

Supplementary Materials: meltPT: A Python package for basaltic whole-rock thermobarometric analysis with application to Hawai'i

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Supplementary Texts

Text S1: Monte Carlo uncertainty analysis for a single sample

In Section 3.4 of the main text, we discuss uncertainties arising from thermobarometric analysis. We note that, if meaningful bounds can be placed on the values of the various required parameters, these uncertainties can be propagated through the analysis to uncertainties in equilibration pressure, equilibration temperature, and mantle potential temperature using a Monte Carlo approach. Here, we perform an illustrative example of such an analysis, using the same Basin-and-Range sample as elsewhere in the main text's Section 2 [Figure S1; Sample UT09DV04; Plank and Forsyth, 2016].

First, we estimate uncertainties for the relevant input parameters: Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, and H_2O wt%. Plank and Forsyth [2016] estimated Fo# for the Basin-and-Range province to be ~ 90 , with a conservative range of 89–91. We represent this range using a normal distribution with mean 90 and standard deviation 0.5. Plank and Forsyth [2016] estimated $\text{Fe}^{3+}/\Sigma\text{Fe}$ on the basis of relationships between it, melt oxidation state, and vanadium partitioning [Kress and Carmichael, 1991; Canil, 2002]. Kelley and Cottrell [2012] used a similar method and showed that, for oxidation states similar to those in the Basin-and-Range, a $\sim 5\%$ error in vanadium concentrations corresponded to a $\sim 5\%$ error in $\text{Fe}^{3+}/\Sigma\text{Fe}$. Vanadium measurements from the Snow Canyon Province, where sample UT09DV04 was collected, have a standard deviation of $\sim 8\%$ so we assume a $\sim 8\%$ standard deviation in $\text{Fe}^{3+}/\Sigma\text{Fe}$. Finally, Plank and Forsyth [2016] measured H_2O concentrations in olivine melt inclusions. They found values ranging from ~ 0.2 wt% to ~ 1.4 wt%, which they attributed to the effects of H_2O diffusion. They identified a cluster of values at the upper end of this distribution which they interpreted as the concentration of the parent melt; we use a normal distribution with a mean of 1.4 wt% and standard deviation of 0.04 wt% to represent this cluster.

We explored the propagation of input uncertainties for a single sample via two sets of Monte Carlo analyses (Figures S1). In the first set, we performed the correction for fractional crystallisation of olivine 1000 times, each time selecting values of source Fo#, source $\text{Fe}^{3+}/\Sigma\text{Fe}$, and melt water concentration at random from their respective probability distributions (Figure S1a–c). Resulting equilibration pressure, equilibration temperature, and mantle potential temperature estimates are shown in Figure S1d–e. Equilibration pressure and temperature estimates spread along two sub-parallel lines in pressure-temperature space (Figure S1e). This pattern arises because all three parameters, but in particular source Fo#, influence the amount of olivine added during the correction for fractional crystallisation: adding more olivine increases sample MgO content leading to deeper and hotter equilibration pressures and temperatures. A temperature correction for the effects of CO_2 applies at pressures ≥ 2 GPa in the Plank and Forsyth [2016]

