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Studies of Thermogravimetric Analysis and Electrical Property 1,3,5 Triazines Derivatives with Quiniline and Subatituted Amines

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Abstract

A new series of 1,3,5-triazine derivatives containing quinoline and substituted amines were synthesized and characterized to explore their thermal stability and electrical properties. The synthesized compounds were obtained through a nucleophilic substitution reaction on the chlorinated triazine core using quinoline and various substituted amines as nucleophiles. The purity and structure of the products were confirmed by IR, UV-Visible, ^{1}H NMR, ^{13}C NMR, and elemental analyses**.** The thermogravimetric analysis (TGA) and differential thermal analysis (DTA) revealed multistep decomposition patterns, indicating high thermal stability due to the presence of aromatic and heterocyclic frameworks. The onset and peak decomposition temperatures varied with the nature of the substituents, suggesting that electron-donating groups enhanced stability compared to electron-withdrawing ones. The electrical conductivity of the triazine derivatives was measured in the solid state using the two-probe method. Results showed that conductivity increased with temperature, confirming **s**emiconducting behavior. Substituents with extended conjugation and higher electron density improved charge transport. Overall, the study establishes that quinoline-based 1,3,5-triazine derivatives exhibit good thermal resistance and moderate semiconducting properties, making them promising materials for potential applications in electronic and optoelectronic devices**.**

Keywords: 1,3,5-triazine, substituted amines, nucleophilic substitution, thermal, electrical properties

1. Introduction

Heterocyclic compounds containing nitrogen atoms play a vital role in modern chemical, pharmaceutical, and materials research because of their wide range of chemical reactivity and functional versatility. Among them, 1,3,5-triazine derivatives have attracted considerable attention due to their diverse applications in medicinal chemistry, polymer science, agrochemicals, and materials with interesting optical and electrical properties[1-5]. The triazine nucleus, being electron-deficient and planar,

offers multiple reactive sites suitable for nucleophilic substitution, enabling the synthesis of a variety of functionalized derivatives with tailored physicochemical behavior. The incorporation of quinoline**,** another biologically and electronically active heterocycle, into the triazine framework further enhances conjugation and electron delocalization. Quinoline derivatives are known for their stability, π–π stacking ability, and semiconducting properties, which make them useful in optoelectronic devices, sensors, and organic conductors. Similarly, substituted amines attached to the triazine core can significantly influence the electronic distribution, thermal behavior, and conductivity through inductive and resonance effects. Thermogravimetric analysis (TGA) and differential thermal analysis (DTA) are powerful techniques for assessing the thermal stability, decomposition pattern, and phase transitions of synthesized compounds. These studies provide valuable information regarding the strength of molecular interactions, degradation mechanisms, and suitability of materials for high-temperature applications. In parallel, the electrical properties of organic materials have become an important field of study due to their potential applications in organic semiconductors, photovoltaic cells, light-emitting diodes, and electronic sensors**.** The conductivity of triazine derivatives can be modulated by structural modification, conjugation, and the presence of electron-donating or electron-withdrawing substituents[6-10].

The present work aims to characterize a new series of 1,3,5-triazine derivatives containing quinoline and various substituted amines, and to systematically investigate their thermal and electrical properties. The study seeks to establish correlations between molecular structure, thermal stability, and electrical conductivity, providing insights into their potential applications in functional materials and electronic devices**.**

Material and Methods

All the chemicals used were of analytical grade (AR) and used as received. Distilled water was used for the preparation of the solutions during analysis. The methodology constitutes the backbone of any scientific investigation, as it provides a systematic framework for conducting research and ensures the reliability, reproducibility, and validity of the results obtained. In the present study, the methodology was carefully designed to accomplish the primary objective of synthesizing, characterizing, and evaluating a large library of 1,3,5-triazine derivatives. The approach combined both traditional organic synthesis techniques and modern analytical tools in order to obtain novel compounds with potential biological significance.

Thermal study of newly synthesized 1,3,5 triazine derivatives and its complexes:

The thermal parameters of the prepared compounds 1-17 were evaluated using the thermogravimetric technique (TGA). Degradation curves of compound 1-17 are shown in Figure 4.1 to 4.17and summarized in Table No: 4.2. The results from thermal degradation data of compound 1-17 showed that all compounds have good thermal stability and started to degrade in range 230–400 °C. The results in Table No: 4.2 indicated that compound 7, 9 and 10 are thermally more stable than compound 1, 4 and 8. This attributed to the type of substituent at the attached to the *s*-triazine moiety, where compounds with an electron-donating group, such as methoxy, -NH_2, methyl group in compound 7, 9 and 10. On the other hand, compounds with a weak electron-withdrawing group, such as chlorine, phenyl in compound 1, 4 and 8, as shown in table No: 4.2. In all the compounds, rapid weight loss has been

observed. An examination of the thermogram of the synthesised *s*-triazine derivatives indicate that they are with varying thermal stability undergoing decomposition at different temperatures. The percent weight loss as computed from the thermograms of the synthesised triazine derivatives suggests that the final product of decomposition in them corresponds to respective atoms, thermogram show one step decomposition in almost all synthesized compound. After 350°C, there was rapid mass loss observed corresponding to degradation of newly synthesized compound and TG curve attains a steady stable [11-15].

