

## Nonisothermal Decomposition Reaction Kinetics, Specific Heat Capacity, Thermodynamic Properties and Adiabatic Time-to-explosion of 4-Amino-1,2,4-triazole Copper Complex

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4-Amino-1,2,4-triazole copper complex (4-ATzCu) was synthesized, and its thermal behaviors, nonisothermal decomposition reaction kinetics were studied by DSC and TG-DTG techniques. The thermal decomposition reaction kinetic equation was obtained as:  $d\alpha/dt = 10^{22.01}(1-\alpha)[-\ln(1-\alpha)]^{1/3} \exp(-2.75 \times 10^4/T)$ . The standard mole specific heat capacity of the complex was determined and the standard molar heat capacity is  $305.66 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$  at 298.15 K. The entropy of activation ( $\Delta S^\ddagger$ ), enthalpy of activation ( $\Delta H^\ddagger$ ), and Gibbs free energy of activation ( $\Delta G^\ddagger$ ) are calculated as  $171.88 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ ,  $225.81 \text{ kJ}\cdot\text{mol}^{-1}$  and  $141.18 \text{ kJ}\cdot\text{mol}^{-1}$ , and the adiabatic time-to-explosion of the complex was obtained as 389.20 s.

**Key Words:** 4-Amino-1,2,4-triazole copper complex (4-ATzCu), Nonisothermal kinetics, Specific heat capacity, Thermodynamic property, Adiabatic time-to-explosion

### Introduction

It is well known that some materials can improve the solid propellant ballistic properties, i.e., the monomeric compound or the composite system of lead oxide, copper oxide, and carbon black, can increase burning rate and decrease the pressure exponent of the burning rate. The organic metal complexes are the important ballistic modifiers used in the solid propellant, and the reactive metals or metal oxide can be generated and released from the complex, showing a more efficient action effect on the combustion process of the propellant than the original metal oxide, as such merit, the organic metal complexes have been extensively used in the solid propellant formulations in these decades. A series of aromatic and acyclic copper salts have been reported in literatures, and the nitrogen heterocycle copper complexes also attracted people's much attention because of the very large positive enthalpy of formation for the nitrogen heterocycle compounds.<sup>1-5</sup> 4-Amino-1,2,4-triazole (4-ATz) is one of the nitrogen heterocycle compounds, and its perchlorate and nitrate, have been reported earlier,<sup>6,7</sup> but 4-amino-1,2,4-triazole copper (4-ATzCu) complex has not been reported.<sup>8,9</sup> In the paper, 4-ATzCu was prepared, and its nonisothermal decomposition reaction kinetics, specific heat capacity, thermodynamic parameters of activation reaction and adiabatic time-to-explosion were studied.

### Experimental

**Sample.** 4-ATzCu complex used in the experiment was prepared according to the following method: an appropriate amount 4-ATz<sup>10</sup> (0.0210 g, 0.25 mmol) was put into 10 mL of water, stirring at 60 °C for 30 min.  $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$  (0.0213 g, 0.125 mmol) was dissolved in 10 mL ethanol and the solution was added into 4-ATz solution slowly and stirring at 60 °C for 120 min. Then

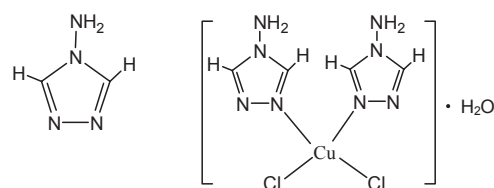


Figure 1. Schemes of 4-ATz and 4-ATzCu.

the blue precipitate was appeared. Finally, the precipitate was washed, filtrated and dried in vacuum at 80 °C, and then the complex was obtained. Yield: 70%. mp 235 ~ 238 °C. Elemental analysis (%): calcd. for  $(\text{C}_2\text{N}_4\text{H}_4)_2\text{CuCl}_2\cdot\text{H}_2\text{O}$ : C 15.84, H 2.64, N 36.96; found: C 15.08, H 2.508, N 34.89. IR (KBr,  $\text{cm}^{-1}$ ): 3389, 3238, 3130, 1640, 1546, 1222, 1081, 1060, 977, 867, and 615. So, the chemical constitution of the complex can be deduced as:  $(\text{C}_2\text{N}_4\text{H}_4)_2\text{CuCl}_2\cdot\text{H}_2\text{O}$ , and the schemes of 4-ATz and 4-ATzCu were shown in Figure 1.

