University of Thi-Qar Journal of Science (UTJsci)
E-ISSN: 2709-0256, P-ISSN: 1991-8690, Vol. 13, No. 1, Jun. 2026

Thermal Decomposition Behavior of 4-Aryl-1,2,3-selenadiazole Derivatives Investigated by Thermogravimetric Analysis

Doaa Rahim Thjeel[1a*], Salih H Abbas[1b], and Ali Jameel Hameed[1c]

[1]*Department of Chemistry, College of Science, University of Basrah, Basrah, Iraq*

[b]Email: salih.hamza@uobasrah.edu.iq , [c]Email: ali.alhamad@uobasrah.edu.iq
[a*]Corresponding author: alamryduaa78@gmail.com

Received: 2025-07-12, Revised: 2025-08-16, Accepted: 2025-08-22, Published: 2026-06-01

***Abstract*— The thermal analysis behavior of some organoselenium compounds based on 4-aryl-1,2,3-selenadiazole was carried out by thermogravimetric analysis. The studied compounds have been selected to be substituted with different electron donating and electron withdrawing groups to investigate the effect of these groups on stability of studied compounds. The thermal analysis (TG and DTG) has been carried out under inert atmosphere by using nitrogen gas. The thermal analysis indicated that the thermal decomposition of the studied compounds is exceedingly affected by both of the steric effects and electronic nature of the substituted groups. The electron with drawing groups such as CN and NO_2 indicate mostly improved thermal stability. On the other hand, the electron donating groups such as CH_3 and OCH_3 indicate reduced thermal stability. Furthermore, there are parameters like the residual mass at high temperatures and steps of decompositions may provide valuable insights on the thermal resistance of the studied compounds. The results highlight the structure property relation of studied compounds and propose their possible for using in polymer stabilization, chemical vapor deposition and high temperature materials.**

Keywords—Organoselenium compounds, Selenadiazole, substituent effect, thermal analysis, styling.

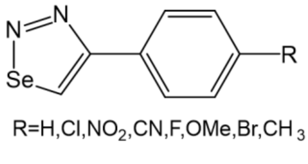
I. INTRODUCTION

Thermogravimetric analysis (TGA) is a technique used to measure changes in the mass of organic and inorganic compounds as function of temperature or time, under controlled atmosphere on inert gas such as nitrogen on argon[1]. The thermogravimetric curve, also known as thermogram, is a graphical showing the change in a sample's mass relative to temperature. This curve provides valuable information about the studied compounds, including their degradation behavior, oxidation resistance, thermal stability, volatile content and moisture content[2].

Recently, there has been a focusing on the developing new materials which are designed to withstand high temperature. Momentous efforts have been achieved to synthesis new organic and inorganic compounds that show high thermal stability against high temperatures for long time. Thermolysis or thermal decomposition is a chemical process of a material produced by heat. The decomposition temperature of materials is the temperature at which it chemically decompose[3]. According to our best knowledge, there are rare studies about the thermal decomposition of organoselenium compounds in the solid state[4-6]. Nevertheless, the literature indicated that during the thermal decomposition organoselenium compounds knowledge reversible of the carbon-selenium bond, causing to formation of radicals of carbon accomplished of responding with numerous radical acceptor[7-9].

Our research focus on the thermal behavior of heterocyclic organo-selenium compounds, specifically five-membered rings containing nitrogen [10-12] , with the aim of correlating their composition and structure with material properties relevant to potential application. Notably, several studies have previously addressed the thermal decomposition of sulfur- and selenium-containing compounds [13-14].

The present work investigates the thermal stability, decomposition patterns, and structural transformations of selected 4-aryl-1,2,3-selenadiazole derivatives, shown in scheme 1, within the temperature range of ambient to 400 °C, using thermogravimetric analysis (TGA) and derivative thermogravimetry (DTG). These compounds are being evaluated for their potential applications as stabilizers in synthetic polymers , reagents in organic synthesis , or as precursors for metal-organic chemical vapor deposition of tellurium[15].Furthermore, this study examines the key factors that influence their thermal stability.