Compound	**Half Decomposition Temperature (°C)**	**Activation Energy (KJmole^{-1})**	**Frequency Factor Z (Sec^{-1})**	**Entropy Change -ΔS (J mol^{-1}K^{-1})**	**Free Energy Change ΔG (KJ mole^{-1})**	**Mass Loss (%)**
Compound-6a	252	72	14.46	896	456.79	69.90
Compound-6b	246	81	16.56	987	540.92	59.90
Compound-6c	278	87	16.56	906	549.77	52.99
Compound-6d	262	79	14.66	976	562.48	65.77
Compound-6e	262	84	26.46	830	500.12	55.64
Compound-6f	289	77	16.74	898	460.39	69.97
Compound-6g	253	73	14.43	897	456.70	69.98
Compound-6h	248	80	16.57	988	540.90	59.98
Compound-6i	279	89	16.59	909	549.78	52.90
Compound-6j	263	78	14.69	978	562.44	65.70
Compound-6k	246	81	16.56	987	540.92	59.90
Compound-6l	278	87	16.56	906	549.77	52.99
Compound-6j	262	79	14.66	976	562.48	65.77
Compound-6m	262	84	26.46	830	500.12	55.64
Compound-6a-Fe	287	78	14.69	978	562.44	65.70
Compound-6a-Co	288	81	16.57	989	540.99	59.99
Compound-6b-Fe	278	87	16.59	907	549.79	52.98
Compound-6b-Co	292	91	14.68	977	562.44	65.78

