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Fitting method for vacuum ultraviolet spectrometer calibration using line ratio technique

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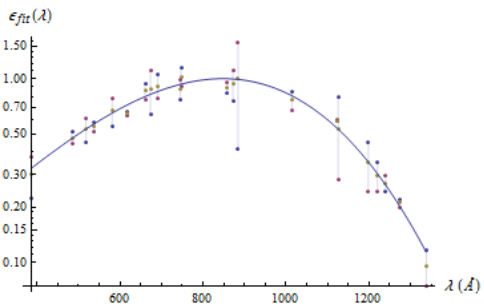
Graphical Abstract



Abstract.

We have developed theoretically a generalized least squared fitting, using as a fitting function the exponential of a cubic polynomial, and as data, the efficiency ratios between different wavelengths in the vacuum ultraviolet spectral range. The fitting function is suggested by the linear interpolation of efficiency ratios whose wavelengths are nearby. We have tested the fitting proposed for data given by different authors in the literature, obtaining a determination coefficient above 98%.

Results and Discussion

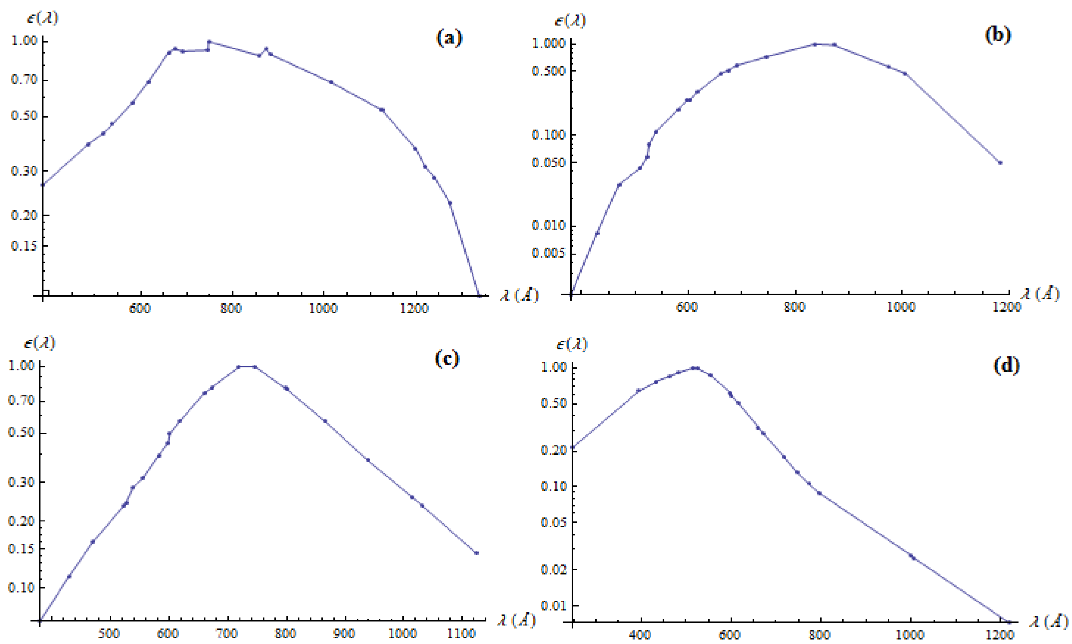


Fig. 1. Graph of the efficiency function in logarithmic scale obtained by linear interpolation according to the data given by (a) Martin et al. [7], (b) Bastert et al. [4], (c) Yang and Cunningham [3] and (d) Sato et al. [5].

