

# How to use RCCM Gibbs energy Database for FactSage

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Research Center of Computational Mechanics, Inc.  
FactSage Support Team



# Preface

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RCCM Gibbs energy Database for FactSage (GeDb) is a collection of thermodynamic databases for FactSage. All of them are distributed free of charge.

GeDb can be used in FactSage Education package. Although FactSage Education package contains some public databases (FTlite, FToxid *etc.*), GeDb allows you to calculate equilibrium and phase diagram with the system that is not included these databases such as Nb-Re, Bi-Se, Ce-Pt.

Furthermore, you can edit parameters in the databases using Compound and Solution apps in FactSage Education. By changing the parameters, please look at the changes in the calculated phase diagram. This will give you a deeper understanding of the thermodynamic database.

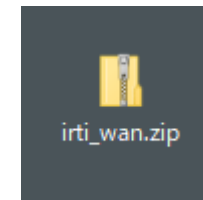
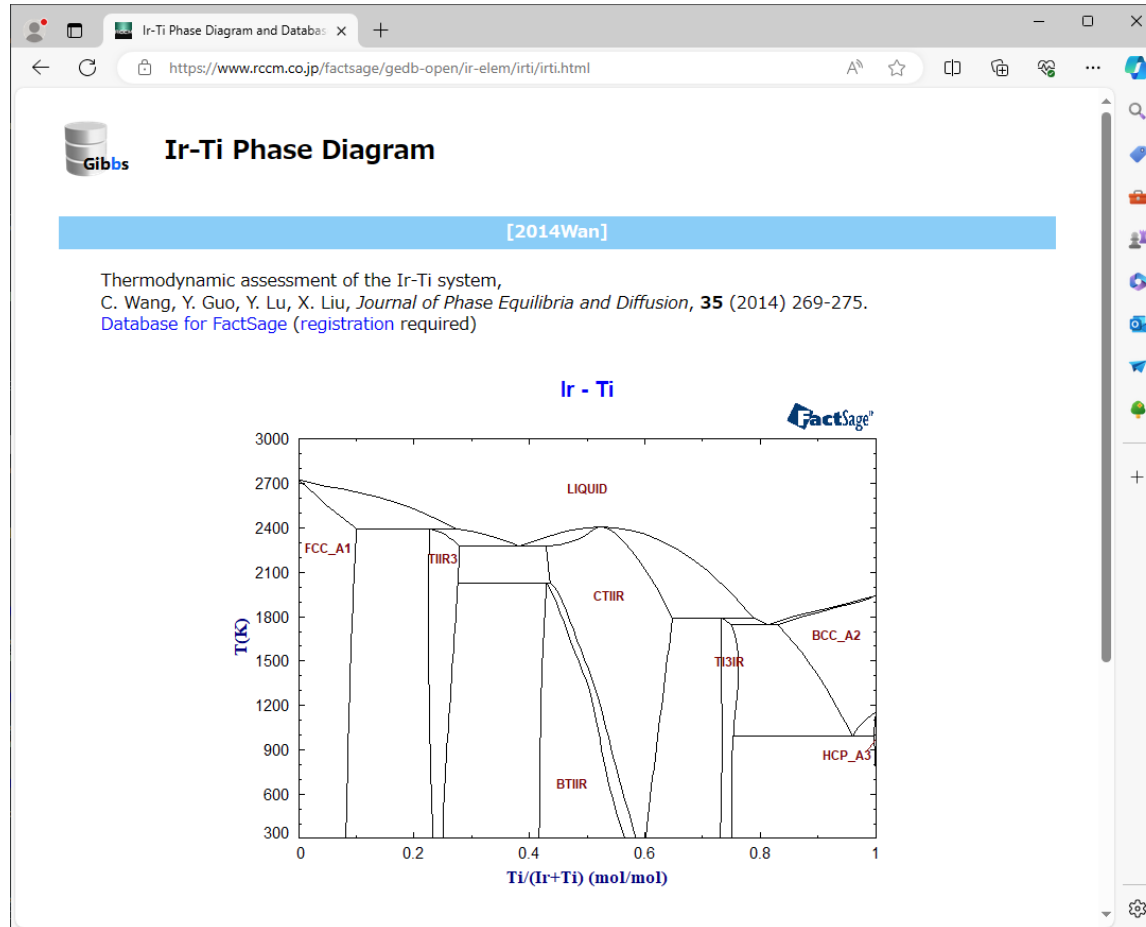
RCCM FactSage Support Team

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# 1. Installing the Thermodynamic Database

# Installing the Thermodynamic Databases

Download the Ir-Ti system database from GeDb to your desktop in advance. Here after, the steps is shown to add this database to FactSage Education. Of course, the same procedure is applicable for the full FactSage package.



