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NOTE

Kinetic Parameters of Ternary Complex of Copper(II) with Amino Acids using Thermogravimetric Analysis

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1 : 1 : 1 Ternary complex of copper(II) using proline and leucine has been synthesized. Kinetic parameters such as apparent activation energy, frequency factor and entropy of decomposition of complex have been determined employing the methods of Sharp-Wentworth and Coats-Redfern using non-isothermal thermogravimetric curves. The values obtained for activation energy, entropy of activation and frequency factor as calculated from Sharp-Wentworth and Coats-Redfern method are in good agreement with each other. The apparent energy of activation, frequency factor and entropy are 9.338 kJ mol^{-1}, 0.2630 s^{-1}, and –31.24 J mol^{-1} K^{-1} respectively.

Key Words: Kinetic, Thermogravimetric analysis. Copper(II) complex, Amino acid.

Thermogravimetric analysis is a continuous non-isothermal method which has many advantages over currently used isothermal methods. The advantages are that a single experimental curve is sufficient to obtain the apparent heat of activation and that the kinetics can be probed over an entire temperature range in a continuous manner without any gap[1–3]. Kinetic constants of the complex have been investigated from thermal analysis procedures[4, 5]. The data obtained are in good agreement.

Freshly precipitated copper hydroxide was mixed with equimolar solutions of proline and leucine. The pH of the solution was kept at 7. The filtrate was concentrated on a water bath. On cooling, blue crystals of ternary complex separated out. These were recrystallized with double distilled water and dried. The elemental analysis was obtained from CDRI Lucknow. The analylical data of the complex consist (%) of C, 38.76 (38.41); H, 5.64 (5.82); N, 7.95 (8.14) and Cu, 18.10 (18.51).

Thermogravimetric analysis of the complex $[Cu(Pro)(Leu)(H_2O)_2]$ in an inert atmosphere was carried out using heating rate of 10°C/min in Mettler-Toledo instrument at NIPER, Mohali.

The thermogravimetric curve was used to calculate the kinetic parameters by using Sharp-Wentworth method[4] (Table-1) and Coats-Redfern method[5].

The thermal analysis data are presented in Tables 1 and 2.

TABLE-1

Temp. (K)	C	(1 – C)	$\log \frac{dc/dt}{(1-c)}$	1000/T
453	0.0709	0.9291	—	—
473	0.1398	0.8602	–2.3975	2.1 14
493	0.2086	0.7914	–2.3616	2.028
513	0.4151	0.5849	–2.0085	.1.949
533	0.5527	0.4473	–1.8709	1.876
553	0.6215	0.3785	–1.8374	1.808
573	0.6731	0.3269	–1.8138	1.745
593	0.7248	0.2752	–1.7705	1.686
613	0.7592	02408	–1.7481	1.631
633	0.7936	0.2064	–1.7110	1.579
653	0.8073	0.1927	–1.7189	1.531
673	0.8142	0.1858	–17404	1.485

$W_o = 2.9060$, $W_t = 0.5400$.

TABLE-2

α	Temp. (K)	log [–log (1 – α)/T^2]	1000/T
0.0870	453	–6.7155	2.207
0.1715	473	–6.4375	2.114
0.2561	493	–6.2771	2.028
0.5097	513	–5.9048	1.949
0.6787	533	–5.7606	1.876
0.7633	553	–5.6890	1.808
0.8267	573	–5.6348	1.745
0.8901	593	–5.5642	1.686
0.9323	613	–5.5069	1.631
0.9746	633	–5.3993	1.579
0.9915	653	–5.3137	1.531

$W_o = 2.9060$, $W_t = 0.5400$, $\alpha = \frac{W_o - W}{W_o - W_t}$

In Coats-Redfern method, the equation deduced for a first order reaction (n = 1)) was used because it gave a straight line over a long range of α values.

$$\log [-\log (1 - \alpha)/T^2] = \log AR/\beta E[1 - 2RT/E] - E/2.303RT$$

In Sharp-Wentworth method, a linear plot was obtained in each case which applied over a wide range of c-values, when order of reaction was taken as one.

$$\log [(dc/dt)/(1 - c)^n] = \log (A/\beta) - E/2.303\ RT$$

The entropy was calculated from Zsako[6] method; the value of ΔS is given by the expression

$$\Delta S = 2.303 \log [Ah/kT_{1/2}]$$

The apparent activation energy as calculated from Sharp-Wentworth method comes out to be 9.338 kJ mol^{-1}. The frequency factor is 0.263 s^{-1} and the entropy is –31.247 J mol^{-1} K^{-1}.

The apparent activation energy as calculated from Coats-Redfern method comes out to be 10.18 kJ mol^{-1}. The frequency factor is 0.1 12 s^{-1} and the entropy is –32.09 J mol^{-1} K^{-1}.

The results obtained from the two methods are in good agreement.

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