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Calculations of Kinetic and Thermodynamic Parameters for Thiourea Single Crystals

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Abstract: Single crystals of Thiourea (NH_2CSNH_2) were obtained through simple and inexpensive evaporation technique. The Differential Scanning Calorimetric analysis was also used to identify the purity and melting point (T_m) of the grown crystal. Thermo Gravimetric Analysis has proved useful for evaluating kinetic parameters of various reactions of materials and provides valuable quantitative information regarding the stability of materials. Using the basic relations of thermodynamically variables, Entropy ΔS, Enthalpy ΔH and Gibb's free energy ΔG were calculated using Horowitz-Metzger relation and summarized in present communication.

Keywords: Thiourea, Thermo Gravimetric Analysis, Differential Scanning calorimetric, Thermodynamic parameters, Horowitz-Metzger relation.

I. INTRODUCTION

In recent trends of technology there has been increased need of organic and semi organic materials for Non Linear optical (NLO) applications. The beauty of single crystals is fascinating. The sharpen of their colors and flatness of shape are very fascinating. Stability and reactivity on the surface of grown crystals are utmost important for their applications. Single crystals of Thiourea (NH_2CSNH_2) were grown using simple and inexpensive evaporation technique. The studies of thermal behavior and more significantly the kinetics of degradation is useful in predicting the behavior of crystals stability and a useful aid in the determination of various bonds within the crystals. Methods for determining the Activation Energy ΔE from a thermo gravimetric curves are available in literature. For the case of Thiourea crystals a small quantity of material is employed in Thermal Gravimetric Analysis, and the barriers between the thermal and diffusion processes are very negligible, hence it is reasonable to assume of the Arrhenius relation. In the present work, the method Horowitz-Metzger relation are used and thermodynamically parameters are calculated.

II. EXPERIMENTAL

Single crystals of Thiourea (NH_2CSNH_2) a promising organic material is grown through simple and inexpensive slow evaporation technique. This material has good chemical flexibility to provide nonlinearity of organic material and strong mechanical property of inorganic material. The thermo grams of grown Thiourea crystals are shown in Fig:1.