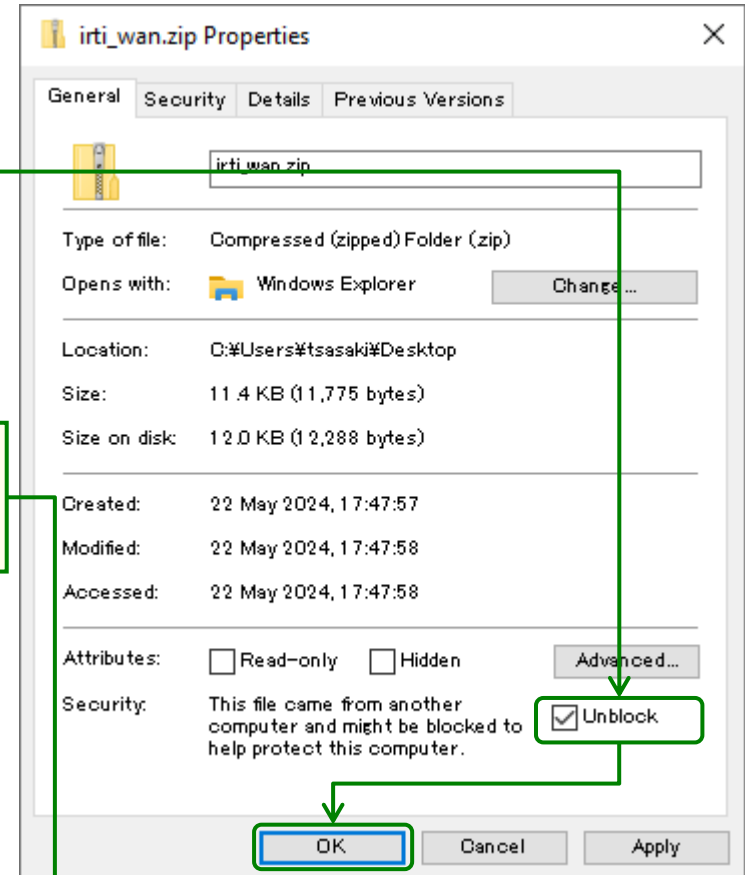
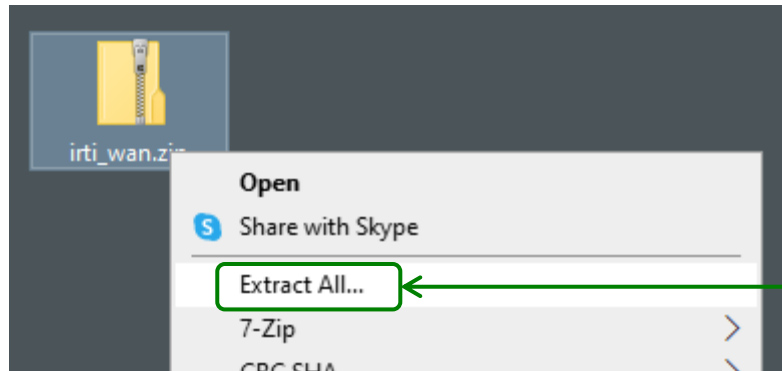
Ir-Ti thermodynamic database saved on the desktop

# Installing the Thermodynamic Databases

1. Right-click on the downloaded zip file ⇒ properties.

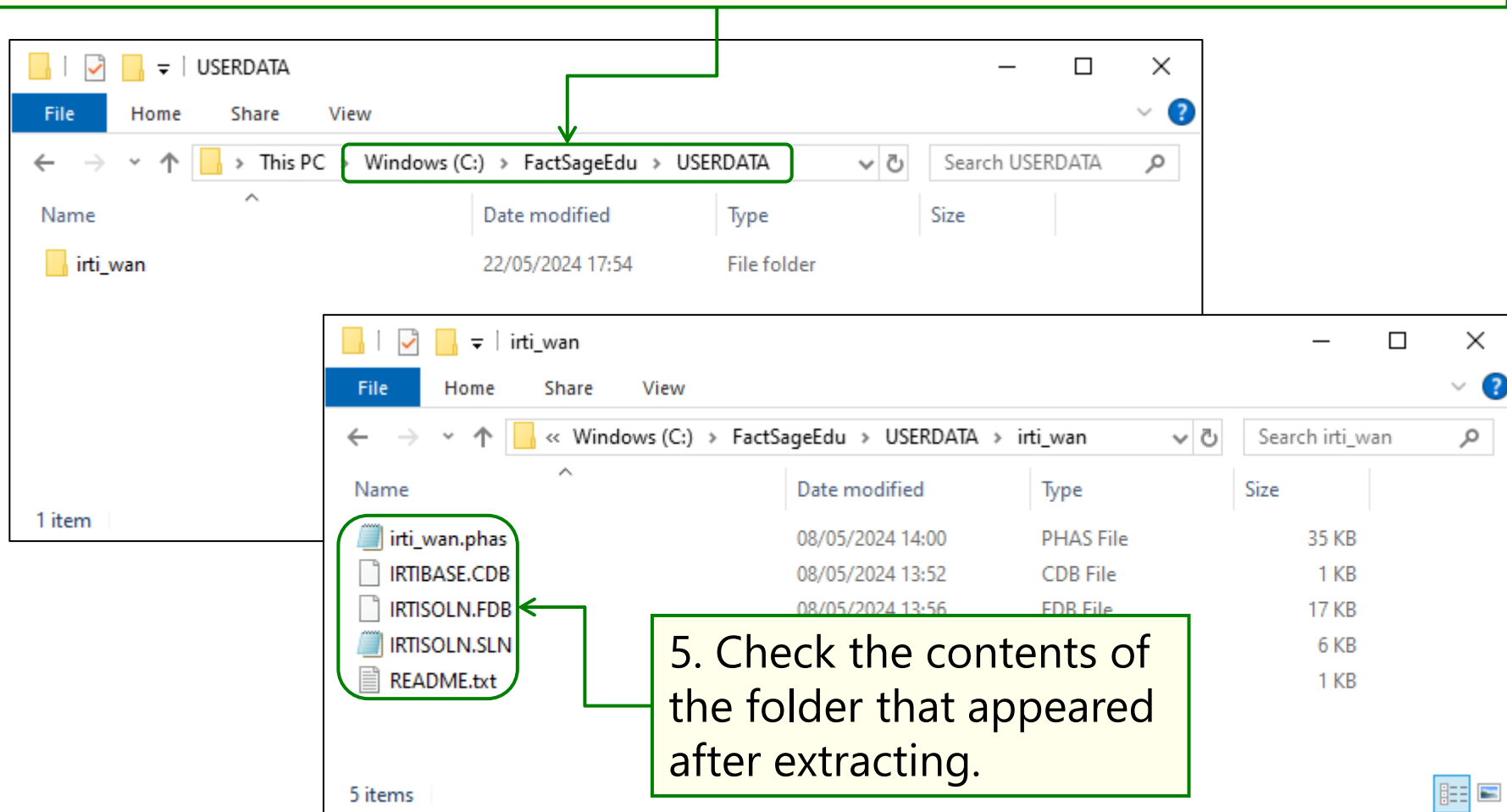
2. Check "Unblock" in Security and click OK.