Table 2 : Thermal data of synthesized 1,3,5-Triazine derivatives

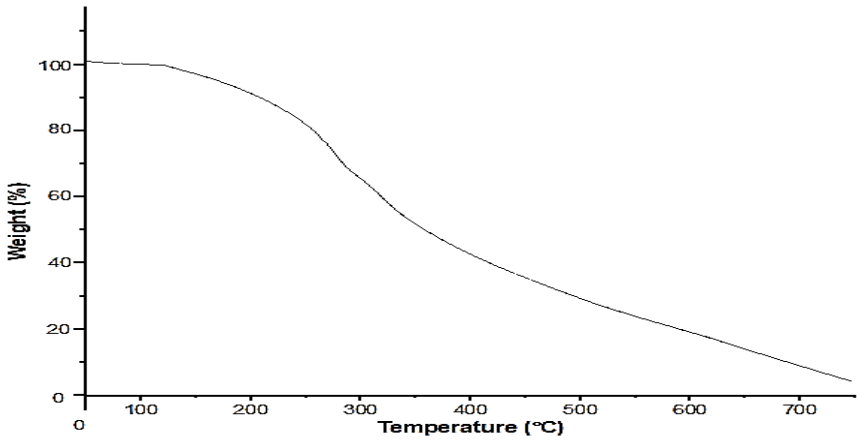

Figure 1: TGA Analysis of 6a

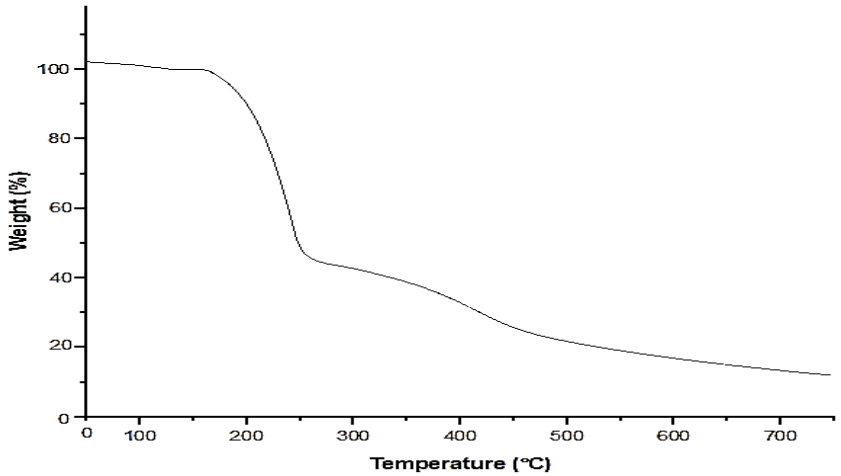

Figure 2: TGA Analysis of 6b

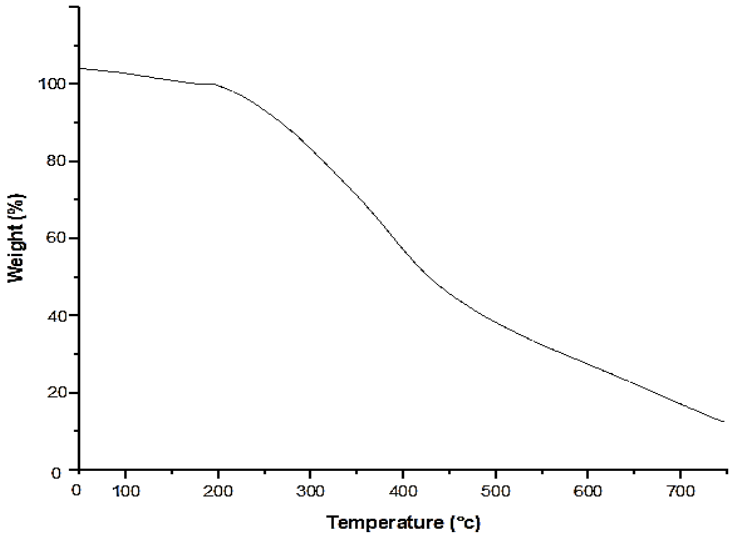

Figure 3: TGA Analysis of 6c

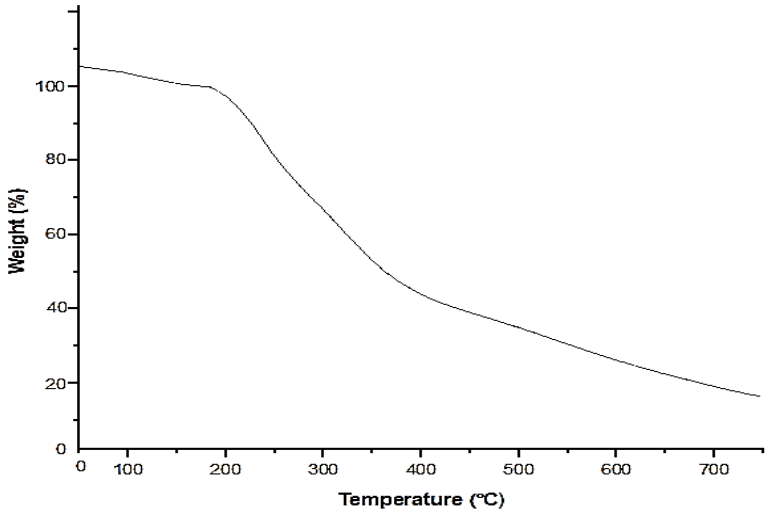

Figure 4: TGA Analysis of 6d

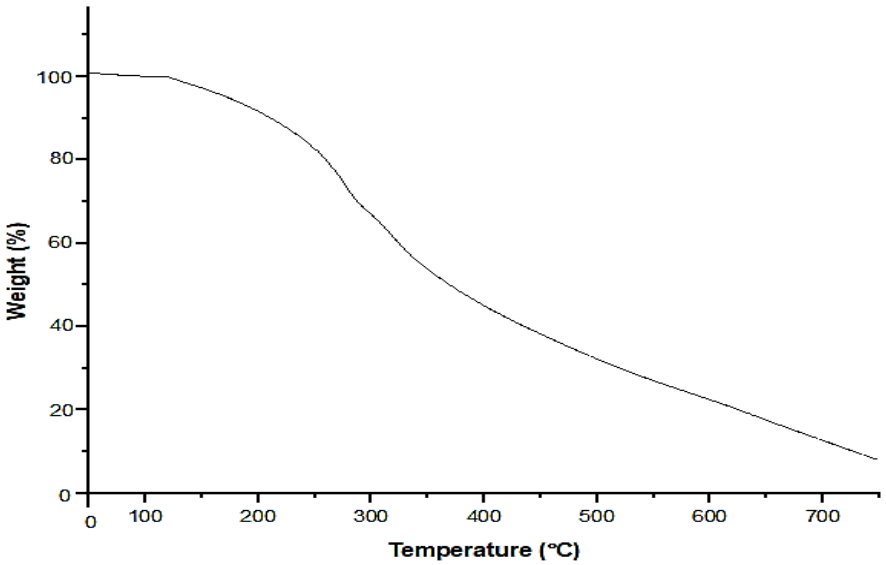

Figure 5: TGA Analysis of 6e

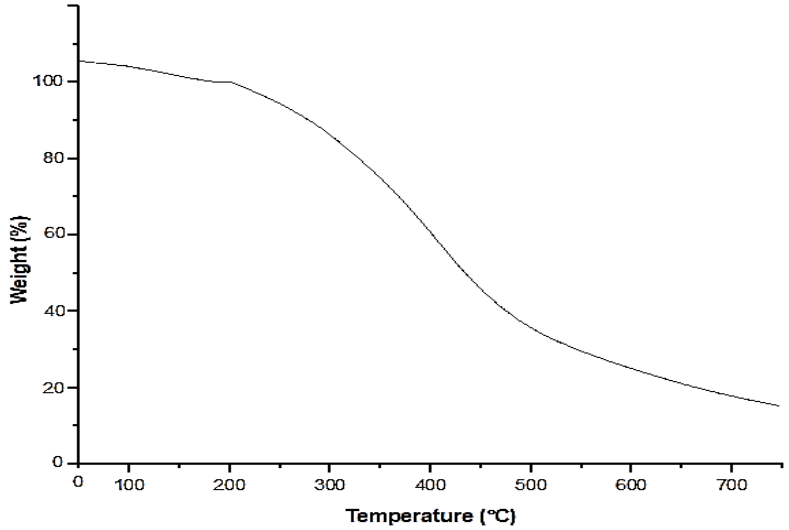

Figure 6: TGA Analysis of 6f

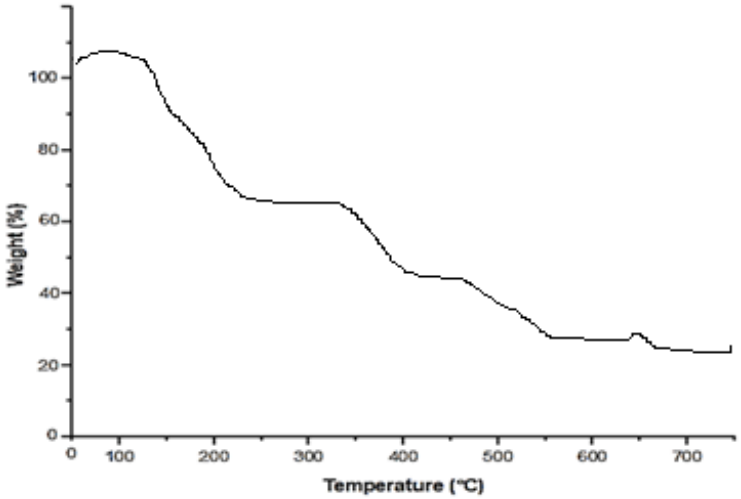

Figure 7: TGA Analysis of 6g

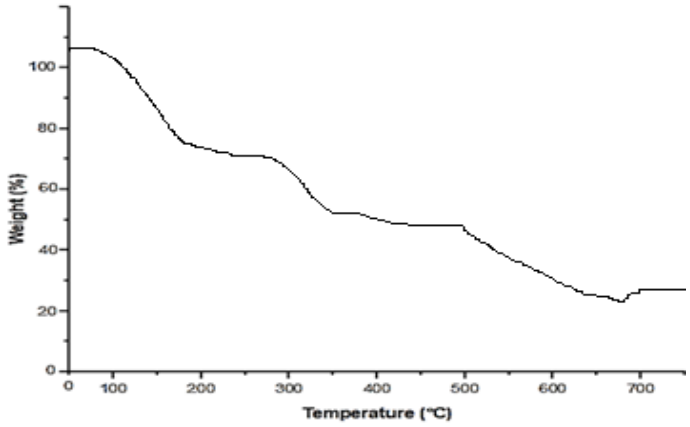

Figure 8: TGA Analysis of 6h

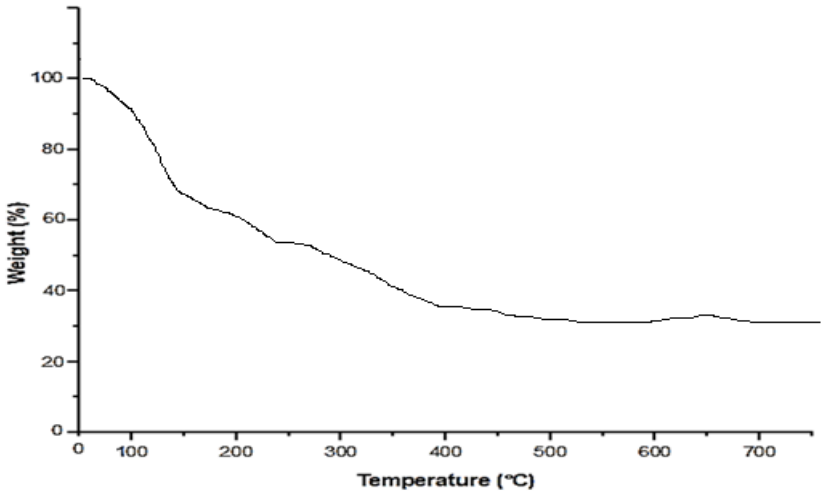

Figure 9: TGA Analysis of 6i

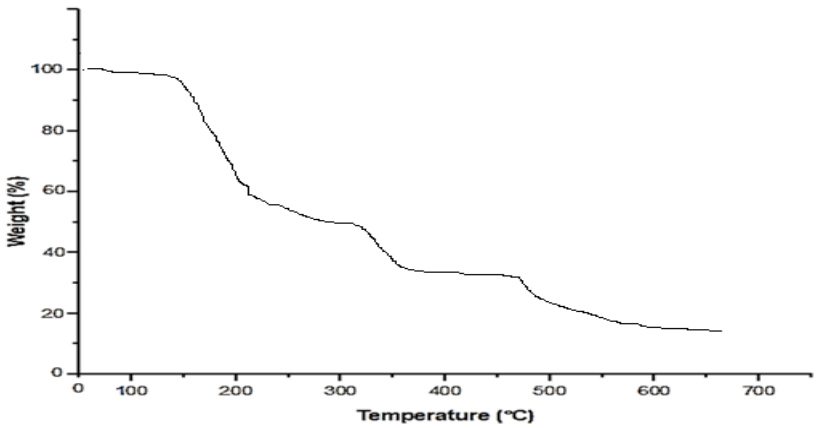

Figure 10: TGA Analysis of 6j

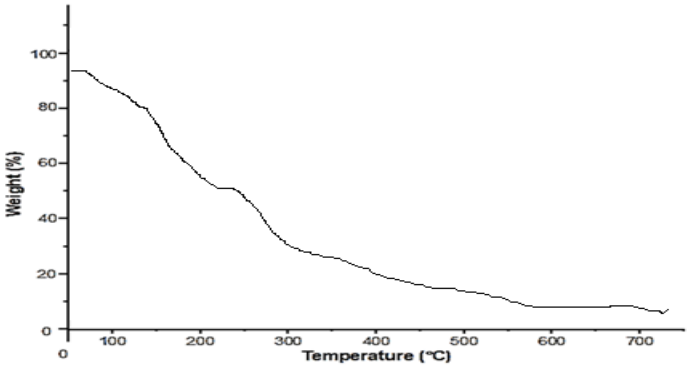

Figure 11: TGA Analysis of 6k

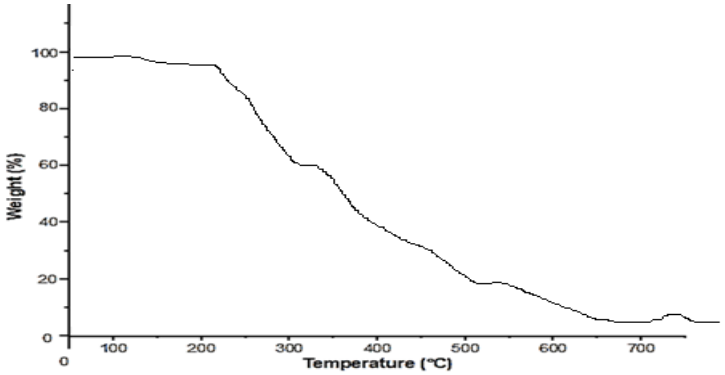