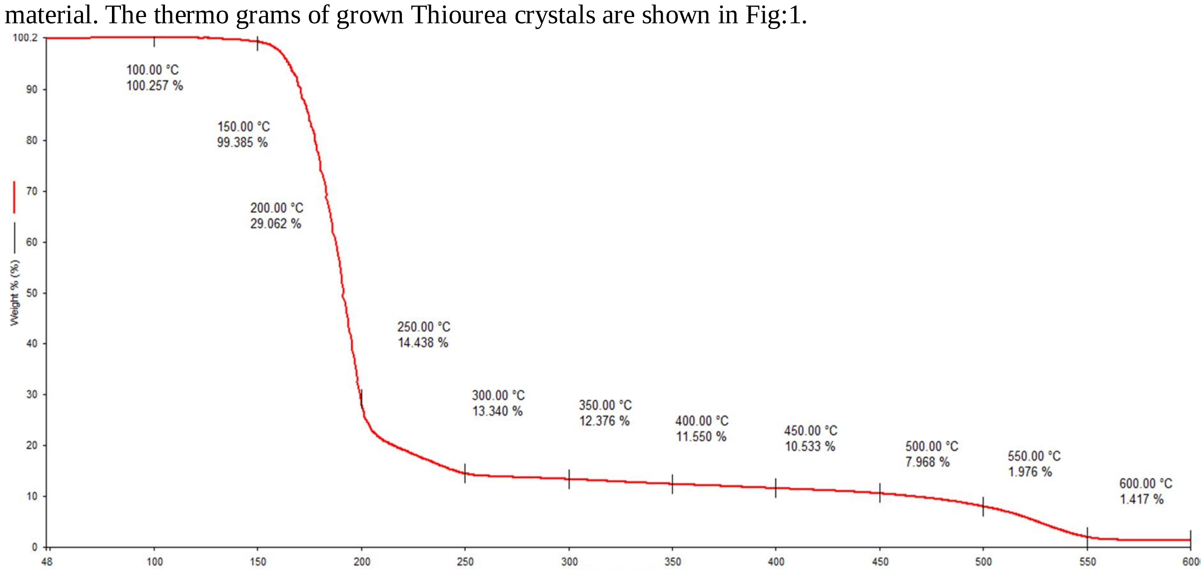

Figure:1: thermogram of thiourea crystal

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Differential scanning calorimetry analysis was used to identify the purity and melting point of the grown crystal. In the thermo gram only one endothermic stage was found. At 179.74°C initiation of phase change started and competed at 182.96°C. Area under the curve was 553.372mJ and heat of transition was 197.9865J/g. Fig: 2.

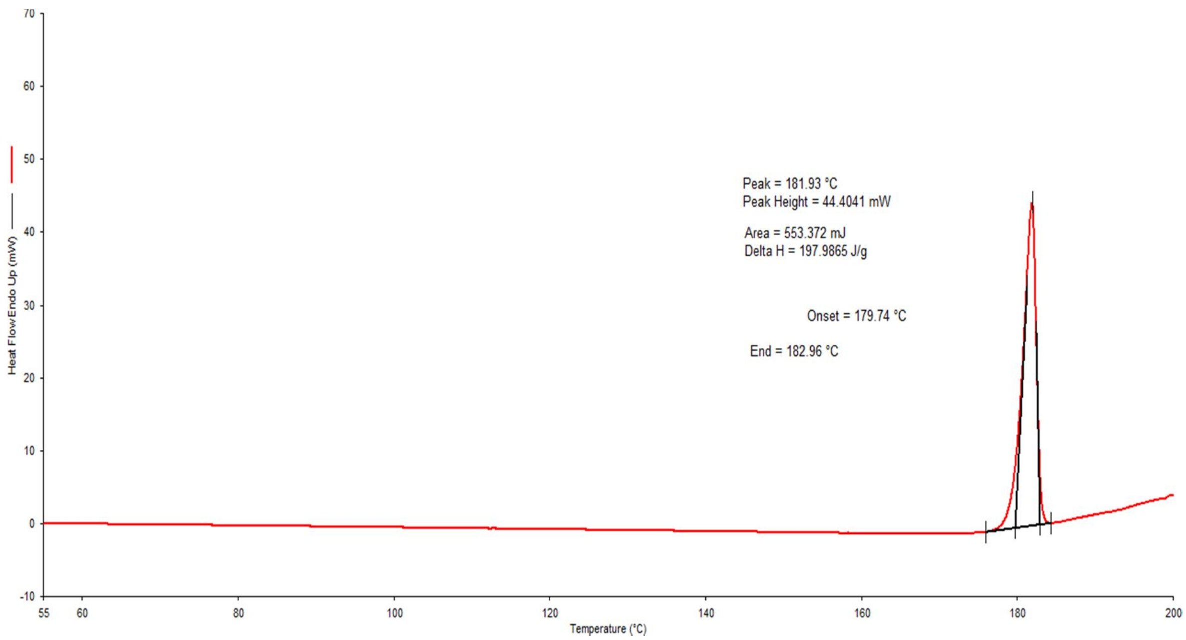

Figure:2: differential scanning calorimetry

III. CALCULLATION

In order to understand the kinetics of solid state reactions leading to the gradual, sequential decomposition of the material for calculation of kinetic and thermodynamic parameter, Horowitz-Metzger relation was used:
Methods for determining activation energy from a thermo gravimetric curve are available in literature. Horowitz and Metzger gave a energy, but this required the order of the reaction to be determined first. Krevelen and co-workers described a method for Interpretation of thermo gravimetric traces, based on the approximate integration of the basic equation.