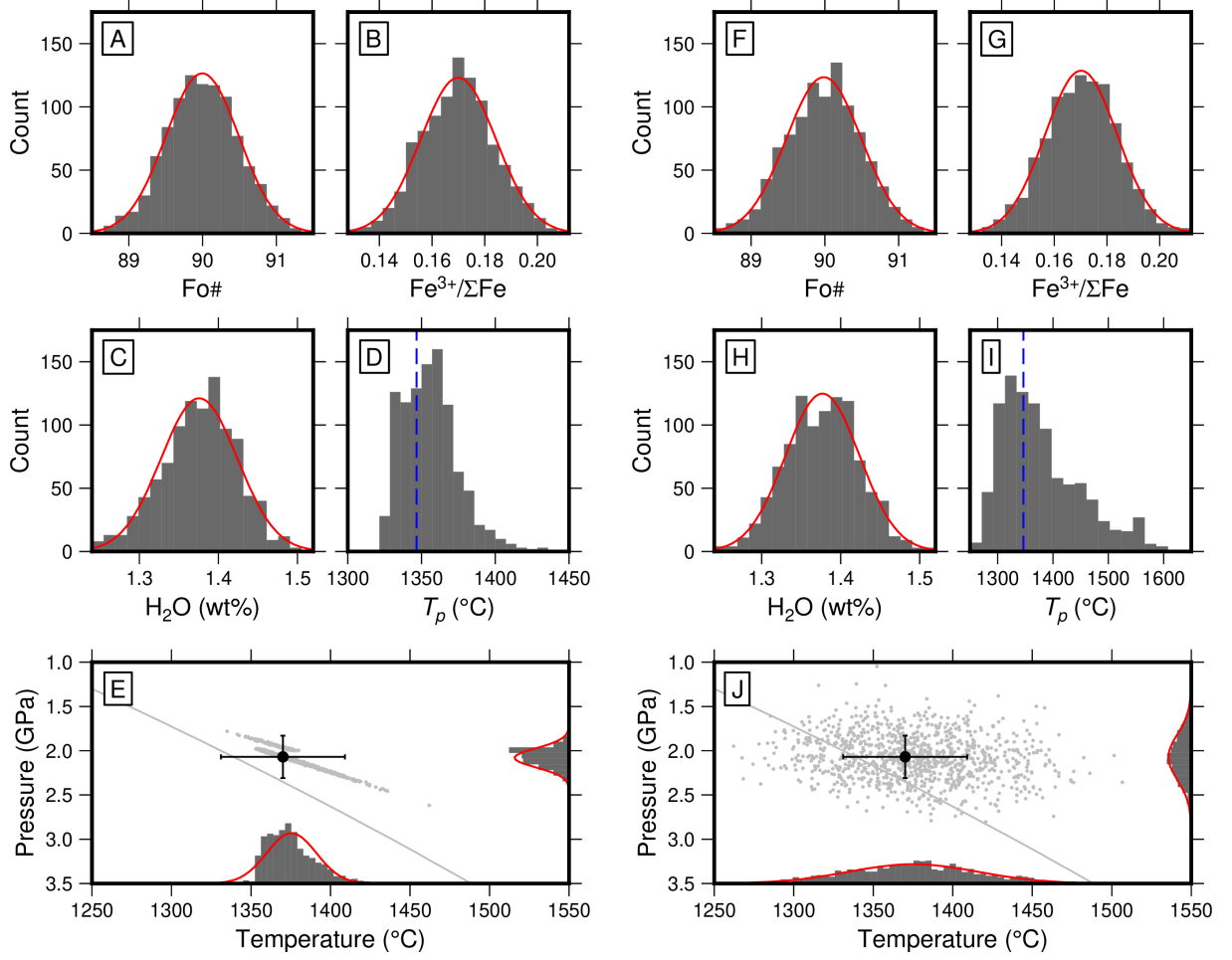


Figure S1: Monte Carlo uncertainty analysis for Sample UT09DV04 [Plank and Forsyth, 2016]. (a–c) Barcharts showing input parameter distributions. Red lines = corresponding normal distributions. Means and standard deviations for each parameter are: (a) $\text{Fo\#} = 90 \pm 0.5$; (b) $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.17 \pm 0.014$; and (c) $\text{H}_2\text{O} = 1.4 \pm 0.048$ wt%. (d) Bar chart showing distribution of resulting mantle potential temperature (T_p) estimates. Blue dashed line = T_p estimate obtained using preferred parameter values. (e) Estimated equilibration pressures and temperatures. Black circle with error bars = equilibration pressure and temperature using preferred parameter values; grey circles = equilibration pressures and temperatures obtained from Monte Carlo analysis; bar charts on horizontal and vertical axes = distributions of temperature and pressure, respectively, obtained from Monte Carlo analysis. (f–j) Same as (a–c) for second set of analyses, in which uncertainty in the thermobarometric parameterisation is also included.

scheme. This correction decreases the temperatures of deeper lying samples, producing two sub-parallel linear equilibration distributions, and causing distributions of equilibration pressures and temperatures to be slightly skewed. Nevertheless, pressure and temperature estimates are reasonably well described by normal distributions with means and standard deviations of $P = 2.08 \pm 0.11$ GPa and $T = 1375 \pm 16$ °C, respectively (Figure S1e). The mean values are close to those obtained using the preferred parameter values (2.07 GPa and 1371 °C). The distribution of mantle potential temperature estimates is also skewed, but there is a broad peak around 1350 °C; the value obtained using the preferred parameter values was 1350 °C (Figure S1d).

In the second set of analyses, we repeated the same steps, but also accounted for uncertainty in the thermobarometric parameterisation by selecting equilibration pressures and temperatures at random from normal distributions with standard deviations of ± 0.24 GPa and ± 39 °C, respectively [as quoted by Plank and Forsyth, 2016]. Results are shown in Figure S1f–j. Equilibration pressure and temperature estimates are much more widely distributed than in the first set of analyses, with means and standard deviations

of 2.07 ± 0.26 GPa and 1375 ± 41 °C, respectively (Figure S1j). These errors are only slightly larger than those introduced by the thermobarometer alone, consistent with the analysis of Plank and Forsyth [2016]. This result implies that, at least in this example, the dominant source of error is in the thermobarometric parameterisation itself. Mantle potential temperature estimates are also much more widely distributed, again with a broad peak around 1350 °C, close to the value obtained using the preferred parameter values (Figure S1i). Note that, in this example, many estimates of equilibration pressure and temperature fall below the solidus, and therefore cannot be used to estimate mantle potential temperature. This effect contributes to a skew towards higher mantle potential temperatures in the distribution.

