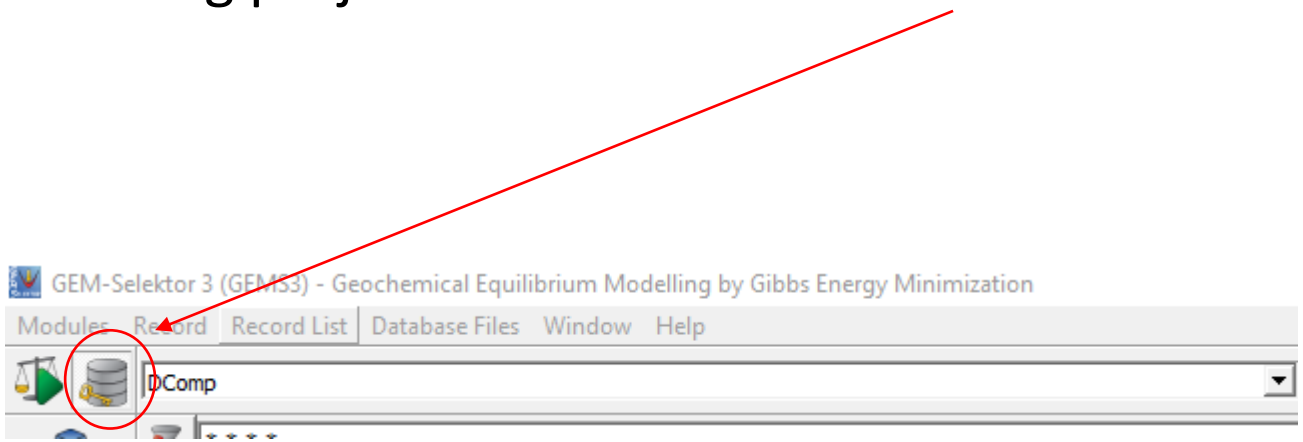
Adding a DCOMP phase in GEMS

Background

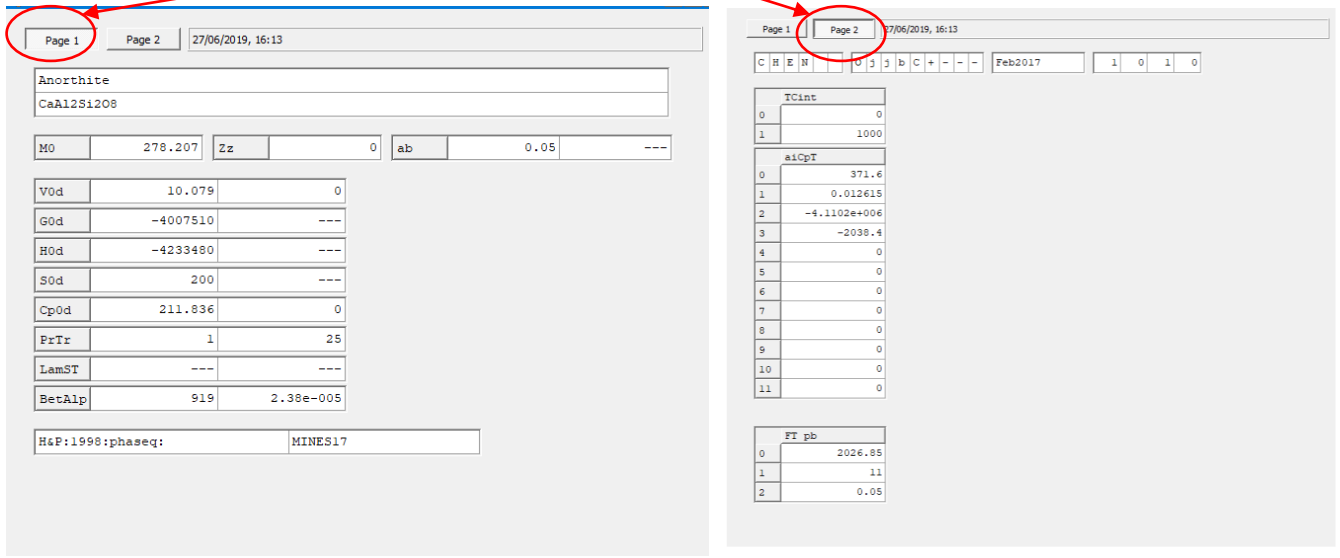
1. In GEMS, it is not recommended (disabled by default) to make changes to the parent thermodynamic database.
2. When a project is created, an editable copy of the database is made by GEMS.
3. It is recommended to make changes on this database.
4. This walkthrough assumes that you already have a project setup.
5. Open an existing project and select the “Database mode” button.