$-dF / F^{n} = k_{0} / a^{*} (e^{-A/T})\, dT$

Where $F = 1 - \alpha$ denotes the fraction of reactant remaining at the end of pyrolysis, n = order of the reaction, k_0 = the pre-exponential part of the rate constant, a = the rate of temperature rise and $A = E/R$.
By applying second approximation we can finally write

$$\log\left[\frac{1-(1-\alpha)^{1-n}}{1-n}\right] = \frac{E\theta}{2.303\, RT_m^2}$$

where, $n \neq 1$ i.e. $n = \frac{1}{2}, \frac{1}{4}, \frac{2}{3}$ etc.
Here $\theta = T - T_m$

where, T_m = temperature at half reaction is over.
A = weight loss up to a particular temperature/total weight loss in the step involved n = fraction of reactant used.
The graph plot of $\log\left[\frac{1-(1-\alpha)^{1-n}}{1-n}\right] \rightarrow \theta$ for each steps are drawn. Then Evidently a fitted linear dependence observed is ½. From the slop of the graph,

Activation energy (E) has been calculated and from the intercept frequency factor is also calculated and recorded.
Activation energy E (eV) = slope x T_m^2 x R (R=Gas Constant)

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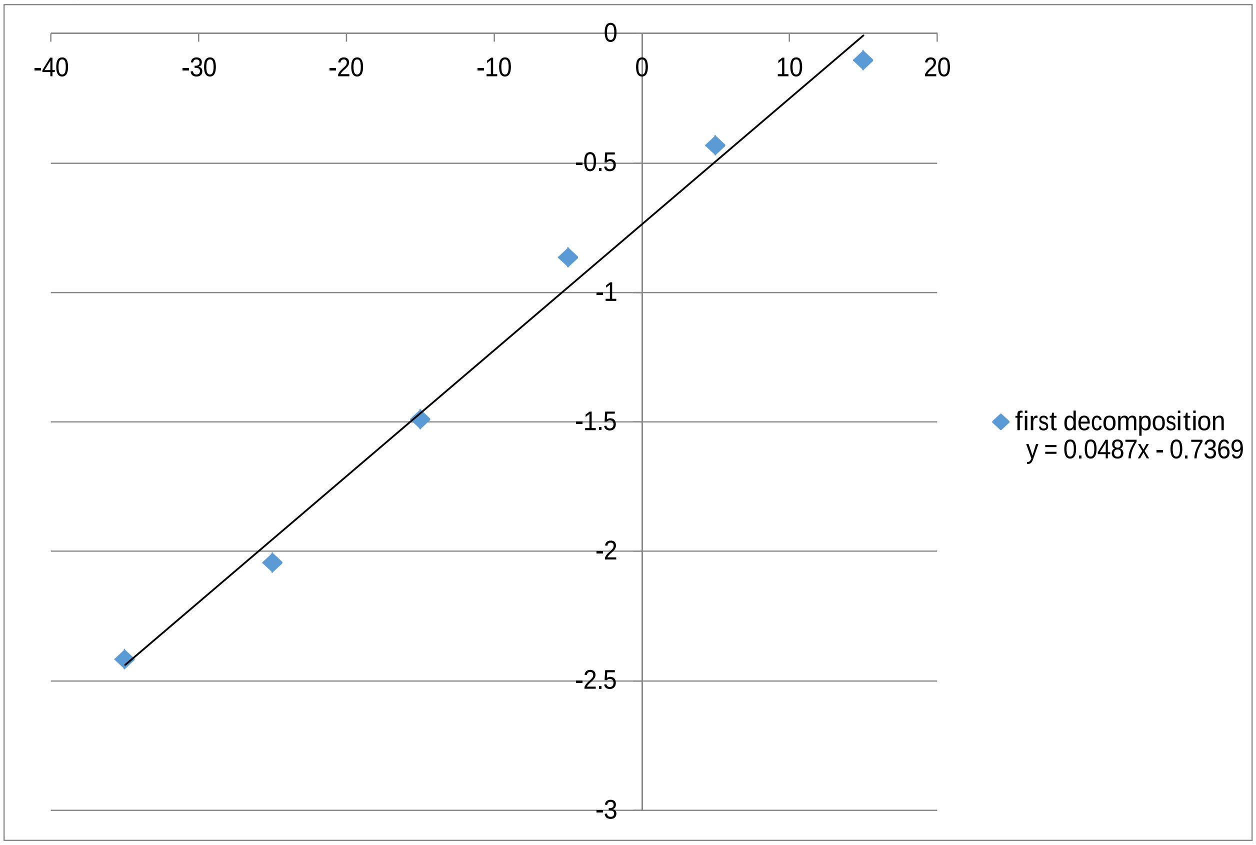

