DISCUSSION ON DECISION LIMIT AND DETECTION LIMIT IN SPECTROSCOPY

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ABSTRACT

Based on fundamental arguments, the expressions for the decision limit and the detection limit both in the count domain and in the count rate domain are derived. These expressions are found to be different from those shown in the existing literature.

Keywords Decision limit, Detection limit, Spectroscopy, Modifications

1 INTRODUCTION

When using a spectroscopic system to get signals (count values or count rate values) from a measured sample in a specified region of interest in the spectrum (usually the area under a specified peak), the decision limit and the detection limit are very important for they help one to determine when one has got detections of signals from the sample or the maximum activity present in the sample if one does not get detections. However, incorrect expressions of these limits occur in some existing literature (e.g. Ref.[1]).

These limits have been defined by Curie in 1968[2]. The decision limit is solely a characteristic of the measuring system itself depending on the background signals obtained, and is totally independent of the activities present or other properties of the samples to be measured. It specifies a net signal level such that when it is exceeded by a detected signal, that detected signal can be said to exceed the background level with a high probability (denoted as 1-α, with α usually very small). On the contrary, the detection limit is dependent on the activity present in the measured sample. To define the detection limit, it is beneficial to first look at the minimum detectable activity (MDA) of the sample (denoted as A_D). When the activity of the sample is greater than A_D, the signal detected by the measuring system (given by εA_D, where ε is the efficiency of the system) will be greater than the decision limit with

Table 1
The K values corresponding to common α and β values

α or β	(1-α) or (1-β)	K_α or K_β
0.01	0.99	2.327
0.02	0.98	2.054
0.025	0.975	1.960
0.05	0.95	1.645
0.10	0.90	1.282
0.20	0.80	0.842
0.50	0.50	0

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a high probability (denoted as 1-β with β usually very small), or it can be said that a detection has been got. The detection limit is defined to be the quantity εA_D.

It is convenient to define K_α and K_β by setting the probability of getting values greater than K_α and K_β in a standard normal distribution to be α and β respectively, which are shown in Table 1. In most cases, one takes $\alpha = \beta$ so that $K_\alpha = K_\beta = K$.

2 COUNT AND COUNT RATE DOMAINS

In fact, for discussions on the decision limits and the detection limits, one frequently encounters two cases, i.e., the case for count values (hereafter referred to case 1) and the case for the count rate values (hereafter referred to case 2). Therefore, L_C and L_D are denoted the decision limit and the detection limit in the count domain, and l_c and l_d in the count rate domain respectively. The background counting time and the sample counting time are T_b and T_s, respectively, which could be but not necessarily equal. In this way, one has

$$L_C/T_s = l_c \tag{1}$$

$$L_D/T_s = l_d \tag{2}$$

$$N_b(T_s)/T_s = N_b(T_b)/T_b = n_b \tag{3}$$

where n_b is the background count rate, $N_b(T_s)$ and $N_b(T_b)$ are background counts obtained by the system for T_s and T_b, respectively.

3 DECISION LIMIT

In deriving the decision limit, we are in fact looking for significant deviations of a detected signal from the background. Therefore, the null hypothesis is that there exists no radioactivity in the measured sample. In mathematical terms, the null hypothesis should then be that the detected value of the total count from the background and the sample ($N_{b,s}$) is equal to the detected value of the count N_b from the background alone (i.e., $N_{b,s} = N_b$) for case 1, i.e. the expectation value of the net count is zero. For $T_s = T_b$, it is obvious to have the standard deviation σ_o given by

$$\sigma_o = [2N_b]^{1/2} \tag{4}$$

so that

$$L_C = K_\alpha [2N_b]^{1/2} \tag{5a}$$

For general discussions ($T_s \neq T_b$),

$$L_C = K_\alpha \left[N_b(T_s) + N_b(T_b)\left(\frac{T_s}{T_b}\right)^2\right]^{1/2} \tag{5}$$

