

APPLICATION OF ISO-TEMPERATURE METHOD OF MULTIPLE RATE TO KINETIC ANALYSIS Dehydration for calcium oxalate monohydrate

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Abstract

A new method of the multiple rate iso-temperature was used to define the most probable mechanism $g(\alpha)$ of a reaction; the iterative iso-conversional procedure has been employed to estimate apparent activation energy E_a , the pre-exponential factor A was obtained on the basis of E_a and $g(\alpha)$. In this new method, the thermal analysis kinetics triplet of dehydration of calcium oxalate monohydrate is determined, which apparent activation energy E_a is $82.83 \text{ kJ mol}^{-1}$, pre-exponential factor A is $1.142 \cdot 10^5 - 1.235 \cdot 10^5 \text{ s}^{-1}$, the most probable mechanism belongs to phase boundary reaction R_n with integral form $g(\alpha) = 1 - (1 - \alpha)^n$ and differential form $f(\alpha) = n(1 - \alpha)^{1-(1/n)}$, where accommodation factor $n = 2.40 - 1.40$.

Keywords: accommodation factor, calcium oxalate monohydrate, iterative iso-conversional procedure, multiple rate iso-temperature method, non-isothermal kinetics

Introduction

The technology of thermal analysis has been widely used in the study of thermal behavior and thermal character of solid-state reaction [1, 2], and the primary intention of thermal analysis kinetics is to establish separate values of E_a , $g(\alpha)$ and A [3, 4], meanwhile the determination of $g(\alpha)$ has gradually been the focus of this field. In this field, there are mostly general kinetics methods used presently, they are integral method of Coats–Redfern [5] differential method of Achar [6], variable iso-conversional method [7] and accommodated model of Gao *et al.* [8]. In this paper, the kinetics of dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ is described by a new method, the most probable mechanism function $g(\alpha)$ of the thermal decomposition reaction is deduced from multiple rate iso-temperature method, the apparent activation energy E_a is obtained from iterative procedure [9], pre-exponential factor A is calculated on the basis of E_a

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and $g(\alpha)$ subsequently. The study of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ using differential scanning calorimetry (DSC) by this new method, the result is satisfactory.

Theoretical

Determination of the most probable mechanism function

Theoretical

According to non-isothermal kinetic theory, thermal decomposition kinetic equation of solid-state material is:

$$\frac{d\alpha}{dT} = \frac{1}{\beta} A e^{E_a/RT} f(\alpha) \quad (1)$$

The Eq. (2) [10] is the integral form of Eq. (1):

$$g(\alpha) = \int_0^\alpha \frac{d\alpha}{f(\alpha)} = \frac{A}{\beta} \int_{T_0}^T e^{-E_a/RT} dT \approx \frac{A}{\beta} \int_0^T e^{-E_a/RT} dT = \frac{AE_a}{\beta R} \int_\infty^x \frac{e^{-x}}{x^2} dx = \frac{AE_a}{\beta R} \frac{e^{-x}}{x} \pi(x) \quad (2)$$

$$\alpha = \frac{\Delta H_i}{\Delta H} \quad (3)$$

where α is the degree of conversion, β is the heating rate, E_a is the activation energy, A is pre-exponential factor, R is the gas constant, $g(\alpha)$ and $f(\alpha)$ are integral and differential expression of kinetics model function. ΔH_i is the enthalpy change of the sample at anyone temperature T_i , ΔH is the total enthalpy change of the sample and $x = E_a/RT$.

The Eq. (4) is derived from the logarithm form of Eq. (2),

$$\ln g(\alpha) = \left[\ln \frac{AE_a}{R} + \ln \frac{e^{-x}}{x} + \ln \pi(x) \right] - \ln \beta \quad (4)$$

Plotting $\ln g(\alpha)$ vs. $\ln \beta$ using a linear regressive of least-square method, if the studied mechanism conforms to a certain $g(\alpha)$, the slope k and the linear correlation coefficient r should be all equal to -1.00000 .

Determination of the most probable mechanism function

The conversions α corresponding multiple rates at the same temperature are put into the left of Eq. (4), combined with thirty-one types of mechanism functions [11], the slope k and correlation coefficient r are obtained from the plot of $\ln g(\alpha)$ vs. $\ln \beta$. The probable mechanism function is that for which the value of the slope k is near to -1.00000 and correlation coefficient r is better. If several $g(\alpha)$ answer for this requirement, the conversions α corresponding to multiple rates at several the same temperatures were applied to calculate the probable mechanism by the same method, the most probable mechanism function is that for which among the results of k and r , the value of k is closest to -1.00000 .