Text S2: Monte Carlo uncertainty analysis for a suite of samples

In Section 4.1 we discuss constraints on and possible ranges of parameter values for the Hawai'ian Islands. Here, we explore implications of uncertainties in these parameter values, using samples from the island of Oahu as an example.

Melts from the Shield and Rejuvenated phases are present on Oahu. We estimate the source Fo# to be ~ 90 for all phases, with plausible upper and lower bounds of ± 1 . We represent this range as a normal distribution with mean 90 and standard deviation 0.5. For the remaining parameters, we estimate means and standard deviations of: $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.15 \pm 0.02$ and $\text{H}_2\text{O}/\text{Ce} = 144 \pm 56$ for the Shield phase; and $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.17 \pm 0.04$ and $\text{H}_2\text{O}/\text{Ce} = 211 \pm 29$ for the Rejuvenated phase. These ranges could reflect (a) variability in the source region; (b) the effects of processes acting during transport to the surface; (c) uncertainties introduced during sample preparation and analysis; or (d) a combination of the three.

First, we test the implications of attributing observed variation in the input parameters to variability in the source region. We performed two sets of 250 analyses. In the first set of analyses, we selected parameter values for each sample individually at random from normal distributions defined by the means and standard deviations outlined above. Distributions of source Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, and $\text{H}_2\text{O}/\text{Ce}$ from an example analysis are shown in Figure S2a–c. Resultant equilibration pressure and temperature estimates are shown in Figure S2d, alongside estimates obtained using preferred parameter values in Figure S2e, for comparison. For the Monte Carlo example, we obtain a similar best-fitting mantle potential temperature to that obtained using the preferred parameter values, but the dispersion of the equilibration pressure and temperature estimates is increased: two thirds of the estimates lie within melting paths with potential temperatures $+54/-42$ °C of the best-fitting value, as opposed to $+35/-31$ °C when the preferred parameter values are used (Figure S2d&e). The same general pattern is obtained for each of the 250 analyses, with average potential temperatures of 1539^{+47}_{-55} °C (Figure S2f). In the second set of analyses, uncertainties introduced by the thermobarometer are also included, again assigned at random for each sample individually (Figure S3). Including uncertainty in the thermobarometer greatly increases the data disparity: in the example shown in Figure S3a–d, two thirds of the data lie within melting paths with potential temperatures $+74/-118$ °C of the best-fitting value. The average potential temperature and upper and lower bounds for these analyses were: 1544^{+77}_{-112} °C. As above, it appears that for this example the effects of uncertainties in the input parameters are comparable to or lower than uncertainties due to the thermobarometric parameterisation. The deterioration in fit between the data and a simple melting path when parameter uncertainties are treated independently for each sample suggests that the plausible ranges in source Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, $\text{H}_2\text{O}/\text{Ce}$, and thermobarometric error most likely do not reflect true source-region variations. Rather, we believe it is more likely that source Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, $\text{H}_2\text{O}/\text{Ce}$ are relatively consistent, that melting occurs at a relatively consistent potential temperature, and that melts follow a relatively consistent melting path.

Second, we test the effects of attributing variation in the input parameters to processes acting during melt transport to the surface and/or uncertainties due to analytical procedures. Again we performed two sets of 250 analyses, each time selecting values of source Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, and $\text{H}_2\text{O}/\text{Ce}$ from normal distributions as described above. In each analysis, single parameter values were selected for the shield and rejuvenated phases and applied to every sample from the respective phase. Distributions of source Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, and $\text{H}_2\text{O}/\text{Ce}$ for the 250 analyses are shown in (Figure S4a–c). The mean potential temperature obtained was 1532 ± 36 °C, with standard deviation 36 °C. The average upper/lower bound on the potential temperature was 46 °C. Whereas allowing input parameters to vary between samples

