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Solid State Kinetics Of Fe(III) Complex Derived From Schiff Base Of 5-Anilino-1,2,3,4-Thiatriazole

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Abstract

Thermal analysis has become an established technique for understanding the thermal stability and decomposition behavior of coordination compounds. The Iron(III) complex $[FeL_2Cl_2]Cl$, where L is a Schiff base derived from 5-anilino-1,2,3,4-thiatriazole (ATT), was synthesized and characterized by elemental analysis and thermogravimetric study. The molecular weight of the complex was found to be 520.25 mg. Thermogravimetric analysis (TGA) revealed a three-step decomposition pattern corresponding to the loss of moisture and chloride ions, decomposition of the ligand, and formation of Fe_2O_3 residue. The kinetic parameters were determined using Freeman–Carroll and Doyle–Zsako methods. The activation energies were found to be 12.99 kcal·mol^{-1} and 12.00 kcal·mol^{-1} respectively, with the order of reaction ≈ 0.1 in both cases. The consistency of results obtained by two methods confirms the reliability of the kinetic evaluation and indicates moderate thermal stability of the complex.

Keywords: Solid state kinetics, thermogravimetric analysis, Schiff base, iron complex, Freeman–Carroll method, Doyle–Zsako method

I.Introduction

Transition metal complexes of Schiff bases containing nitrogen, oxygen, and sulphur donor atoms have gained importance due to their structural diversity and wide range of applications in catalysis, materials chemistry, and bioinorganic processes. Thermal decomposition studies of such complexes provide essential data regarding their stability, decomposition mechanism, and bonding environment in the solid state.

Thermal analysis methods such as the Freeman–Carroll and Doyle–Zsako approaches are widely used for calculating kinetic parameters like activation energy, order of reaction, and frequency factor.

In the present study, a Schiff base derived from 5-anilino-1,2,3,4-thiatriazole was coordinated with Iron(III) chloride to form a complex $[FeL_2Cl_2]Cl$. The thermal behavior and kinetic parameters of this complex were studied to understand its decomposition mechanism and thermal stability.

II. Experimental

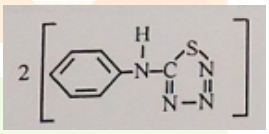
The Schiff base ligand was synthesized by the condensation of 5-anilino-1,2,3,4-thiatriazole with the appropriate aldehyde in ethanol under reflux. The Iron(III) complex was prepared by refluxing an ethanolic solution of $FeCl_3$ (1 mmol) with an ethanolic solution of the ligand (2 mmol) for 3–4 hours. The obtained precipitate was filtered, washed with ethanol and distilled water, and dried in a desiccator.

Thermogravimetric analysis (TGA) of the complex was carried out in air at a constant heating rate of 10°C/min, and the data were analyzed using the Freeman–Carroll and Doyle–Zsako methods for kinetic parameter determination.

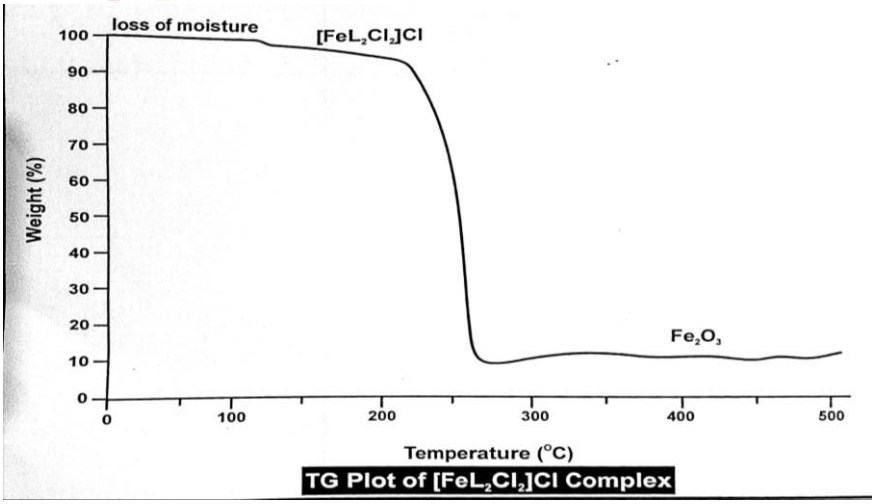
III. Results and Discussion

III.I Thermal Decomposition Profile

Table:1

S.No.	Temperature Range (°C)	Species Decomposed	% Weight Loss (Found)	% Weight Loss (Calculated)
1	100–200	Loss of moisture and $3Cl^-$ ions	19.10	20.12
2	200–250	Loss of whole ligand moiety 	62.52	63.00
3	260–300	Formation of Fe_2O_3 residue	10.24	10.88

- **TG Curve of $[FeL_2Cl_2]Cl$ Complex:**



TG Plot of $[FeL_2Cl_2]Cl$ Complex

Fig.1

• Initial weight at 100°C = 0.96118 mg

• Final weight at 260°C = 0.20817 mg

The total weight loss corresponds closely with calculated values, confirming a three-step decomposition pattern. The TG curve shows smooth weight reduction, indicating homogeneous decomposition and formation of Fe_2O_3 residue.