3. Right-click on the downloaded zip file ⇒ Extract All ...



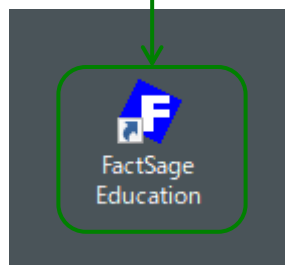
# Installing the Thermodynamic Databases

4. Save the extracted folder in the FactSage or FactSage Education installation folder. You can make subfolders in the installation folder. However, the folder name must be alphanumeric (*i.e.*, not include any Japanese characters). In the example below, a new subfolder named USERDATA is created and saved.

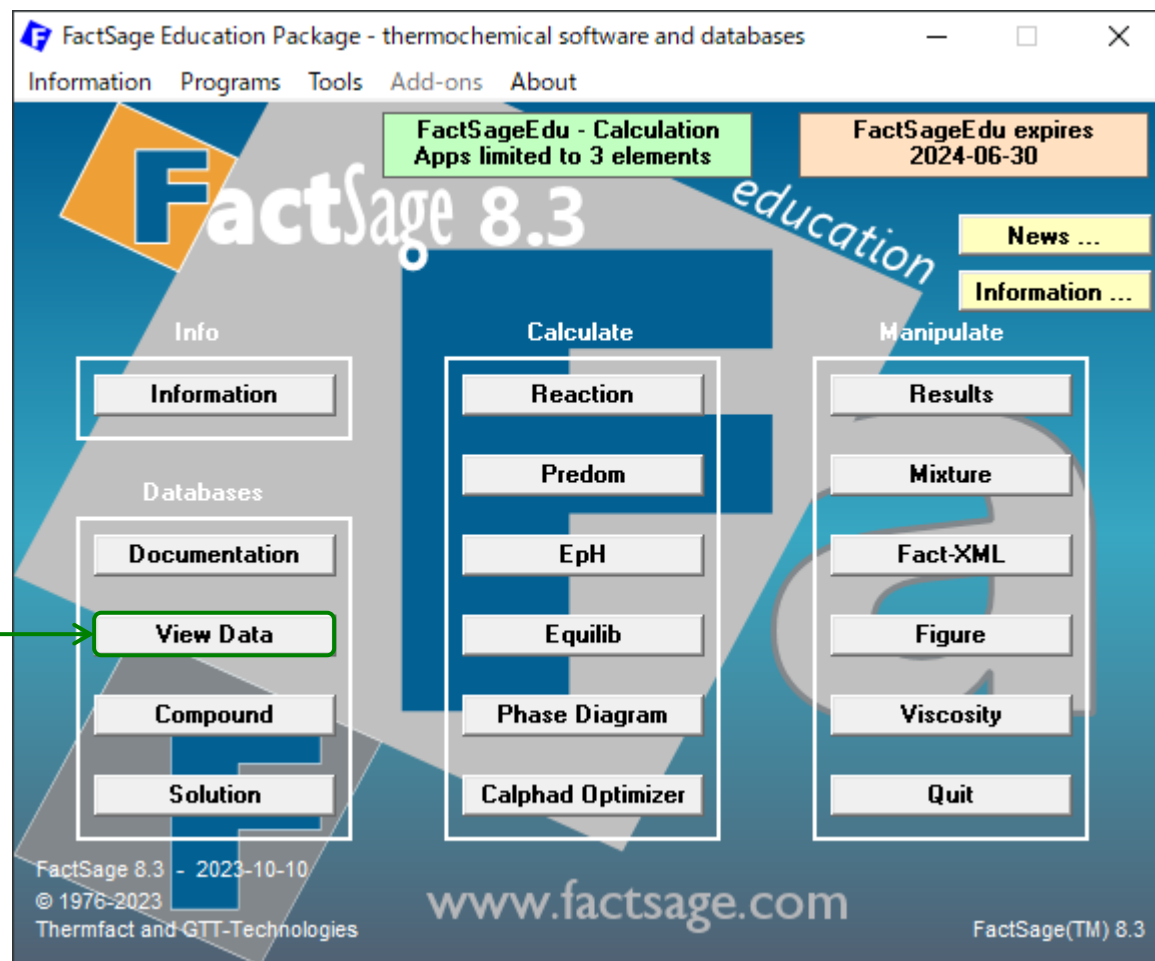


# Installing the Thermodynamic Databases

6. Launch FactSage Education.



7. Start View Data.



# Installing the Thermodynamic Databases

**View Data**

View compounds - enter a list of elements or a compound or ALL

Examples: Al, Ca and/or O

8. Click "Add".

Cu[++] - cation  
OH[-] - anion  
ALL - all compounds  
ALL Fe - all compounds of Fe  
ALL SO4 - all compounds with SO4  
ALL Fe S O - all compounds with Fe, S and O

Pressure  
☒ atm  
☐ bar

Energy  
☒ J  
☐ cal

Data  
☒ compound ☐ solution  
minimum solution components  
☒ 1 ☐ 2 cpts

Compound Databases (14)

Summary ... **Add ...** Remove ... FactPS

C:\FactSageEdu\FACTDATA\F553base.cdb  
FactPS - FACT pure substances database (2023)

Elements or Compound or ALL: Ca

Exit Assessments ... Information ... **OK**

10. Click "Browse" ⇒ Select the database file (IRTIBASE.CDB) and click "OK". You can also select IRTISOLN.SLN instead. Either one is fine.