Calculation of activation energy E_a by iterative procedure

Ozawa Eq. [12] and KAS Eq. [13] are shown below:

$$\text{Ozawa Eq.:} \quad \ln \beta = \ln \left[\frac{0.0048 A E_a}{g(\alpha) R} \right] - 1.0516 \frac{E_a}{RT} \quad (5)$$

$$\text{KAS Eq.:} \quad \ln \frac{\beta}{T^2} = \ln \left[\frac{A E_a}{g(\alpha) R} \right] - \frac{E_a}{RT} \quad (6)$$

The iterative procedure is used to approach the actual value of E_a , the Eqs are expressed:

$$\ln \frac{\beta}{H(x)} = \ln \left[\frac{0.0048 A E_a}{g(\alpha) R} \right] - 1.0516 \frac{E_a}{RT} \quad (7)$$

$$\ln \frac{\beta}{h(x) T^2} = \ln \left[\frac{A E_a}{g(\alpha) R} \right] - \frac{E_a}{RT} \quad (8)$$

where

$$H(x) = \frac{\exp(-x) h(x) / x^2}{0.0048 \exp(-1.0516x)} \quad (9)$$

$$h(x) = \frac{x^4 + 18x^3 + 86x^2 + 96x}{x^4 + 20x^3 + 120x^2 + 240x + 120} \quad (\text{Seman-Yang function}) \quad (10)$$

Evaluation of pre-exponential factor A

Pre-exponential factor A can be estimated from the intercept B of the plot of $\ln g(\alpha)$ vs. $\ln \beta$, where $\pi(x) \approx 1$.

Experimental

Measurement

The dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ (AR grade, Beijing Chemical plant, China) was carried out in a differential scanning calorimetry (DSC) (Mettler-Toledo DSC822^o, Switzerland). The selected heating rates were 1.5, 3, 5, 6, 7, 8 and 10 K min⁻¹. Pure gas was nitrogen gas of high purity, flowing at 20 mL min⁻¹. The sample cells are aluminium pans with pierced lid. Sample mass was around 5.00 mg and the temperature was recorded from 375 to 550 K. (The results presented in the paper were calculated by the programs compiled by ourselves.)

Experimental data

DSC curves corresponding to the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ at different heating rates are shown in Fig. 1.

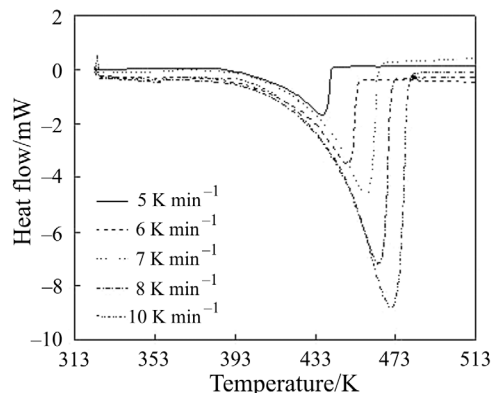


Fig. 1 DSC curves of the dehydration for $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ at different heating rates

The curves corresponding to the conversion for the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ at different heating rates are shown in Fig. 2.

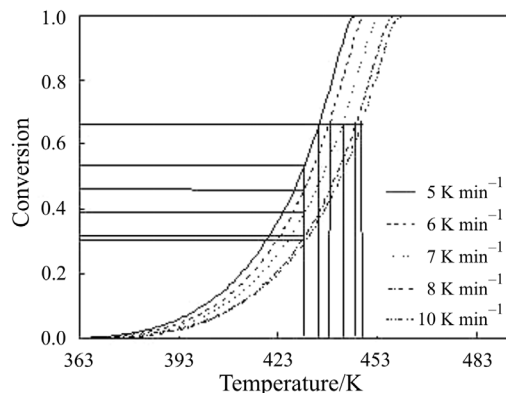


Fig. 2 The conversion degree for the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ at different heating rates

Result and discussion

Determination of kinetic mechanism

Determination of kinetic mechanism by multiple rate iso-temperature method roughly