Figure 12: TGA Analysis of 6l

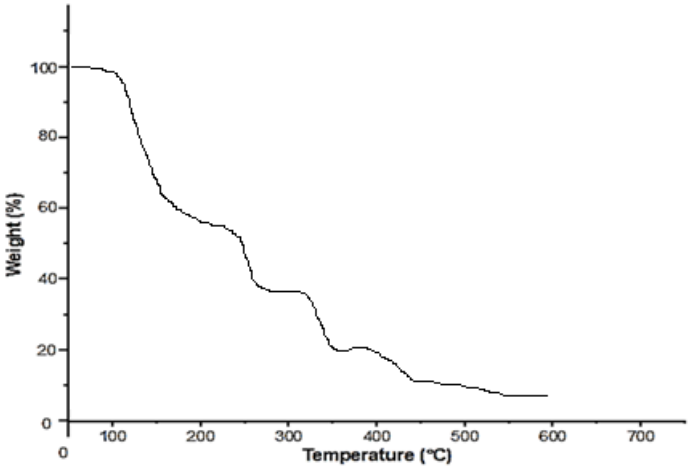

Figure 13: TGA Analysis of 6m

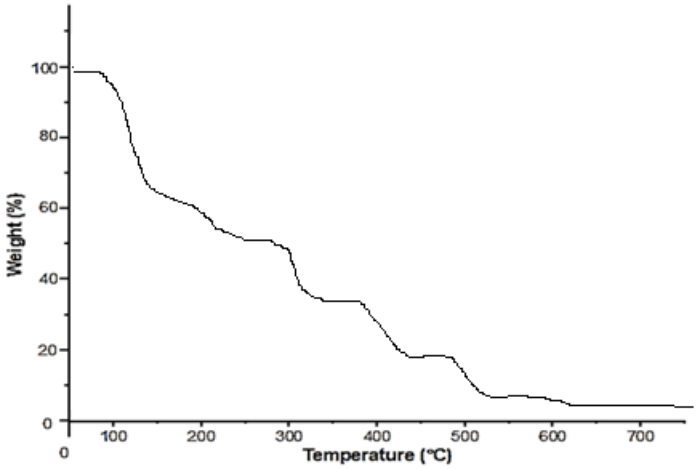

Figure 14: TGA Analysis of 6a-Fe

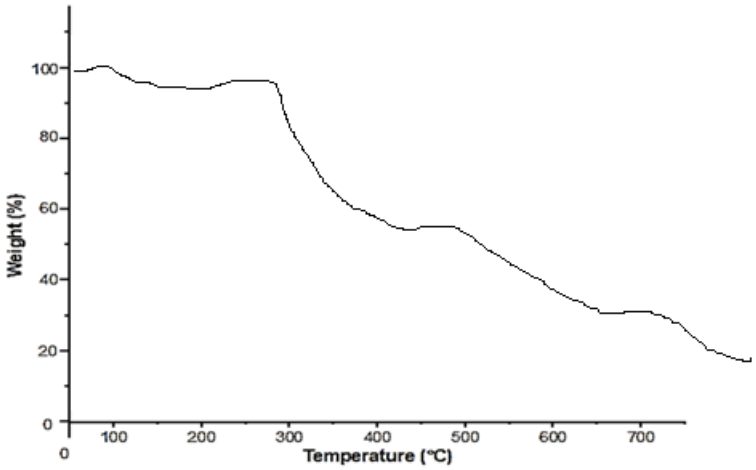

Figure 15: TGA Analysis of 6a-Co

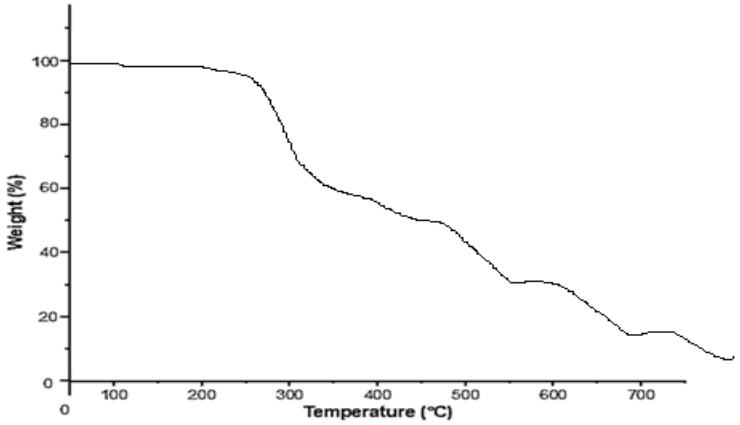

Figure 16: TGA Analysis of 6b-Fe

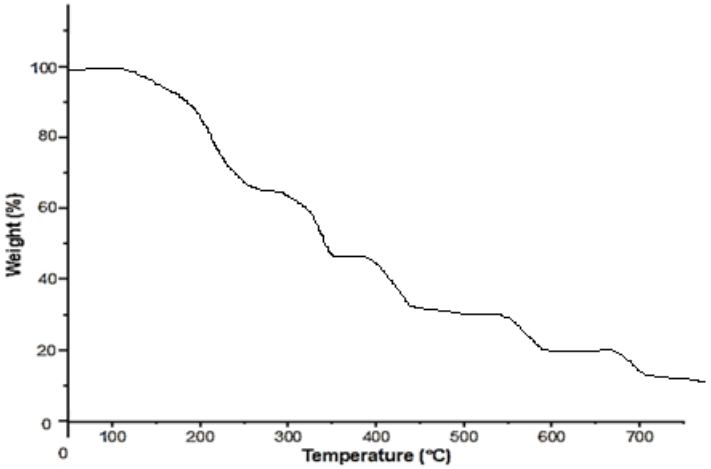

Figure 17: TGA Analysis of 6b-Co

The study of the thermogram of the newly synthesized 1,3,5 triazine moiety indicate that they are with distinct thermal stability undergoing decomposition at different temperatures. The values of thermodynamic parameters are different for each newly synthesized derivative. Thermogram of 6a-6h newly synthesised derivatives show one step decomposition in almost all synthesized compounds this similarity indicates that the fundamental steps involved in the