Supplementary Online Material for

EntraPT: an online platform for elastic geothermobarometry

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Example

Here we show how EntraPT can be used in practice to: (i) interpret the residual strain measured in several inclusions; (ii) calculate the residual pressure and the entrapment conditions evaluating the uncertainties for each step of the calculation; (iii) store all of the data in a consistent way and use them for further analysis. In this example we will focus on the data published by Bonazzi et al. (2019), obtained from hydrothermal synthesis experiments with a piston-cylinder press to produce quartz inclusions in pure almandine garnet (>99%) at eclogite facies metamorphic conditions. In the study two experiments were performed and labelled Alm-1 (synthesis performed at P = 3.0 GPa and T= 775 °C) and Alm-2 (at P= 2.5 GPa and T= 800 °C). From each experiment they recovered several host crystals, each containing one or more crystals of quartz as inclusions. Isolated, fully-enclosed quartz inclusions in the recovered garnets were then investigated using micro-Raman spectroscopy. The changes in the Raman peak positions were measured at the central

point of the inclusion and interpreted by applying the phonon-mode Grüneisen tensors of quartz (Murri et al., 2018) to obtain the full strain state of each inclusion, using the program stRAinMAN (Angel et al., 2019). From the residual strain they calculated the full residual anisotropic stress state and the mean stress by using the elastic properties of quartz. The authors showed that the entrapment pressures calculated from this mean stress with the isotropic model for host-inclusion systems differ from the known synthesis pressure by <0.2 GPa, which is on the order of the combined experimental uncertainties. Their results show that the most significant effect of the elastic anisotropy of quartz is on the Raman shifts of the inclusion, and not on the subsequent calculation of entrapment conditions.

Add new analyses: set the host-inclusion system and import the measured residual strains

The user can add new *analyses* from the *Add New Analyses* tab. This tab has a panel on the right to navigate through the *Host&Inclusion*, *Geometry*, *Orientation* and *Strain* pages where all of the parameters that define an *analysis* can be set. Since all of the measurements refer to quartz inclusions in almandine, the user has first to set these phases as host and inclusion in the *Host&Inclusion* page (Fig. OM1d). The analysis in the current version of EntraPT is based on the assumptions that the inclusion is spherical and far away from fractures and the external surface of the host. Therefore, we will show the application to those inclusions measured by Bonazzi et al. (2019) that have an "ideal" geometry (almost spherical and far from the surface of the host). As a consequence, the geometry can be left as a sphere in the *Geometry* page (Fig. OM1e). Since the orientation between the host and inclusion is not relevant for isotropic elastic geobarometry, the *Orientation* page (Fig. OM1f) is set by default to an inclusion unrotated with respect to the host.
Once all of the parameters are set, the user needs to confirm them from the *Orientation* page and moves to the next page, *Strain* (Fig. OM2a). Since we want to analyse multiple measurements all belonging to the same host-inclusion systems with the same features (mineral phases, geometry and orientation) we can choose to import the strains for multiple *analyses* (Fig. OM2b). By clicking on *Import File* (Fig. OM2c), a file-dialog is opened to choose an input file (with **.dat* extension) from the computer of the user. In Bonazzi et al.(2019) the residual strain of each inclusion was obtained from the stRAinMAN program using the measured Raman shifts. Since the inclusion (quartz) is uniaxial, the values $\varepsilon_1 = \varepsilon_2$ and ε_3 (together with their esd and covariance) are given in

the output file of stRAinMAN. It was formatted into the input file for EntraPT (Table 2) using a spreadsheet editor and is available in the Deposit items. The input file is then loaded to the server and the consistency check is performed (see the main article for details). If the check is passed, the imported data will be listed in the application. The user can now click on *Add Analyses to Workspace* (Fig. OM2d) and all the imported *analyses* will appear in the *Workspace* on the left side of the app (Fig. OM2e).