Pavan Akula

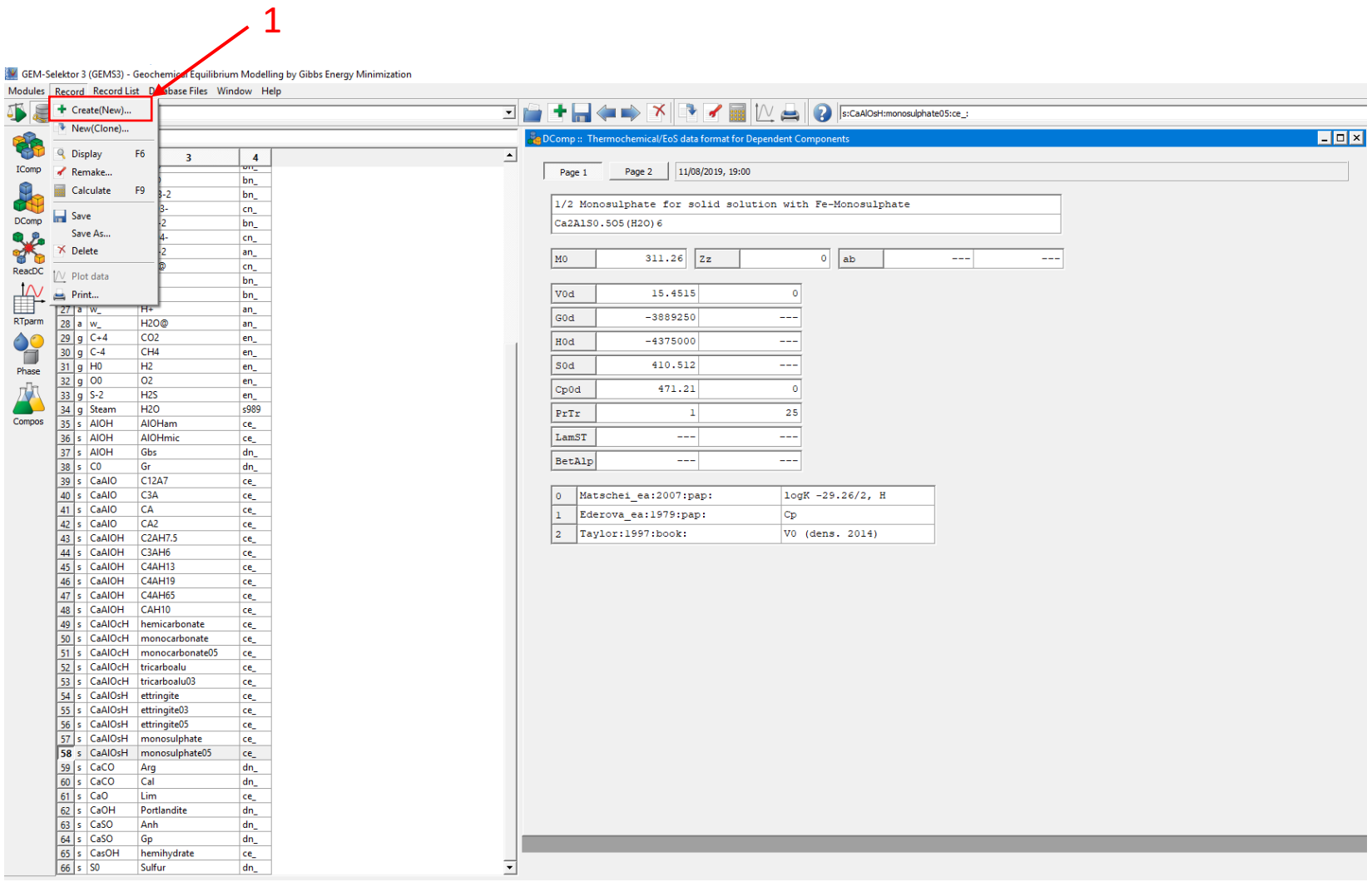
Adding a DCOMP phase in GEMS

1. We will add anorthite as a DCOMP phase.
2. The thermodynamic parameters for anorthite can be adopted from literature and databases (e.g. MINES; http://tdb.mines.edu/)