Scheme 1: Structure of para-substituted -1,2,3-selenazole compounds

II. EXPEREMENTAL PART

The studied compounds: 4-phenyl-1,2,3-selenadiazole (1), 4-(4-cyanophenyl)-1,2,3-selenadiazole (2), 4-(4-Chlorophenyl)-1,2,3-selenadiazole (3), 4-(3-nitrophenyl)-1,2,3-selenadiazole (4), 4-(4-fluorophenyl)-1,2,3-selenadiazole (5), 4-(4-bromophenyl)-1,2,3-selenadiazole (6), 4-(4-methoxyphenyl)-1,2,3-selenadiazole (7), 4-(4-

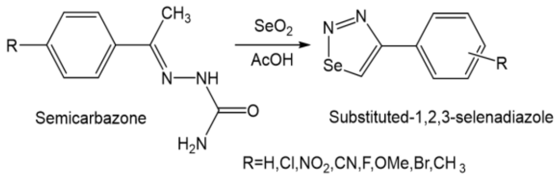
https://doi.org/10.32792/utq/utjsci/v13i1.1448

methylphenyl)-1,2,3-selenadiazole(8) were prepared purified and characterized as previously reported [10-11].

Thermal analysis was conducted using a SHIMADZU-TGA-50 thermoanalyzer, which simultaneously records thermogravimetric (TG) and derivative thermogravimetric (DTG) data. All experiments were performed under a nitrogen atmosphere using α-Al_2O_3 as the reference material. The samples were heated from room temperature 25°C to 550°C at a constant rate of 20 °C per minute. The resulting TG-DTG profiles are presented in Figures 1- 8.

III. RESULT AND DISCUSSION

The studied compounds were synthesized through the cyclization of semicarbazone derivatives with selenium dioxide as an oxidizing agent, in the presence of glacial acetic acid as an acidic medium, leading to the formation of a five-membered heterocyclic ring containing two nitrogen atoms and one selenium atom, as illustrated in scheme 2.Keep your text and graphic files separate until after the text has been formatted and styled. Do not use hard tabs, and limit use of hard returns to only one return at the end of a paragraph. Do not add any kind of pagination anywhere in the paper. Do not number text heads-the template will do that for you.



Scheme 2: Synthesis diagram of preparation para-substituted-1,2,3-selenazole compounds

Figures 1-8 show the TG and DTG of the studied compounds. Table 1 presents the thermal decomposition data for the studied selenadiazole derivatives.

Compound 1 exhibits four decomposition steps at 102 °C, 200 °C, 246 °C, and 312 °C. The residual mass at 575 °C is 12.11%, with a total mass loss of 87.89%. Compound (2) shows two decomposition steps at 171 °C and 513 °C, with 13% residue remaining at 550 °C and a mass loss of 87%. Compound (3) undergoes three decomposition steps at 171 °C, 300 °C, and 493 °C, with 19.5% of the material remaining at 275 °C and 80.5% lost. Compound (4) displays two decomposition stages at 158 °C and 473 °C, leaving 25% of the material at 575 °C and a mass loss of 75%. Compound 5 also shows two decomposition steps at 292 °C and 493 °C, with a residue of 20% at 575 °C and a loss of 80%. Compound 6 exhibits three decomposition stages at 142 °C, 335 °C, and 500 °C, with 20% residue at 575 °C and 80% mass loss. Compound 7 undergoes three decomposition steps at 121 °C, 279 °C, and 411 °C, also leaving 20% residue at 575 °C and a loss of 80%. Finally, Compound 8 shows three decomposition steps at 314 °C, 390 °C, and 485 °C, with 23% of the sample remaining at 575 °C and a mass loss of 77%.