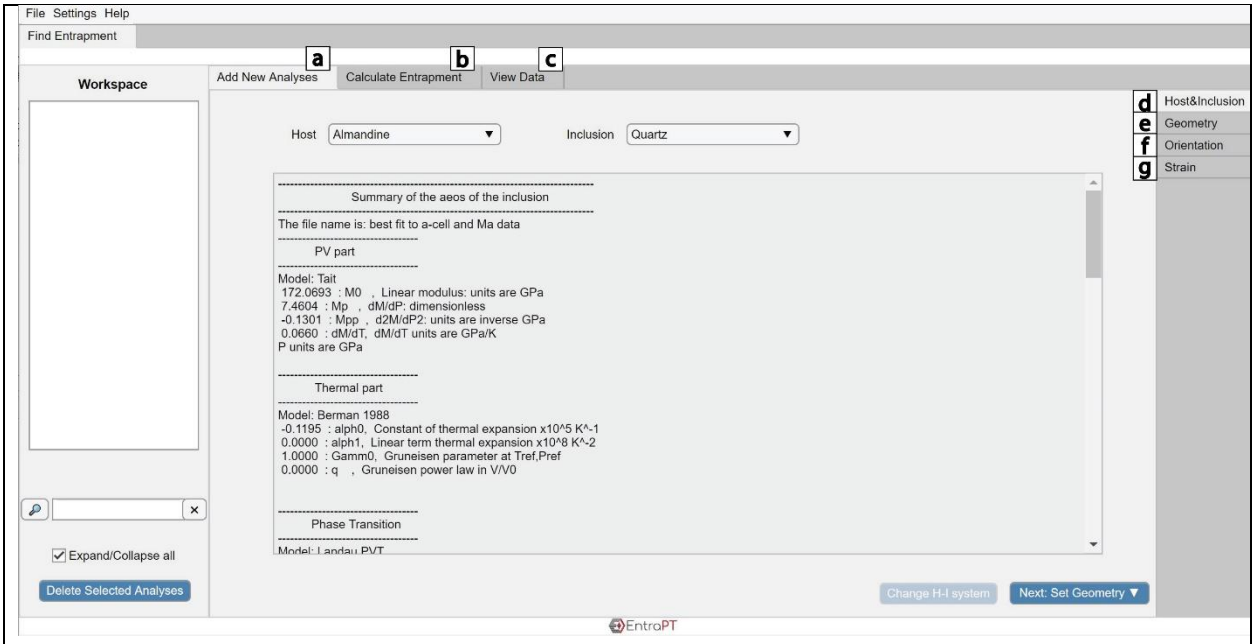

Figure OM1. EntraPT is structured with three main tabs: *Add New Analyses* (a), *Calculate Entrapment* (b) and V*iew Data* (c). The user has first to define one or more new analyses from the *Add New Analyses* tab. Using the panel on the right side the user can set the host and inclusion minerals (d), the geometry (e), the orientation (f) and the measured residual strains (g). This figure shows the Host&Inclusion page (d) where the host and the inclusion minerals are set, and a summary of their EoS is shown to the user.

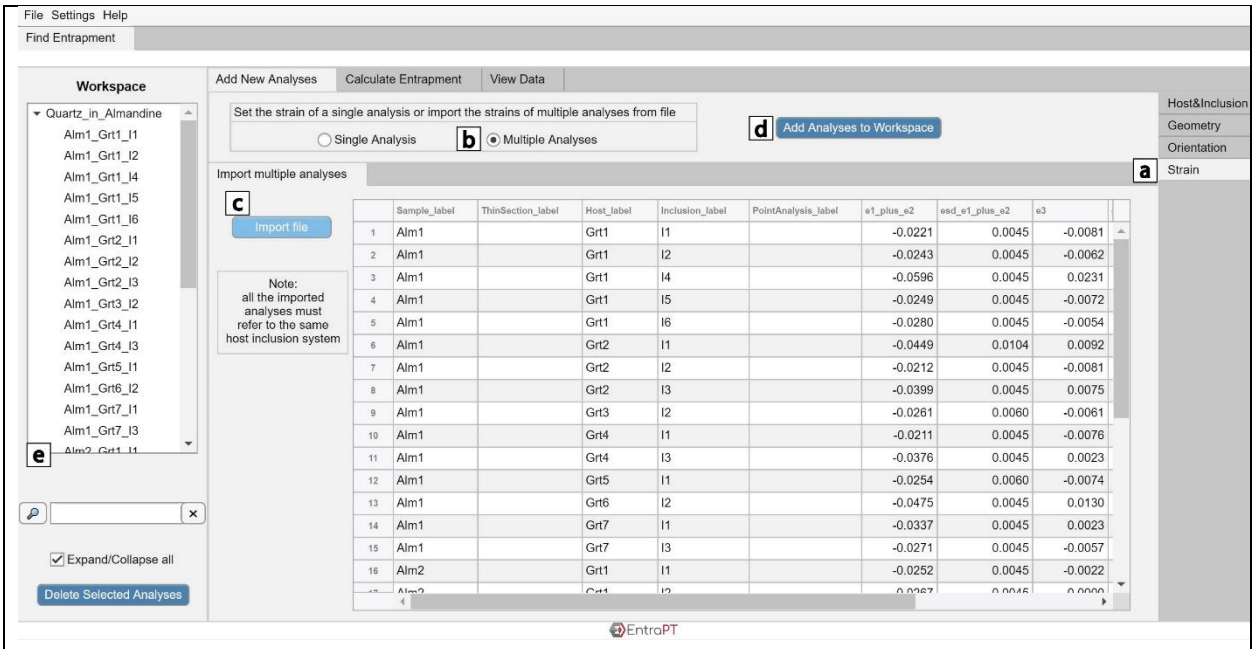

Figure OM2. The user can import several measurements of the residual strain measured in the same host inclusion system (i.e. same minerals, geometry and orientation) from the *Strain* page (a) under *Add New Analyses.* The user has first to choose the option *Multiple analyses* (b) and then click on *Import file* (c). A file dialog is opened to choose the input file (with *.dat extension) from the user's computer. If the file is imported successfully, the imported data are listed in the app and the analyses can be added to the current project by clicking on *Add Analyses to Workspace* (d). The analyses will appear in the *Workspace* (e).