Figure:3(a): Plot of Log{(1-(1-α)(1-n)/(1-n)} Vs ϴ (first decomposition n=1/2 Tm=448.15 We=70.966)

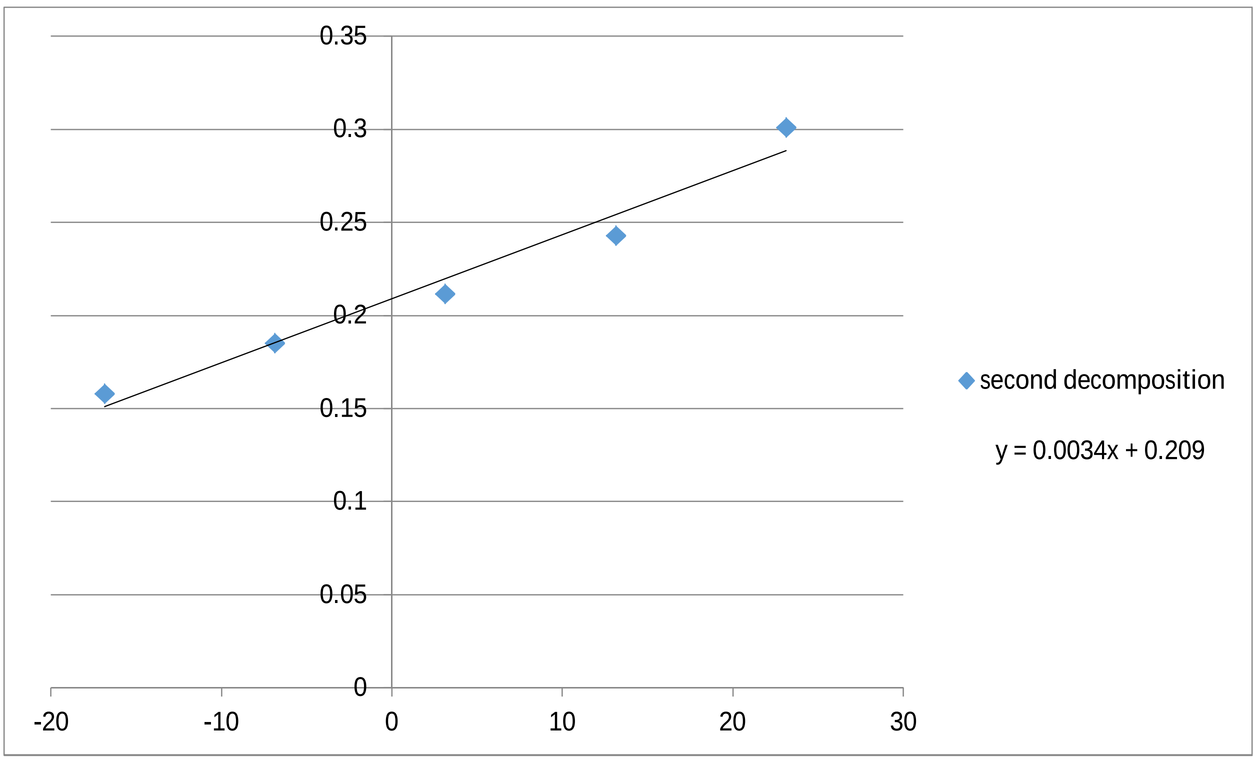

Figure:3(b): Plot of Log{(1-(1-α)(1-n)/(1-n)} Vs ϴ second decomposition n=1/2 Tm=500 We=85.59