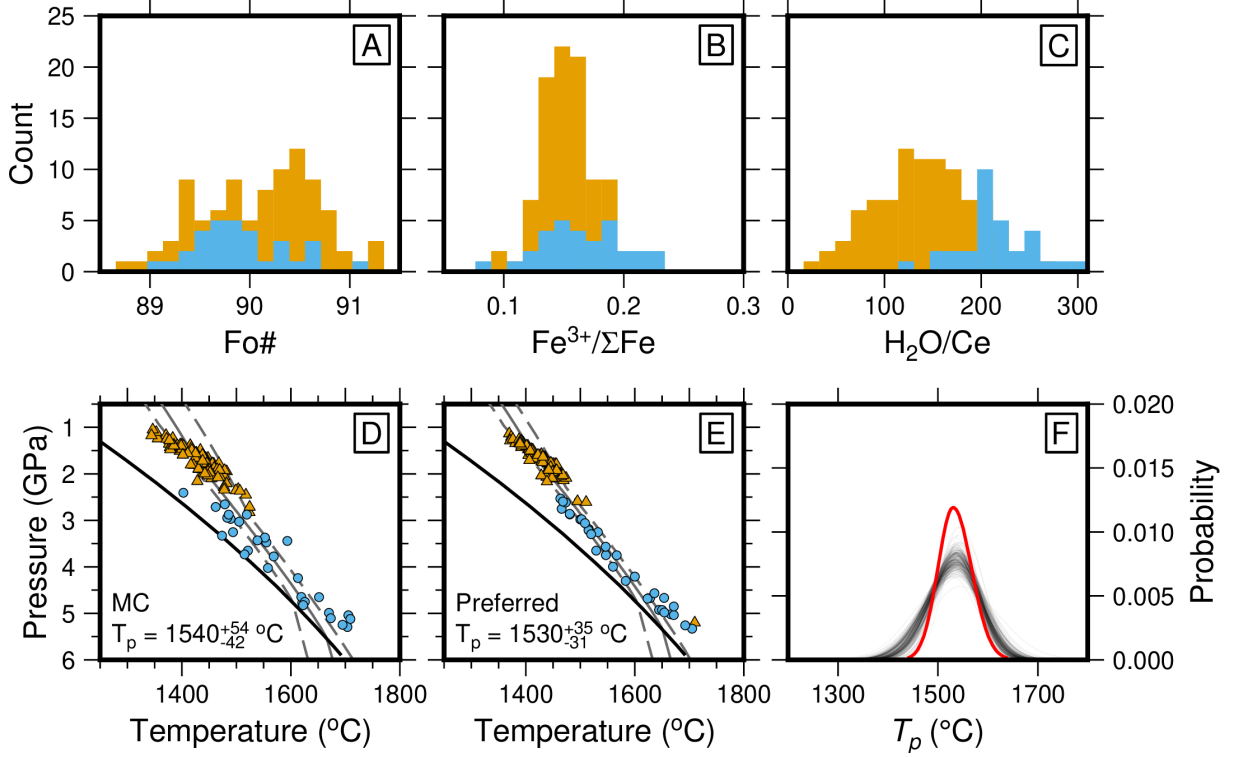


Figure S2: Monte Carlo uncertainty analysis for Oahu in which input parameters for each individual sample were drawn at random. (a) Histogram showing example distribution of source Fo# selected for shield (orange) and rejuvenated phase (blue) samples from a normal distribution with mean and standard deviation of $\text{Fo}\# = 90 \pm 0.5$. (b) As (a) for $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.15 \pm 0.02$ (shield phase samples) and $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.17 \pm 0.04$ (rejuvenated phase samples). (c) As (a) for $\text{H}_2\text{O}/\text{Ce} = 144 \pm 56$ (shield phase samples) and $\text{H}_2\text{O}/\text{Ce} = 211 \pm 29$ (rejuvenated phase samples). (d) Example estimated equilibration pressures and temperatures with input parameter distributions shown in (a-c). Orange triangles = shield phase; blue circles = rejuvenated phase; black line = anhydrous solidus; gray line = best-fitting melt pathway; dashed gray lines = bounding melt pathways. (e) As (d) for example when every sample is assigned mean values of input parameters. (f) Distributions of mantle potential temperature estimates. Red line = mantle potential temperature estimate for example when every sample is assigned mean values of input parameters, represented by a two-sided (Fechner) normal distribution with mean and upper and lower standard deviations of $1530^{+35}_{-31} \text{ }^\circ\text{C}$; gray transparent lines = same for 250 analyses where input parameters for each individual sample were drawn at random.

within an analysis resulted in consistent best-fitting potential temperatures but wider data dispersion, this procedure shifts the samples systematically, so that a wider range of potential temperatures are obtained, but the dispersion can remain small. Large dispersion can arise when shield and rejuvenated phase samples diverge. Finally, we repeated the analysis including uncertainty in the thermobarometer, again applying the same error to each shield-phase sample within an analysis, and another error to each rejuvenated-phase sample (Figure Figure S5). This procedure resulted in a similar pattern with a wider range of results: the mean potential temperature was $1547 \pm 53 \text{ }^\circ\text{C}$, with average upper/lower bounds of $45 \text{ }^\circ\text{C}$.

