

# Thermal analysis on potential risk of cosmetic materials by DSC

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**Abstract.** To explore the potential risk of usage on daily chemicals, the product which most contact for human directly, cosmetics, were selected as study object. In this study, common cosmetic materials, such as propylene glycol, ethanolamine, silicon dioxide, iron oxide, and copper oxide were discussed for potential hazard. According to results of differential scanning calorimetry experiments, the apparent activation energy and SADT were calculated out as 779.22 kJ mol<sup>-1</sup> and 45°C, respectively.

## 1 Introduction

The desire to look attractive is universally accepted. The origin of cosmetics can be tracked back to ancient Egyptians nearly 4,000 years ago. It was a badge of an honourable position. Today it has evolved into a way of decoration. In the mid-1970s, mineral make-up began revolutionizing cosmetics, especially when nanomaterial technology matured. Using nano-grade materials as additions is the latest approach and is an effective way to cover flaws on face and other parts of the body. However, this modern technology has had doubts about its safety for human health within last decade [1]. Even though cosmetic products are supervised strictly by the World Health Organization, it is still worrisome since they are interrelated closely in life. There are numerous cases in which people have been burned or developed an allergy by cosmetic mask, gel, toner, creams, lotion, and powder. That is not only because of their allergies, but also from unsafe applications and storage or unknown potential risk. Generally, approximately 50 kinds of composition are added to a cosmetic product. Furthermore, several products are usually used at the same time. A tiny interaction may inevitably cause the above hurt.

In this study, common cosmetic materials, such as propylene glycol, ethanolamine (ETA), SiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, and CuO were discussed for potential hazard. Differential scanning calorimetry (DSC) was used to ascertain the matrix relation and DSC curve of above substances. It is believed that the results of this study can contribute to recommendations or references for cosmetic composition for future applications.

## 2 Experiments and methods

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Nano graded TiO<sub>2</sub>, propylene glycol, ETA, and benzophenone (Ph<sub>2</sub>CO) are the most common materials used in sun block, moisturizer, color make-up, and so on. ETA is a common material which is a wetting agent in lotions and creams.

Thermogravimetry (TG) and TA8000 system DSC821e were used to for non-isothermal experiments out. TG has the ability to acquire the parameters of pyrolysis substances. It is a way to select the scope of temperature in DSC tests, which are from 30.0 to 300.0°C. Through DSC experiments, various thermokinetic parameters can be obtained, such as onset temperature, maximum temperature, heat of decomposition, and self-heating rate. Moreover, considering assessment theory, reproducibility in each experiment of DSC was performed and validated.

Reactions in some cosmetic materials generally belong to an autocatalytic reaction, such as benzoyl peroxide [2]. To determine a non-isothermal kinetic model on the above cosmetic materials, the activation energy is an indispensable parameter. Therefore, the Arrhenius equation was used to calculate for nth order reaction. The Arrhenius equation describes the temperature versus reaction rate. An indefinite integral type Arrhenius equation is shown in Eq. (1).

$$k = Ae^{-E_a (RT)^{-1}} \quad (1)$$

where  $k$  is reaction rate constant,  $A$  is Arrhenius constant,  $E_a$  is activation energy which is usually displayed by kilojoule per mol ( $\text{kJ mol}^{-1}$ ),  $R$  is air constant, and  $T$  is absolute temperature, which is displayed by degree Kelvin (K).

According to the Arrhenius equation,  $k$  is proportional to  $T$  and  $E_a$ . That is, when  $E_a$  receives a higher value,  $k$  rises faster as  $T$  is augmented;  $k$  is more sensitive with  $T$ . For different  $T$ , the plot of  $\ln k$  versus  $T^{-1}$  presents a straight line, with the slope and intercept  $-E_a R^{-1}$  and  $\ln A$ , respectively. Therefore,  $E_a$  can also be expressed as in Eq. (2).

