

Creating a New Reaction Database

1. Choose **File > New > Reaction Database**. The File dialog appears.
 2. In the dialog, specify a database file path and click the Open button.
- A window with an empty reaction table will appear.

Opening a Reaction Database

The user can process several reaction databases simultaneously. To open a reaction database:

1. Choose **File > Open**. The File dialog appears.
 2. In the dialog, select the database file path and click the Open button.
- The window with reaction table appears.

Note. Make sure the reaction database file is not read-only.

Entering Reactions

Paste Reactions

This method is used when data is available in an electronic form, for example as a text file. In addition the data should have the internal Chemked units: A-units are mol-cm-sec, E-units are cal/mol. Copy the data to the clipboard and then carry out the following steps.

1. In the reaction table select a row.
2. Choose **Edit > Paste**
or on the toolbar, click the **Paste** button
or right click mouse on the selected row and choose **Paste** from the pop-up menu.

The reactions will be pasted in the reaction table below the selected row.

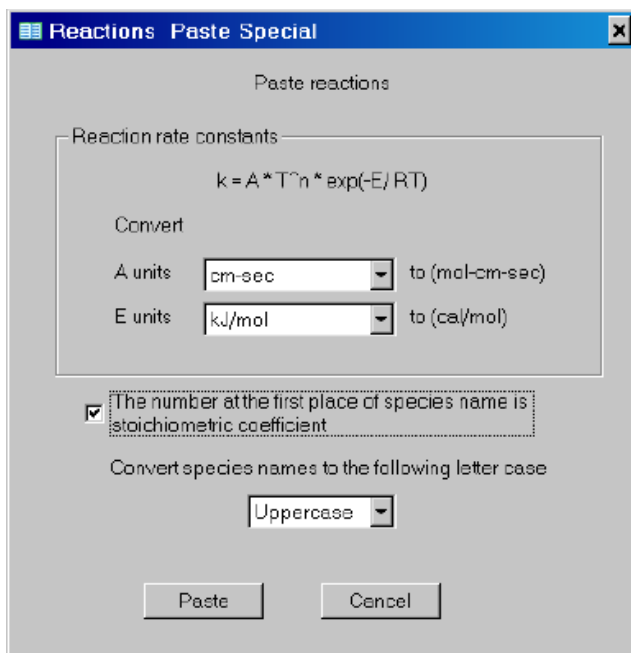
Remark -----

If you need to enter a large volume of data (more than a few hundred reactions), we recommend you to enter the data in parts.

Paste Special

If the data you want to paste does not have the internal Chemked units, they should be converted to these units. Some help can be get using the special pasting the data. Copy the data to the clipboard and then carry out the following steps.

1. In the reaction table select a row.
2. Choose **Edit > Paste Special**. The Paste Special dialog appears.



Here you can convert

A-units from cm-sec (concentration in 1/cm³)
to mol-cm-sec (concentration in mol/cm³),
E-units from kcal/mol, J/mol, kJ/mol or K
to cal/mol.

Important. If the units have been entered erroneously, all ensuing unit conversions in the program will be incorrect.

3 To take into account stoichiometric coefficients, check the corresponding check box. The number on the first position of species names will be interpreted as stoichiometric coefficients.

The reaction

2H + M <=> H2 + M 1.000E+18 -1.000 0

will be pasted as

H + H + M <=> H2 + M 1.000E+18 -1.000 0

The maximum number of reactants is 3 and the maximum number of products is 6 including stoichiometric coefficients.

4. If it is needed, change letter case of species names.

After clicking the Paste button the reactions will be pasted in the reaction table below the selected row.

References and Comments

The information behind exclamation mark (!) in the first line of the reaction description is a reference. It will be written in the Reference field of the reaction table. A reference may have maximum length of 64 characters.

Lines with the exclamation mark (!) in the first position are comments; they will be written in the Comment field of the reaction table. A comment for one reaction may have maximum length of 256 characters.