3. A screenshot of the required thermodynamic parameters for anorthite (from MINES database) is shown in figure below.
4. Save the screenshot of Page 1 and Page 2.



Required thermodynamic parameters for a DCOMP phase

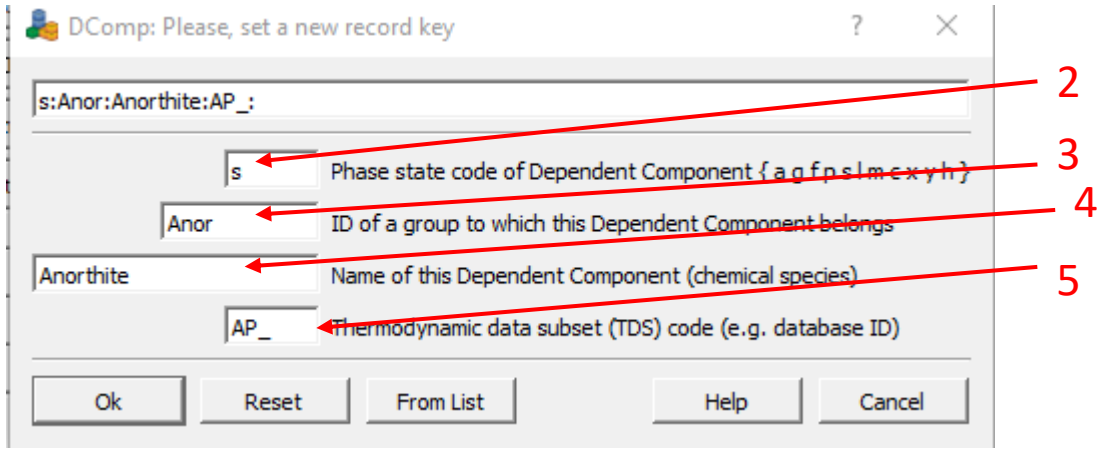
STEP 1



In this manual we will add kaolinite as a DCOMP in GEMS.