Visual analysis of the residual strain

Once the measured strains are stored in the project, the user can at any time perform a visual analysis of the residual strain from *Plot Strain* (Fig. OM3a) in the *View Data* tab. By selecting all of the *analyses* from the *Workspace* (Fig. OM3b), their strains are shown by default in a plot of ε_1 vs ε_3 with error bars and confidence ellipses obtained from the esd and covariances on the residual strain (Fig. OM3c). Other choices for the axes can be done, e.g. $\varepsilon_1 + \varepsilon_2$ vs ε_3. The isochors and the lines of isotropic strain and hydrostatic stress can be added to the plot (Fig. S3e) and the range of the axes can be modified as needed by using the Plot Settings (Fig. OM3f). The user can show the plot of specific groups of analyses by using the search field (Fig. 3g) below the *Workspace*.

For example, searching for the keyword "Alm1" will display in the *Workspace* only those analyses belonging to the sample Alm1, which can be selected and displayed in the current plot. As already noted by Bonazzi et al., (2019), the measured strain values lie sub-parallel to the isochors and are clustered above the line of hydrostatic conditions (Fig. OM3c). The presence of a non-hydrostatic stress in these inclusions is expected from the symmetry of the inclusion and purely elastic behavior: when the quartz is trapped in a cubic host such as garnet, the inclusion will be subject to isotropic strains imposed by the host and therefore, because it is elastically anisotropic, the inclusion will develop deviatoric stresses unless the deviatoric stress is decreased by a plastic deformation (e.g. Zhong et al., 2018; Zhong et al., 2020).