TABLE 1. Thermal stability parameters of substituted -1,2,3-selenazole compounds from TG curves

No.	Substituent	Highest Decomposition Temp.	Temperature of 25 % mass loss/°C	Temperature of 50 % mass loss/°C	Temperature of 75 % mass loss/°C	Char content % at 575 °C
1	H	102,200,246,312	225	263	365	12.11
2	CN	171,513	175	185	477	13.2
3	Cl	171,300,493	162	395	503	19.5
4	NO_2	158,473	165	360	560	25
5	F	292,493	275	335	459	20.12
6	Br	142,335,500	275	477	514	20
7	OCH_3	52,350	364	517	557	23
8	CH_3	135,300,485	370	468	555	24

The thermogravimetric data presented in Table1 indicate notable differences in the thermal stability and decomposition patterns of the studied 4-aryl-1,2,3-selenadiazole derivatives. These variations can be rationalized by examining the electronic nature and steric influence of the substituents on the phenyl ring.

Compound (1), the unsubstituted 4-phenyl-1,2,3-selenadiazole, exhibits four distinct decomposition steps, indicating a relatively complex thermal degradation pathway likely influenced by the unsubstituted of electron withdrawing or electron donating groups, which leads to moderate thermal stability with 12.11% residue remaining at 575 °C.

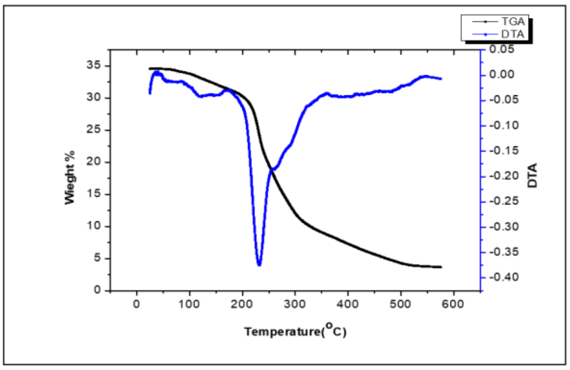


Fig. 1: TG-DTG curves of Compound 1

In Compound 2, bearing a strong electron-withdrawing cyano group (CN) at the para position, only two decomposition steps were observed, but with a higher decomposition temperature (up to 513 °C), suggesting enhanced thermal stability. This is consistent with the stabilizing effect of the cyano substituent, which delocalizes electron density of the aromatic bonds and enhances the aromatic ring's resistance to thermal degradation.

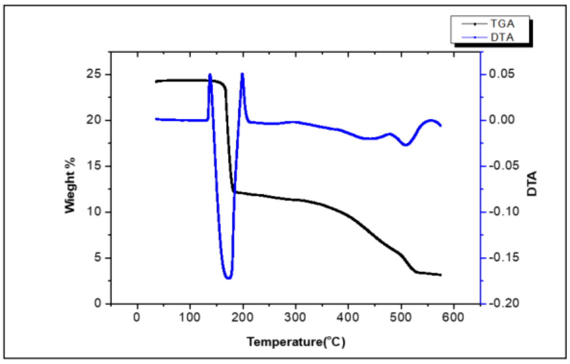


Fig. 2: TG-DTG curves of Compound 2

Compound 3, substituted with a para-chloro group (Cl), undergoes three decomposition steps, with a residue of

19.5% at 275 °C. The chloro substituent is moderately electron withdrawing group, but it seems to stabilize the molecule less effectively than that the cyano group. As a result, the Compound 3 being decompose earlier than Compound 2.

Compound 4, with a meta-nitro group (NO_2), displays only two decomposition steps, but leaves a relatively high residue (25%) at 575 °C. The nitro group is strongly electron withdrawing, yet its meta positioning limits conjugative interaction with the selenadiazole core. This could make the structure more rigid and less sensitive to heat, which would slow down its overall degradation.