III.II Freeman–Carroll Method

Table:2

S.No.	Temp (°C)	Weight	$\frac{\Delta \log \frac{dw}{dt}}{\Delta \log Wr}$	$\frac{\Delta T^{-1} \times 10^{-3}}{\Delta \log Wr}$
1	200	0.83764	-2.50001	1.09989
2	210	0.77034	-1.0124	0.40882
3	220	0.70262	-0.04004	0.20001
4	230	0.62625	-0.71648	0.57636
5	240	0.53208	-0.82098	0.34972
6	250	0.40921	-0.55773	18.29680

•Freeman–Carroll Plot of $FeL_2Cl_2]Cl$ Complex:

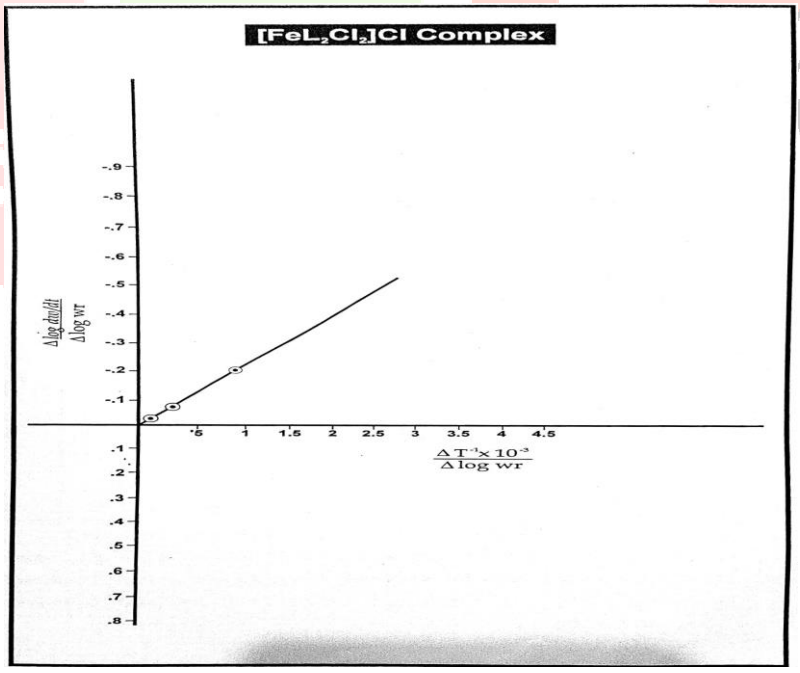


Fig.2

• Initial weight at 180°C = 0.96118 mg

• Final weight at 260°C = 0.20817 mg

From the Freeman–Carroll plot, the slope corresponds to an activation energy (Ea) = 12.99 kcal·mol^{-1} and the intercept indicates an order of reaction n = 0.1. The linearity of the plot confirms a single-step kinetic process.

III.III Doyle–Zsako Method

• Average activation energy (Ea) = 12.00 kcal·mol⁻¹

• Order of reaction (n) ≈ 0.1

The close agreement between Freeman–Carroll and Doyle–Zsako results confirms reproducibility. The reaction proceeds with a low activation barrier, reflecting moderate stability of Fe–ligand coordination.

III.IV Comparison of Kinetic Parameters

Table:3

Method	Order of Reaction	Activation Energy (kcal·mol⁻¹)
Freeman–Carroll	0.1000	12.99897
Doyle–Zsako	0.1	12.0000

Both kinetic models yielded comparable activation energies and reaction orders. The slight deviation is within acceptable experimental limits, confirming data reliability. The Fe(III)–ligand bond system shows moderate stability typical of Schiff base complexes.

IV. Conclusion

The Fe(III) complex $[FeL_2Cl_2]Cl$ undergoes a three-step thermal decomposition as confirmed by TGA. Kinetic parameters obtained by both Freeman–Carroll and Doyle–Zsako methods show good agreement, confirming the reliability of these models. The moderate activation energy indicates a stable but not highly refractory complex, supporting its suitability for comparative kinetic studies among transition metal Schiff base systems.

V. Future Scope

1. Comparative thermal and kinetic studies of Co(II), Ni(II), Cu(II), and Zn(II) analogues.
2. Study of spectral and magnetic behavior to correlate structure and bonding.
3. Investigation of antimicrobial and catalytic activity of Fe(III)–Schiff base complexes.
4. DFT-based computational modeling to understand stability and electronic transitions.

VII. References

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