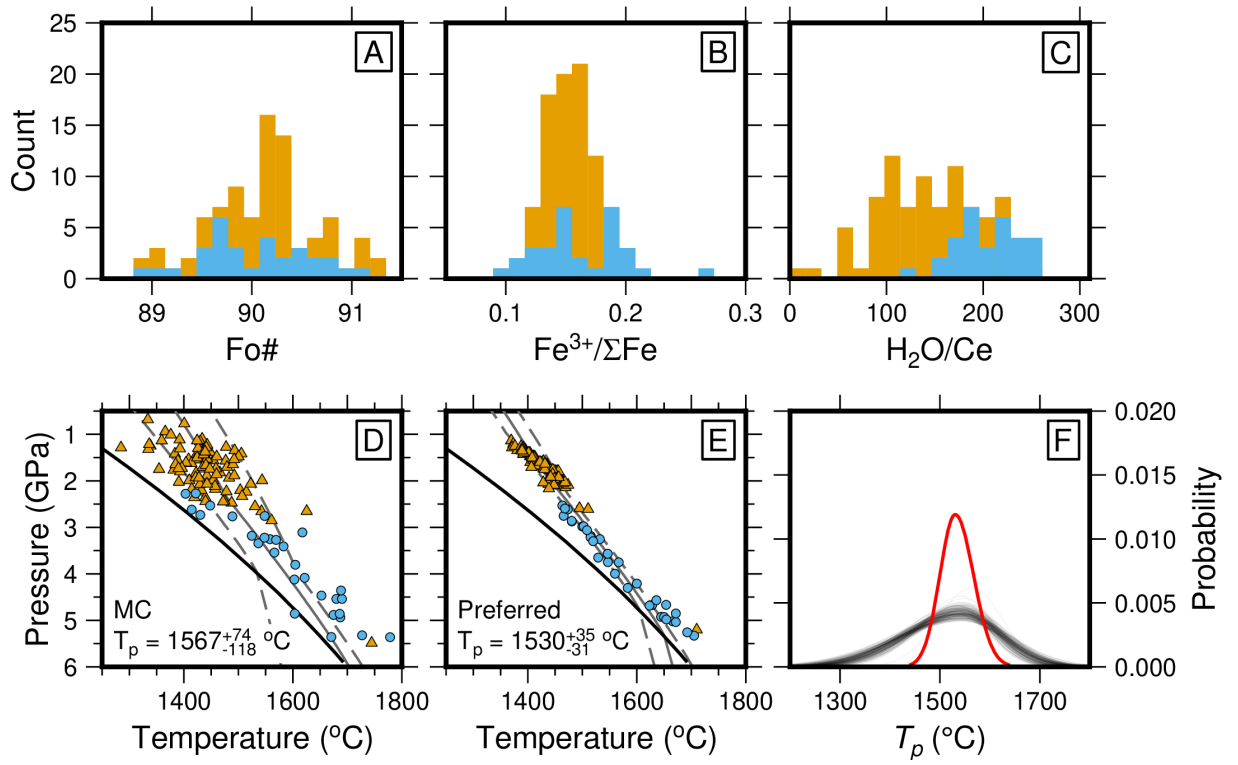


Figure S3: Same as Figure S2, with uncertainties introduced by the thermobarometer are also included. For each sample, once an equilibration pressure and temperature were estimated, uncertainties were drawn from normal distributions with standard deviations of ± 0.24 GPa and ± 39 $^{\circ}\text{C}$ for pressure and temperature, respectively, and added on to the initial value.