**Equipment and conditions.** The specific heat capacity of the complex was determined by a Micro-DSCIII instrument (Setaram Co., France) with a continuous  $C_p$  mode within 283 K to 353 K at a heating rate of  $0.15 \text{ K}\cdot\text{min}^{-1}$ . Sample mass, 209.67 mg; Precisions of temperature and heat flow,  $10^{-4}\text{ }^\circ\text{C}$  and  $0.2 \mu\text{W}$ . The microcalorimeter was calibrated with  $\alpha\text{-Al}_2\text{O}_3$  (calcined), the math expression is  $C_p(\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1})(\alpha\text{-Al}_2\text{O}_3) = 0.1839 + 1.9966 \times 10^{-3} T$  ( $283 \text{ K} < T < 353 \text{ K}$ ), and the standard heat capacity  $C_{p,m}(\alpha\text{-Al}_2\text{O}_3)$  at 298.15 K was determined as  $79.44 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ , which is in an agreement with the value ( $79.02 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ ) reported in Ref. 11.

DSC and TG-DTG curves for the complex under the condition of flowing nitrogen gas (purity, 99.999%; atmospheric pressure) were obtained by using a 204HP differential scanning calorimeter (Netzsch Co., Germany) and a Q600SDT thermal analyzer (TA Co., USA), respectively. The conditions of DSC

analyses were: sample mass, about 1 mg; N<sub>2</sub> flowing rate, 50 cm<sup>3</sup> min<sup>-1</sup>; heating rate, 5, 10, 15, and 20 K min<sup>-1</sup>; furnace pressures, 0.1 MPa; reference sample,  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>; type of crucible, aluminum pan with a pierced lid. The conditions of TG-DTG were: sample mass, about 1 mg; N<sub>2</sub> flowing rate, 100 cm<sup>3</sup> min<sup>-1</sup>; heating rate ( $\beta$ ), 5, 10, 15, and 20 K min<sup>-1</sup>.

## Results and Discussion

**Specific heat capacity.** The determination result of specific heat capacity of the complex is shown in Figure 2, from which one can see that the specific heat capacity of the complex presents a good quadratic relationship with temperature in the determined temperature range, and the  $C_p$  vs  $T$  equation is obtained as:

$$C_p(\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}) = 1.475 - 7.027 \times 10^{-3}T + 1.770 \times 10^{-5}T^2 \quad (283 \text{ K} < T < 353 \text{ K}) \quad (1)$$

The standard molar specific heat capacity of the complex is 305.66 J·mol<sup>-1</sup>·K<sup>-1</sup> at 298.15 K. Although only 70 K range was taken in the determination process, the specific heat capacity equation obtained is a stable and continuous equation, which can provide a reference and some help for the wide temperature application.

**Thermodynamic properties.** The enthalpy change, entropy change and Gibbs free energy change of the complex were calculated by Eqs. (2)-(4) at 283 ~ 353 K, from the ambient temperature to thermal decomposition temperature, taking 298.15 K as the benchmark. The results were listed in Table 1.

$$H_T - H_{298.15} = \int_{298.15}^T C_p dT \quad (2)$$

$$S_T - S_{298.15} = \int_{298.15}^T C_p \cdot T^{-1} dT \quad (3)$$

$$G_T - G_{298.15} = \int_{298.15}^T C_p dT - T \int_{298.15}^T C_p \cdot T^{-1} dT \quad (4)$$

**Thermal behaviors.** Typical DSC and TG-DTG curves for the complex are shown in Figures 3 and 4. The DSC curve indicates that the thermal decomposition of the complex was composed of two exothermic processes with the peak temperatures of 505.1 K and 899.3 K, corresponding to two mass-loss stages in TG curve and two peaks in DTG curve.

The first mass-loss stage in TG curve begin at about 473.2 K and completed at 525.0 K with a mass loss of 34.6%, the second stage begin from 592.2 K to 921.9 K, with a mass loss of 29.3%. The first stage is caused by the main exothermic decomposition reaction.