9. Select "both".

**List of Databases**

**Database Type**  
☐ compound  
☐ solution  
☒ both

**Summary of files**  
Click for a summary of all database files including those not on the FactSage list:  
Summary ...

**Add database to the list**

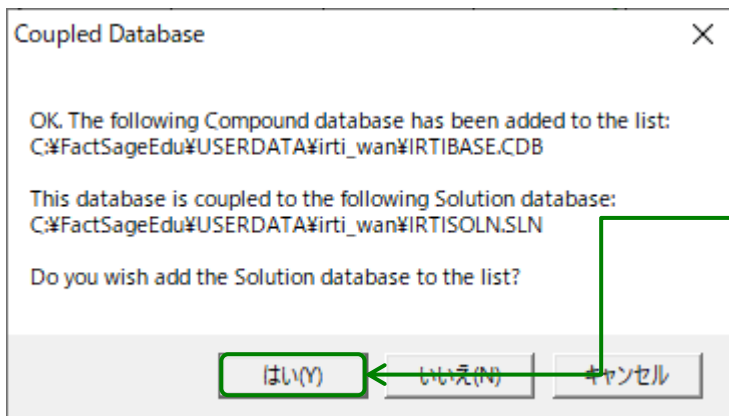
file: C:\FactSageEdu\USERDATA\virt\_i\_wan\IRTIBASE.CDB  
dir: C:\FactSageEdu\USERDATA\virt\_i\_wan\...  
nickname IRTI version 8.0  
info: IRTI compound database  
Click on 'OK' to add to the list.  
You may edit and change the info.

Quit

Browse ...  
Scan ...  
**OK**

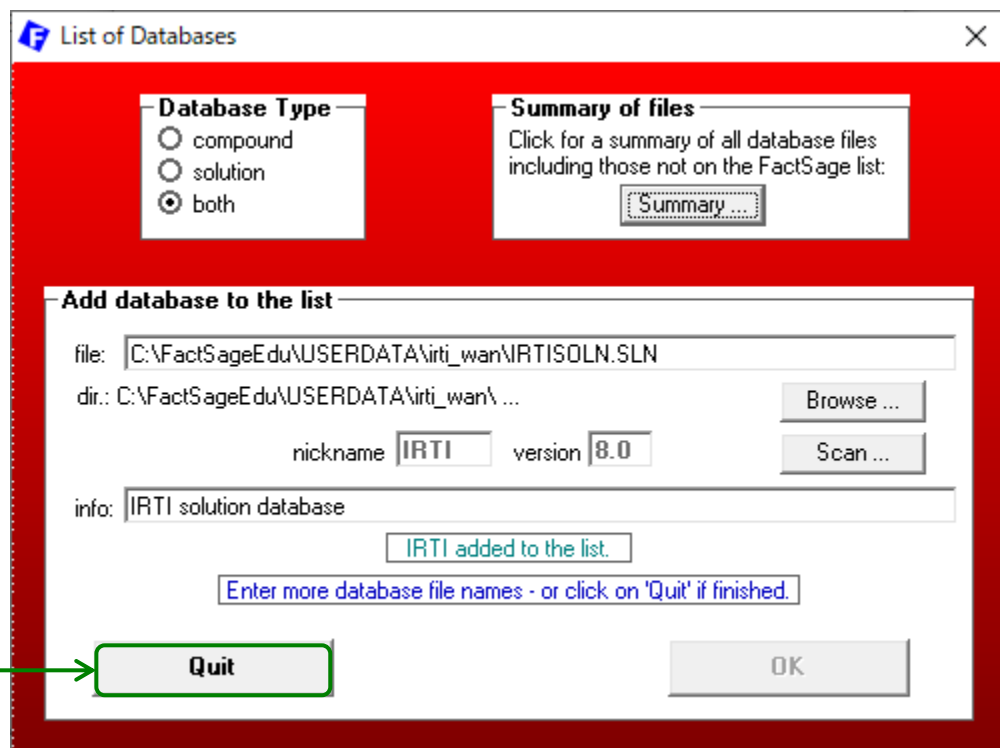


# Installing the Thermodynamic Databases



11. Click "Yes" to add both of compound and solution databases at the same time. It will take a few seconds.

12. Click "Quit".



# Installing the Thermodynamic Databases

## 13. Verify that IRTI database is added.

**View Data**

View compounds - enter a list of elements or a compound or ALL

Examples:

- Al Ca O - compounds of Al, Ca and/or O
- SiO2 - compound
- Fe2(SO4)3 - compound
- Cu[++] - cation
- OH[-] - anion
- ALL - all compounds
- ALL Fe - all compounds of Fe
- ALL SO4 - all compounds with SO4
- ALL Fe S O - all compounds with Fe, S and O

Pressure: ☒ atm ☐ bar

Energy: ☒ J ☐ cal

Data: ☒ compound ☐ solution

minimum solution components: ☒ 1 ☐ 2 cpts

Compound Databases (15)

Summary ... Add ... Remove ... **IRTI**

C:\FactSageEdu\USERDATA\irti\_wan\IRTIBASE.CDB

IRTI compound database

Elements or Compound or ALL: ALL

Exit Assessments ... Information ... **OK**

**View Data**

View solutions - enter a list of elements or ALL

Examples:

- Ca Al O S - solutions with Ca, Al, O and/or S
- H O Fe S - solutions (including aqueous) of H, O, Fe and/or S
- ALL - ALL solutions

Pressure: ☒ atm ☐ bar

Energy: ☒ J ☐ cal

Data: ☐ compound ☒ solution

minimum solution components: ☒ 1 ☐ 2 cpts

Solution Databases (14)