1: Select Record → New Record

STEP 2



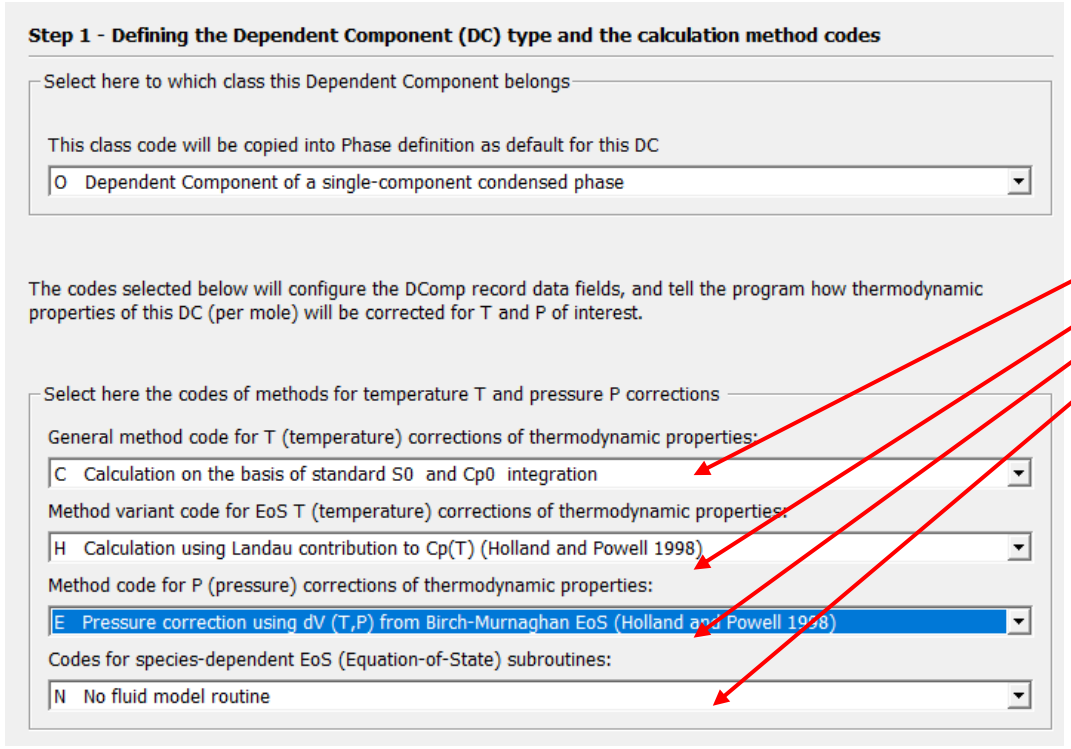
2: Select the phase state code. For crystalline solids (e.g. Anorthite), select s. You can refer to the complete list of available codes by selecting the Help button (bottom right).

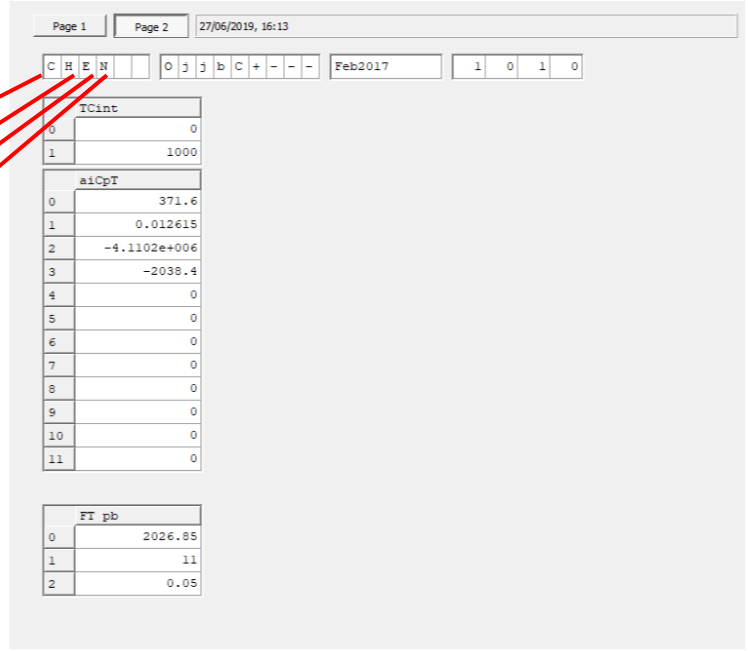
3: Enter a ID.

4: Enter the name of the phase

5: This is for the reference of the user. It is recommended to enter a unique identifier (e.g. your initials). You can use the identifier to locate phases that were added by you. It is really helpful if there is an error.