**Nonisothermal reaction kinetics.** To explore the reaction mechanisms of the main exothermic decomposition processes of the complex, five integral methods [Eqs. (5)-(9)] and one differential method [Eq.(10)] in Table 2 are employed.<sup>12-15</sup>

In these equations,  $\alpha$  is the conversion degree of the main exothermic reaction,  $T$  is the absolute temperature,  $T_p$  is the peak

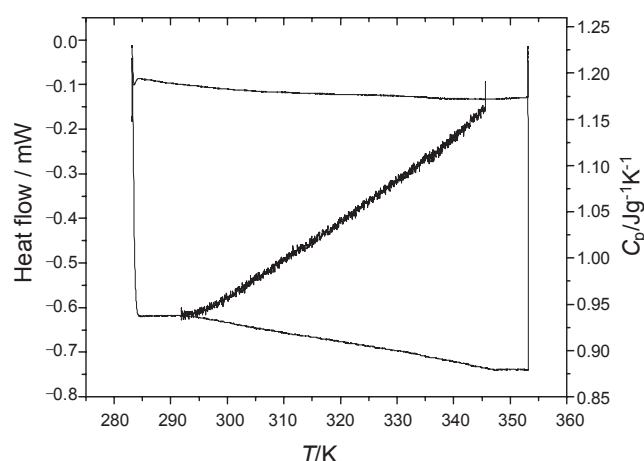


Figure 2. Determination results of the continuous  $C_p$  of the complex.

Table 1. Thermodynamic functions of the complex

$T/(\text{K})$	$H_T - H_{298.15} / (\text{kJ}\cdot\text{mol}^{-1})$	$S_T - S_{298.15} / (\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	$G_T - G_{298.15} / (\text{kJ}\cdot\text{mol}^{-1})$
283	-4.5038	-0.0155	-0.1174
288	-3.0436	-0.0104	-0.0527
293	-1.5581	-0.0053	-0.0136
298	-0.0458	-0.0002	-0.0000
303	1.4947	0.0050	-0.0121
308	3.0649	0.0101	-0.0498
313	4.6661	0.0153	-0.1132
318	6.2999	0.0204	-0.2025
323	7.9674	0.0257	-0.3177
328	9.6704	0.0309	-0.4590
333	11.4100	0.0361	-0.6266
338	13.1878	0.0414	-0.8206
343	15.0051	0.0468	-1.0411
348	16.8634	0.0522	-1.2885
353	18.7642	0.0576	-1.5628

temperature,  $A$  is the pre-exponential factor,  $R$  is the gas constant,  $\beta$  is the linear heating rate,  $E$  is the apparent activation energy.  $f(\alpha)$  and  $G(\alpha)$  are the differential model function and the integral model function,  $\alpha$  is the conversion degree. The data needed for the equations of the integral and differential methods,  $i, \alpha_i, \beta_i, T_i, T_p, i = 1, 2, 3, \dots, n$ , are obtained from the DTG curves and summarized in Table 3.

The values of  $E_a$  were obtained by Ozawa's method [Eq. (9)] from the isoconversional DSC curves at the heating rate of 5, 10, 15, and 20 K·min<sup>-1</sup>, and the  $E_a - \alpha$  relation is shown in Figure 5. From Figure 5, one can see that the activation energy changes slightly in the section of 0.10 - 0.90 ( $\alpha$ ), and the section was selected to calculate the nonisothermal reaction kinetics.

Forty-one types of kinetic model functions in Ref. 13 and the original data tabulated in Table 3 were put into Eqs. (5)-(10) for calculation. The values of  $E_a$ ,  $\lg A$ , linear correlation coefficient ( $r$ ), and standard mean square deviation ( $Q$ ) were calculated with the linear least-squares method at various heating rates 5,

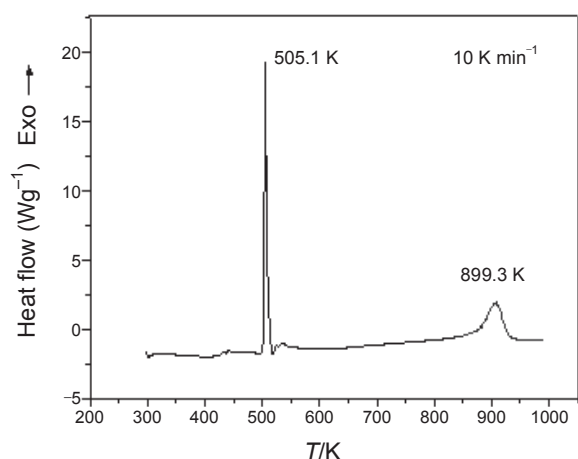


Figure 3. DSC curve for the complex at a heating rate of 10 K·min<sup>-1</sup>.

