# Notes

## ON THE METHOD OF COATS AND REDFERN FOR THE KINETIC ANALYSIS OF THERMOANALYTICAL DATA

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In a recent issue of this journal, Judd and Pope [1] dealt with the kinetic analysis of the thermal decompositions of calcium, strontium and barium carbonates. The following equation was used for the kinetic analysis of experimental data, according to Coats and Redfern [2], when a first-order reaction is assumed;

$$\log_{10}\left[-\log_{10}\frac{(1-\alpha)}{T^2}\right] = \log_{10}\frac{AR}{aE}\left[1-\frac{2RT}{E}\right]-\frac{E}{2.303\,RT} \tag{1}$$

where $\alpha$ = fraction of sample decomposed at time $t$
$T$ = temperature (°K)
$A$ = pre-exponential factor
$R$ = the gas constant
$E$ = activation energy
$a$ = conversion factor to transfer from a time scale to a temperature scale,

i.e.
$$a = \frac{\mathrm{d}T}{\mathrm{d}t} \tag{2}$$

Equation (1) was actually printed in the paper of Coats and Redfern [2]. However, this equation is incorrect, presumably due to misprinting since correct expressions are found in the other parts of the paper.

The correct equation can be derived from the following fundamental equation:

$$\int_0^{\alpha}\frac{\mathrm{d}\alpha}{(1-\alpha)^n} = \frac{A}{a}\int_0^{T}\exp\left(-\frac{E}{RT}\right)\mathrm{d}T \tag{3}$$

where $n$ is the order of reaction. The integration for $n = 1$ gives

$$-\log_e(1-\alpha) = \frac{ART^2}{aE}\left[1-\frac{2RT}{E}\right]\exp\left(-\frac{E}{RT}\right) \tag{4}$$

where the integral of the right-hand side of Eq. (3) is approximated. Taking logarithms, we obtain

$$\log_{10}\left[-\frac{\log_e(1-\alpha)}{T^2}\right] = \log_{10}\frac{AR}{aE}\left[1-\frac{2RT}{E}\right]-\frac{E}{2.303\,RT} \tag{5}$$

Thus, not $\log_{10}\left[-\log_{10}\frac{(1-\alpha)}{T^2}\right]$ but $\log_{10}\left[-\frac{\log_e(1-\alpha)}{T^2}\right]$ should be plotted against $1/T$ for a reaction of the first order.

Although Judd and Pope obtained the result that the reactions are of order 2/3 for the three substances, revision may be necessary since an incorrect method was applied to analyse the experimental data.

## References

1. M. D. JUDD and M. I. POPE, J. Thermal Anal., 4 (1972) 31.
2. A. W. COATS and J. P. REDFERN, Nature, 201 (1964) 68.