In the example, 'Marinov 1998' is a reference. The last two lines are comments.

```
ch2oh+h=ch3+oh      1.00E+13 0.0      0.0  !Marinov 1998
!Marinov, N. M, Int. J. Chem. Kinet. 31:183-220 (1999).
!Review and release date: May 19, 2004.
```

In the following example, the line with the Arenius parameters of the reverse reaction is commented out; it will be written in the Comment field of the reaction table.

```
ch3oh(+m) = ch3+oh(+m) 1.900E+16    0.00  9.173E+04
!      rev / 9.181E+10 1.00 7.450E+02 /
      low / 2.95E+44 -7.35 9.546E+04 /
      troe/0.414 279. 5459. 1.00E+15/
      h2/2/ h2o/16/ co/2/ co2/3/
```

Remark -----

In the CHEMKIN standard representation the reactions are written as a sequence of lines where the first and last lines contain the key words REACTIONS and END respectively. To use this data you should copy all the text between, not including, the key words. An error will occur if the data contains the key words (REACTIONS, END) or another auxiliary information (MOLES, CAL/MOLE).

Manual Input

1. In the reaction table select a row.
2. Choose **Edit > Insert New Row**
or on the toolbar, click the **Insert New Row** button
or right click mouse on the selected row and choose **Insert New Row** from the pop-up menu.
A new row will be created below the selected row.
3. Double click a field in the new row; the input window appears.
4. Type data in the text boxes of the input window; click OK.

The screenshot shows a software window titled "REAC_H2 .mdb" with a sub-header "No 14" and an "Irreversible" checkbox. It features five tabs: "General", "Third Bodies", "Pressure Effects", "Ref.", and "Tips". The "General" tab is active, displaying a chemical reaction table with three rows. The first row shows H2O2 as a reactant and O2 as a product. The second row shows HO2 as a reactant and HO2 as a product. The third row is empty. Below the table, the rate law is given as $K_{for} = A \cdot T^n \cdot \exp(-E/RT)$. There are two columns of input fields: "Forward" and "Reverse". The "Reverse" checkbox is checked. The "Forward" column has values: A = 4.63E+16 cm³/mol s, n = -0.35, and E = 50670 cal/mol. The "Reverse" column has values: A = 4.20E+14 cm³/mol s, n = 0, and E = 11980 cal/mol. At the bottom are "OK", "Cancel", and "Show Species" buttons.

	Forward	Reverse
A	4.63E+16 cm ³ /mol s	4.20E+14 cm ³ /mol s
n	-0.35	0
E	50670 cal/mol	11980 cal/mol

Important. Make sure that the pasted data have A-units mol-cm-sec and E-units cal/mol.

Editing Reactions

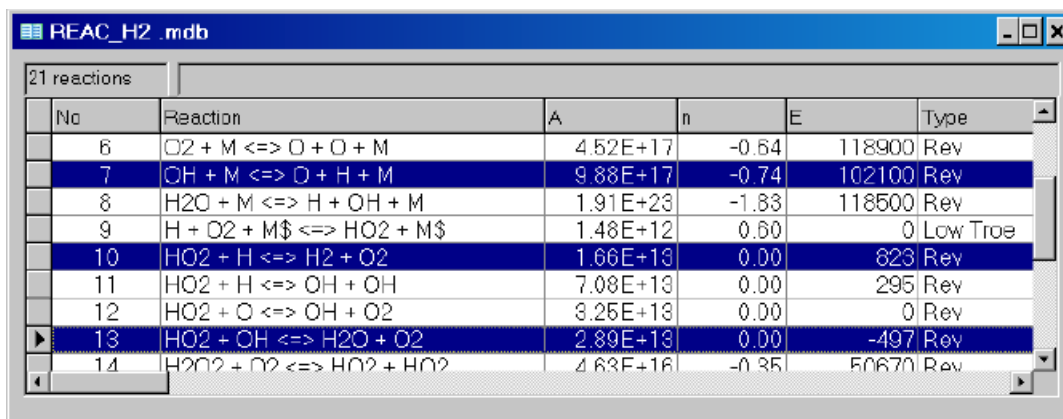
Ordering Reactions

The reactions can be ordered by values in each table column. To do that, click column header. If you click the header some times, the reactions will be sorted in ascending or descending order sequentially.