Summary ... Add ... Remove ... **IRTI**

C:\FactSageEdu\USERDATA\irti\_wan\IRTISOLN.SLN

IRTI solution database

Elements or ALL: ALL

Exit Assessments ... Information ... **OK**

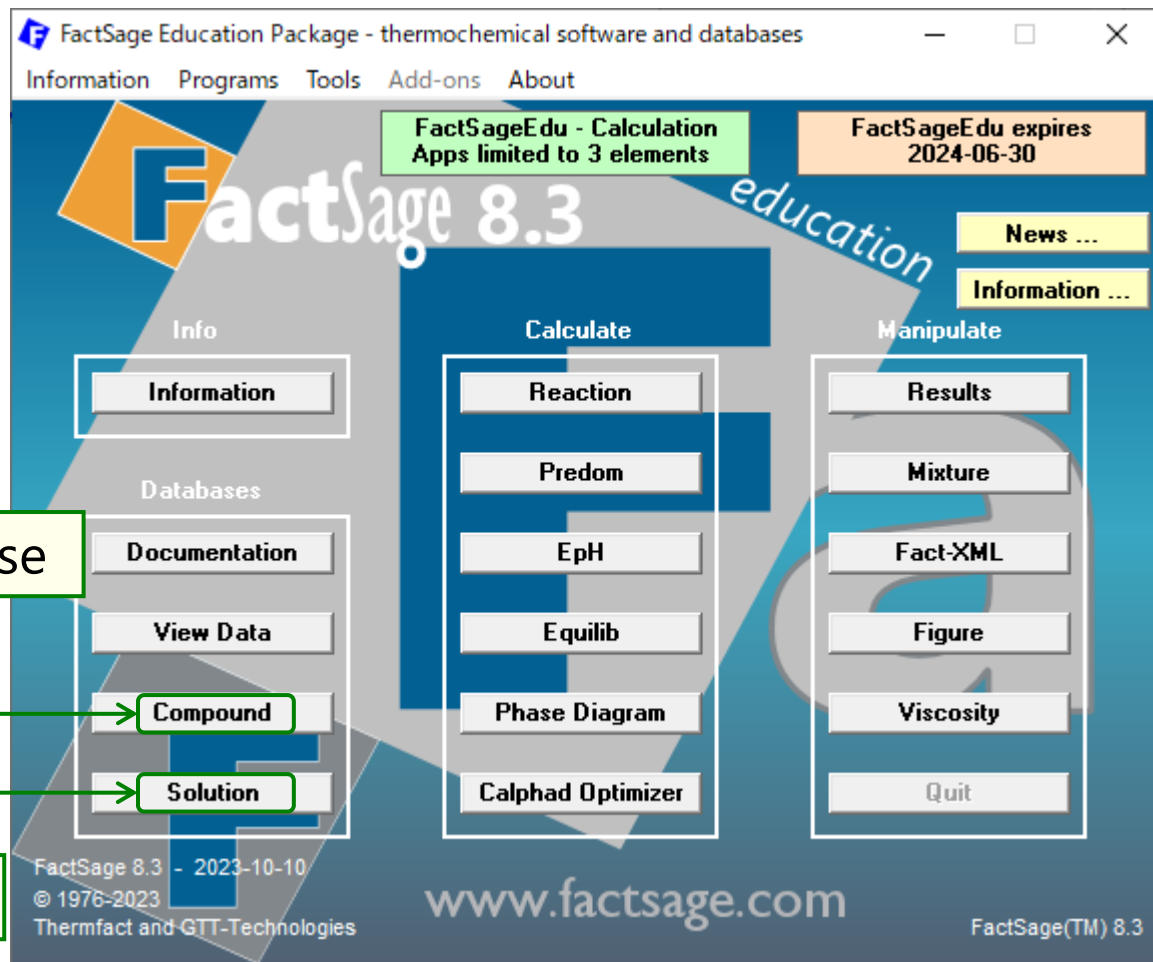
# Installing the Thermodynamic Databases

You can edit thermodynamic databases by Compound and Solution apps. Here, we look at the contents of the database (details on how to use the apps are omitted).

Note: IRTI database consists only of solution phases, hence IRTI compound database is empty.