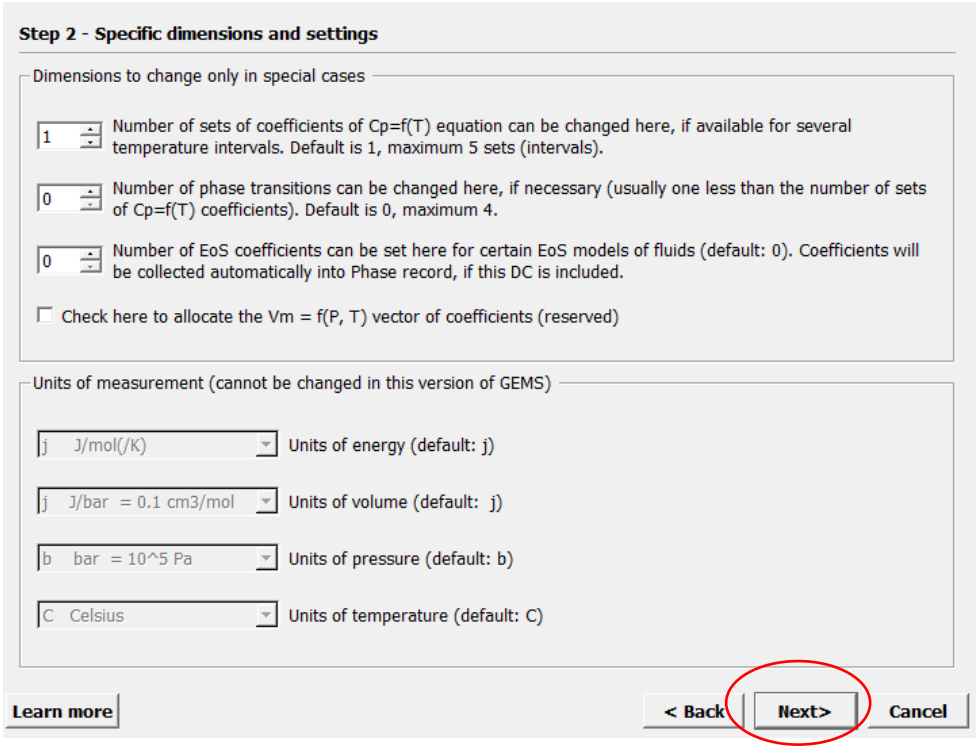
STEP 3

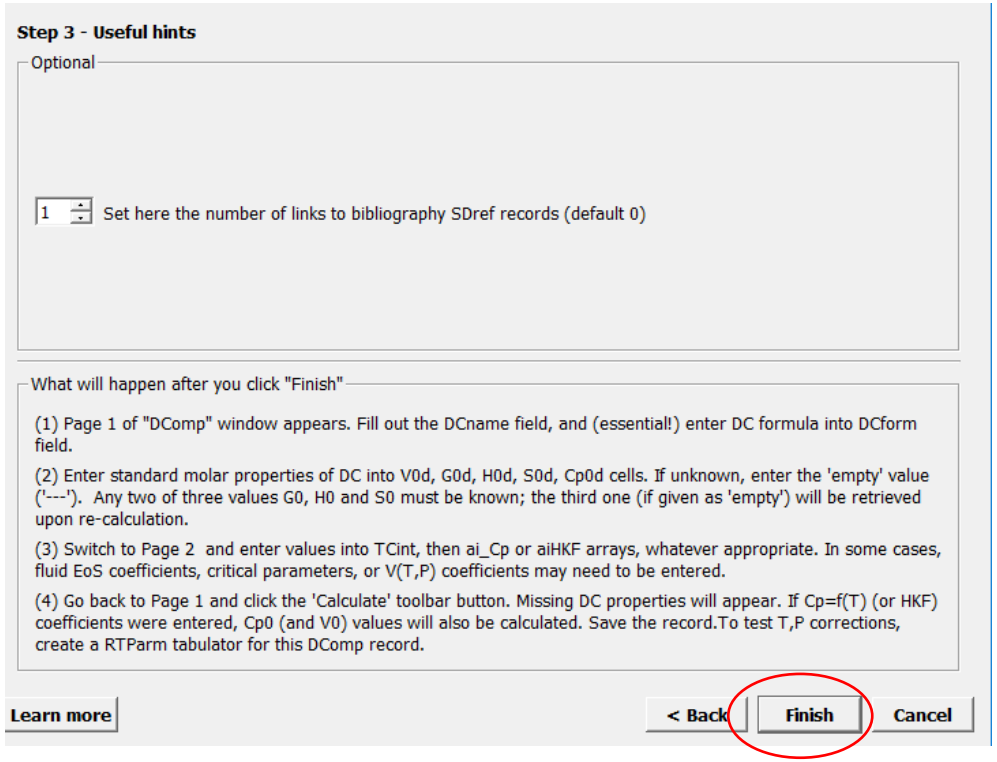




Use the screenshot as reference to select the calculation method codes

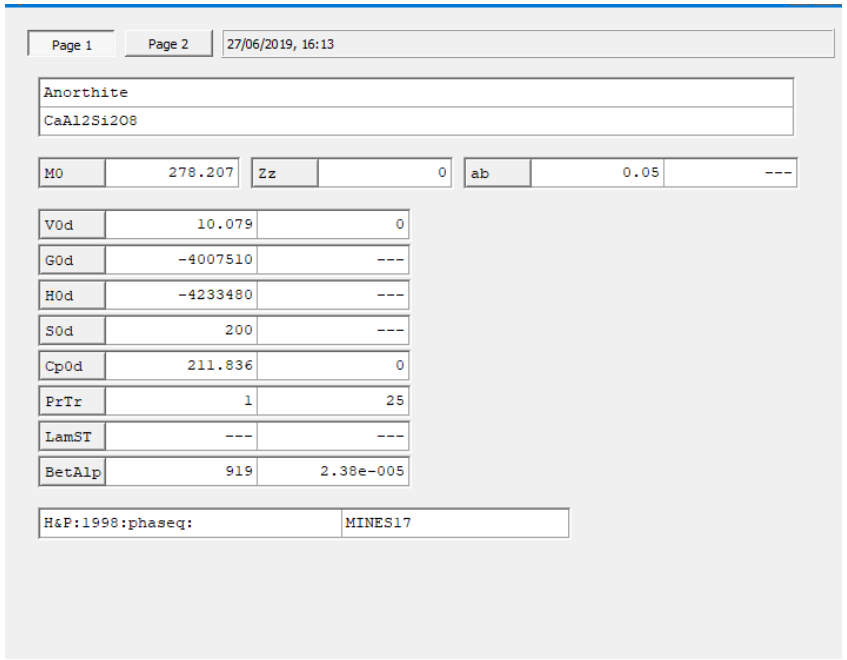
STEP 4

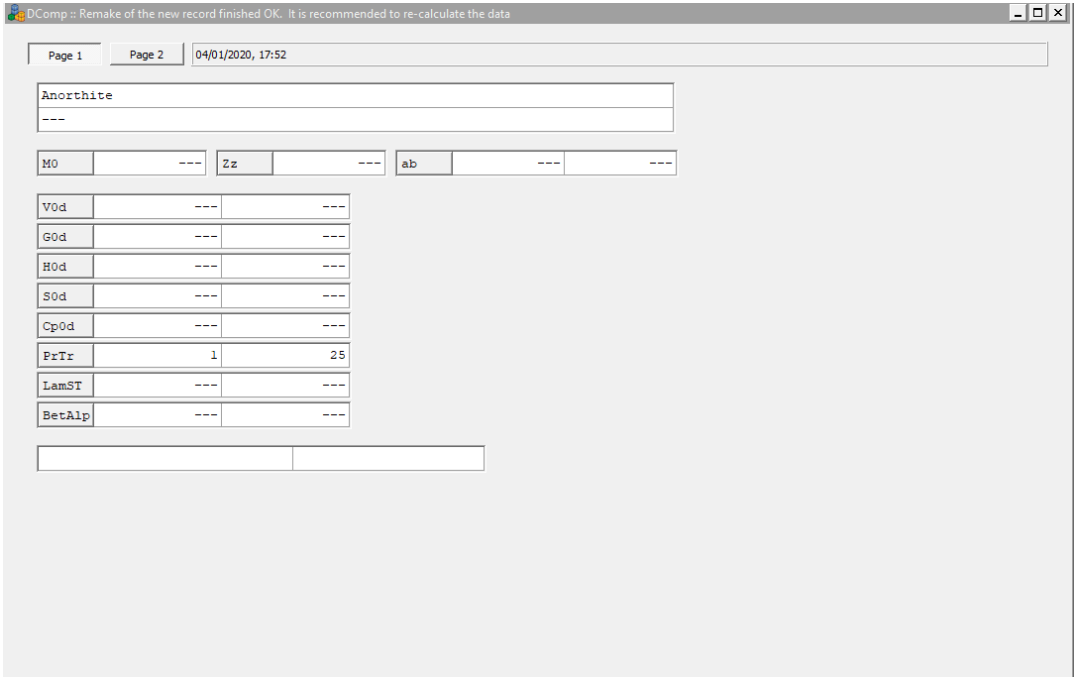




- For most phases, it is usually not necessary to change the default values in this step. Select “Next” on the “Step 2 - Specific dimensions and settings dialogue box” followed by “Finish” on the Step 3 – Useful hints dialogue box.
- Select “Learn more” if you are not sure.

