## addenda and errata



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## Iterative energy self-calibration of Fe XANES spectra. Erratum

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A correction is made to the paper by Jones *et al.* (2020). [*J. Synchrotron Rad.* 27, 207–211].

In the paper by Jones *et al.* (2020), the authors have noted that an incorrect value was published for the calibrated  $\text{Fe}^{3+}/\Sigma\text{Fe}$ for the rafted pumice sample from the 2012 Havre eruption. The correct value is 0.257 (0.010) and is included in the updated Table 2 below and updated in the inset in Fig. 3(*c*) (overleaf).

## Table 2

Summary of uncalibrated and self-calibrated values for the data presented in Fig. 3, where the uncalibrated, self-calibrated and expected Fe<sup>3+</sup>/ $\Sigma$ Fe ratios are presented together with the required energy change ( $\Delta E$ ).

Sample	$\mathrm{Fe}^{3+}/\Sigma\mathrm{Fe}$			
	Uncalibrated	Self-calibrated	Expected	$\Delta E (eV)$
MORB VG 3450	0.591 (0.018)	0.129 (0.004)	0.132	0.8
RGM-2	0.535 (0.037)†	0.231 (0.016)	0.262 (0.015)‡	0.3§
Havre pumice	0.452 (0.031)†	0.257 (0.010)	_	0.5§

 $\dagger$  Manually offset to be within calibration range.  $\ddagger$  RGM-1 values. \$ After manual offset.

## References

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Cottrell, E., Kelley, K. A., Lanzirotti, A. & Fischer, R. A. (2009). *Chem. Geol.* 268, 167–179.

Jones, M. W. M., Mallmann, G., Wykes, J. L., Knafelc, J., Bryan, S. E. & Howard, D. L. (2020). *J. Synchrotron Rad.* **27**, 207–211.



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Figure 3

Demonstration of iterative energy calibration correction. (*a*) A MORB glass spectra (Smithsonian Institute sample number VG 3450), as collected by Berry *et al.* (2018) (orange dot–dashed line), iteratively self-corrected (solid black line) to the basaltic glass standards. Also shown for reference are the spectra for the 0.011 and 0.775 Fe<sup>3+</sup>/ $\Sigma$ Fe ratio standards (black dotted lines). The Fe<sup>3+</sup>/ $\Sigma$ Fe ratio (inset) for Method A (solid orange lines) and B (dashed blue lines) as a function of iteration number shows convergence to a single Fe<sup>3+</sup>/ $\Sigma$ Fe ratio. Similar treatment is shown for the RGM-2 reference standard (*b*) and an experimental section of pumice from the 2012 Havre eruption (*c*), both iteratively self-corrected to the rhyolite glass standards (Cottrell *et al.*, 2009). Also shown for reference are the spectra for the 0.238 and 0.806 Fe<sup>3+</sup>/ $\Sigma$ Fe ratio standards (black dotted lines). The vertical dashed lines in (*a*)–(*c*) refer to the two points *E*<sub>1</sub> and *E*<sub>2</sub> in each case.