Editing compound database

Editing solution database

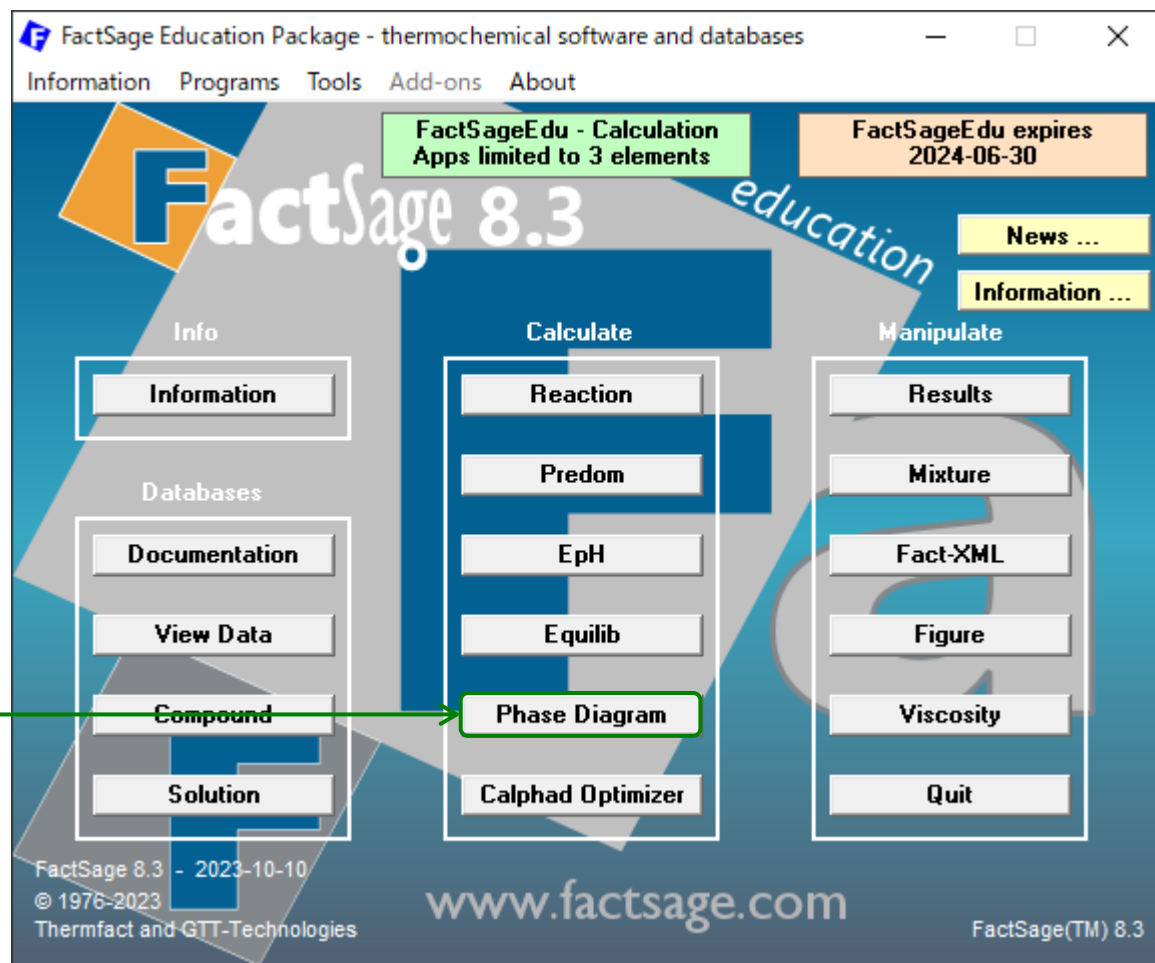


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## 2. Phase Diagram (Using configuration files)

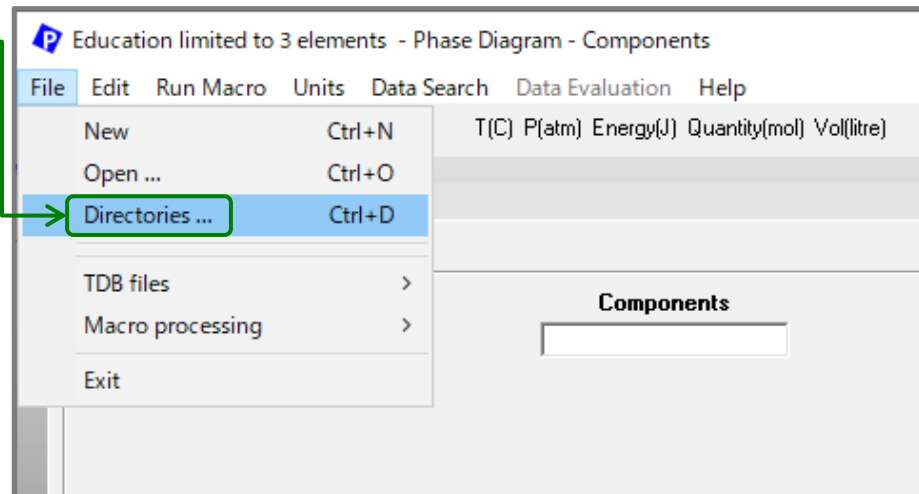
# Phase Diagram(Using configuration files)

1. Launch "Phase Diagram".

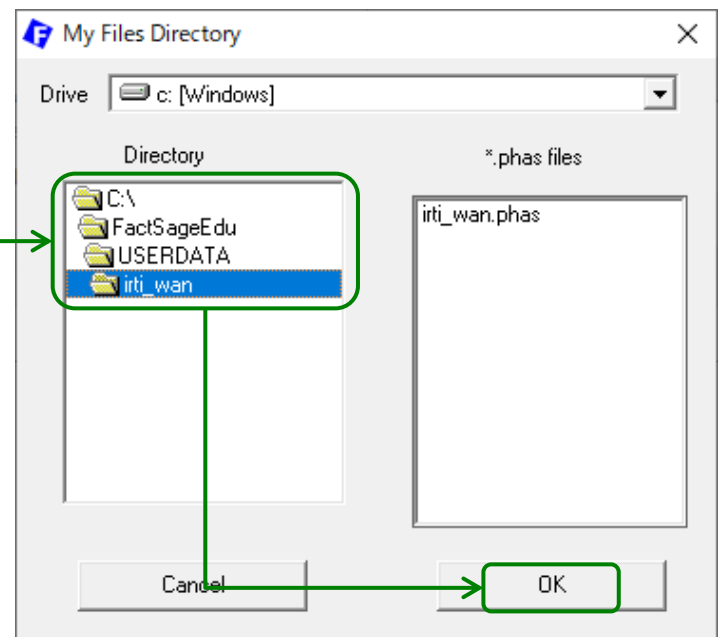
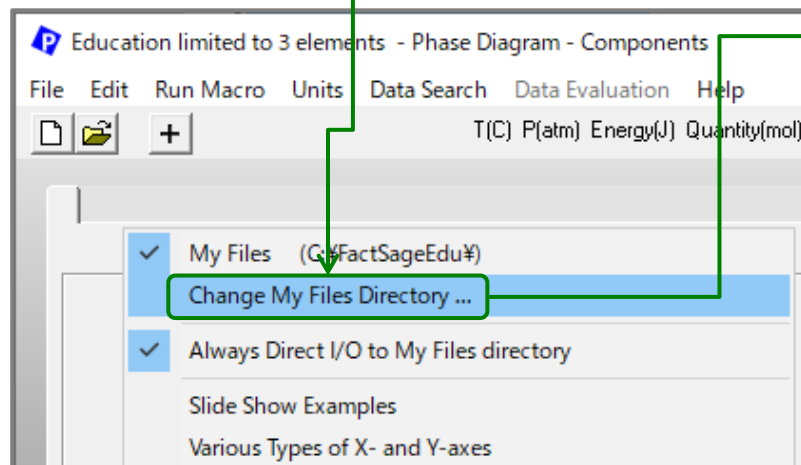


