PTGIBBS-

An EXCEL[™] Visual Basic program for computing and visualizing thermodynamic functions and equilibria of rock-forming minerals.

by

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System requirements:

PTGIBBS requires complete Microsoft EXCELTM installation (version 8.0 or version 9.0) on an IBM-compatible personal computer. The minimum system requirements are a Pentium III 1000 Mhz processor (or equivalent) and 128 RAM memory. For good performance a minimum screen resolution of 1024 x 768 is recommended.

VERY Important INSTRUCTIONS FOR FIRST TIME USE

IT IS STRONGLY ADVISED THAT YOU print THESE INSTRUCTIONS SO YOU CAN REFER TO THEM as you follow the steps below.

To use PTGIBBS, the Excel Solver package must be installed on your system and Excel must be able to trust add-ins and templates.

To avoid error messages based on solver incompatibilities, please follow these steps:

- 1) Open a new Excel-Workbook.
- 2) Click on the Tools Menu in Excel.
 - 1. If Solver is not installed (you do not see the word Solver in the list of tools), open

the Tools/Add-ins menu;

2. If Solver is missing, run the Office Setup program with the Add/Remove option, and install the Solver add-in.

3. Also read the Microsoft documentation.

3) Modify the security configurations

Excel 97-Users:

 Click on menu item Tools > Options and then select the General tab and disable the Macro virus protection.

– Click OK.

Excel 2000-Users:

- On the Tools menu, point to Macro and click Security.
- In the Security dialog box, click Low to change your macro security level.
- Then click the Trusted Sources (also labeled Trusted Publishers) tab.
- On the lower left, click to select the <u>Trust all installed add-ins and templates</u> check box.

– Click OK.

Excel XP,2002,2003-Users: (PTGIBBS should also work with these versions)

- On the Tools menu, point to Macro and click Security.
- In the Security dialog box, click Low to change your macro security level.
- Then click the Trusted Sources (also labeled Trusted Publishers) tab.

- On the lower left, click to select the <u>Trust all installed add-ins and templates</u> check box and the <u>Trust Access to Visual Basic Project</u> check box.

- Click OK.

4) Close the opened Excel Workbook.

5) Copy the rest of this paragraph for reference, then click on the next words to <u>run</u> <u>PTGIBBS</u> for the first time (or you can return to <u>Tools and Applications</u> and click on the name PTGIBBS in the Tools menu). This will send PTGIBBS – an Excel program – to a temporary folder on your computer and open the program.

1. A VBAProject Password message box may appear. If it does, do not enter a password, just click on the Cancel button.

2. Click on <u>Solver</u> in the Tools menu. The solver window should open. Next simply

close solver, by clicking on the button 'close'.

3. Click <u>Save As</u> in the File menu to designate the directory into which you wish to save the PTGIBBS workbook on your computer (name of the workbook can be changed). This may take a little time.

4. Close PTGIBBS. (If asked whether you want to save the changes check No.)

INSTRUCTIONS

For complete instructions and examples please refer to:

PTGIBBS-an EXCELTM Visual Basic program for computing and visualizing thermodynamic functions and equilibria of rock-forming minerals A.Brandelik* & H.J. Massonne Computers & Geosciences, v. 30, # 9-10, p. 909-923.

To **RUN** PTGIBBS – open <u>the workbook saved on your computer</u>. If you have not saved PTGIBBS to your computer, refer to the instructions above!

After starting PTGIBBS the worksheet **INPUT** is automatically activated. In this worksheet mineral equilibria can be entered for computation. Three command bars appear in the upper portion of the screen as separate windows (command bars). They allow simple navigation in the workbook and the start of different computation routines.

1. Example

The routine CALCULATE 3D enables the display of diverse thermodynamic data of a selected phase as a function of P and T in a chart.

1. No input within the range of the worksheet **INPUT** is necessary.

2. After clicking on the control button CALCULATE 3D in the command bar **PTGIBBS CALCULATION** select a phase and a function in the opening dialogue (The P-T range can also be defined).

3. The result will appear by clicking on the button **CREATE 3D PLOT**.

4. The spatial orientation of the chart can easily be changed by means of the scroll bars.

5. By clicking on the button COPY 3D DATA, the computed data are copied to the clipboard.

6. You can reach the worksheet **INPUT** after computation, by closing the control dialogue (window "3D-Functions") and clicking on the control button **RETURN** in the command bar.

2. Example

By clicking on the button LOAD EXAMPLE in the command bar SHEET CONTROL, the user can view the input structure using selected examples.

1. Load example 4.

2. Click on the control button "Calculate equilibria" in the command bar **PTGIBBS** CALCULATION.

3. After starting the routine "Calculate equilibria" the button SELECT ALL has to be clicked in the opening dialogue. This carries out the calculation on all the listed reactions.

4. In the next dialogue, the P-T range for the computation can be defined.

5. After calculation, the result is automatically displayed in the worksheet PT_PLOT.

6. An ActiveX list box is located at the top of the worksheet PT_PLOT listing the equations of the calculated reactions. By selecting a reaction there, the corresponding curve is automatically assigned in the chart (or vice versa).

7. Additional procedures can be run by clicking on one of several control buttons arranged in the command bar. By means of an interactively operating system, it is possible, for example, to calculate the intersection between two curves, to display only selected curves, or to save the results of the calculation in a new workbook.

8. You can reach the worksheet **INPUT** after computation, by clicking on the control button **RETURN** in the command bar.

Return to **Tools**