

Enter number of species and elements

Number of Species	Number of Elements
<input type="text" value="9"/>	<input type="text" value="4"/>
<input type="button" value="Next"/>	

Figure 1: Java applet window for entering number of species and elements

6 Java Applet JSTOICH

6.1 Getting Started

JSTOICH is a Java applet; your browser must be capable of running Java classes (incorporated, for example, in Netscape version 3.0 or later, and in Internet Explorer version 3.0 or later).

To implement JSTOICH, the steps are as follows:

- Enter the number of species and number of elements in the initial window (Figure 1).
 - Click the **Next** button.

A new window will appear for the entry of the species names and their molecular formulas in a table (Figure 2).

- Enter the species names in the first column as indicated, using any desired notation (*e.g.*, H₂O(g) for gaseous water and H₂O(l) for liquid water; i-C₄H₈ for isobutene, *etc.*).
 - Enter the names of the elements across the top row of the table, using any desired notation (*e.g.*, Na for sodium, H for hydrogen, *etc.*).
 - Enter the (total) subscripts to each of the elements for each species in the row of the table to the right of its name (*e.g.*, for H₂O, enter 2 for H, 1 for O, and 0 for any other element in the system; for

Species Names	N	H	Cl	O
NH ₄ ClO ₄	1	4	1	4
Cl ₂	0	0	2	0
N ₂ O	2	0	0	1
NOCl	1	0	1	1
HCl	0	1	1	0
H ₂ O	0	2	0	1
N ₂	2	0	0	0
O ₂	0	0	0	2
ClO ₂	0	0	1	2

Calculate

Java Applet Window

Figure 2: Java applet window for entering species names and formulas

(CH₃)₂CO enter 3 for C, 6 for H, 1 for O, and 0 for any other element in the system.)

- Click the **Calculate** button.

The window is over-written with the results of the calculation (Figure 3).

3. The window contains:

- C , the number of components
- R , the number of independent chemical equations in a proper set
- a list of any chemically inert species (those that are not contained in any chemical equation), if any

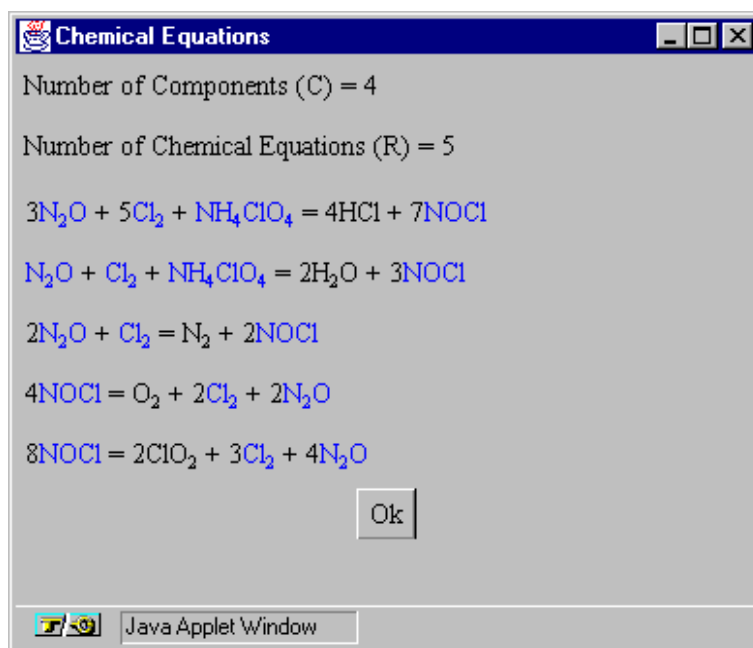


Figure 3: Java applet window containing results of the calculation

- a proper set of chemical equations in conventional canonical chemical form.
- the component species indicated in the equations in blue, and the noncomponent species indicated in the usual text color, typically black.

Click on the **Ok** button to close the window.

4. To terminate JSTOICH, choose the **Exit** item on the menu bar of the window under Step 2 above.

Example 9:

Figures 1-3 show the three windows for the example problem (Segraves and Wickersham, 1991): $\{(\text{NH}_4\text{ClO}_4, \text{Cl}_2, \text{N}_2\text{O}, \text{NOCl}, \text{HCl}, \text{H}_2\text{O}, \text{N}_2, \text{O}_2, \text{ClO}_2), (\text{N}, \text{H}, \text{Cl}, \text{O})\}$, relating to the explosion of ammonium perchlorate. The component species are NH_4ClO_4 , Cl_2 , N_2O , and NOCl .

6.2 Capabilities

JSTOICH:

- allows any number of species, N
- allows any number of elements, M
- allows for:
 - inert species
 - multiphase system
 - charged species
 - problem modification by addition of a species or element to a given list
 - problem modification by deletion of a species or element from a given list

6.3 Help File for JSTOICH

Optional actions may be performed by clicking on any of the items in the menu bar of the final window, as follows:

- **Options:**
 - Enter zero values:
instead of entering 0 values for element subscripts, only the non-zero ones need be entered; this option fills in the remaining entries with zeros.
- **Delete:**
 - Clear all matrix entries:
All the species formulas are erased from the table.
 - Clear all entries:
The species names and formulas, and the element names are erased from the table.
 - Species:
A row in the table is deleted corresponding to the selected species.

- Element:
A column in the table is deleted corresponding to the selected element.
- **Add:**
 - Species:
A row in the table is added for an additional species
 - Element:
A column in the table is added for an additional element
- **Exit:**
 - The Java applet is terminated.
- **Help:**
 - Instructions are given to perform specific tasks (displays this file).

Some Additional Hints:

- After entering each element name, pressing the Enter key will move the cursor to the next element.
- The cursor (arrow) keys allow you to move around the cells of the table for the species and element names, and their formulas.
- For systems involving charged species, enter a symbol for the protonic charge (*e.g.*, “p”) and enter the signed charge of each species in the corresponding column of the table for its formula; *e.g.*, for H⁺ the charge is 1; for OH⁻, the charge is -1. The charge entry for a neutral species is 0.
- You can save the output windows of the applet to a file in the usual way. For example, to insert CRS output into a wordprocessor in Windows (*e.g.*, Word or WordPerfect), do the following:
 1. When the appropriate window of the applet is active (as indicated by the highlighted bar at its top), press Alt-Print Scrn to copy its contents to the Windows Clipboard.
 2. In the wordprocessor, place the cursor at the desired location and press Control-V.