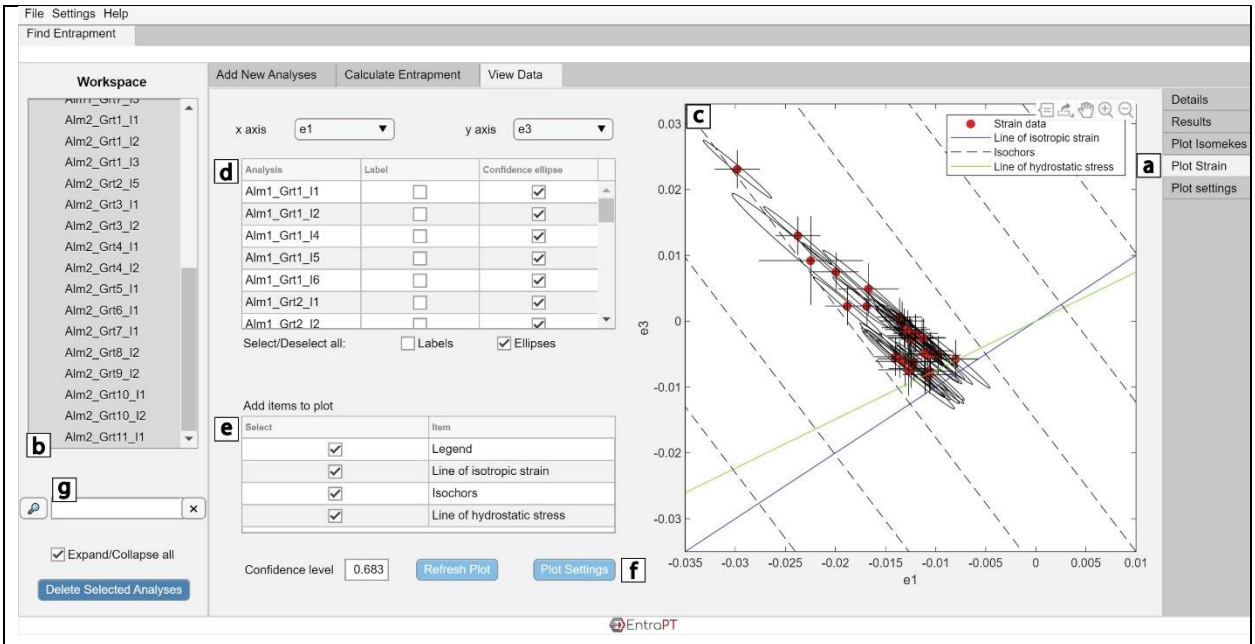

Figure OM3. Once the analyses are added to the current project, a visual inspection of the measured residual strains can be performed from the *Plot Strain* page (a) under *View Data*. Here the user needs to select one or more analyses from the *Workspace* (b). By default, the strain data are shown in a ε_3 vs ε_1 plot (c), but other choices of axes can also be made in the app. The values of the strains are plotted together with their error bars and confidence ellipses obtained from their covariance matrices. The labels of the analyses and the confidence ellipses can be shown or hidden (d). The lines of isotropic strain and hydrostatic stress and the isochors can be also added to the plot (e). The range of the axes can be adjusted as needed (f). The search field (g) allows the user to search for specific analyses by typing a full label or part of it. The searched

analyses are listed in the *Workspace*. The strain components determined at room temperature for quartz inclusions from experiments Alm-1 and Alm-2 by Bonazzi et al. (2019) are shown in the plot with the confidence ellipses corresponding to one standard deviation. They lie sub-parallel to the isochors and are clustered above the strains for hydrostatic conditions.

Calculate the entrapment isomekes

The entrapment conditions are calculated in the *Calculate Entrapment* tab. The user has to select one or more *analyses* from the *Workspace* to calculate their entrapment isomekes (Fig. OM4a). The user can set the range of temperatures for the calculation of the entrapment isomeke using the Tmin, Tmax and Tstep fields in the application (Fig. OM4b). Initially, the units for temperature (Tscale) and for the pressure (Pscale) are set to °C and GPa respectively, but they can be set to K and kbar, respectively, from the Settings menu. Since the inclusions were synthetized by Bonazzi et al. (2019) in two experiments conducted at 3 GPa, 775 °C (Alm1) and 2.5 GPa, 800 °C (Alm2), in our example we choose *Tmin* = 750 °C, *Tmax*=850 °C, *Tstep* =5 °C as the temperature range for the calculation of the entrapment isomeke. The final conditions at which the residual strain was measured are always assumed to be room conditions (T = 25 °C or 298 K, P = 0 GPa or 0 kbar, Fig. OM4c). One or both of the models discussed in the section *Calculation of the entrapment isomeke with uncertainties* of the main article can be chosen to get the residual pressure from the measured strain (Fig. OM4d), by enabling the *Expert Mode* panel from the *Settings* menu. The chosen residual pressure(s) will be used for the calculation of the entrapment isomeke. For the current example, the residual pressure was calculated using both methods. By selecting all the *analyses* from the *Workspace*, the calculation of the entrapment isomeke is run at once (Fig. OM4e) and the results are saved to the project. However, the user can calculate the entrapment isomekes for each *analysis* independently by selecting one at time from the *Workspace* and setting the appropriate calculation parameters.

