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Thermal Decomposition Kinetics of Cobalt(II) and Nickel(II) Complexes of Substituted Isoxazole and their Antibacterial Activity

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5-Amino-3(4-dimethyl amino phenyl) isoxazole-4 carboxylic acid complexes of cobalt(II) and nickel(II) have been subjected to thermal decomposition studies in air using TG and DTG techinique. The kinetic parameters for all the stages of decomposition of these complexes were computed by a weighted least squares method—the Coats-Redfern equation.

Isoxazole with suitable substitution constitute an interesting class of chelating agents capable of co-ordination with one or more metal ions and thus forms mononuclear metal complexes. As a part of our studies on the thermal decomposition studies of transition metal complexes, we have synthesized and characterized cobalt(II) and nickel(II) complexes of 5-amino-3(4-dimethyl amino phenyl) isoxazole-4-carboxylic acid. Thermal behaviour and decomposition kinetics of these complexes have been studied and the results of these studies are described in this paper.

The ligand and its metal complexes were prepared by the procedure reported earlier[1, 2] respectively.

Thermal studies were carried out with Perkin-Elmer 3700 thermal analyzer. The operational charactersitcs were as follows: heating rate 10°C/min; sample size 2 to 6 mg; atmosphere static air; crucible platinum; the evaluation of kinetic parameters order (n); energy of the activation (E_a); entropy of activation (ΔS) and pre-exponential factor (A), using the Coats-Redfern equation.[3] These were based on a computer programme.

The molecular formulae of the complexes were found to be $(C_{12}H_{12}N_3O_3)_2M{\cdot}2H_2O$ ($M = Co^{2+}$ or Ni^{2+}). The proposed structure of the complexes is shown in Fig. 1.

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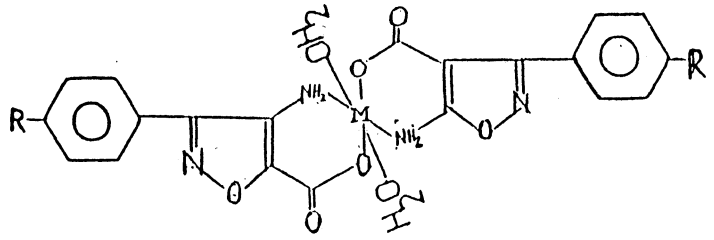

R = —N $\begin{matrix} CH_3 \\ CH_3 \end{matrix}$ M = Co^{2+} or Ni^{2+}

Fig. 1

The thermal behaviour of the complexes is shown in Fig 2. The complexes are stable upto 100°C. Thermo-analytical data for complexes are presented in Table-1. The percentage mass loss and probable composition of lost groups are given in this Table-1.

TABLE-1
THERMAL DECOMPOSITION DATA OF THE COMPLEXES

Complexes	Decomposition temperature range in TG (°C)	Peak temperature in DTG (°C)	Total loss of weight (%)		Probable composition of lost groups
			From TG	Theoretical	
Co complex	100–160	120	3.75	6.25	$2H_2O$
	160–380	310	45.00	43.65	$2CO_2$, $2NH_2$, $2N<\begin{matrix} CH_3 \\ CH_3 \end{matrix}$
	450–610	570	88.30	89.45	L
Ni complex	100–300	211	47.12	43.67	$2H_2O$, $2CO_2$, $2NH_2$, $2N<\begin{matrix} CH_3 \\ CH_3 \end{matrix}$
	440–580	539	88.04	89.49	L

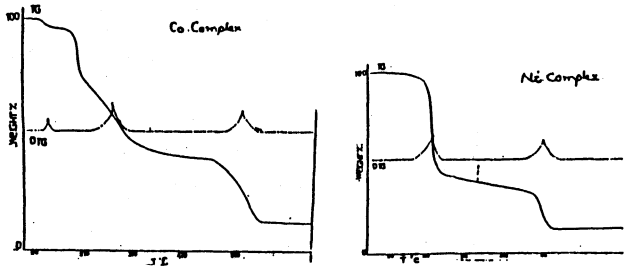

Fig. 2 TG and DTG curves.

Decomposition Kinetics

Various methods have been used for the calculation of kinetic parameters from TG data.[4,5] In the present case, the kinetic parameters n, E_a, ΔS and A for the

complexes have been calculated using the Coats-Redfern equation and results are presented in Table-2. The kinetic parameters were evaluated under the similar experimental conditions[6,7] (same heating rate, furnace atmosphere and sample weight etc.).[6,7]

TABLE-2
KINETIC DATA

Complexes	Stage	Order "n"	Ea (kJ mol^{-1})	ΔS (kJ mol^{-1} K^{-1})	A (S^{-1})
Co complex	I	1.23	20.8	–293	0.394×10^{-2}
	II	1.25	37.4	–283	0.189×10^{-1}
	III	0.94	253.5	–59	0.142×10^{11}
Ni complex	I	1.40	109.8	–139	0.550×10^{6}
	II	1.03	270.7	–30	0.484×10^{12}

In nickel(II) complex,—E_a values for the first stage decomposition were found to be lower than the second stage of decompositin. This shows that the rate of reaction is fast during the first decomposition. The negative ΔS value indicates a more ordered activated structures than the reactants.

In cobalt(II) complex, the three stage decomposition has successively lower values for E_a. The activation of energy indicats faster rate for the successive decomposition. The negative ΔS values for this complex indicate a more ordered activated structure than the reactants.

Evaluation of Antibacterial Activity

The anti-bacterial activity of the test compounds was carried out against four microorganisms (one gram –ve and three gram +ve). The tests were carried out by the cup-plate method.[8–11] The results of antibacterial testing were presented in Table-3.

TABLE-3
ANTIBACTERIAL ACTIVITY OF COMPOUNDS

Name of the compounds	Zone of inhibition after 24 h (in mm)			
	Escherichia coli	*Bacillus subtilis*	*Bacillus vulgaris*	*Staphylococcus aureus*
Ligand	14	13	14	16
Co complex	17	18	20	17
Ni complex	15	15	15	15
Ampicillin	32	25	28	28
Chloramphenicol	30	36	28	34
Norfloxacin	32	33	32	40
Ciprofloxacin	30	27	28	40

The antibacterial activity of the ligand and its complexes were compared with standard drugs. It was observed that the activity of the ligand and complexes is less than the activity shown by the standard drugs.

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