Appendix 2 - Error analysis

The uncertainties associated with *y*, estimated composition, are computed as follows:

$$\sigma_y^2 = \sigma_{SE}^2 + \sigma_{y\,uc}^2$$

Where:

$$\sigma_{SE}^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Where *n* is the number of datasets in the regression; y_i and $\hat{y}_i$ are the observed and calculated *y* values of the regression data, respectively.

and

$$\sigma_{y\,uc}^2 = \frac{1}{m}\sum_{j=1}^{m}(\hat{y}_j - \hat{y}_{j\,\sigma_{uc}})^2$$

Where m is the number of unit-cell parameters in the function (e.g., five in plagioclase), $\hat{y}_j$ is the composition calculated with your input unit-cell parameters, $\hat{y}_{j\,\sigma_{uc}}$ is the calculated composition calculated with the error associated with your unit-cell parameter added to the unit-cell parameter [e.g., $a_{\sigma_{uc}}$ = (a+σ_a)].

Errors associated with arithmetical equations were computed with the following formula:

$$\sigma_{y_i}^2 = \sum_{i}^{n}\sigma_{x_i}^2$$

Where σ_{x_i} is the uncertainty associated with each coefficient in the equation.

Root-Mean-Square Error (RMSE) = $\sqrt{\frac{\sum_{i=1}^{n}(y_i-\hat{y}_i)^2}{n}}$

Where *n* is the number of datasets in the regression; y_i and $\hat{y}_i$ are the observed and calculated *y* values of the equation, respectively.