$$E_a = RT^2 d \ln k (dT)^{-1} \quad (2)$$

### 3 Results and discussion

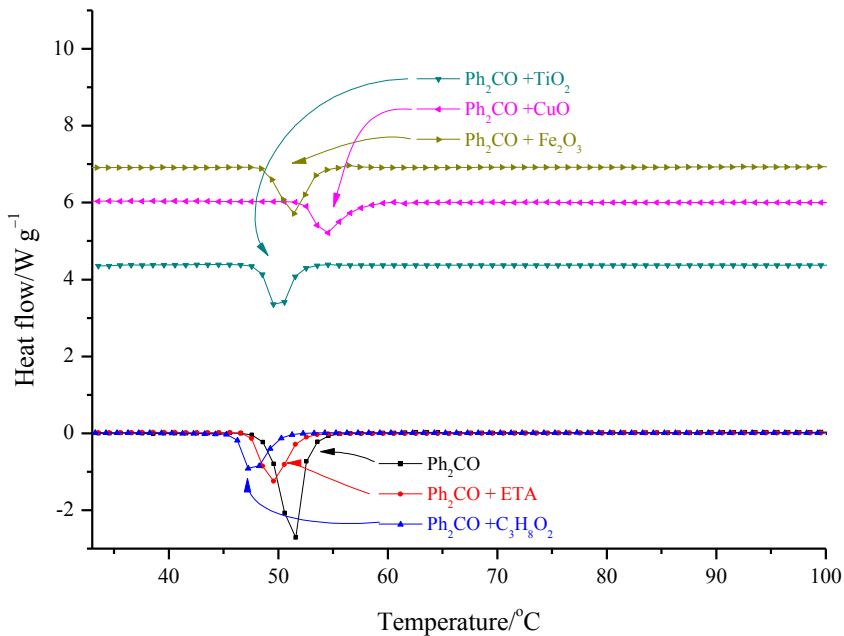
Common cosmetic materials were tested by DSC at a heating rate of  $4^\circ\text{C min}^{-1}$  with matrix relation randomly. Overall, the results on thermal stability of materials have been positive. To summarize the salient features of the tests, several findings are of interest. Different substances seem to be closely connected to onset temperature and their reaction intensities. The pure materials and materials mixed with mineral make-up powder for DSC tests are shown in Fig. 1.

As expected, some reactions happened when the pure materials were mixed with others. The findings suggest that these materials are not necessarily mutually exclusive. Not surprisingly, the results of study did not show extreme danger since these substances are used on body and skin closely. Nevertheless, a phase change may cause the quality variation to become lower, even inferior. Interestingly, when the Ph<sub>2</sub>CO mixed with propylene glycol and ETA, respectively, onset temperatures decreased. In regards to mining-make up materials with Ph<sub>2</sub>CO, onset temperatures also decreased. The difference is that the onset temperature of Ph<sub>2</sub>CO mixed with CuO compared higher with pure Ph<sub>2</sub>CO. The initial reaction of Ph<sub>2</sub>CO mixed with propylene glycol was low to  $46.08^\circ\text{C}$ . It means that the quality deterioration will occur because this temperature is as low as ambient surroundings. To explore more deeply concerning different situations, Ph<sub>2</sub>CO mixed with propylene glycol was tested at heating rates of 0.5, 1.0, 2.0, 4.0, and  $8.0^\circ\text{C min}^{-1}$ .

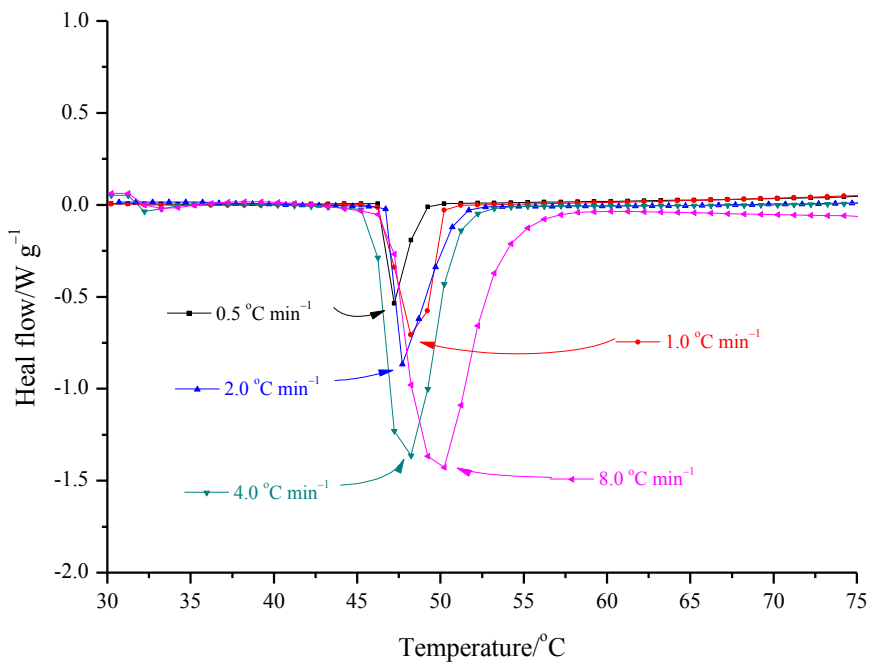
$$d\alpha (dt)^{-1} = Ae^{-E_a (RT)^{-1}} f(\alpha) \quad (3)$$

