227	-0.178	-0.165	186.71	181.12
	3-21G	-6.267	-1.669	4.598	-3367551.6		0.735	-0.695	-0.627	228.29	224.08
I	PM3	-9.157	-1.335	7.822	-1872.87	60.57	0.225	-0.179	-0.165	188.45	182.2
	3-21G	-6.113	-1.68	4.433	-6083834.1		0.735	-0.694	-0.627	228.48	224.07
CN	PM3	-9.705	-1.636	8.069	-2116.98	74.83	0.235	-0.175	-0.162	183.40	178.52
	3-21G	-6.794	-2.162	4.632	-1817991.5		0.75	-0.692	-0.624	221.47	219.01
NO2	PM3	-10.019	-1.966	8.053	-2108.47	31.57	0.248	-0.166	-0.16	178.61	175.07
	3-21G	-7.002	-2.515	4.487	-1887994.5		0.756	-0.689	-0.624	219.22	217.49

Table 2. Various reactivity indices of studied 4-(4-Substituted phenyl)-1,2,5-Selenadiazole Derivatives[6].

	IP	EA	μ	X	η	S	ω
NMe_2	4.994	1.09	-3.042	3.042	1.952	0.512	2.37
NH_2	5.187	1.091	-3.139	3.139	2.048	0.488	2.405
OCH_3	5.786	1.337	-3.561	3.561	2.224	0.449	2.851
OH	5.825	1.353	-3.589	3.589	2.236	0.447	2.88
CH_3	6.153	1.432	-3.792	3.792	2.36	0.423	3.046
CF_3	6.819	1.985	-4.402	4.402	2.417	0.413	4.008
H	6.215	1.351	-3.783	3.783	2.432	0.411	2.942
Ph	5.794	1.874	-3.834	3.834	1.96	0.51	3.749
F	6.308	1.593	-3.95	3.95	2.357	0.424	3.309
Cl	6.385	1.72	-4.052	4.052	2.332	0.428	3.52
Br	6.267	1.669	-3.968	3.968	2.299	0.434	3.424
I	6.113	1.68	-3.896	3.896	2.216	0.451	3.424
CN	6.794	2.162	-4.478	4.478	2.316	0.431	4.329
NO_2	7.002	2.515	-4.758	4.758	2.243	0.445	5.046

Table 3. The calculate values of global hardness (η) and global softness(S)for the substituted groups.

	η	S
NMe2	1.952	0.512
Ph	1.960	0.510
NH2	2.048	0.488
I	2.216	0.451
OCH3	2.224	0.449
OH	2.236	0.447
NO2	2.243	0.445
Br	2.299	0.434
CN	2.316	0.431
Cl	2.332	0.428
F	2.357	0.424
CH3	2.360	0.423
CF3	2.417	0.413
H	2.432	0.411

4. Conclusion

This study provides a comprehensive computational analysis of 4-(4-substituted phenyl)-1,2,3-selenadiazole derivatives, examining their electronic properties, reactivity indices, and proton affinities using PM3 and B3LYP/3-21G methods. The findings reveal that electron-donating and electron-withdrawing substituents have significant and systematic impacts on the molecules' electronic behavior and reactivity. Key conclusions include:

1. HOMO-LUMO Analysis: Substituents influence the energy band gap, with electron-donating groups, particularly NMe2, significantly reducing the gap. This suggests that such substituents enhance the electronic reactivity of the derivatives.
2. Charge Distribution and Proton Affinities: The distribution of partial charges across selenium and nitrogen atoms demonstrates subtle effects of substituents, while proton affinities highlight N2 as the more basic site. Notably, electron-donating groups systematically increase basicity, indicating their potential for enhancing catalytic properties.
1. Reactivity Indices: Parameters such as chemical potential, hardness, softness, and electrophilicity index reveal distinct trends, with NMe2-substituted derivatives exhibiting the highest softness and lowest hardness, making them excellent electron donors. Conversely, derivatives with NO2 show strong electrophilic tendencies.
2. Comparison of PM3 and DFT Methods: The study underscores the reliability of DFT in capturing detailed electronic effects, as evidenced by its consistent predictions of higher proton affinities and reactivity indices.

5. Implications and Future Directions:

The insights into electronic and reactivity properties of 1,2,3-selenadiazole derivatives provided by this study pave the way for their application in diverse fields such as catalysis, material science, and drug design. The observed trends in proton affinities and reactivity indices could guide the development of tailored derivatives with specific chemical behaviors.

Future research should focus on experimental validation of the computational predictions, particularly for proton affinities and reactivity indices. Additionally, exploring a broader range of substituents and using advanced computational methods could provide deeper mechanistic insights and uncover novel applications.

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الخواص الإلكترونية وتفاعلية جزيئات 4-(بارا-فينيل مستبدل)-1,2,5-سيلينياديازول

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معلومات البحث

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الكلمات المفتاحية

1,2,5-سيلينياديازول،تقارب البروتون، مؤشرات التفاعل، نظرية DFT.

الملخص

تبحث هذه الدراسة في سلسلة من جزيئات 4-(فينيل مستبدل بارا)-1,2,5-سيلينياديازول من خلال طرق نظرية. تم إجراء تحسين هذه الجزيئات في البداية باستخدام طريقة PM3 شبه التجريبية، تليها تحسين هندسي أكثر تفصيلاً باستخدام نظرية الكثافة الوظيفية (DFT) عند مستوى G21-3. تم اختيار بدائل مانحة ومستقبلة مختلفة للاستبدال في موضع بارا لحلقة الفينيل لاستكشاف تأثيرات التغييرات البنيوية على الخصائص الإلكترونية وتفاعلية الجزيئات المدروسة في المجال الطبي. تم حساب وتحليل المعلمات الرئيسية مثل تقارب البروتون، ومؤشرات التفاعل، والتوزيع المكاني لأعلى مدار جزيئي مشغول (HOMO) وأدنى مدار جزيئي غير مشغول (LUMO).

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