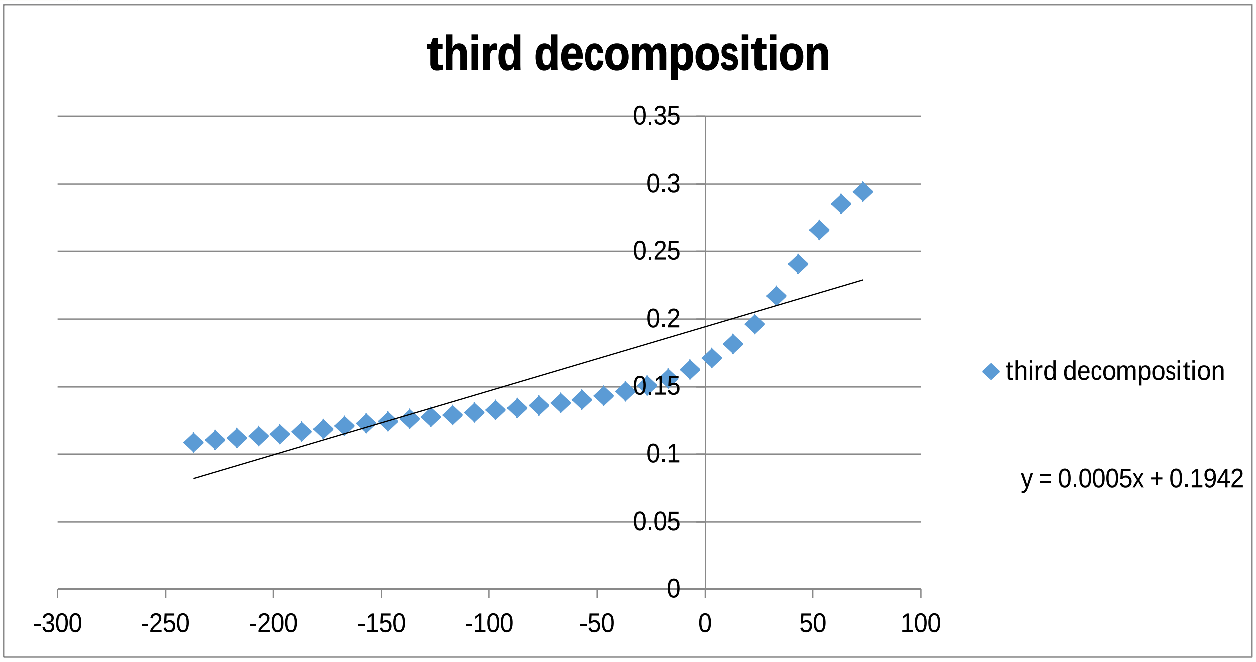

Figure:3(c): Plot of Log{(1-(1-ɑ)(1-n)/(1-n)} Vs ϴ third decomposition n=1/2 Tm=770 We=98.642

IV. RESULTS

The graph is shown in Figure: 3(a), 3(b),3(c) and the calculated parameters are summarized in table: 1

Stage	Entropy ΔS eV/K	Enthalpy ΔH eV/mole	Gibb's Free Energy ΔG Ev
1	-1.5337×10^{21}	-4.5473×10^{22}	63.3876×10^{22}
2	-1.6375×10^{21}	-5.2221×10^{22}	77.3951×10^{22}
3	-1.6572×10^{21}	-7.0899×10^{22}	106.1422×10^{22}

Table: 1 calculated parameters using Horowitz-Metzger relation.

V. CONCLUSION

Thiourea (NH_2CSNH_2) organic single crystals are successfully grown by using relatively simple and inexpensive slow evaporation of aqueous solution technique. This material has good chemical flexibility to provide non linearity of organic material and strong mechanical property of inorganic material. Kinetic parameters like, Entropy ΔS, Enthalpy ΔH and Gibb's free Energy ΔG are calculated using basic thermodynamically relations.