Figure 2 illustrates that when heating rate became higher, the endothermic onset temperatures on DSC were oppositely getting lower. It is noteworthy that the endothermic peak heat flow of  $0.5$  and  $8.0^\circ\text{C min}^{-1}$  is  $-0.54$  and  $-1.43 \text{ W g}^{-1}$ , respectively. Apparently, the maximum endothermic peak heat flow is approximately three-fold higher than the minimum one. To obtain  $E_a$  and other parameters, the

method from the American Society for Testing and Materials E698-5 was adopted, as shown in Eq. (3) [3].

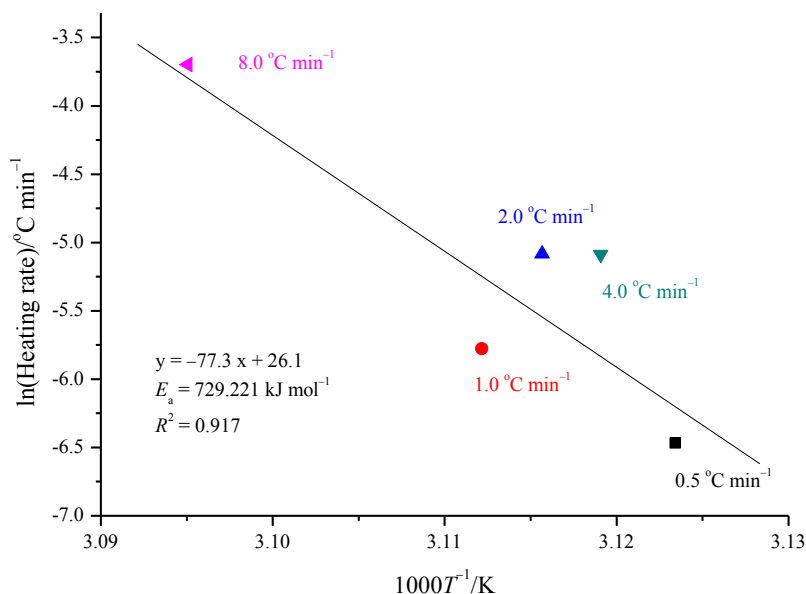


**Figure 1.** DSC curve during heating process for pure  $\text{Ph}_2\text{CO}$  and  $\text{Ph}_2\text{CO}$  mixed with common ingredients of cosmetic, respectively, at heating rate of  $4.0^{\circ}\text{C min}^{-1}$ .



**Figure 2.** DSC curve during heating process for  $\text{Ph}_2\text{CO}$  mixed with  $\text{C}_3\text{H}_8\text{O}_2$  at heating rates of  $0.5$ ,  $1.0$ ,  $2.0$ ,  $4.0$ , and  $8.0^{\circ}\text{C min}^{-1}$ .

To refer to Eq. (3), the  $E_a$  between different heating rates was calculated. The linear regression was adopted to figure out the R-square of relationship in different heating rates, as shown in Fig. 3.



**Figure 3.** Apparent activation energy calculation with  $\text{Ph}_2\text{CO}$  mixed with  $\text{C}_3\text{H}_8\text{O}_2$ .

In the end, SADT was assessed in this study to consider the thermal stability of  $\text{Ph}_2\text{CO}$  mixed with propylene glycol. The SADT is steady at  $45.0^{\circ}\text{C}$  for 50.0, 100.0, 200.0, and 500.0 kg.

## 4 Conclusion

The findings of this study pointed out that  $\text{Ph}_2\text{CO}$  has an advance reaction and phase alternation when it is mixed with propylene glycol. It should be noted that the heat flow between different heating rates is a several-fold gap. It is conceivable that when this kind of combined cosmetic product deteriorates in quality it becomes indisposed for people to reuse. The parameters of thermokinetic technology used in this study can be applied in usage and storage mechanism for cosmetics of interest.

## Acknowledgments

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## References

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