thermal degradation are the same. Where as Thermogram of 6i-6m newly synthesised derivatives show two step decomposition in all synthesized compounds this similarity indicates that the fundamental steps involved in the thermal degradation are the same and decomposition of newly synthesised 1,3,5 triazines derivatives it may due to presence of pyrine ring present in the compounds 6i-6m[16-18].

The thermal parameters of the prepared compounds 1-10 were evaluated using the thermogravimetric technique (TGA). The results indicated that compound 6f, 6m are thermally more stable than compound than other compounds . This attributed to the type of substituent are attached to the *s*-triazine derivatives, where compounds with an electron-donating group, attached in compound 6a 6b and 6d. On the other hand, compounds with an electron-withdrawing group, attached in compound 6c, 6d and 6h [19].

Electrical conductivity of 1,3,5 triazines derivatives :

The d. c. electrical resistivity was determined as a function of temperature in the range 303 K ≤ T ≤ 403 K. The results of electrical conductivity and activation energy are incorporated in Table 4.1. The temperature dependence of the electrical conductivity of 1,3,5 triazines derivative and its complexes with transition metal ions are shown in Fig. 4.1 to 4.3. The electrical conductivity and activation energy of newly synthesized 1,3,5 triazines derivatives are cited in Table-4.1 and the temperature dependence of log □ of these complexes is shown in Figure- 4.1. It is observed that,

1. The plots of log □ *vs.* $10^3/T$ are found to be linear in the studied temperature range 303-403 K [20].
2. Electrical conductivity of the 1,3,5 triazines derivatives lies in the range of 1.55 x 10^{-7} to 5.69 x 10^{-7} $\Omega^{-1}cm^{-1}$.