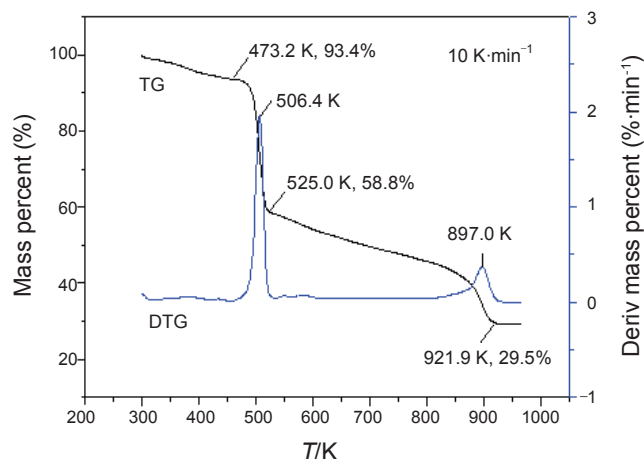


Figure 4. TG-DTG curve for the complex at a heating rate of 10 K·min<sup>-1</sup>.

Table 2. Kinetic analysis methods

Method	Equation
Ordinary-integral	$\ln[G(\alpha)/T^2] = \ln[(AR/\beta E)(1 - 2RT/E)] - E/RT$ (5)
Mac Callum-Tanner	$\lg[G(\alpha)] = \lg(AE/\beta R) - 0.4828E^{0.4357} - (0.449 + 0.217E)/(0.001T)$ ( $E$ in kcal·mol <sup>-1</sup> ) (6)
Šatava-Šesták	$\lg[G(\alpha)] = \lg(A_s E_s/\beta R) - 2.315 - 0.4567E_s/RT$ (7)
Agrawal	$\ln[G(\alpha)/T^2] = \ln\left\{ \frac{AR/\beta E}{[1 - 5(RT/E)^2]} \right\} - E/RT$ (8)
Flynn-Wall-Ozawa	$\lg\beta = \lg\left\{ \frac{AE}{[RG(\alpha)]} \right\} - 2.315 - 0.4567E/RT$ (9)
Kissinger	$\ln(\beta_i/T_{pi}^2) = \ln(A_k R/E_k) - E_k/RT_{pi}$ , $i = 1, 2, \dots, 4$ (10)

10, 15, and 20 K·min<sup>-1</sup>, and they are listed in Table 4. The most probable mechanism function is selected by the better values of  $r$ , and  $Q$  taken from Ref. 13. The results of satisfying the conditions mentioned above are also listed in Table 4.

From Table 4, one can find that the values of  $E_a$ , and  $\lg A$  obtained from nonisothermal curve are in approximately good agreement with the calculated values obtained by Kissinger's method and Ozawa's method. Therefore, one can conclude that the reaction mechanism of exothermic main decomposition process of the complex is classified as Avrami-Erofeev equation ( $n = 2/3$ ) and the mechanism function is:  $f(\alpha) = (3/2)(1 - \alpha)[- \ln(1 - \alpha)]^{1/3}$ .

Substituting  $f(\alpha)$  with  $(3/2)(1 - \alpha)[- \ln(1 - \alpha)]^{1/3}$ ,  $E$  with 228.89 kJ·mol<sup>-1</sup> and  $A$  with  $10^{21.83}$  s<sup>-1</sup> into Eq. (11):

$$d\alpha/dt = A f(\alpha) \exp(-E/RT) \quad (11)$$

and the kinetic equation of the main exothermic decomposition reaction of the complex is obtained and described as:

$$d\alpha/dt = 10^{22.01} (1 - \alpha)[- \ln(1 - \alpha)]^{1/3} \exp(-2.75 \times 10^4/T) \quad (12)$$

**Thermodynamic parameters of activation reaction.** The entropy of activation ( $\Delta S^\ddagger$ ), enthalpy of activation ( $\Delta H^\ddagger$ ), and Gibbs free energy of activation ( $\Delta G^\ddagger$ ) corresponding to  $T = T_{p0} = 492.38$  K,  $E = E_k = 229900$  J·mol<sup>-1</sup>,  $A = A_k = 10^{21.99}$  s<sup>-1</sup>

obtained by Eqs. (13)-(15)<sup>13,14</sup> are 171.88 J·mol<sup>-1</sup>·K<sup>-1</sup>, 225.81 kJ·mol<sup>-1</sup> and 141.18 kJ·mol<sup>-1</sup>, respectively. The positive value of  $\Delta G^\ddagger$ , indicates that the exothermic decomposition reaction for the complex must proceed under the heating condition.

$$A = \frac{k_B T}{h} \exp\left(\frac{\Delta S^\ddagger}{R}\right) \quad (13)$$

$$\Delta H^\ddagger = E - RT \quad (14)$$

$$\Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger \quad (15)$$

where  $k_B$  is the Boltzmann constant ( $1.3807 \times 10^{-23}$  J·K<sup>-1</sup>) and  $h$  is the Planck constant ( $6.626 \times 10^{-34}$  J·s).