For Compounds 5 and 6, bearing para-fluoro (F) and para-bromo (Br) substituents respectively, the decomposition proceeds in two and three stages, with both leaving around 20% residue at 575 °C. Halogen (F, Cl and Br) substituents can affect thermal behavior through their size and electronegativity, using both inductive and steric effects. In Compound 6, the bulkier bromine atom may cause steric hindrance, slightly weaken the ring system and cause it to decompose earlier.

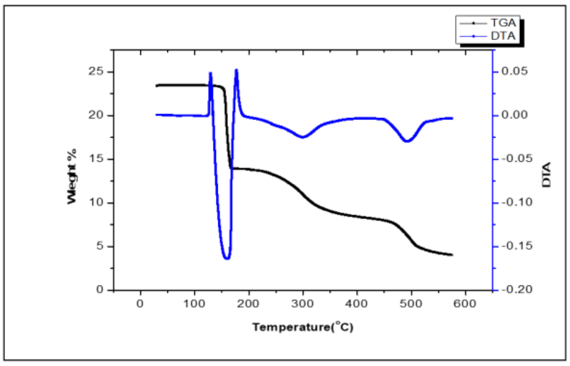


Fig. 3: TG-DTG curves of Compound 3

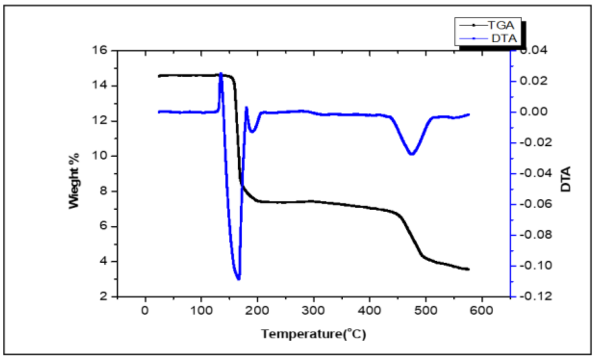


Fig. 4: TG-DTG curves of Compound 4

Compound 7, containing a para-methoxy group (OCH_3), and Compound 8, with a para-methyl group (CH_3), both show three decomposition stages with 20% and 23% residue, respectively.

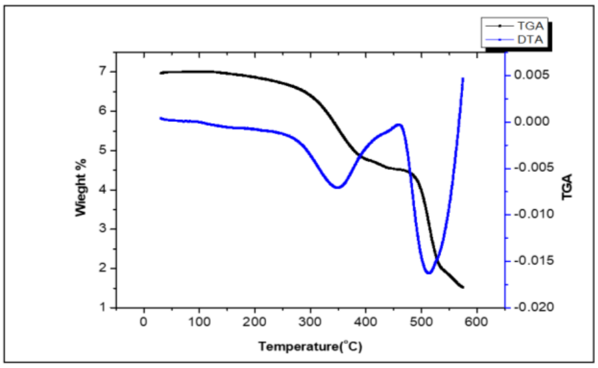


Fig. 5: TG-DTG curves of Compound 5

These electron donating groups activate the aromatic ring, increasing its electron density and maybe making the selenadiazole derivative more vulnerable to thermal degradation. However, the slightly higher residue in Compound 8 suggests that the methyl group, being less electron donating than the methoxy group, gives slightly greater thermal resistance. In general, the thermal behavior of these compounds appears to be affected by the electronic nature of the substituents group. It can be seen clearly that the electron withdrawing groups such as CN, NO_2, Cl tend to enhance thermal stability. Nevertheless, the electron donating groups such as CH_3, OCH_3 slightly reduce thermal resistance. In the case of bromine substituent, the bulkier bromine atom may cause steric hindrance, slightly weaken the ring system and cause it to decompose earlier.

