

The program *epidotefull.m* is a simple routine running under MATLAB™ environment (tested for the R2022a version). It calculates the amount of iron in epidotes using the equations reported in the article.

In input it requires the positions of the peaks at around 570, 980, 1090, 3370 cm⁻¹.

They should be given as argument, between round brackets, comma separated (e.g. *epidotefull* (570.5, 980.3, 1090.5, 3365)). The order of the peaks is not important.

The equations used for the calculation change according to the number of input arguments.

If three numbers are present in input, then they are considered as the position of the low-frequency peaks (at 570, 980, and 1090 cm⁻¹) and only the three corresponding equations are used to determine XFe (amount of iron). The obtained value *xfe_lf* is the weighted average of the results obtained from the three equations. The weight of the three equations are contained in the vector *wg*. By default, all equations have the same weight (1). The weights can be changed in case the experimental results produce results of different quality for the different peaks.

In case of a single input value, it is considered as the position of the OH stretching band at nearly 3370 cm⁻¹ and only the equation related to OH stretching is used to determine XFe (*xfe_oh*).

In case of four numbers in input, all the equations are used, and iron amount (XFe) is calculated as the average mean of the values obtained from the low-frequency equations (*xfe_lf*) and the one obtained from the OH stretching equation (*xfe_oh*). The relative weight used for the OH stretching part in the mean average is *wg-oh*. Its default value is 0.5 (same weight for both parts). It can be changed if the experiments produce spectra of different quality or reliability in the low-frequency part and high-frequency (OH stretching) part of the spectrum.