# Phase Diagram(Using configuration files)

2. Click "File ⇒ Directories".

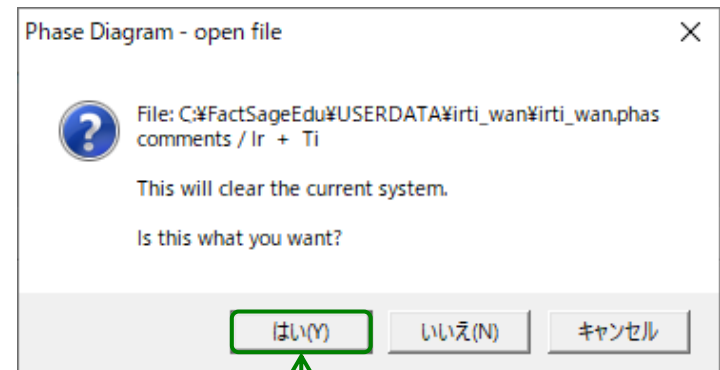
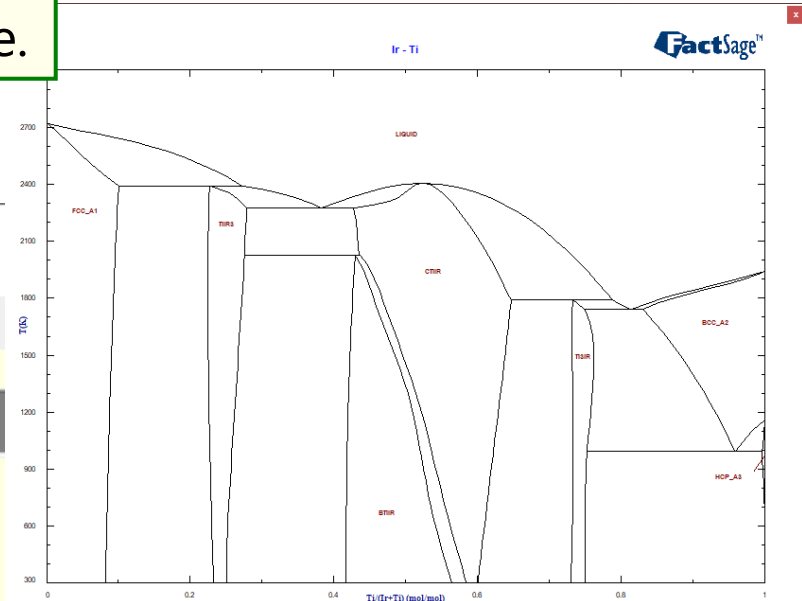
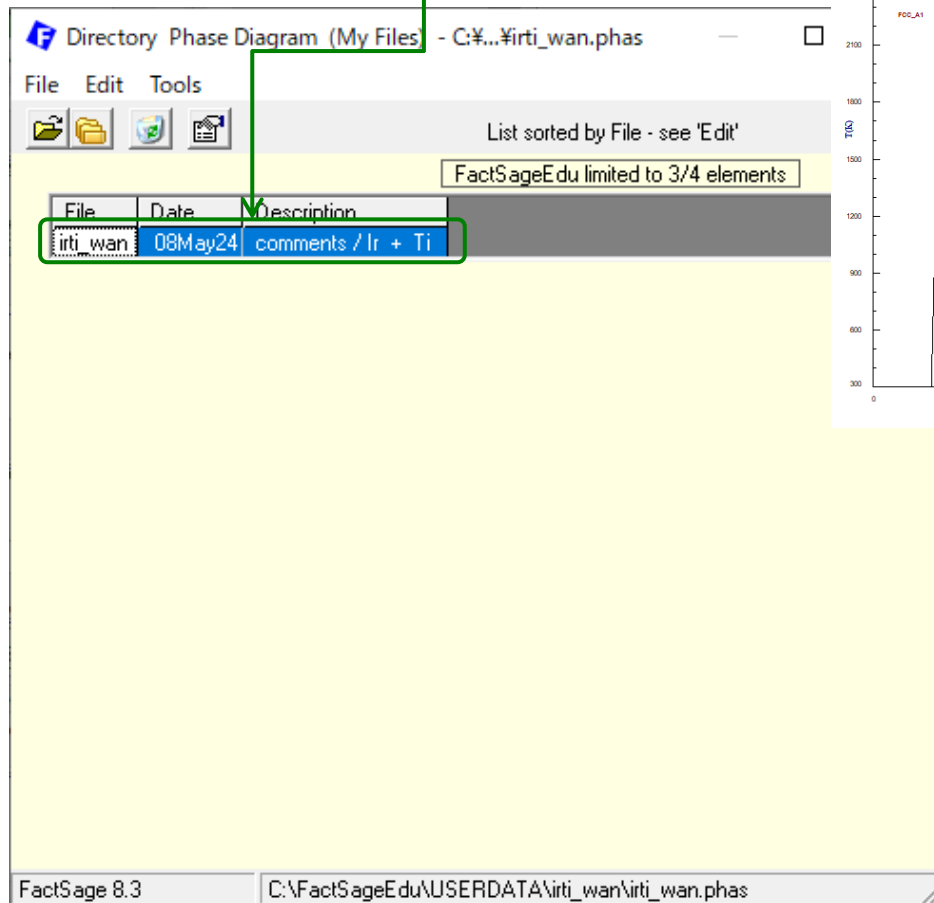


3. Click "Change My Files Directory ...". Find and double-click the folder in which IRTI database is saved. Then click "OK".



# Phase Diagram(Using configuration files)

4. Double-click the configuration file.



5. Click "Yes" to clear the current setting for the calculation.

# Phase Diagram(Using configuration files)

6. Click "Yes" to show the phase diagram stored in the \*.phas file.

If the message "- no product species selected" was shown and any figure did not appear, click "File  $\Rightarrow$  Open" again and reload the configuration file. Otherwise, click "No" and click Calculate button.