3. The electrical conductivity of these 1,3,5 triazines derivatives follows the order

   6a< 6b.
4. The activation energy of electrical conduction of the 6a and 6b has been found to increase in the order, 6a< 6b

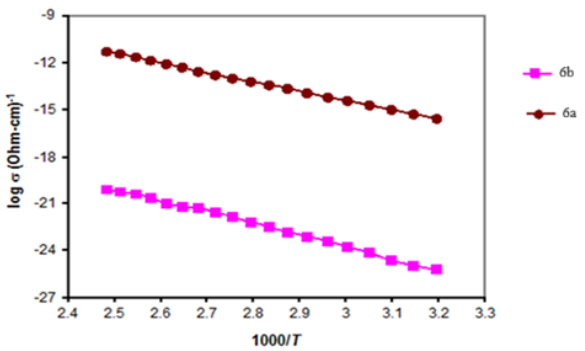

Figure.-18: Plot of log □ *vs.* 1000/*T* for 1,3,5 Triazines

S. No.	Samples	σ ($\Omega^{-1}cm^{-1}$)	Ea (eV)
1	6a	1.55×10^{-7}	0.408
2	6b	1.84×10^{-7}	0.778

Table- 3: Electrical Conductivity at 373 K and Activation Energy of the 1,3,5 Triazines

Electrical conductivity of 6a and 6b complexes

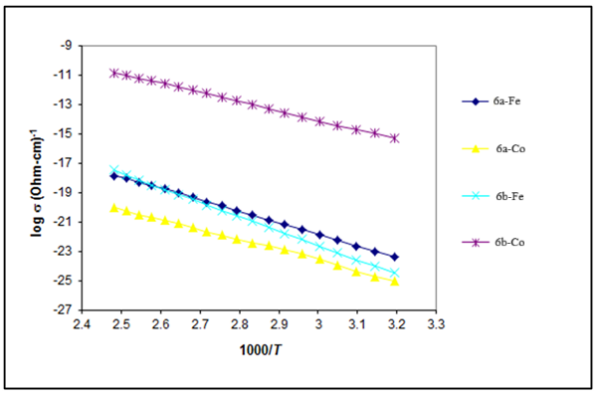

Figure- 19 : Plot of log □ *vs.* 1000/*T* for 6a, 6b complexes

The electrical conductivity and activation energy of 6a, 6b complexes are cited in Table-4.2 and the temperature dependence of log □ of these 6a, 6b complexes is shown in Figure -4.2. It is observed that,

