Quick Guide

This is a brief 'how-to' guide. It is hoped that PASCal is relatively self-explanatory, however this file contains extra detail. A paper providing a full rationale and computational detail is available at the arXiv: http://arxiv.org/pdf/1204.3007.pdf. Please cite it if you use PASCal to analyse your data. PASCal might not be the most appropriate method for full analysis of your data, so please read the caveats if you have particularly precise needs.

Input:

The input consists of whitespace or comma separated values with each row representing a single data point and each column in turn containing: temperature or pressure data, error in the temperature or pressure data, followed by the cell parameters a, b, c, alpha, beta, gamma. No errors in cell parameters are needed or used by PASCal, as often the scatter in the data and error in temperature or pressure dominate the resultant errors. Data should be for a single phase only.

For pressure data, there is option to include a nonzero critical pressure. This is not fitted, and is especially relevant where there is a phase transition above ambient pressure. There is also the advanced option to use finite strain rather than infinitesimal strains.

The data is stripped of all non-number characters, and further, comments beginning with # are also ignored. Note this means that input of the form 1E-4 will produce unexpected and unwanted results!

Output:

Topping the page is a summary table of the coefficients of thermal expansion (CTEs)/median compressibilities for each of the principal directions. This also includes the projections of the principal axes onto each of the crystallographic axes, i.e. giving the [UVW] direction of each of the principal axis.

For pressure, there then follows a table showing various fits to the widely used Birch-Murnaghan equation of state. It should be noted that different equations of state have different value, especially where data are highly anomalous. The value of B' can indicate anomalous behaviour, especially pressure induced softening (B' < 0) and rapid stiffening (B' >> 4).

Below is the interactive indicatrix – this shows the variation of the coefficient of thermal expansion/median compressibility with direction. Red indicates positive magnitude, blue, negative. If the indicatrix doesn't update, first make sure you haven't disabled javascript. If you have javascript enabled, please also make sure you have the latest version of your browser – problems have been reported with earlier versions of Firefox.

Various interactive plots follow. Clicking on the plot area will give the position of your cursor, and clicking on the legend switches on and off lines/data series. The plot of the variation of compressibility with pressure shows a derived curve for compressibility – this is not accessible directly from the data. The graphs are in the vector '.svg' format and should be easily editable in Adobe Illustrator or in Inkscape.

Tables giving the values used to calculate the plots follow, including the basis of PASCal, the calculated strains. Copying these tables should allow you to create your own plots. The parsed input ends the output. This is primarily of interest in the event that PASCal produces unexpected results, for confirmation that the parsed input is correct.