The screenshot shows the FactSage 8.3 software interface. The main window displays the 'Components' (Ir + Ti) and 'Products' (Compound species) sections. A 'Phase Diagram' dialog box is open, asking 'Show the figure calculated last time?'. The 'はい(Y)' (Yes) button is highlighted with a green box and an arrow. The dialog also shows a table of 'Solution phases' with columns for 'Base-Phase' and 'Full Name'. The 'Legend' section indicates 2 immiscible and 6 selected species. The 'Variables' section shows a table with columns for T(K) and Ti/(Ir+Ti). The 'Phase Diagram' section at the bottom right shows a plot area with axes Y and X, and a 'Calculate >>' button.

**Components [2]**

Ir + Ti

**Products**

Compound species

gas ☒ ideal ☐ real 0  
aqueous 0  
pure liquids 0  
pure solids 0

species: 0

**Target**

- none -  
Estimate T(K): 1000

**Variables**

| T(K)     | Ti/(Ir+Ti) |  |  |  |
|----------|------------|--|--|--|
| 300 3000 | 0 1        |  |  |  |

T(K) vs Ti/(Ir+Ti)

**Solution phases**

| * | + | Base-Phase | Full Name |
|---|---|------------|-----------|
| + |   | IRTI-LIQU  | LIQUID    |

**Phase Diagram**

Show the figure calculated last time?

はい(Y) いいえ(N) キャンセル

**Legend**

I - immiscible 2  
+ - selected 6

☒ Show ☒ all ☐ selected

species: 32  
solutions: 10 **Select**

**Custom Solutions**

☐ fixed activities  
☐ ideal solutions **Details ...**

**Pseudonyms**

apply ☐ **Edit ...**

**Volume and physical prop data**

☒ assume molar volumes of solids and liquids = 0  
☐ use only molar volume data  
☐ use V & phys. property data

☐ paraequilibrium & Gmin **edit**

**Total Species (max 936)** 32  
**Total Solutions (max 200)** 10  
**Total Phases (max 1500)** 10

**Phase Diagram**

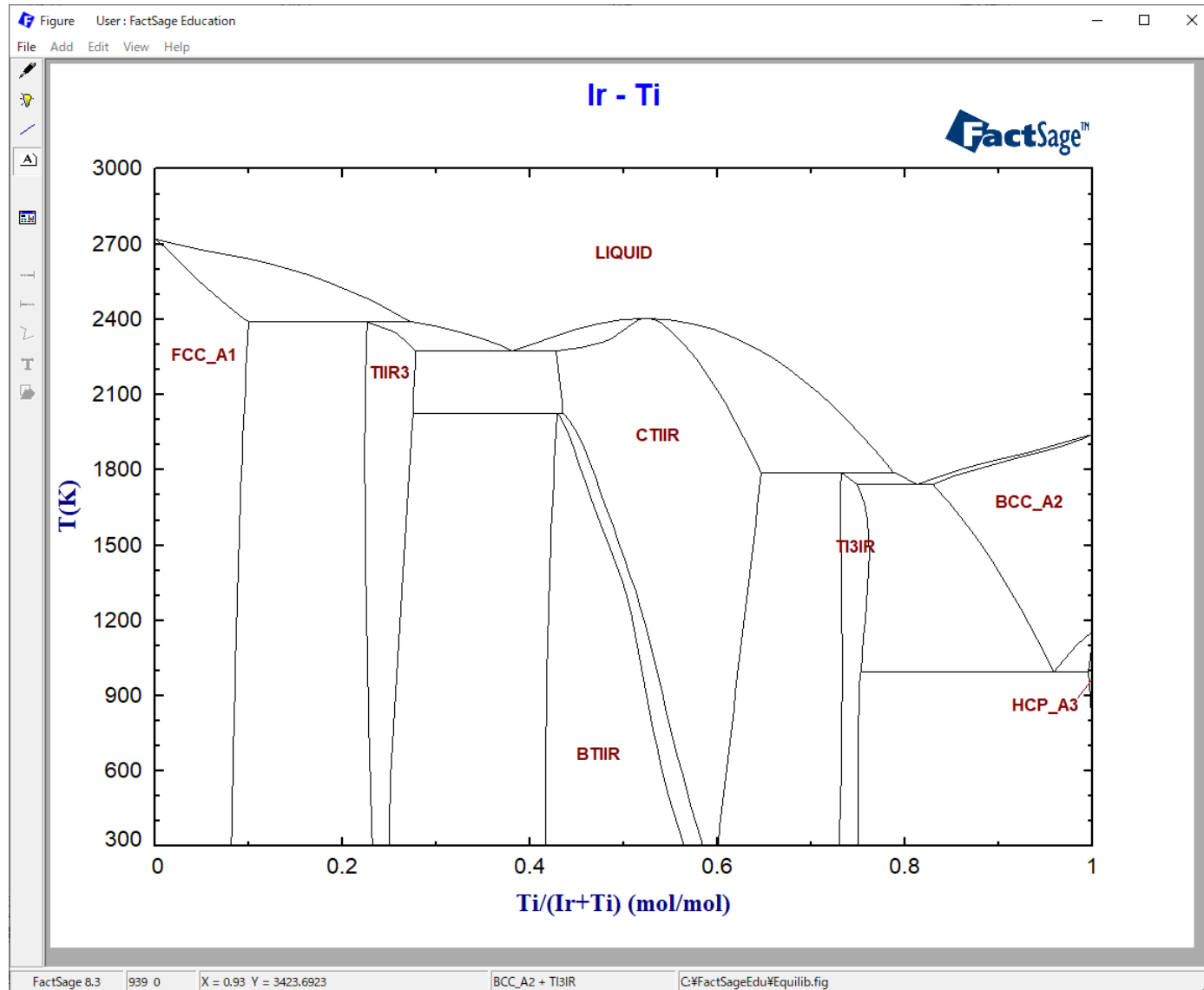
Y  
X  
- no time limit - **Calculate >>**

FactSage 8.3 C:\FactSageEdu\USERDATA\irti\_wan\irti\_wan.phas



# Phase Diagram(Using configuration files)

## Displayed phase diagram



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Edition / 2024 May 30

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