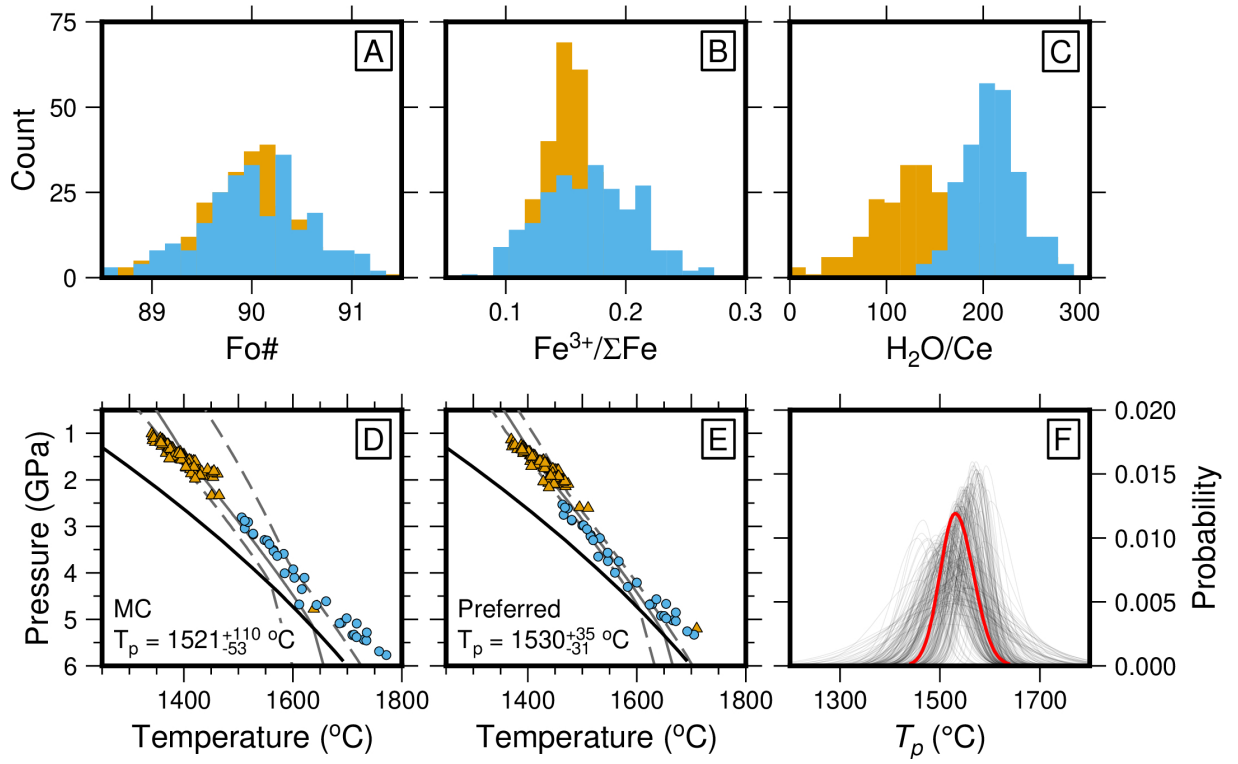


Figure S4: Same as Figure S2, where in each analysis values of source Fo#, $\text{Fe}^{3+}/\Sigma\text{Fe}$, and $\text{H}_2\text{O}/\text{Ce}$ are selected at random and applied to the entire suite (treating shield and rejuvenated phases separately).

