

## ***The Journal of Gemmology Data Depository***

Spectral deconvolution of the optical absorption spectra of laurenthomasite to accompany the article:

Pignatelli, I., Ferraris, C. & Schaniel, D. 2023. Origin of the colour and dichroism in laurenthomasite. *Journal of Gemmology*, **38**(7), 2023, 708–716, <https://doi.org/10.15506/JoG.2023.38.7.708>.

In Figure DD-1, the absorption spectrum of laurenthomasite has been simulated using seven Gaussian peaks and a constant baseline. The purpose of this simulated spectrum is not to perform a fit, but to provide a possible deconvolution of the spectrum of laurenthomasite carried out perpendicular to the *c*-axis ( $E \perp c$ ) based on a reasonable assumption of peak positions and peak widths. For example, the two peaks in the near-infrared region (referred to as peaks 0 and 1) have been placed at  $7700 \text{ cm}^{-1}$  (1300 nm) and  $11000 \text{ cm}^{-1}$  (909 nm), a reasonable assumption for their positions due to the  $E_g$  state of  $\text{Fe}^{2+}$  (see Amthauer & Rossman 1984). For this simulation, we consider the spectrum saturated between  $9000\text{--}13000 \text{ cm}^{-1}$  (1111–769 nm), an assumption justified by the poor signal-to-noise ratio at an elevated absorbance value of nearly four in this spectral region. (The crystal is rather thick, 4.41 mm, and the spectrum was acquired without cutting or other preparation of its surfaces.)

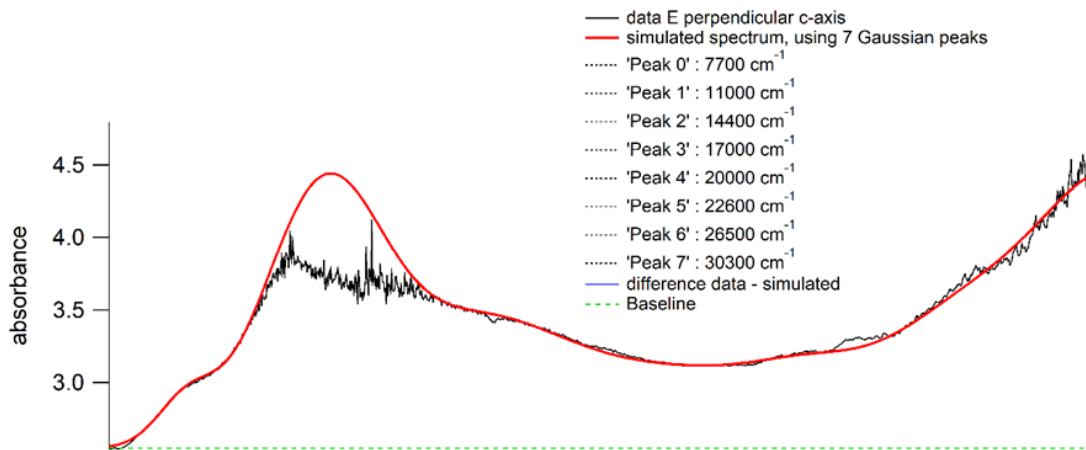
From this simulation, it is clear that the visible region of the spectrum cannot be fitted by a single peak. Instead, at least three or four peaks are needed to describe the observed spectrum. These peaks are placed at  $14400$ ,  $17000$ ,  $20000$  and  $22600 \text{ cm}^{-1}$ , corresponding to 694, 588, 500 and 442 nm. The two bands at  $14400$  and  $17000 \text{ cm}^{-1}$  (the latter with a FWHM of  $4163 \text{ cm}^{-1}$ ) are consistent with assignment to  $\text{Fe}^{2+}\text{--Fe}^{3+}$  intervalence charge transfer (IVCT). Mattson and Rossman (1987) listed the IVCT as between  $14100$  and  $16500 \text{ cm}^{-1}$ , with FWHM values ranging from  $3150$  to  $6600 \text{ cm}^{-1}$ .

