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Note

INTEGRAL DEPENDENT ON PARAMETER "E" IN CLASSICAL NON-ISOTHERMAL KINETICS WITH LINEAR HEATING RATE, II.

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In a previous paper [1] the derivative with respect to the activation energy E of the integral

$$I(T,E) = \int_0^T e^{-\frac{E}{Ry}} dy \tag{1}$$

was considered.
Taking into account the temperature dependence of the preexponential factor

$$A = A_r T^r \qquad (r = \text{const}) \tag{2}$$

this note deals with the derivative with respect to E of the integral:

$$I(T,E,r) = \int_0^T y^r e^{-\frac{E}{Ry}} dy \tag{3}$$

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To obtain the derivative $\frac{\partial I(T,E,r)}{\partial E}$ the following relationships [2]

$$I(T,E,r) = \frac{RT^{r+2}}{E} e^{-\frac{E}{RT}} Q_r\left(\frac{E}{RT}\right) \tag{4}$$

$$Q'_r\left(\frac{E}{RT}\right) - Q_r\left(\frac{E}{RT}\right)\left(1 + \frac{r+2}{\frac{E}{RT}}\right) + 1 = 0 \tag{5}$$

will be used.

Relationship (5) is obtained taking the derivative with respect to T of relationship (4) and $Q'_r\left(\frac{E}{RT}\right)$ means derivative of Q_r with respect to $-\frac{E}{RT}$.

From relationship (4) one obtains:

$$\frac{\partial I(T,E,r)}{\partial E} =$$

$$= -\frac{RT^{r+2}}{E^2} e^{-\frac{E}{RT}} Q_r\left(\frac{E}{RT}\right) - \frac{T^{r+1}}{E} e^{-\frac{E}{RT}} Q_r\left(\frac{E}{RT}\right) + \frac{T^{r+1}}{E} e^{-\frac{E}{RT}} Q'_r\left(\frac{E}{RT}\right) \tag{6}$$

The substitution of $Q'_r\left(\frac{E}{RT}\right)$ from (5) in (6) leads to:

$$\frac{\partial I(T,E,r)}{\partial E} = \frac{RT^{r+2}}{E^2} e^{-\frac{E}{RT}} \left((r+1)\, Q_r\left(\frac{E}{RT}\right) - \frac{E}{RT}\right) \tag{7}$$

It is easy to see that for $r = 0$ relationship (7) turns into relationship (12) from reference [1]. As far as the form of the function $Q_r\left(\frac{E}{RT}\right)$ is concerned, among the approximations considered in reference [2] we mention in these note only one, namely

$$Q_r(x) \cong \frac{x^2 + x(4+r)}{x^2 + x(6+2r) + (r+3)(r+2)} \tag{8}$$

References

1 E. Urbanovici and E. Segal, J. Thermal Anal., 35 (1989) 215.
2 E. Urbanovici and E. Segal, Thermochim. Acta, in print