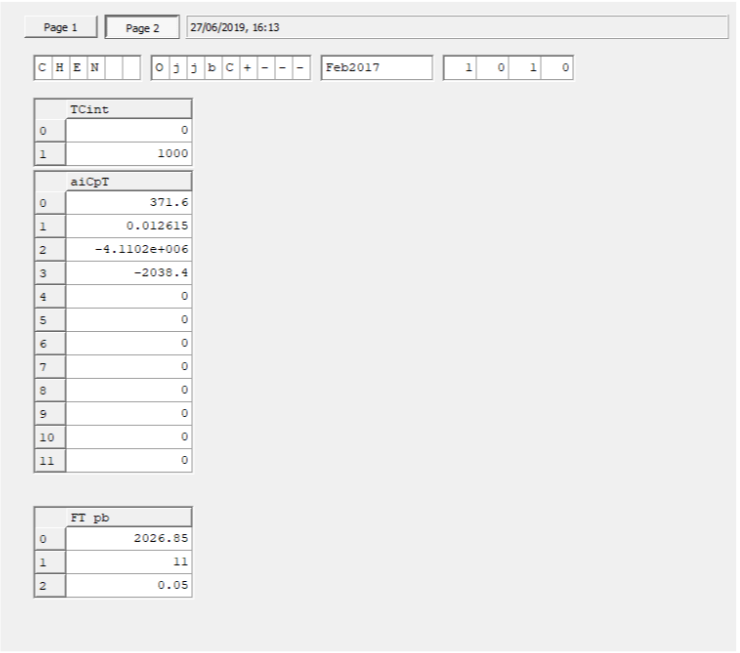
STEP 5

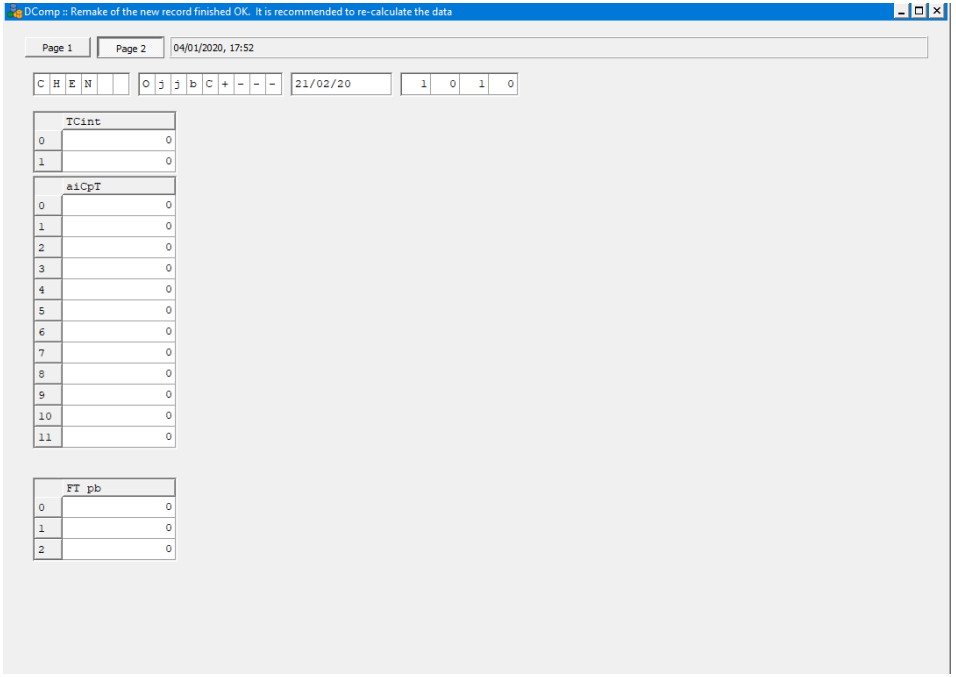




- Manually enter the database parameters.
- In this example we use the parameters from MINES database for anorthite.

STEP 6





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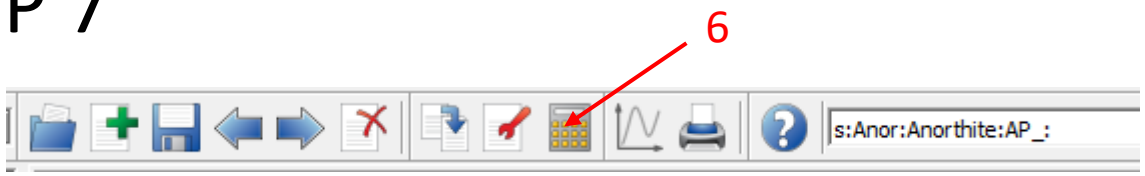
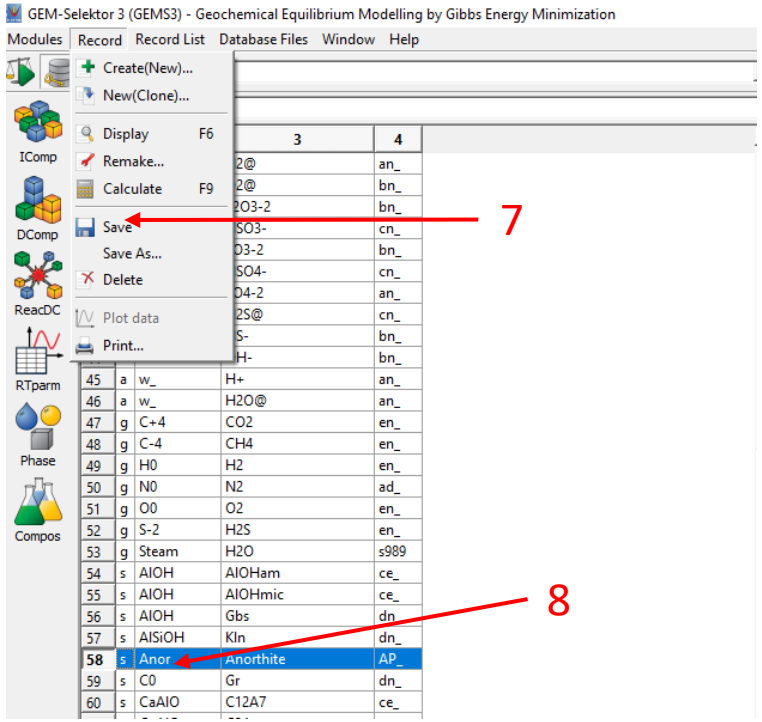
- In this example we use the parameters from MINES database for anorthite.

STEP 7



Select the calculate record button (6).



- Select Record → Save (7)
- Check DCOMP list for anorthite (8)

STEP 8

1. It is important to open the same project again.
2. A dialogue box will pop up when the project is opened.
    - Select “Yes” Add for all. (This will add the DCOMP phase to the project)
3. Run a recipe with the DCOMP and check for convergence.