Note. The reaction numbers are sorted always in ascending order.

Selecting Rows in Reaction Table

In the reaction tables, most of the edit operations are performed on selected rows. To select a row, click its header. To use the multiple-selection mode, hold down the Ctrl key and click the row headers. To select all rows, choose **Edit > Select All**.



REAC_H2.mdb

21 reactions

No	Reaction	A	n	E	Type
6	O2 + M <=> O + O + M	4.52E+17	-0.64	118900	Rev
7	OH + M <=> O + H + M	9.88E+17	-0.74	102100	Rev
8	H2O + M <=> H + OH + M	1.91E+23	-1.83	118500	Rev
9	H + O2 + M\$ <=> HO2 + M\$	1.48E+12	0.60	0	Low Troe
10	HO2 + H <=> H2 + O2	1.66E+13	0.00	823	Rev
11	HO2 + H <=> OH + OH	7.08E+13	0.00	295	Rev
12	HO2 + O <=> OH + O2	3.25E+13	0.00	0	Rev
13	HO2 + OH <=> H2O + O2	2.89E+13	0.00	-497	Rev
14	H2O2 + O2 <=> HO2 + HO2	4.63E+16	-0.35	50670	Rev

Multiple-selection mode

Deleting Reactions

Select reactions you want to delete. Press the Del key or choose **Edit > Delete Rows**.

Copying Reactions

Select reactions you want to copy.

Choose **Edit > Copy**

or on the toolbar, click the **Copy** button

or right click mouse on a selected row and choose **Copy** from the pop-up menu.

Reactions will be stored in the clipboard.

Note. In the clipboard, the reactions have the CHEMKIN text format. You can view the reactions in any text editor.

Changing Reaction Parameters

1. Double click the field of the reaction table with a value you want to change. The input window appears.
2. In the corresponding text box of the input window, change the value; click OK.

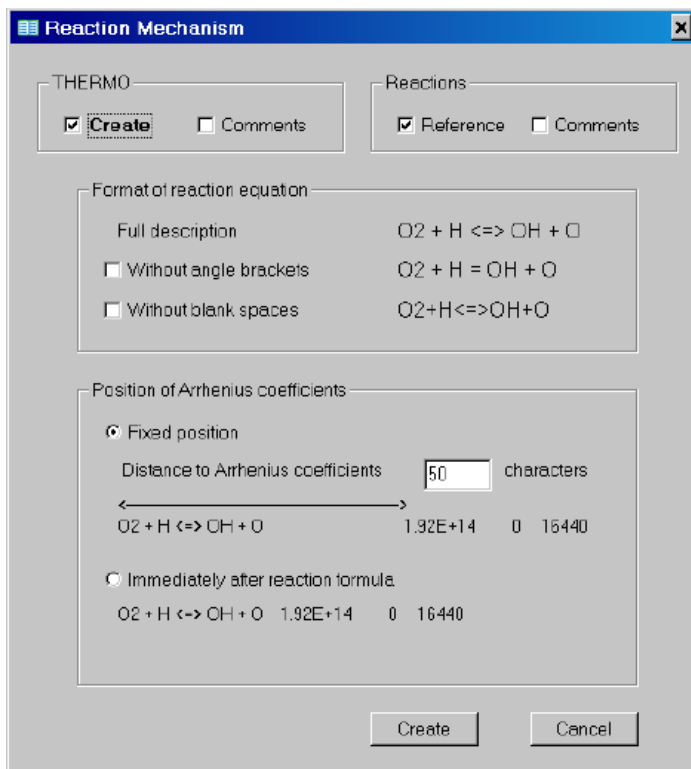
Reaction Mechanism in CHEMKIN Format

1. Choose **File > Reaction Mechanism in CHEMKIN Format**.

The Reaction Mechanism dialog appears.

2. In the dialog, select the items you **want** to include in the document, choose the format; click OK.

Reaction mechanism appears in a text window; you can print this or save it to a file.