**Adiabatic time-to-explosion ( $t_{Tlad}$ ).** The adiabatic time-to-explosion ( $t_{Tlad}$ ) of energetic materials (EMs) is the time of decomposition transiting to explosion under the adiabatic conditions and is an important parameter for assessing their thermal stability and the safety.<sup>12,16-18</sup> The estimation formula of adiabatic time-to-explosion as Eqs. (16) and (17), and  $t_{Tlad}$  value obtained by the definite integral equation is 389.20 s.

$$t_{Tlad} = \int_0^{t'} dt = \frac{1}{Q_d A} \int_{T_1}^{T_2} \frac{C_p \exp(E/RT)}{f(\alpha)} dT \quad (16)$$

$$\alpha = \int_{T_1}^{T_2} \frac{C_p}{Q_d} dT \quad (17)$$

**Table 3.** Data for the decomposition process of the complex determined by DTG curve

$\alpha$	$T_5/K$	$T_{10}/K$	$T_{15}/K$	$T_{20}/K$	$\alpha$	$T_5/K$	$T_{10}/K$	$T_{15}/K$	$T_{20}/K$
0.00	468.1	473.2	477.2	480.6	0.52	498.2	505.5	508.8	512.7
0.02	479.6	487.2	490.2	494.6	0.54	498.6	505.9	509.2	513.1
0.04	483.2	490.6	493.7	497.9	0.56	498.9	506.2	509.5	513.5
0.06	485.2	492.8	495.9	499.8	0.58	499.3	506.5	509.8	513.8
0.08	486.7	494.3	497.4	501.2	0.60	499.6	506.9	510.2	514.2
0.10	487.9	495.5	498.6	502.3	0.62	500	507.2	510.5	514.6
0.12	488.9	496.4	499.6	503.2	0.64	500.3	507.5	510.9	515
0.14	489.7	497.3	500.4	504.0	0.66	500.6	507.9	511.2	515.4
0.16	490.4	498	501.1	504.6	0.68	501.0	508.2	511.6	515.8
0.18	491.1	498.6	501.8	505.3	0.70	501.4	508.6	512.0	516.2
0.2	491.7	499.2	502.3	505.8	0.72	501.7	509.0	512.4	516.7
0.22	492.2	499.7	502.9	506.4	0.74	502.1	509.3	512.8	517.1
0.24	492.7	500.2	503.4	506.9	0.76	502.5	509.7	513.2	517.6
0.26	493.2	500.6	503.9	507.3	0.78	502.8	510.2	513.6	518.0
0.28	493.6	501.1	504.3	507.8	0.80	503.2	510.6	514.0	518.5
0.30	494.0	501.5	504.7	508.3	0.82	503.7	511.1	514.5	519.0
0.32	494.5	501.9	505.2	508.7	0.84	504.1	511.6	515.0	519.6
0.34	494.9	502.3	505.6	509.1	0.86	504.6	512.1	515.5	520.2
0.36	495.3	502.7	505.9	509.5	0.88	505.1	512.7	516.1	520.9
0.38	495.6	503.1	506.3	510.0	0.90	505.7	513.3	516.8	521.6
0.40	496.0	503.4	506.7	510.4	0.92	506.3	514.0	517.5	522.5
0.42	496.4	503.8	507.1	510.8	0.94	507.1	514.9	518.4	523.6
0.44	496.8	504.2	507.4	511.2	0.96	508.3	516.0	519.5	524.9
0.46	497.1	504.5	507.8	511.5	0.98	510.3	517.7	521.1	526.8
0.48	497.5	504.8	508.1	511.9	1.00	518.5	525.0	526.6	533.3
0.50	497.9	505.2	508.5	512.3		499.7( $T_p$ )	506.4( $T_p$ )	509.1( $T_p$ )	512.3( $T_p$ )

$T$  with the subscript 5, 10, 15, and 20 is the temperature obtained at the heating rates of 5, 10, 15, and 20  $K \cdot min^{-1}$ , respectively.

where  $t_{Tlad}$ , the adiabatic time-to-explosion in s;  $C_p$ , the specific heat capacity in  $J \cdot g^{-1} \cdot K^{-1}$ ;  $f(\alpha)$ , differential mechanism function;  $E$ , activation energy in  $J \cdot mol^{-1}$ , and  $E = E_k$ ;  $A$ , pre-exponential constant in  $s^{-1}$ , and  $A = A_k$ ;  $Q_d$ , decomposition heat in  $629.36 J \cdot g^{-1}$ ;  $R$ , the gas constant;  $\alpha$ , the conversion degree; the integral lower limit  $T_1 = T_{00} = 462.28 K$ , the upper limit  $T_2 = T_{p0} = 492.38 K$ .