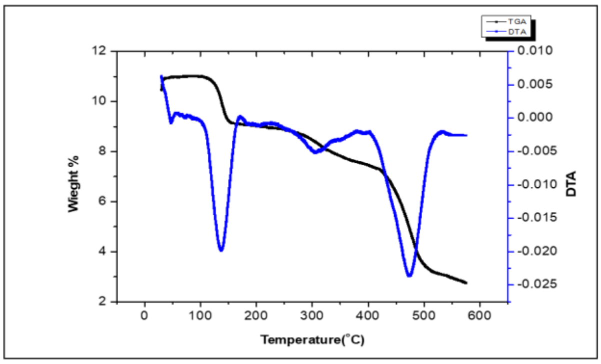


Fig. 6: TG-DTG curves of Compound 6

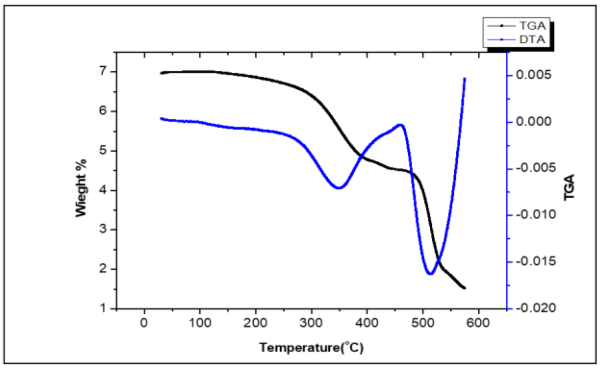


Fig. 7: TG-DTG curves of compound 7

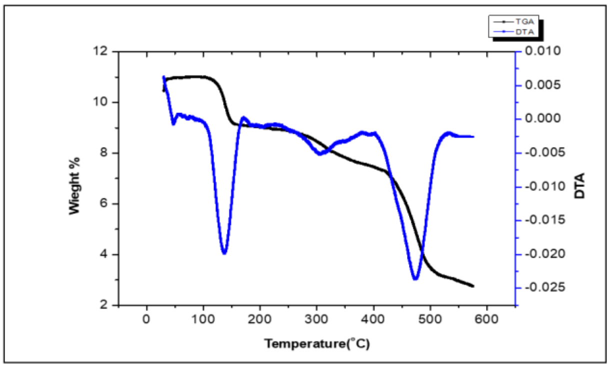


Fig. 8: TG-DTG curves of compound 8

IV. CONCLOSIN

The thermal analysis behavior of some organoselenium compounds based on 4-aryl-1,2,3-selenadiazole was carried out by thermogravimetric analysis. The thermal analysis behavior of 4-aryl-1,2,3-selenadiazole indicated thermal decomposition affected by the steric effects and the nature of the substituted group (electron donating or withdrawing group). The electron with drawing groups such as CN and NO2 showed mostly improved thermal stability. Alternatively, the electron donating groups such as CH3 and OCH3 indicate reduced the thermal stability. Additionally, the residual mass at high temperatures and steps of decompositions may afford valuable insights on the thermal resistance of the studied compounds. Selenium compounds containing species may be released during high-temperature decomposition such as H2Se gas, and we recommend strict safety protocols and environmental precautions during handling and processing. All in all, the results highlight the structure property relation of studied compounds and propose their possible for using in polymer stabilization, chemical vapor deposition and high temperature materials. Further research especially with a broader range of substituents groups and computational study will strengthen the predictive understanding.

ACKNOWLEDGMENT

The authors would like to thank the Department of Chemistry, College of Science, University of Basrah for their financial support of this project .

CONFLICT OF INTEREST

Authors declare that they have no conflict of interest.

REFERENCES

[1] A. Ari, M. Karahan, H. A. M. Ahmed, O. Babiker, and R. M. A. Dehşet, "A review of cellulosic natural fibers' properties and their suitability as reinforcing materials for composite panels and applications," *AATCC J. Res.*, vol. 10, no. 3, pp. 163–183, 2023.

[2] C. Wang, C. Chazallon, S. Braymand, and P. Hornych, "Thermogravimetric analysis (TGA) for characterization of self-cementation of recycled concrete aggregates in pavement," *Thermochim. Acta*, vol. 733, p. 179680, 2024.