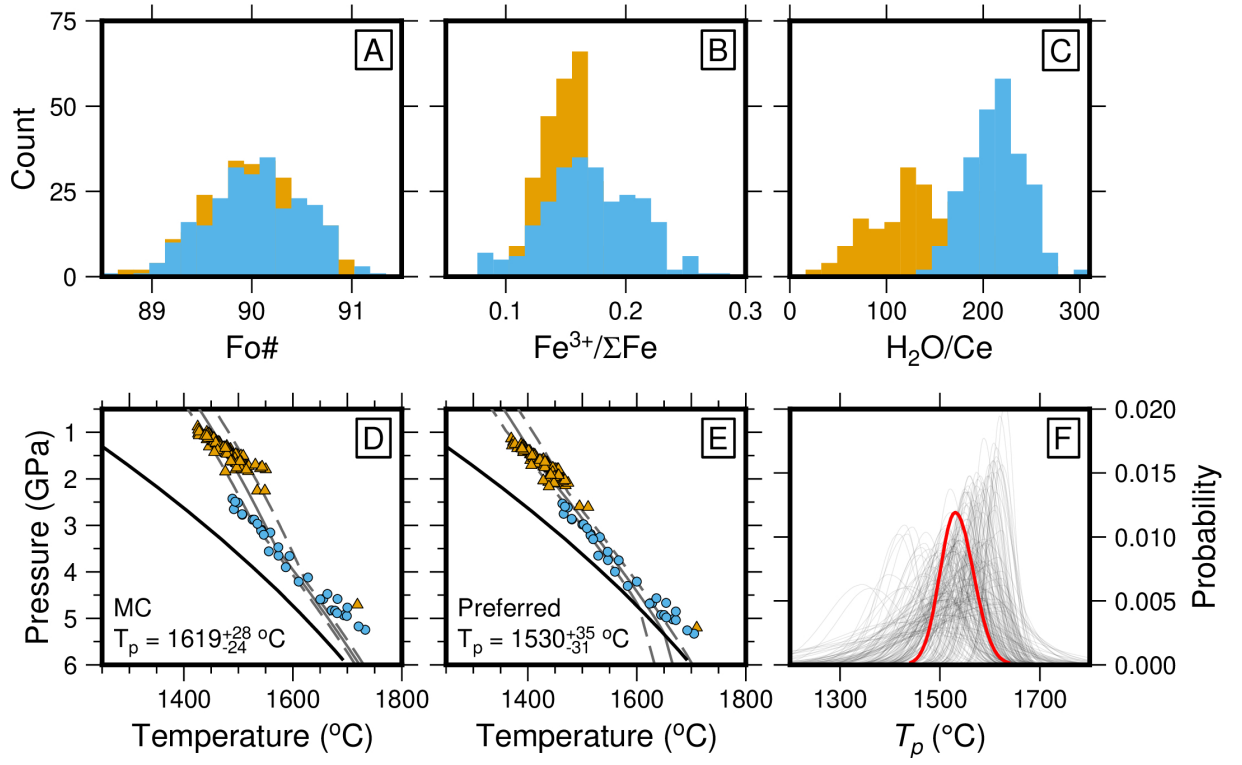


Figure S5: Same as Figure S4, with uncertainties introduced by the thermobarometer are also included. For each analysis, uncertainties in pressure and temperature were drawn from normal distributions with standard deviations of ± 0.24 GPa and ± 39 $^{\circ}\text{C}$ for pressure and temperature, respectively, and added on to the initial values. Shield and rejuvenated phases were again treated separately.

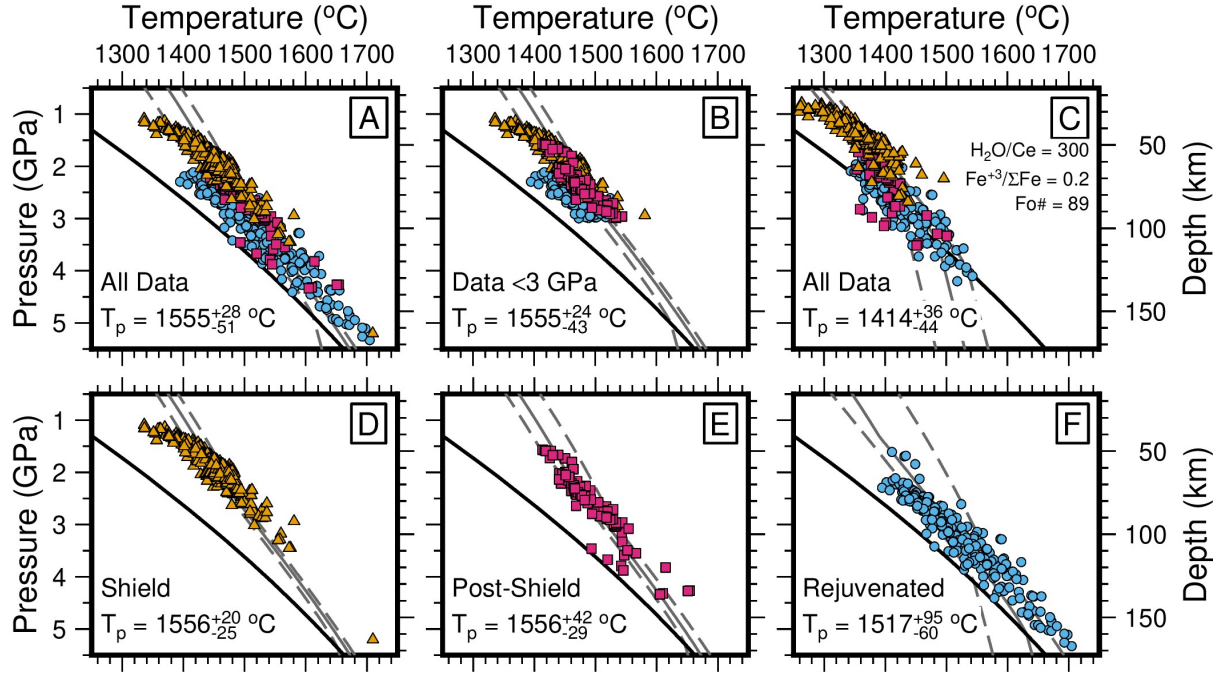


Figure S6: (a) Temperature plotted as function of depth/pressure. Symbols = equilibration pressure/temperature estimates determined for all Hawai'ian Islands samples using formulation of Plank and Forsyth [2016] and parameters in Table 2 of main text. Orange/pink/blue symbols = shield/post-shield/rejuvenated phase data. Black line = anhydrous solidus; gray line = best-fitting melt pathway; dashed gray lines = minimum and maximum melt pathways for which misfit value at global minimum is double [Katz et al., 2003]; optimal value of T_p shown bottom right. (b) Fit for samples with < 3 GPa. (c) Pressures and temperatures calculated using extreme values for parameters shown top left of panel. (d) Shield phase samples. (e) Post-shield phase samples. (f) Rejuvenated phase samples.

