

## Notes for Use of *Cpx/Liq Calcs* and *P-T Calcs* Spreadsheets Last Updated: 6/1/03

The spreadsheet *Cpx/Liq Calcs* can be used to obtain cation fractions for nominal liquid compositions (whole rock, glass, matrix etc.), and to calculate cation assignments for clinopyroxenes. These data can then be input (using cut-and-paste commands) into *P-T Calcs* to obtain estimates of pressures and temperatures of crystallization (using the models of Putirka et al. 1996, and new models from Putirka et al., 2003 –Am. Min., in press). *P-T Calcs* also includes cpx-saturation models of Putirka (1999) so that you may check whether or not your cpx-liquid match and *P-T* estimates are consistent with experimental determinations of cpx-liquid equilibrium. The spreadsheets are not linked, so you need not enter data into one, to use the other. The spreadsheets are also set up so that you can enter as many data as you, like - just use the “fill down” command to complete the calculations. The models labeled New 1/15/02” (from the Am. Min. paper) can be used for a wider range of liquid compositions (basalt – dacite) and hydrous liquid compositions than the 1996 models. The 1996 models, though, may be more precise for dry basaltic bulk compositions. If you receive a ‘circular reference’ error while using *P-T Calcs*, make sure that in the Tools-Preferences-Calculation window (in Excel) that the Iteration box is checked, or that your spreadsheet preferences are otherwise set up to handle iterative calculations.

### Convert Weight %'s; Calculate P& T

1. Enter the weight % values from XRF or electron microprobe data into columns C-L in *Cpx/Liq Calcs*.

(a) If you have input nominal liquid compositions, the necessary cation fraction values appear in columns AA-AJ.

(b) If you have input cpx compositions, the necessary cation assignment calculations appear in BR-CC. Fe<sup>3+</sup> calculations are calculated using the formula of Lindsley (1986). Be aware that Fe<sup>3+</sup> calculations are highly unreliable due to error in SiO<sub>2</sub> measurements (see McGuire et al. 1989), and hence are not used for any part of the calculations scheme.

2. Copy the contents of columns AA-AJ from *Cpx/Liq Calcs* and paste them into columns C-L in the spreadsheet *P-T calcs*.

3. Copy the contents of columns BR-CC of *Cpx/Liq Calcs* and paste them into columns N-Y in *P-T Calcs*. ‘Fill down’ columns Z - BV

### Reading the Results

1. Caveat: As noted above, the spreadsheet *P-T calcs* is set up so that the Tools-Preferences-Calculation window has the Iteration box checked. This allows Excel to solve two equations 'simultaneously', without giving a circular reference error. You may need to change the preferences in your spreadsheet program.

2. Output of P(kb) & T(K) appear in columns BJ-BQ of *P-T calcs*. The columns labeled NEW, contain estimates for a revised model that can be applied to basalt to dacite compositions (Putirka et al., 2003). The 1996 models are applicable only to basaltic liquids.

3. Tests of equilibrium: The values in columns BA-BF in *P-T Calcs* are predicted values and component totals for cpx compositions (Putirka, 1999), using the liquid composition, and calculated values of *P* & *T* as input. As a check on whether you have the best liquid match, you may compare these values to the 'measured' cpx components, which appear in columns AC-AH. The calculated and observed totals should approach unity. And, understanding that there is some error in the calculation of cpx components, predicted and measured values should be close. How close is a matter for you to determine. An error of 2% or 3% (see Putirka, 1999, figures 4 and 5 for error on these models) is probably not unreasonable, though you might in some cases want to apply more stringent tests. I usually compare predicted values of CaTs, EnFs and DiHd, and look for data from large data sets to cluster about a one-to-one line when measured vs. predicted values of CaTs, EnFs and DiHd components are plotted on the same graph. I also will plot the cpx component sums on the same graph, to check whether they approach 1.0. Column BU reports the *T(K)* of saturation from the models of Putirka (1999); recent tests indicate that this model is not as precise as the model presented in column BJ, but it should still be helpful as rough check on temperature.

4. Olivine and cpx crystallization temperatures need not match, but the Fe-Mg exchange model of Putirka et al. (1996), and the olivine thermometer of Putirka (1997) can be used to compare olivine crystallization conditions to those for cpx. In practice, I have found that for some whole rock liquids that appear not to be liquids (due cumulus olivine), adding or subtracting olivine can be quite helpful in adjusting whole rock compositions. One can then check whether the amount of olivine removed matches modal proportions (although there are some obvious complications to this approach). Adjusting cumulate whole rock compositions until either (a) olivine-liquid Fe-Mg exchange values approach 0.3 (Roeder and Emslie, 1971), or (b) cpx Fe-Mg approaches either a constant value of 0.27 (or values predicted from equation 3.3 in Table 3 of Putirka (1999)), might at times be useful.

### References Cited

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- Roeder, P.L. and Emslie, R.F. (1970) Olivine-liquid equilibrium. *Contributions to Mineralogy and Petrology*, 29, 275-289.

Final Note: These spreadsheets were not specifically designed for public dissemination, but having received a large number of requests, I have tried to put together something useful. They thus still contain quite some 'junk' calculations (extraneous calculations that are not needed for *P-T* estimation) that I am still trying to clean up. However, I am happy to send these spreadsheets out to anyone who contacts me with such a request. Since the number of such requests is growing, I would greatly appreciate feedback from you if you find errors, or have suggestions for improvement or added clarity. Thank you for your interest in this work!

Cheers,

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