The conversions for $\beta=1.5, 3, 5, 7$ and 10 K min^{-1} at the same temperature were illustrated in Table 1. An appropriate temperature is randomly selected, the range of the conversions of this temperature should be within 0.10–0.90 we choose the corresponding

Table 1 The relation of temperature and conversion α of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ at different heating rates β (K min^{-1})

T/K	α				
	$\beta=1.5$	$\beta=3$	$\beta=5$	$\beta=7$	$\beta=10$
410	0.15	0.08	0.05	0.04	0.02
415	0.23	0.12	0.08	0.06	0.03
430	0.59	0.32	0.21	0.15	0.10
431	0.63	0.34	0.22	0.16	0.10
432	0.67	0.36	0.23	0.17	0.12
433	0.71	0.38	0.25	0.18	0.12
434	0.75	0.40	0.26	0.19	0.13
435	0.79	0.43	0.27	0.20	0.14
436	0.84	0.44	0.29	0.21	0.15
437	0.88	0.47	0.30	0.23	0.16
439	0.97	0.52	0.34	0.25	0.18
440	0.99	0.55	0.34	0.26	0.19

conversions of $T=435$ K for example to put into thirty-one types of mechanism functions (part of basic models of solid-state reactions as shown in Table 2), the slope k , correlation coefficient r and intercept B of linear regression of $\ln g(\alpha)$ vs. $\ln \beta$ are obtained (as shown in Table 3). The parameters in Table 3 show that the slopes of No. 13, 14 and 15 are closer to -1.00000 than others and with better correlation coefficient r , but which type of mechanism is the most probable one, it needs further research.

Table 2 Part of basic models of solid state reactions

Function No.	Name of function	Mechanism	Integral form $g(\alpha)$	Differential form $f(\alpha)$
12	n th order	$n=1/4$	$1-(1-\alpha)^{1/4}$	$4(1-\alpha)^{3/4}$
13	Contracting sphericity, (volume)	Phase boundary reaction, sphericity symmetry, R_3	$1-(1-\alpha)^{1/3}$	$3(1-\alpha)^{2/3}$
14	Contracting cylindrical, (area)	Phase boundary reaction, cylindrical symmetry, R_2	$1-(1-\alpha)^{1/2}$	$2(1-\alpha)^{1/2}$
15	Mample power law	Phase boundary reaction, one-dimensional, R_1	α	1
16	Mample power law	$n=3/2$	$\alpha^{3/2}$	$2/3\alpha^{-1/2}$

Table 3 $\ln g(\alpha)$ vs. $\ln \beta$ curves of 31 types of mechanism functions at $T=435$ K ($\beta=1.5, 3, 5, 7$ and 10 K min^{-1})

Function No.	Integral form $g(\alpha)$	B	$-k$	$-r$
1	α^2	0.27048	1.80364	0.99964
2	$\alpha+(1-\alpha)\ln(1-\alpha)$	-0.00385	1.98176	0.99948
3	$[1-(1-\alpha)^{1/3}]^2$	-1.01175	2.19957	0.99805
4	$(1-2\alpha/3)-(1-\alpha)^{2/3}$	-1.34358	2.05380	0.99911
5	$[1+\alpha]^{1/3}-1]^2$	-2.38470	1.63318	0.99913
6	$[(1-\alpha)^{-1/3}-1]^2$	0.07422	2.68244	0.99249
7	$-\ln(1-\alpha)$	0.85357	1.21500	0.99569
8	$[-\ln(1-\alpha)]^{2/3}$	0.56810	0.80949	0.99567
9	$[-\ln(1-\alpha)]^{1/2}$	0.42605	0.60721	0.99566
10	$[-\ln(1-\alpha)]^{1/3}$	0.28411	0.40485	0.99568
11	$[-\ln(1-\alpha)]^{1/4}$	0.21394	0.30422	0.99574
12	$1-(1-\alpha)^{1/4}$	-0.72814	1.12827	0.99770
13	$1-(1-\alpha)^{1/3}$	-0.50560	1.09984	0.99807
14	$1-(1-\alpha)^{1/2}$	-0.22249	1.04639	0.99886
15	$1-(1-\alpha)^{1/1}=\alpha$	0.13587	0.90211	0.99962
16	$\alpha^{3/2}$	0.20328	1.35295	0.99963
17	$\alpha^{1/2}$	0.06730	0.45063	0.99963
18	$\alpha^{1/3}$	0.04511	0.30081	0.99957
19	$\alpha^{1/4}$	0.03337	0.22519	0.99966
20	$-\ln(1-\alpha)$	0.85357	1.21500	0.99569
21	$(1-\alpha)^{-1/2}-1$	0.59150	1.40825	0.99065
22	$(1-\alpha)^{-1}-1$	1.76512	1.62695	0.98449
23	$(1-\alpha)^{-2}$	3.25930	1.44995	0.92569
24	$1-(1-\alpha)^2$	0.28576	0.67805	0.99345
25	$1-(1-\alpha)^3$	0.28039	0.52050	0.97898
26	$1-(1-\alpha)^4$	0.24830	0.40784	0.96062
27	$[-\ln(1-\alpha)]^2$	1.70577	2.42935	0.99568
28	$[-\ln(1-\alpha)]^3$	2.55934	3.64435	0.99568
29	$[-\ln(1-\alpha)]^4$	3.41199	4.85887	0.99569
30	$[1-(1-\alpha)^{1/2}]^{1/2}$	-0.11188	0.52263	0.99886
31	$[1-(1-\alpha)^{1/3}]^{1/2}$	-0.25302	0.54984	0.99804