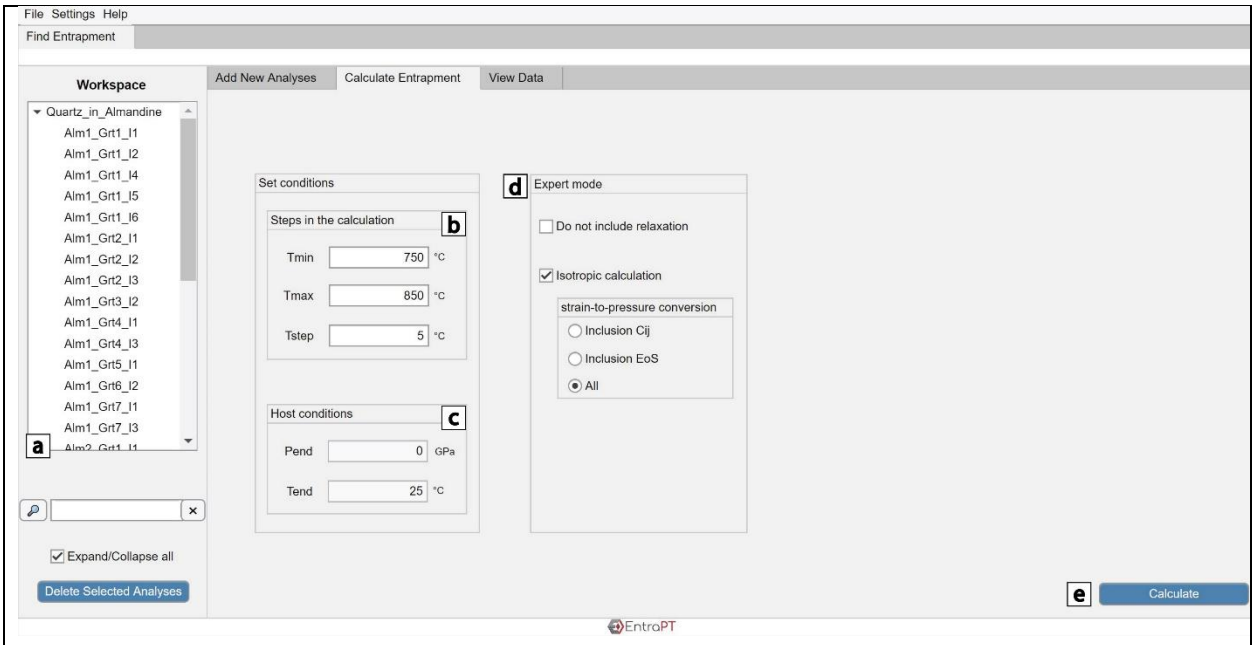

Figure OM4. In the *Calculate Entrapment* tab the user can calculate the entrapment isomekes of one or more analyses by selecting them from the *Workspace* (a). The T limits and steps in the calculation of the isomekes can be adjusted as needed (b). Other P and T scales (K and kbar) can be selected from the *Settings* menu. The final conditions of the host are always assumed to be room conditions (c). The *Expert mode* panel (d) allows the user to not include the elastic relaxation (see Angel, Mazzucchelli, et al., 2014) in the calculation and to choose the model to obtain the residual pressure from the measured strain (see the main article for more details). Once the parameters are set, the calculation is started by clicking on the *Calculate* button (e).

View and plot the results

The results from each *analysis* can be viewed in the *View Data* tab (Fig. OM5). By selecting one *analysis* from the *Workspace* (Fig. OM5a), the *Details* page (Fig. OM5b) shows all of the details of the selected analysis such as the label, the notes, the host-inclusion system, and the residual strain. The *Results* page (Fig. OM5c) shows all of the numerical results (residual pressure found with each model, *P-T* points on the isomekes, and all of the uncertainties). The *Plot Isomekes* page (Fig. OM5d) shows a *P-T* graph reporting the isomekes obtained using models (1) and (2) described in the section *Calculation of the entrapment isomeke with uncertainties* of the main

article, with their estimated uncertainties shown as a shaded area (Fig. OM5e). As discussed there, the uncertainties on the isomekes are estimated assuming an uncertainty equal to one standard deviation on the residual pressure. The user can selectively choose to hide one or more objects from the plot (isomekes, shaded area of the uncertainty, legend, labels, see Fig. OM5f and g), and set the *P* and *T* range for the plot (Fig. OM5h). The plot can be exported to the user's computer using the toolbar at the top-right of the plot (Fig. OM5i). The buttons in the toolbar allow the user to select any point on the plot to get its coordinates, zoom in and out, and export the plot as a picture. Plots can be customized and exported to various formats (png, jpeg). They can also be exported as pdf which can be easily edited in common vector graphics programs to produce publication-quality plots. The user can also generate a plot with the isomekes of multiple *analyses* by selecting two or more from the *Workspace*. Specific *analyses* or groups of *analyses* can be searched by using the tool (Fig. OM5j) below the *Workspace*.

The entrapment conditions determined using EntraPT agree with those reported by Bonazzi et al., 2019 (e.g. compare the P_{trap} calculated at 775 °C in Fig. OM6 with Fig. 6a in Bonazzi et al., 2019). For each *analysis* the isomekes calculated from the two different definitions of residual pressure, can be plotted simultaneously. As noted by Bonazzi et al. (2019), the isomekes calculated using the P_{inc}^{V} obtained from the inclusion EoS (model 2) tend to overestimate the expected entrapment pressure, especially for those inclusions with a high differential residual strain (inclusions in the top left sector of the plot in Fig. OM3). This is because the effective bulk modulus of quartz is lower in presence of differential stresses and strains that fall above the hydrostatic line in ε_3 vs ε_1 plots (e.g. as shown in Fig OM3). Therefore, for such inclusions the P_{inc}^{V} becomes larger as a consequence of the Reuss bulk modulus of the EoS being larger than that of the strained inclusion. For the same reason, the uncertainty on the P_{inc}^{V} obtained from eq. (11) is in general larger than the uncertainty on the P_{inc}^{strain} (found with the stiffness tensor and eq. 9), especially for soft inclusions under differential stress. This is illustrated in Fig. OM5e taking as an example the quartz Alm1_Grt6_I2 which has a high measured differential strain (≈ 0.037). Its P_{inc}^{V} is 1.453 ± 0.079 GPa while the pressure P_{inc}^{strain} obtained from the strain through the stiffness tensor (eq. 4 and 5) is 1.104 ± 0.038 GPa. As a consequence, the isomeke calculated from P_{inc}^{V} overestimates the synthesis pressure of P_{trap} = 3 GPa at T_{trap} = 775°C (Fig. OM5e), and has a larger associated uncertainty compared to the isomeke obtained from P_{inc}^{strain}. The same observation is shown

synthetically in Fig. OM6 for all of the *analyses* belonging to the synthesis Alm1 of Bonazzi et al. (2019). Because the residual pressure P_{inc}^{V} obtained from the volume strain is overestimated in presence of large differential stresses in the inclusion, the entrapment pressures P_{trap}^{V} calculated from P_{inc}^{V} clearly diverge from the synthesis conditions with the increasing differential stress in the inclusion (Fig. OM6). On the other hand, the P_{trap}^{strain} obtained from the measurements of strain are in good agreement with the experimental pressure of the synthesis, independently of the degree of differential stress in the inclusion.