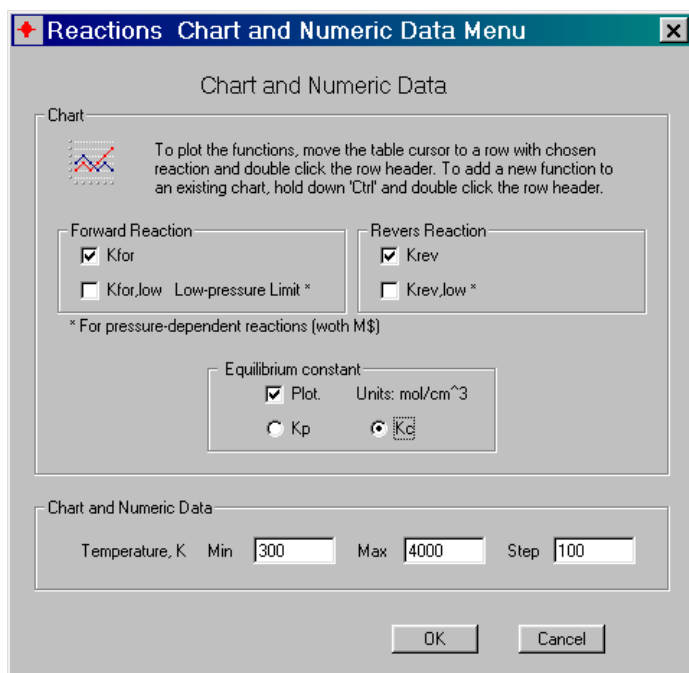
Creating Charts and Viewing Numeric Data

You can create charts and view numeric data of the following functions: forward and reverse rate constants (including low pressure limit for pressure dependent reactions), equilibrium constant.

Selecting Functions

1. Choose **View > Chart and Numeric Data Dialog**
or on the toolbar, click the **Chart and Numeric Data Dialog** button.
The dialog appears.

2. In the dialog, select the functions you want to plot, and specify the interval and step of temperature; click OK.



Dialog for choosing functions

Plotting Functions

1. In the reaction table, select the row with a reaction whose functions you want to plot.
2. Double click the row header; the curves of the functions appear in Temporary Chart.

No	Reaction	A	n	E	Type
7	OH + M <=> O + H + M	9.88E+17	-0.74	102100	Rev
8	H2O + M <=> H + OH + M	1.91E+23	-1.83	118500	Rev
9	H + O2 + M\$ <=> HO2 + M\$	1.48E+12	0.60	0	Low Troe
10	HO2 + H <=> H2 + O2	1.66E+13	0.00	823	Rev
11	HO2 + H <=> OH + OH	7.08E+13	0.00	295	Rev
12	HO2 + O <=> OH + O2	3.25E+13	0.00	0	Rev
13	HO2 + OH <=> H2O + O2	2.89E+13	0.00	-497	Rev
14	H2O2 + O2 <=> HO2 + HO2	4.63E+16	-0.35	50670	Rev
15	H2O2 + O2 <=> HO2 + HO2	1.43E+13	-0.35	37060	Rev
16	H2O2 + M\$ <=> OH + OH + M\$	2.95E+14	0.00	48430	Low Troe

Double click here to plot the functions

If this procedure is repeated for different reactions the existing curves will be replaced with new ones. If you want to add new curves to Temporary Chart, hold down the Ctrl key and then double-click the row header.

Saving Temporary Chart

Temporary Chart is deleted when the program closes. To save the chart you should carry out the following steps.

1. Activate the Temporary Chart window.
2. Choose **File > Save As**. A file dialog appears.
3. In the dialog, specify a file path; click the Save button.

Important. The file name should have the '.pg' extension.

Viewing Numeric Data

1. In the reaction table select the row with a reaction whose data you want to view.
 2. Choose **View > Numeric Data of Current Reaction**
or right click mouse on the selected row and choose **Numeric Data of Current Reaction** from the pop-up menu.
- Numeric data of rate constants and equilibrium constant vs. temperature appear in a text window. You can print this or save it to a file.