B , k and r are the intercept, slope and correlation coefficient of linear regression of $\ln g(\alpha)$ vs. $\ln \beta$ respectively, the following are the same

Determination of kinetic mechanism by multiple rate iso-temperature method precisely

We randomly choose several temperatures (Table 1) which corresponding conversions $0.10 < \alpha < 0.90$ to calculate the slope k , correlation coefficient r and intercept B of No. 13, 14 and 15 mechanism function by the same method. The results are listed in Table 4, they illustrate that the slope of No. 14 be the most adjacent to -1.00000 and correlation coefficient r be better. So we can determine that No.14 mechanism function is the most probable one of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$, with integral form $g(\alpha) = 1 - (1 - \alpha)^{1/n}$ and differential form $f(\alpha) = n(1 - \alpha)^{1-(1/n)}$, belongs to the mechanism of phase boundary reaction, R_n ; $n = 2.00$.

Table 4 $\ln g(\alpha)$ vs. $\ln \beta$ curves of 3 types of probable mechanism functions when $0.10 < \alpha < 0.90$ ($\beta = 1.5, 3, 5, 7$ and 10 K min^{-1})

T/K	Function No.	B	$-k$	$-r$
430	13	-0.94044	1.03624	0.99946
	14	-0.61084	1.00418	0.99950
	15	-0.13367	0.91397	0.99900
431	13	-0.86041	1.04468	0.99938
	14	-0.53808	1.00918	0.99951
	15	-0.07891	0.91123	0.99917
433	13	-0.69100	1.06737	0.99899
	14	-0.38578	1.02419	0.99937
	15	-0.02872	0.90581	0.99945
434	13	-0.60103	1.08216	0.99860
	14	-0.30590	1.03430	0.99916
	15	0.08275	0.90420	0.99955

The influence of temperature selection on the mechanism function

We randomly choose several temperatures (Table 1) which corresponding conversions $\alpha < 0.10$ or $\alpha > 0.90$ to calculate the slope k , correlation coefficient r and intercept B of linear regression of $\ln g(\alpha)$ vs. $\ln \beta$, the values of the slopes which are close to -1.00000 are all listed in Table 5. The probable mechanism function have been changed when $\alpha < 0.10$ or $\alpha > 0.90$, the reaction is in the initial stage or finished stage, they can not represent the whole process of reaction truly, so we can conclude that the selection of temperature be very important, its corresponding conversions must be in the range of $0.10-0.90$.

The influence of combination of different heating rates on the mechanism function

Randomly combined of different heating rates of 5, 6, 7, 8 and 10 K min^{-1} , when $0.10 < \alpha < 0.90$, the slope k , correlation coefficient r and intercept B of linear regres-

Table 5 $\ln g(\alpha)$ vs. $\ln \beta$ curves of the probable mechanism functions when $\alpha < 0.10$ or $\alpha > 0.90$ ($\beta = 1.5, 3, 5, 7$ and 10 K min^{-1})