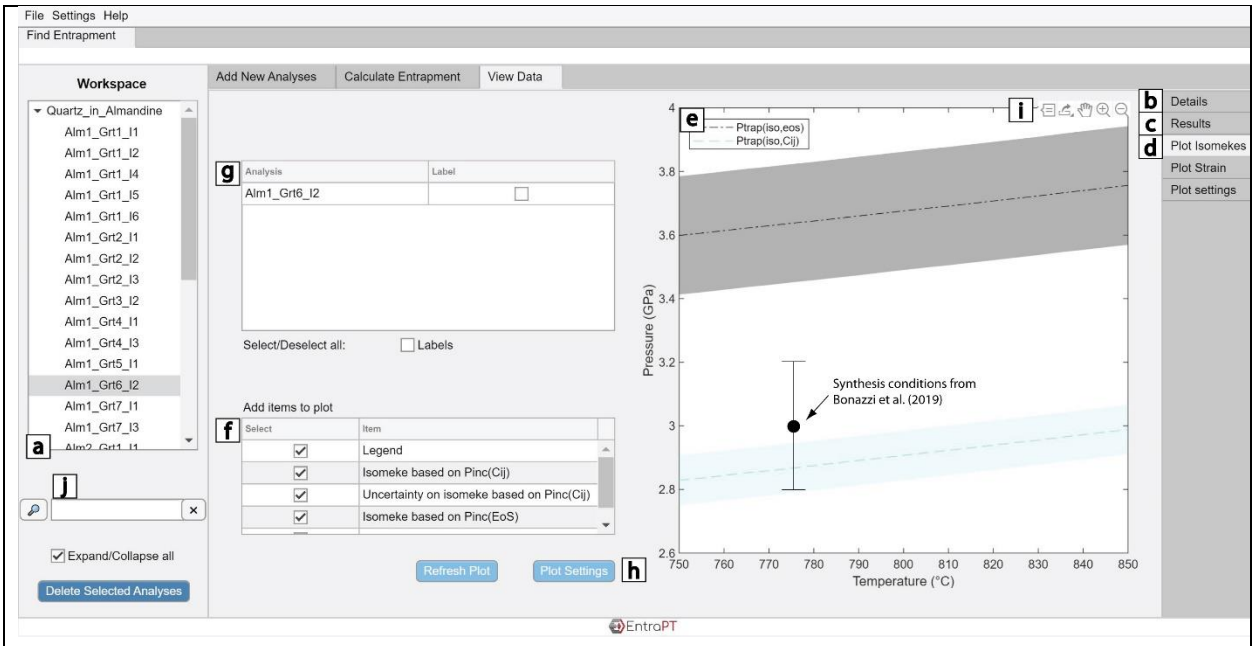

Figure OM5. The data relative to each analysis and the results of the calculation of the entrapment conditions can be viewed at any time from the *View Data* tab.When the user selects one analysis from the *Workspace* (a) its details are shown in the *Details* page (b). The numerical results of the calculation are shown under *Results* (c). The isomeke(s) can be plot from *Plot Isomekes* (d). In the *Plot Isomekes* page, the graph (e) reports one or two isomekes depending on the models chosen for the calculation (see panel in Fig. OM4d) together with the estimated uncertainties on them represented by a shaded area. The isomekes, the shaded areas and the labels of the analysis can be optionally hidden from the specific panels (f and g). The range of the axes can be adjusted as needed (h). A toolbar on the right-top side of the plot (i) allows the user to get the coordinates on the plot of the selected points, to export the figure in various formats and to enable the zoom. The search field (j) allows the user to search for specific

analyses by typing a full label or part of it. The searched analyses are listed in the *Workspace*. The plot in (e) shows the isomekes and the associated uncertainties for the *analysis* Alm1_Grt6_I2 of Bonazzi et al. (2019) calculated starting from P_{inc}^{V} (black line) and P_{inc}^{strain} (light blue line). The point at 3 GPa, 775 °C is added as visual reference to represent the synthesis conditions of the experiment Alm1, with the error bar associated with the experimental uncertainties.