For case 2, the standard deviation s_o is

$$s_o = \left[\frac{n_b}{T_s} + \frac{n_b}{T_b}\right]^{1/2} \tag{6}$$

so that

$$l_c = K_\alpha \left[\frac{n_b}{T_s} + \frac{n_b}{T_b}\right]^{1/2} \tag{7}$$

When $T_s = T_b = T$,

$$l_c = K_\alpha \left[\frac{2n_b}{T}\right]^{1/2} \tag{7a}$$

4 DETECTION LIMIT

The discussions on the detection limit are similar to those on the decision limit. The detection limit should be given by $L_D = L_C + K_\beta \sigma_\alpha$, where σ_α is the standard deviation of the net count distribution for the sample obtained by the measuring system.

In deriving the detection limit, the null hypothesis (no detection) should be that the detected signal from the measured sample is (at most) L_D. In mathematical terms, the null hypothesis should then be $N_{b,s} = N_b + L_D$ for case 1. For $T_s = T_b$, it is obvious to have the standard deviation σ_α given by

$$\sigma_\alpha = [N_{b,s} + N_b]^{1/2} \tag{8}$$

so that

$$L_D = L_C + K_\beta \sigma_\alpha = K_\alpha [2N_b]^{1/2} + K_\beta [N_{b,s} + N_b]^{1/2}$$

when $K_\alpha = K_\beta = K$, one obtains

$$L_D = L_C + K(N_{b,s} + N_b)^{1/2} = L_C + K[(L_D + N_b) + N_b]^{1/2}$$

Recalling $L_C^2 = 2N_b$, we arrive at

$$L_D = K^2 + 2L_C = K^2 + 2K[2N_b]^{1/2} \tag{9a}$$

For general discussions ($T_s \neq T_b$), when $K_\alpha = K_\beta = K$,

$$L_D = K^2 + 2K \left[N_b(T_s) + N_b(T_b)(\frac{T_s}{T_b})^2\right]^{1/2} \tag{9}$$

For case 2, the standard deviation s_α is

$$s_\alpha = \left[\frac{n_b}{T_b} + \frac{n_b + l_d}{T_s}\right]^{1/2} \tag{10}$$

so that

$$l_d = K_\alpha \left[\frac{n_b}{T_s} + \frac{n_b}{T_b}\right]^{1/2} + K_\beta \left[\frac{n_b}{T_s} + \frac{n_b}{T_b} + \frac{l_d}{T_s}\right]^{1/2}$$

When $K_{\alpha} = K_{\beta} = K$, one has

$$l_{\mathrm{d}} = \frac{K^2}{T_{\mathrm{s}}} + 2l_{\mathrm{c}} = \frac{K^2}{T_s} + 2K\left[\frac{n_{\mathrm{b}}}{T_{\mathrm{s}}} + \frac{n_{\mathrm{b}}}{T_{\mathrm{b}}}\right]^{1/2} \tag{11}$$

when $T_{\mathrm{s}} = T_{\mathrm{b}} = T$,

$$l_{\mathrm{d}} = \frac{K^2}{T} + 2K\left[\frac{2n_{\mathrm{b}}}{T}\right]^{1/2} \tag{11a}$$

5 CONCLUSIONS

The decision limit and the detection limit are very important for they help one to determine when one has got detections of signals from the sample and the maximum activity present in the sample if one does not get detections. Based on fundamental arguments, we have arrived at expressions for the limits both in the count domain (case 1) and in the count rate domain (case 2).

For case 1, the decision limit L_{C} and the detection limit L_{D} are respectively given by Eq.5 and (when $K_{\alpha} = K_{\beta} = K$) Eq.9. For case 2, the decision limit l_{c} and the detection limit l_{d} are respectively given by Eq.7 and (when $K_{\alpha} = K_{\beta} = K$) Eq.11. When $T_{\mathrm{s}} = T_{\mathrm{b}} = T$, these equations can be simplified to Eqs.(5a), (9a), (7a) and (11a), respectively. These equations are different from those shown in some existing literature (e.g. Ref.[1]).

REFERENCES

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