[3] R. Golabiazar, M. A. HamaYali, M. A. Hamadamin, and S. R. Saadi, "Green synthesized photocatalyst ethylenediaminetetraacetic acid@ SiO2/CeO2/Fe3O4 nanocomposites by the Echinops L. plant for removal eriochrom black-T dye: focus on photodegradation, scavengers, kinetics, and antibioactivity," *React. Kinet. Mech. Catal.*, pp. 1–30, 2025.

[4] J. M. Sonego, S. I. De Diego, S. H. Szajnman, C. Gallo-Rodriguez, and J. B. Rodriguez, "Organoselenium compounds: Chemistry and applications in organic synthesis," *Chem. Eur. J.*, vol. 29, no. 52, p. e202300030, 2023.

[5] A. A. Heredia, L. M. Bouchet, W. D. Castro-Godoy, and J. E. Argüello, "Synthesis of organoselenium compounds using electrochemical and photochemical methods as novel approaches in organic chemistry," *Tetrahedron*, vol. 148, p. 133667, 2023.

[6] S. Purohit, P. Oswal, A. Tyagi, A. Bahuguna, N. Bhatt, and A. Kumar, "Organoselenium Compounds as an Emerging Class of Stabilizers of applied Nanomaterials for Applications in the Catalysis of Organic Reactions," *Asian J. Org. Chem.*, vol. 13, no. 9, p. e202400174, 2024.

[7] J. Ścianowski, A. J. Pacuła-Miszewska, A. Laskowska, and M. Obieziurska-Fabisiak, "Synthesis and applications of new chiral terpenyl organoselenium compounds," *Phosphorus. Sulfur. Silicon Relat. Elem.*, vol. 199, no. 1, pp. 2–9, 2024.

[8] S. Lai, X. Liang, and Q. Zeng, "Recent progress in synthesis and application of chiral organoselenium compounds," *Chem. Eur. J.*, vol. 30, no. 16, p. e202304067, 2024.

[9] J. T. Stadel and T. G. Back, "Asymmetric Synthesis with Organoselenium Compounds–The Past Twelve Years," *Chem. Eur. J.*, vol. 30, no. 21, p. e202304074, 2024.

[10] D. H. Alsawad, A. A. Al-Riyahee, and A. J. Hameed, "Simulation Study of Structural and Electronic Properties for Adducts complexes of Bis (Acetylacetonato) oxoVandium (IV) with 4-(Para-substituted phenyl)-1, 2, 3-Selenadiazole," in *Journal of Physics: Conference Series*, IOP Publishing, 2021, p. 12002.

[11] S. A. Abdullah, D. S. Ali, and A. J. Hameed, "A study of the biological activity of 4-(Para-Substituted phenyl)-1, 2, 3-Selenadiazole derivatives as anti-oxidant and anti-breast cancer," *Basrah J. Sci.*, vol. 38, no. 3, pp. 480–496, 2020.

[12] A. T. Abdulwahid and A. J. Hameed, "Synthesis, Characterization and Theoretical Study of 2, 4-diaryl-1, 3-Selenazole," *Biomed. Chem. Sci.*, vol. 3, no. 1, pp. 9–17, 2024.

[13] S. J. Dansereau and J. Sheng, "Heavy chalcogen properties of sulfur and selenium enhance nucleic acid-based therapeutics," *Biomolecules*, vol. 15, no. 2, p. 218, 2025.

[14] B. S. Patial, N. Thakur, and S. K. Tripathi, "Crystallization study of Sn additive Se–Te chalcogenide alloys," *J. Therm. Anal. Calorim.*, vol. 106, no. 3, pp. 845–852, 2011.

[15] P. G. Joshi, M. S. More, A. A. Jadhav, and P. K. Khanna, "Materials and biological applications of 1,2,3-selenadiazoles: a review," *Mater. Today Chem.*, vol. 16, p. 100255, 2020, doi: 10.1016/j.mtchem.2020.100255.