Supplementary Datasets

Dataset S1

Dataset of whole-rock geochemical compositions of Hawai'ian basaltic rocks compiled by Ball et al. [2021] with some additional data. Includes data from: Arevalo and McDonough [2008]; Bergmanis et al. [2000]; Bohrson and Clague [1988]; Casadevall and Dzurisin [1987]; Chen and Frey [1983]; Chen et al. [1990, 1991]; Chen [1993]; Chen et al. [1996]; Clague et al. [1980]; Clague and Beeson [1980]; Clague and Frey [1982]; Clague [1988]; Clague et al. [1995]; Clague and Moore [2002]; Clague et al. [2006, 2016]; Coombs et al. [2004, 2006]; Cousens and Clague [2015]; Crocket [2000, 2002]; Davis et al. [2003]; Desilets et al. [2006]; Dixon et al. [2008]; Dzurisin et al. [1995]; Feigenson et al. [1983]; Feigenson [1984]; Fekiacova et al. [2007]; Ferguson et al. [2016]; Fodor et al. [1987, 1992]; Frey et al. [1990, 1994, 2016]; Fodor and Bauer [2014]; Gaffney [2002]; Gaffney et al. [2004, 2005]; Garcia et al. [1986, 1992, 1995]; Garcia [1996]; Garcia et al. [1998, 2000, 2003, 2008, 2010, 2015, 2016, 2017]; Guillou et al. [2000]; Gurriet [1988]; Hammer et al. [2006]; Hanano et al. [2010]; Hanyu et al. [2010]; Haskins and Garcia [2004]; Hauri and Kurz [1997]; Hauri [2002]; Helz [1980]; Helz and Thornber [1987]; Huang et al. [2005]; Ireland et al. [2009]; Jackson et al. [1999]; Johnson et al. [2002]; Kauahikaua et al. [2002]; Kimura et al. [2006]; Lanphere and Frey [1987]; Leeman et al. [1994]; Lipman et al. [1990, 2006]; Maaløe et al. [1989, 1992]; Mangan et al. [1995]; Marske et al. [2007, 2008]; Moore [1983]; Moore and Campbell [1987]; Moore et al. [1987, 1990]; Moore and Clague [1992]; Morgan et al. [2007]; Mukhopadhyay et al. [2003]; Nichols et al. [2009]; Norman and Garcia [1999]; Norman et al. [2002, 2004]; Phillips et al. [2016]; Pietruszka et al. [2013]; Presley et al. [1997]; Quane et al. [2000]; Reiners and Nelson [1998]; Ren et al. [2004, 2009]; Rhodes [1983]; Rhodes and Hart [1995]; Rhodes [1996]; Rhodes and Vollinger [2004]; Rhodes et al. [2012]; Riker et al. [2009]; Roden et al. [1984]; Roeder et al. [2003]; Sherrod et al. [2003, 2007]; Sides et al. [2014]; Sisson et al. [2002]; Sinton et al. [2014]; Spengler and Garcia [1988]; Sobolev and Nikogosian [1994]; Stone and Fleet [1991]; Stolper et al. [2004]; Tagami et al. [2003]; Tanaka et al. [2002]; Tanaka and Nakamura [2005]; Thornber et al. [2002]; Thornber [2003]; Van Der Zander et al. [2010]; Vinet and Higgins [2010, 2011]; Weinstein et al. [2004]; Wallace [1998]; Wallace et al. [2015]; Walton and Schiffman [2003]; Wanless et al. [2006]; Weinstein et al. [2004]; West et al. [1992]; West and Leeman [1994]; Wilkinson and Stolz [1983]; Wilkinson and Hensel [1988]; Wolfe et al. [1987, 1988]; Wright [1984]; Xu et al. [2005, 2007, 2014]; Yamasaki et al. [2011]; Yang et al. [1994]; Yokose et al. [2005].

Dataset S2

H₂O and Ce concentrations of olivine-hosted melt inclusions; forsterite content of host olivine; Mg# of the whole rock calculated using cation values [Dixon and Clague, 2001; Dixon et al., 2008; Garcia et al., 2015, 2016, 2022; Moore et al., 2021; Sakyi et al., 2012; Sides et al., 2014; Tucker et al., 2019; Wieser et al., 2019].

Dataset S3

Melt inclusion and volcanic glass compositions including H₂O, S and Fe⁺³/ΣFe [Brounce et al., 2017; Dixon et al., 1997; Helz et al., 2017; Moussallam et al., 2016].

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