Export project: save data to the user's computer and further processing

The data can be exported to the computer of the user from the *File>Export Project* menu. By default, the project is saved to a binary file with *.*ept* extension that contains all of the *analyses* with their data. Project files can be imported back into EntraPT, using the *File>Import Project* menu, to view the data, generate the plots. Importing a project file puts EntraPT in the same configuration as when the project file was created. Once a project is loaded, new *analyses* can be added or existing *analyses* can be deleted. Moreover, multiple project files can be merged in EntraPT to create larger databases. Such project files can be easily shared, making the checking and the comparison of data and results reliable. The *.*ept* project file can be opened and processed using MATLAB®. Short scripts can be implemented to rapidly produce custom plots that are not directly displayed in EntraPT, taking advantage that all of the data are structured consistently in the project file. An example is the plot of the entrapment pressures as a function of the residual differential stress (Fig. OM6) that was generated externally with the MATLAB® script provided in the Deposit items using the data contained in the project file. During the export procedure from EntraPT, the user can also choose to save the data to spreadsheets (with *.*xlsx* extension) that can be read by any commonly used spreadsheet application, such as Microsoft Excel® or LibreOffice®. In this case an individual spreadsheet is created for each *analysis*. A compressed folder, with *.*zip* extension, is created that contains the *.*ept* project file and one or more folders containing the spreadsheet files. To preserve the privacy of the users and the complete control of their data, all of the data are deleted from the server when the EntraPT session is terminated and cannot be recovered even by the server administrators. Therefore, downloading the project to the

users computer is the only way to have access to the data after the EntraPT session is terminated. The upload and the download of the data to and from the server is always performed over a secure SSL connection.

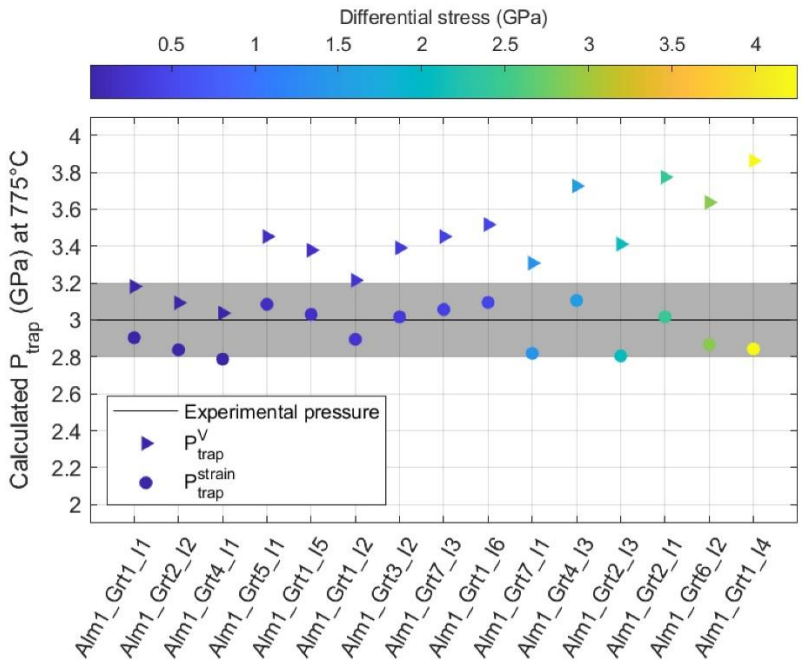

Figure OM6. Entrapment pressure P_{trap} calculated at 775 °C for all the analyses belonging to the experiment Alm1 of Bonazzi et al. (2019), reported as a function of the residual differential stress measured in the inclusion. The quartz inclusions in garnet were synthetized at 3± 0.2 GPa at 775 °C (black line in the plot). The shaded area represents the maximum estimated uncertainty propagated through the calculation of P_{trap}. The pressures P^{V}_{trap} calculated from P^{V}_{inc} (triangles) always overestimate the synthesis conditions, especially in presence of large differential stress in the inclusion. The P^{strain}_{trap} obtained from the measurements of strain show a good agreement with the experimental pressure of the synthesis, independently of the differential stress in the inclusion. The plot was generated with an external MATLAB® script provided in the Deposit items together with the project file with all the data.