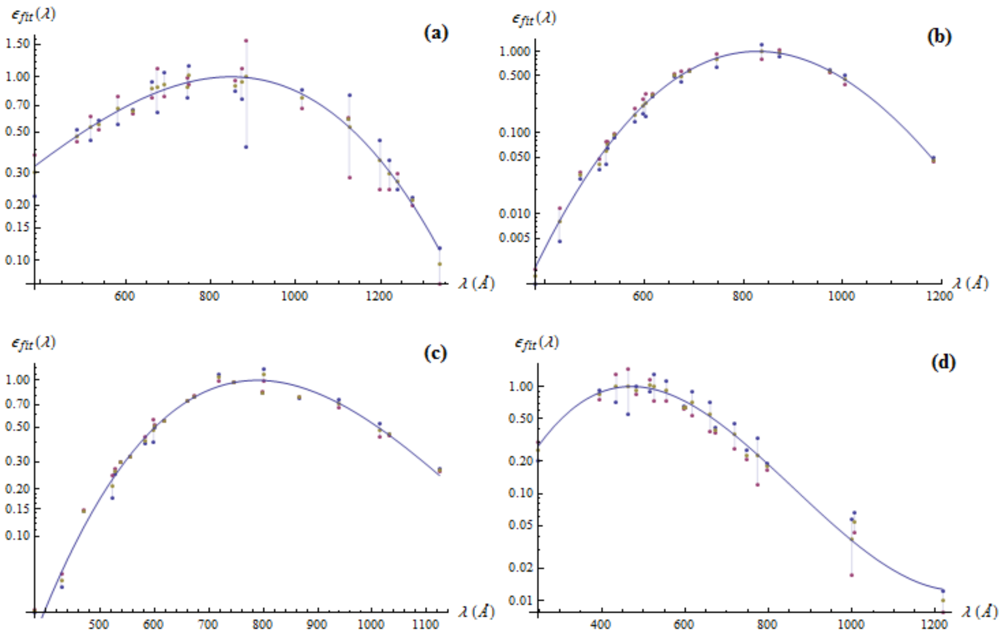


Fig 2. Efficiency curves fitted by generalized least squares in logarithmic scale obtained from the data offered by (a) Martín et al. [7], (b) Bastert et al. [3], (c) Yang and Cunningham [4] and (d) Sato et al. [5].

Table 1: Fitting parameters and determination coefficients for different authors.

Ref.	a_1 (Å^{-3})	a_2 (Å^{-2})	a_3 (Å^{-1})	K	λ_{max} (Å)	$\overline{R}_\rho$	R_y
[7]	$-3{,}999\times10^{-9}$	$3{,}069\times10^{-6}$	$3{,}424\times10^{-3}$	$6{,}912\times10^{-2}$	848,1	0,9586	0,9855
[3]	$1{,}340\times10^{-8}$	$-4{,}871\times10^{-5}$	$5{,}183\times10^{-2}$	$3{,}556\times10^{-8}$	788,6	0,9426	0,9824
[4]	$7{,}397\times10^{-9}$	$4{,}532\times10^{-5}$	$5{,}988\times10^{-2}$	$1{,}374\times10^{-10}$	828,8	0,9951	0,9984
[5]	$1{,}851\times10^{-8}$	$-4{,}779\times10^{-5}$	$3{,}269\times10^{-2}$	$1{,}195\times10^{-3}$	470,8	0,9311	0,9896

Conclusions

We have developed a fitting method to calculate the efficiency curve of a spectrometric system as a function of wavelength $\varepsilon(\lambda)$ from experimental line ratios between different wavelengths. The efficiency ratios are obtained by the line ratio method [1]. The method presented in the literature, Sato et al [5], of linear interpolation to reconstruct the efficiency function from the efficiency ratios, has the disadvantage that depends on the order of the efficiency ratios, since it is an iterative process. In any case, the linear interpolation method applied to different spectrometric systems in the spectral range of the vacuum ultraviolet (see Fig. 2) suggests that the efficiency function fits to the exponential of a cubic polynomial,

$$\varepsilon(\lambda) \approx \varepsilon_{fit}(\lambda) = K \exp\left(a_1\lambda^3 + a_2\lambda^2 + a_3\lambda\right).$$

The proposed method has the advantage that all efficiency ratios are fitted simultaneously and not iteratively as in the linear interpolation method. In addition, using generalized least squares (7), we take into account the experimental error of each efficiency ratio, so that the ratios with less error have more weight in the fitting and vice versa. The comparison of the results obtained by linear interpolation and by the proposed method (Figs. 1 and 2) suggests that the linear interpolation method is indeed a first approximation to the efficiency function. Also, a method has been developed to visualize how efficiency ratios would fit with its corresponding error in the proposed fitting curve. Finally, we have found a fitting level over 98% for different authors given in the literature (Table 1).

References

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