T/K	Function No.	B	$-k$	$-r$
410	14	-2.03210	1.04082	0.98940
	15	-1.38400	1.02268	0.98974
	24	-0.77992	0.98647	0.98709
415	13	-2.02992	1.02966	0.99461
	14	-1.64813	1.01988	0.99437
	15	-1.02369	0.99179	0.99355
439	8	1.05985	0.97979	0.98280
	14	0.16988	1.12896	0.99589
	15	0.32658	0.88725	0.99986
440	8	1.34186	1.10681	0.97118
	14	0.29772	1.16580	0.99415
	15	0.35703	0.87519	0.99983

sion of $\ln g(\alpha)$ vs. $\ln \beta$ are obtained (Table 6). The parameters in Table 6 prove that the most probable mechanism function of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ is also No.14 no matter what the combination of different heating rates. So we can conclude that different heating rates have little influence on the most probable mechanism function, meanwhile this method have randomness and the result possesses uniqueness.

Table 6 $\ln g(\alpha)$ vs. $\ln \beta$ curves of 3 types of probable mechanism functions when $0.10 < \alpha < 0.90$ ($\beta = 5, 6, 7, 8$ and 10 K min^{-1})

T/K	Function No.	B	$-k$	$-r$
441	13	-1.09746	1.01230	0.95656
	14	-0.72904	0.99957	0.95692
	15	-0.14043	0.96452	0.95695
445	13	-0.85725	1.00881	0.96296
	14	-0.50059	0.99189	0.96307
	15	0.05442	0.94451	0.96302
450	13	-0.55168	1.01332	0.96824
	14	-0.21181	0.99054	0.96847
	15	0.29458	0.92670	0.96851
453	13	-0.35426	1.02525	0.97084
	14	-0.02670	0.99820	0.97057
	15	0.43985	0.92037	0.97096

The calculation of optimal value n of the accommodation function

During the course of determining the most probable mechanism function about the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$, we have successfully found that No. 13, 14 and 15 mechanism function are all belong to phase boundary reaction, R_n , with integral form $g(\alpha) = 1 - (1 - \alpha)^{1/n}$, n equals to 3.00, 2.00 and 1.00 respectively, the results of Table 3 show that the smaller of the value of n , the smaller of the value of $-k$. So we can conclude that the probable optimal range of n is 2.00–1.00 with the slope k approach to -1.00000 . In order to make certain optimal value of n further, we decrease the value of n among 2.00–1.00 with decrement of 0.10. Take β of 1.5, 3, 5, 7 and $10 \text{ K} \cdot \text{min}^{-1}$ for example, plotting $\ln g(\alpha)$ vs. β using a linear regressive of least-square method, the results are listed in Table 7.

Table 7 $\ln g(\alpha)$ vs. $\ln \beta$ curves of accommodation functions when $T=430 \text{ K}$ ($\beta=1.5, 3, 5, 7$, and $10 \text{ K} \cdot \text{min}^{-1}$)

n	B	$-k$	$-r$
2.00	-0.61084	1.00418	0.99950
1.90	-0.57149	0.99939	0.99949
1.80	-0.52941	0.99375	0.99949
1.70	-0.48823	0.98762	0.99948
1.60	-0.44342	0.98840	0.99946

n is the accommodation factor of mechanism function of R_n , the followings are the same

Table 7 shows that when $T=430 \text{ K}$ and $n=1.90$, the slope k is closest to -1.00000 .

By the same method, when $0.10 < \alpha < 0.90$, the corresponding results of accommodation function R_n under other temperatures are listed in Table 8.

Table 8 $\ln g(\alpha)$ vs. $\ln \beta$ curves of accommodation functions when $0.10 < \alpha < 0.90$ ($\beta=1.5, 3, 5, 7$ and $10 \text{ K} \cdot \text{min}^{-1}$)

T/K	n	B	$-k$	$-r$
432	1.80	-0.38692	1.00304	0.99952
434	1.60	-0.16206	1.00009	0.99944
436	1.50	0.02229	1.00360	0.99923
437	1.40	0.12659	0.99565	0.99924

When $0.10 < \alpha < 0.90$ under the combination of different heating rates ($\beta=5, 6, 7, 8$ and $10 \text{ K} \cdot \text{min}^{-1}$), the results of accommodation function R_n at the same temperature are listed in Table 9, the optimal range of n is 2.40–2.00.

From the general results of Table 7–9 we can conclude that the optimal range of n is 2.40–1.40 under the combination of different heating rates, as found in [8].