File formats

Input file. The input file must have a **.dat* extension, and be a tab-delimited text file. Template files are provided with the program on the website mineralogylab.com and can be edited with a spreadsheet editor, to preserve the tab delimited structure. Each row of this file stores the data of one analysis, i.e. of one measurement (see Table OM1). All of the analyses in one input file must belong to the same host-inclusion system (i.e. same host and inclusion phases). The content of each column is specified by the headers. Five columns are reserved for the labels to identify the *analysis* (sample, thin section, host, inclusion and point analysis) and one column for the notes associated to the *analysis*. The content of the remaining columns depends on the symmetry of the residual strain, which corresponds to the symmetry of the inclusion in absence of symmetry breaking. A general-purpose file, suitable for any symmetry of the strain, contains one column for each strain component (6 columns), and one column for each independent entry of the covariance matrix (21 columns). If the inclusion is uniaxial without symmetry breaking both the strain and the covariance matrix have fewer independent components. In this case a specific template is provided (see Table OM1 and the **.dat* file included in the Deposit items for an example). For uniaxial inclusions without symmetry breaking the measured strain components and the statistical parameters (esd, covariances) can be easily copied and pasted from the stRAinMAN logfile to this input file using any spreadsheet editor. When the inclusion is cubic (without symmetry breaking), the volume strain is sufficient to describe the strain state of the inclusion (e.g. Angel et al., 2019). Therefore, the volume strain and its esd can be specified in the appropriate input file for cubic inclusions.

Project files. By default, the project is saved to a binary MAT-file of MATLAB® with a custom **.ept* extension. The project file contains all of the *analyses* with their data (elastic parameters, EoS, strain, calculation parameters, results). The user can optionally choose to save the data to spreadsheets with **.xlsx* extension. **.xlsx* is a Microsoft proprietary binary format that can be opened with Microsoft Excel® or with free programs such as LibreOffice®. All the output files are compressed in a **.zip* folder before the downloading to the computer of the user.

Table OM1. Example of input file to import into EntraPT the components of the residual strain and the associated esd and covariances of uniaxial inclusions without symmetry breaking. In this example, the Raman shifts were measured in quartz inclusions in almandine host synthetized by Bonazzi et al. (2019), and they were converted into residual strains using the program stRAinMAN (Angel et al., 2019). The first row reports the headers that must be included in the input file even when the associated columns are not used. The labels allow the user to identify each *analysis* by giving the codes of the sample, thin section, host and inclusion to which it belongs. The *PointAnalysis_label* can be used when more than one *analysis* are measured in the same inclusion. To keep consistency with the label scheme of the original data of Bonazzi et al. (2019), in this example the columns corresponding to the *ThinSection_label* and the *PointAnalysis_label* are intentionally left empty. The complete template **.dat* file is included in the Online Material.

Sample_label	ThinSection_label	Host_label	Inclusion_label	PointAnalysis_label	e1_plus_e2	esd_e1_plus_e2	e3	esd_e3	cov_e1_plus_e2_e3
Alm1		Grt1	I1		-0.02210	0.00451	-0.00810	0.00291	-1.2995E-05
Alm1		Grt1	I2		-0.02430	0.00451	-0.00620	0.00291	-1.2995E-05
Alm1		Grt1	I4		-0.05960	0.00451	0.02310	0.00291	-1.2995E-05
Alm1		Grt1	I5		-0.02490	0.00451	-0.00720	0.00291	-1.2995E-05
Alm1		Grt1	I6		-0.02800	0.00451	-0.00540	0.00291	-1.2995E-05
Alm1		Grt2	I1		-0.04490	0.01041	0.00920	0.00673	-6.9345E-05
Alm1		Grt2	I2		-0.02120	0.00451	-0.00810	0.00291	-1.2995E-05
Alm1		Grt2	I3		-0.03990	0.00451	0.00750	0.00291	-1.2995E-05
Alm2		Grt1	I1		-0.02520	0.00451	-0.00218	0.00291	-1.2995E-05
Alm2		Grt1	I2		-0.02670	0.00451	0.00004	0.00291	-1.2995E-05
Alm2		Grt1	I3		-0.02630	0.00451	-0.00100	0.00291	-1.2995E-05
Alm2		Grt2	I5		-0.02720	0.00451	0.00063	0.00291	-1.2995E-05
Alm2		Grt3	I1		-0.02480	0.00451	-0.00262	0.00291	-1.2995E-05
Alm2		Grt3	I2		-0.02500	0.00451	-0.00244	0.00291	-1.2995E-05
Alm2		Grt4	I1		-0.01600	0.00451	-0.00574	0.00291	-1.2995E-05
Alm2		Grt4	I2		-0.02100	0.00451	-0.00449	0.00291	-1.2995E-05
Alm2		Grt5	I1		-0.01950	0.00451	-0.00517	0.00291	-1.2995E-05
Alm2		Grt6	I1		-0.02400	0.00451	-0.00185	0.00291	-1.2995E-05
Alm2		Grt7	I1		-0.02270	0.00451	-0.00247	0.00291	-1.2995E-05
Alm2		Grt8	I2		-0.03340	0.00601	0.00491	0.00388	-2.3131E-05
Alm2		Grt9	I2		-0.02240	0.00451	-0.00254	0.00291	-1.2995E-05

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