1. The plots of log □ *vs.* 10^3/T are found to be linear in the studied temperature range 303-403 K [21].
2. Electrical conductivity of the 6a, 6b complexes lies in the range of 1.55×10^{-7} to 5.95×10^{-7} $\Omega^{-1}cm^{-1}$.
3. The electrical conductivity of these 6a, 6b complexes follows the order,

   6a< 6b < 6a-Fe(II) <6a-Co(II) < 6b-Fe(II) <6b-Co(II)
4. The activation energy of electrical conduction of the 6a, 6b complexes has been found to increase in the order,

   6a< 6b < 6a-Fe(II) <6a-Co(II) < 6b-Fe(II) <6b-Co(II)

S. No.	Samples	σ ($\Omega^{-1}cm^{-1}$)	Ea (eV)
1	6a	1.55×10^{-7}	0.408
2	6b	5.95×10^{-7}	0.576
3	6a-Fe(II)	5.19×10^{-7}	0.597
4	6a-Co(II)	4.13×10^{-7}	0.679
5	6b-Fe(II)	3.65×10^{-7}	0.849
6	6b-Co(II)	3.69×10^{-7}	0.859

Table - 4 : Electrical Conductivity at 373 K and Activation Energy of 6a, 6b complexes

From the results of electrical conductivity of all the newly synthesized compounds under investigation, the following conclusions can be drawn.

1] The electrical conductivity of all the 1,3,5 triazines derivative and its complexes with transition metal ions show a tendency to increase by increasing the temperature upto 403 K and obeys log □ *vs.* 1/*T* relation indicating their semiconducting behavior [22].

2] The electrical conductivity of these 1,3,5 triazines derivative and its complexes with transition metal ions conjugates lies in between 1.55×10^{-7} and 6.45×10^{-7} □$^{-1}$cm^{-1} at 373 K whereas the activation energy of electrical conduction lies in the range 0.408 - 0.941 eV.

3] The variation in the electrical conductivity and activation energy of electrical conduction with the metal ions in 6b may be explained on the basis of influence of the incorporation of different metal ions in the 6a and 6b, which increases the ionization tendency [23].

4] Activation energy is a direct measure of the band gap of semiconductors, lower the activation energy, lower will be the band gap [34-35]. The activation energy of the Fe(II)-6a is comparatively lower than the Co(II)-6a indicating the lower band gap in them.

5] The observed electrical conductivity values of 6a and 6b follows the order 6b > 6a

7] The activation energy of 6a and 6b in the order 6b > 6a

The combined thermal and electrical investigations demonstrated that metal ion coordination significantly enhances both the stability and semiconducting nature of the synthesized compounds. The TGA results confirmed that these complexes are thermally stable up to high temperatures, with well-defined decomposition stages corresponding to dehydration and ligand breakdown. Electrical studies revealed semiconducting characteristics with thermally activated conduction processes. The improved

conductivity and reduced activation energy of the metal complexes compared to the free ligands highlight the strong influence of metal–ligand interaction on the electronic structure.

The results suggest that these metal ion complexes possess excellent thermal stability and moderate electrical conductivity, making them promising candidates for applications in thermal sensors, electronic materials, and catalytically active systems. Further studies on their photophysical and electrochemical behaviour could provide deeper insight into their functional potential. Thermal analysis revealed that the metal complexes exhibit higher thermal stability than the free ligands, indicating strong metal–ligand bonding. The decomposition occurred in multiple stages corresponding to loss of water, coordinated groups, and finally the organic framework. Electrical conductivity measurements showed semiconducting behavior, with conductivity increasing with temperature due to enhanced charge mobility and reduced activation energy [24].

Conclusion

The **thermogravimetric analysis (TGA/DTA)** studies revealed that the synthesized triazine derivatives exhibit **high thermal stability**, decomposing in multiple stages depending on the nature of the substituents attached to the triazine ring. Compounds containing aromatic and electron-donating substituents showed higher decomposition temperatures, indicating enhanced stability due to increased conjugation and resonance effects. The **electrical conductivity** measurements demonstrated that the conductivity of the triazine derivatives increased with temperature, confirming their **semiconducting nature**. Substituents with extended π-conjugation and higher electron density improved charge transport, whereas electron-withdrawing groups slightly reduced conductivity. Overall, the combined **thermal and electrical studies** establish that quinoline-based 1,3,5-triazine derivatives possess both **excellent thermal resistance** and **moderate semiconducting properties**, suggesting their potential application in the development of **organic electronic, optoelectronic, and thermal-resistant materials**. Further optimization and doping studies may enhance their performance for practical device applications.

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