The values of  $T_{00}$  and  $T_{p0}$  were calculated by Eq. (18).

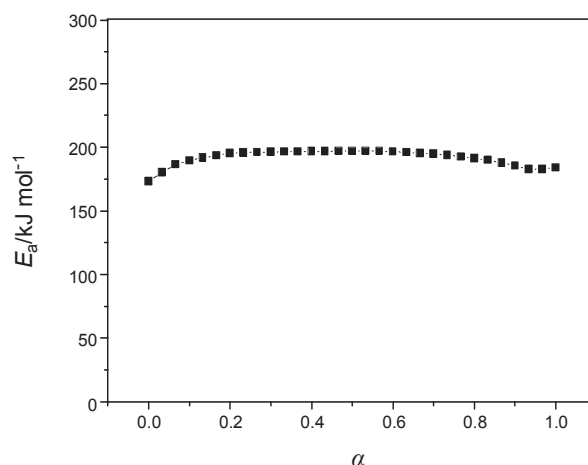
$$T_{(0 \text{ or } p)_i} = T_{(00 \text{ or } p0)} + b\beta + c\beta^2 \quad i = 1 - 4 \quad (18)$$

where  $b$  and  $c$  are coefficients.

### Conclusions

(1) The main thermal decomposition reaction kinetics of the complex was studied under the nonisothermal conditions by DSC and TG-DTG methods, and the kinetic equation is  $d\alpha/dt = 10^{22.01}(1-\alpha)[- \ln(1-\alpha)]^{1/3} \exp(-2.75 \times 10^4/T)$ .

(2) The specific heat capacity equation is  $C_p(J \cdot g^{-1} \cdot K^{-1}) = 1.475 - 7.027 \times 10^{-3}T + 1.770 \times 10^{-5}T^2$  ( $283 K < T < 353 K$ ), and the molar heat capacity is  $305.66 J \cdot mol^{-1} \cdot K^{-1}$  at  $298.15 K$ . The



**Figure 5.** The  $E_a$ - $\alpha$  curve for the decomposition of the complex by Ozawa's method.

enthalpy change, entropy change and Gibbs free energy change were calculated at 283 - 353 K.

(3) The entropy of activation ( $\Delta S^\ddagger$ ), enthalpy of activation ( $\Delta H^\ddagger$ ), and Gibbs free energy of activation ( $\Delta G^\ddagger$ ) are 171.88

**Table 4.** Calculated values of kinetic parameters of decomposition of the complex ( $\alpha = 0.10 - 0.90$ )

Method	$\beta/(\text{K}\cdot\text{min}^{-1})$	$E_a/(\text{kJ}\cdot\text{mol}^{-1})$	$\lg A/\text{s}^{-1}$	$r$	$Q$
Ordinary-integral	5	226.83	21.65	0.9986	0.0317
	10	236.24	22.58	0.9976	0.0531
	15	234.66	22.43	0.9976	0.0549
	20	219.64	20.81	0.9951	0.1103
Mac Callum-Tanner	5	228.11	21.78	0.9987	0.0059
	10	237.71	22.74	0.9978	0.0099
	15	236.18	22.59	0.9977	0.0103
	20	221.12	20.95	0.9954	0.0207
Šatava-Šesták	5	223.56	21.35	0.9986	0.0059
	10	232.62	22.26	0.9978	0.0099
	15	231.18	22.12	0.9977	0.0103
	20	216.96	20.56	0.9954	0.0207
Agrawal	5	226.83	21.65	0.9986	0.0317
	10	236.24	22.58	0.9976	0.0531
	15	234.66	22.43	0.9976	0.0549
	20	219.64	20.81	0.9951	0.1103
Mean		228.89	21.83		
Flynn-Wall-Ozawa		226.62		0.9988	0.0005
Kissinger		229.90	21.99	0.9987	0.0026

$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ , 225.81  $\text{kJ}\cdot\text{mol}^{-1}$  and 141.18  $\text{kJ}\cdot\text{mol}^{-1}$ , respectively.

(4) The adiabatic time-to-explosion of the complex is 389.20 s.

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