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Short Communication

AN ALTERNATIVE METHOD FOR THE EVALUATION OF INTEGRAL DEPENDENT ON PARAMETER E IN CLASSICAL NON-ISOTHERMAL KINETICS WITH LINEAR HEATING RATE

R. K. Gartia, Th. Subodh Chandra Singh and P. S. Mazumdar

DEPARTMENT OF PHYSICS, MANIPUR UNIVERSITY, CANCHIPUR, IMPHAL - 795 003 MANIPUR, INDIA

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We have suggested a straightforward method for the determination of the derivative of the temperature integral with respect to the activation energy.

Recently Urbanovici and Segal [1] have proposed a method for the evaluation of the first derivative of the temperature integral with respect to the activation energy. Here we plan to propose an alternative straightforward method to obtain the first derivative of the temperature integral with respect to the activation energy, which is needed for the evaluation of the kinetic parameters by the method of least squares [1].

The temperature integral can be written as [1]

$$I(T,E) = \int_{0}^{T} e^{-E/RT'} \mathrm{d}T' \qquad (1)$$

where the symbols have their usual meanings. If we put $u' = E/RT'$ [2] we get

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$$I(u,E) = \frac{E}{R}\int_u^\infty \frac{e^{-u'}}{u'^2}\,du' \tag{2}$$

The integral in (2) can be expressed in terms of the second exponential integral [3] as

$$E_2(u) = \int_1^\infty \frac{e^{-ut}}{u^2}\,dt = u\int_u^\infty \frac{e^{-u'}}{u'^2}\,du' \tag{3}$$

From (2) and (3) we have

$$I(u,E) = \frac{E}{R}\frac{E_2(u)}{u} \tag{4}$$

From (4) we get

$$\frac{dI}{dE} = \frac{1}{R}\left[\frac{E_2(u)}{u} - \frac{e^{-u}}{u}\right] \tag{5}$$

where we have used the following relations [3]

$$\frac{d}{du}\left[E_2(u)\right] = -E_1(u) \tag{6}$$

$$E_2(u) = e^{-u} - uE_1(u) \tag{7}$$

$E_1(u)$ is the first exponential integral.

The expression (5) for dI/dE can be evaluated quite accurately by using suitable rational approximations for $E_2(u)$ [2-5].

One such rational approximation as used by Gartia *et al.* [6, 7] is

$$E_2(u) = e^{-u}\frac{f(u)}{g(u)} \qquad (\text{for, } 1 \leq u < \infty) \tag{8}$$

where,

$$f(u) = 0.999993\,u^3 + 7.5739\,u^2 + 12.464892\,u + 3.690723 \tag{9}$$

$$g(u) = u^4 + 9.573322\,u^3 + 25.632956\,u^2 + 21.099653\,u + 3.958497 \tag{10}$$

$$E_2(u) = e^{-u} + u\ln u + u\,(0.577216 - 0.999992\,u + 0.249911\,u^2 - 0.055200\,u^3 + 0.009760\,u^4 - 0.001079\,u^5) \quad (\text{for, } 0 \leq u \leq 1) \tag{11}$$

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