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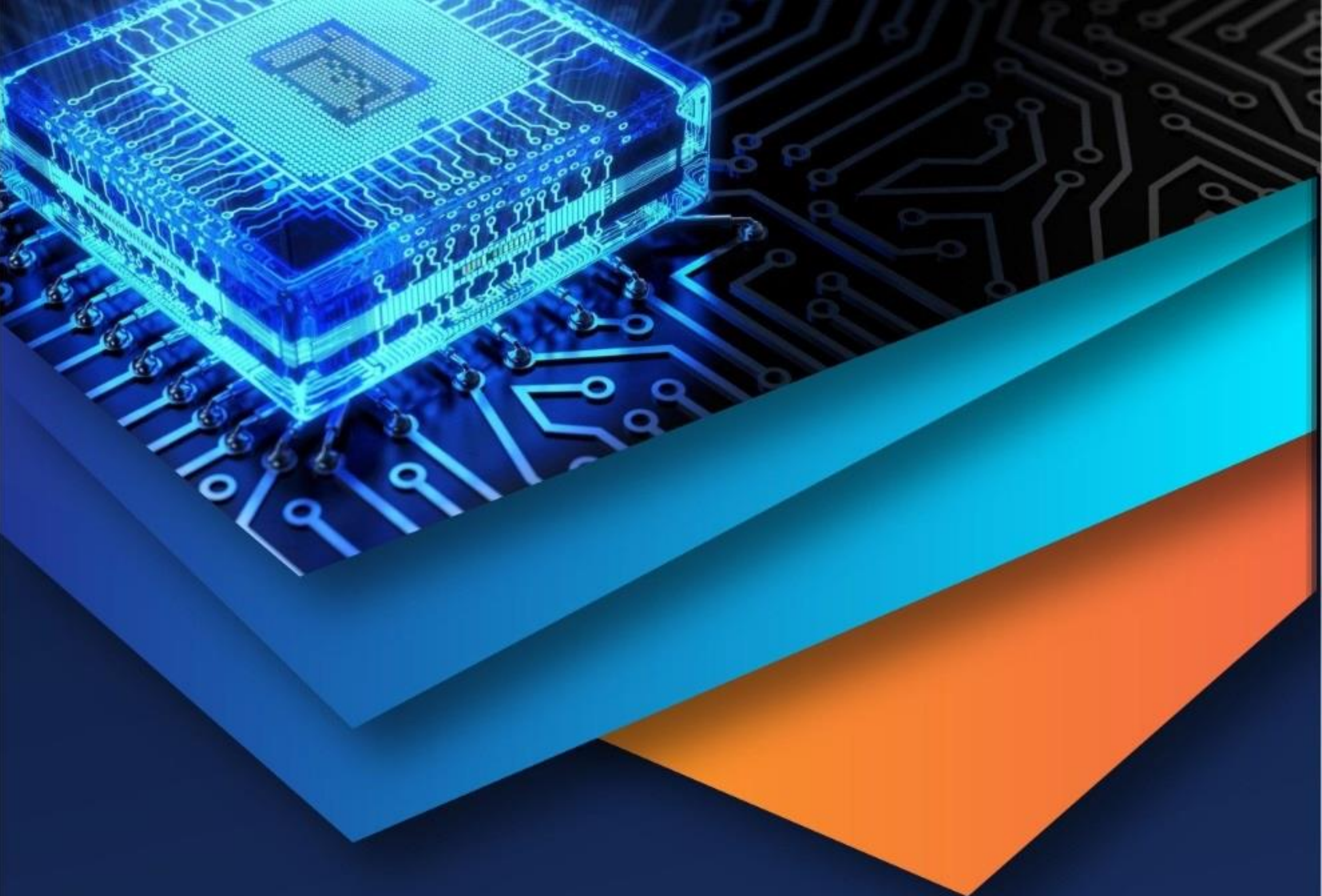

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