Table 9 $\ln g(\alpha)$ vs. $\ln \beta$ curves of accommodation functions when $0.10 < \alpha < 0.90$ ($\beta=5, 6, 7, 8$ and 10 K min^{-1})

T/K	n	B	$-k$	$-r$
441	2.00	-0.72904	0.99957	0.95692
445	2.40	-0.65901	0.99948	0.94304
450	2.40	-0.36147	1.00161	0.96834
453	2.10	-0.06414	1.00240	0.97084

Calculation of activation energy E_a by iterative procedure

The values of E_a of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ are obtained by the above method, the values of E_a corresponding to different conversions α are shown in Table 10.

Table 10 E_a of the $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ by different methods ($\beta=5, 6, 7, 8$ and 10 K min^{-1})

α	$E_a/\text{kJ mol}^{-1}$			
	Ozawa method	KAS method	$\ln[\beta/H(x)]$ vs. $1/T$	$\ln[\beta/h(x)T^2]$ vs. $1/T$
0.10	88.24	85.45	85.80	85.82
0.20	86.76	83.79	84.06	84.01
0.30	85.57	82.43	82.70	82.70
0.40	85.30	82.03	82.32	82.32
0.50	85.05	81.74	82.00	81.95
0.60	85.11	81.69	82.00	82.00
0.70	85.23	81.71	82.07	82.01
0.80	85.37	81.80	82.17	82.15
0.90	85.75	82.28	82.53	82.53
Average	85.82	82.55	82.85	82.83

$\ln[\beta/H(x)]$ vs. $1/T$ and $\ln[\beta/h(x)T^2]$ vs. $1/T$ are iterative method of Ozawa method and KAS method respectively.

As shown in Table 10, compared with the values of E_a obtained by iterative method and KAS method or Ozawa method, that obtained by Ozawa method is general higher (excessing about $2.44\text{--}3.22 \text{ kJ mol}^{-1}$), however, the results obtained by iterative method and KAS method are very close to each other (differing about $0.25\text{--}0.37 \text{ kJ mol}^{-1}$). Meanwhile, we discover that the values obtained from the plot of $\ln[\beta/H(x)]$ vs. $1/T$ or $\ln[\beta/h(x)T^2]$ vs. $1/T$ by iterative procedure are very close to each other (the biggest one only differs about 0.02 kJ mol^{-1}), it is not difficult to find that the values of E_a obtained from iterative method or KAS method are more reliable, so the suggestion that the values obtained from these two methods determined the range of E_a is reasonable, while the heating rates are 5, 6, 7, 8 and 10 K min^{-1} , the value of E_a is equal to $82.83 \text{ kJ mol}^{-1}$ at $0.10 < \alpha < 0.90$, which is accord with the values presented in [8, 14].

The calculation of pre-exponential factor A

By the intercept B listed in Table 6, the range of pre-exponential factor A is $1.142 \cdot 10^5 \sim 1.235 \cdot 10^5 \text{ s}^{-1}$.

Conclusions

A new method of using multiple rate iso-temperature method combined with thirty-one types of mechanism function is used to define the most probable mechanism $g(\alpha)$, iterative iso-conversional procedure has been applied to estimated apparent activation energy E_a , the pre-exponential factor A is obtained on the basis of E_a and $g(\alpha)$. Using this method to calculate thermal analysis kinetic triplet, it have many excellences such as simplicity, convenience and reappearance, the result is credible and comparable.

From the experiment results, we can conclude that when $\alpha < 0.1$ or $\alpha > 0.90$, the probable mechanism functions do not completely focus in No.13, 14 and 15, for the reasons that they are probably in the initial stage and finished stage of reaction, they can not represent the whole process of reaction truly. When $0.10 < \alpha < 0.90$, the parameters of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ are as follow: $E_a = 82.83 \text{ kJ mol}^{-1}$, $A = 1.142 \cdot 10^5 \sim 1.235 \cdot 10^5 \text{ s}^{-1}$, the most probable mechanism function belongs to phase boundary reaction with integral form $g(\alpha) = 1 - (1 - \alpha)^{1/n}$ and the differential form $f(\alpha) = n(1 - \alpha)^{1-(1/n)}$, and accommodation function R_n with $n = 2.40 \sim 1.40$, the kinetic equation of the dehydration of $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ is $d\alpha/dt = Ae^{-E_a/RT} n(1 - \alpha)^{1-(1/n)}$.

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