### **References**

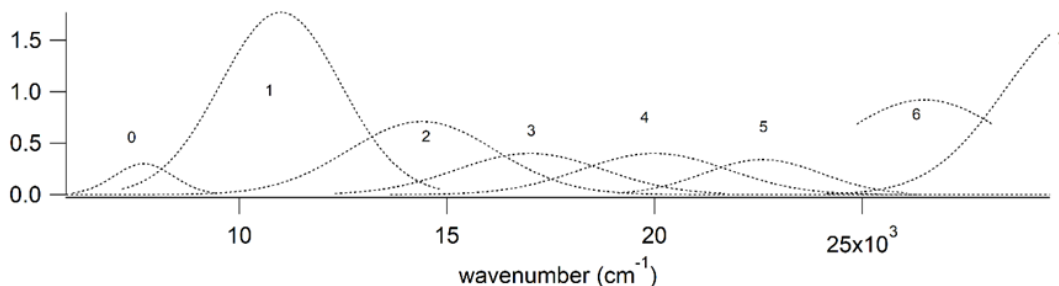
- Amthauer, G. & Rossman, G.R. 1984. Mixed valence of iron in minerals with cation clusters. *Physics and Chemistry of Minerals*, **11**(1), 37–51, <https://doi.org/10.1007/bf00309374>.
- Mattson, S.M. & Rossman, G.R. 1987. Identifying characteristics of charge transfer transitions in minerals. *Physics and Chemistry of Minerals*, **14**(1), 94–99, <https://doi.org/10.1007/bf00311152>.

Figure DD-1: (a) Comparison between experimental spectrum (black line) and simulated one (red line). (b) The simulated spectrum is obtained using seven Gaussian peaks (dotted lines). (c) The difference between experimental and simulated data is shown as the blue line.

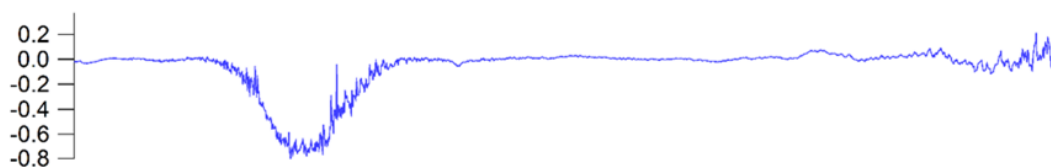
a)



b)



c)



Baseline Type: Constant

$$y_0 = 2.5473 \pm 1.079e-60$$

Peak 0 Type: Gauss

Location = 7700 [1300 nm]  
 Height = 0.3  
 Area = 531.74  
 FWHM = 1665.1

Peak 1 Type: Gauss

Location = 11000 [909 nm]  
 Height = 1.77  
 Area = 6431.3  
 FWHM = 3413.5

Peak 2 Type: Gauss

Location = 14400 [694 nm]  
 Height = 0.71  
 Area = 3146.1  
 FWHM = 4162.8

Peak 3 Type: Gauss

Location = 17000 [588 nm]  
 Height = 0.4  
 Area = 1772.5  
 FWHM = 4162.8

Peak 4 Type: Gauss

Location = 20000 [500 nm]  
 Height = 0.4  
 Area = 1772.5  
 FWHM = 4162.8

Peak 5 Type: Gauss

Location = 22600 [442 nm]  
 Height = 0.34  
 Area = 1205.3  
 FWHM = 3330.2

Peak 6 Type: Gauss

Location = 26500 [377 nm]  
 Height = 0.92  
 Area = 4892  
 FWHM = 4995.3

Peak 7 Type: Gauss

Location = 30300 [330 nm]  
 Height = 1.7  
 Area = 7834.2  
 FWHM = 4329.3