

Chapter 2. Periodic table of the elements

2.1 Introduction

The basis of the [periodic table](#) is the electron configurations of the elements, which can be used for a discussion of some of properties of elements, including atomic radii, ionization energies, and electron affinities. These atomic properties also form the rationale basis of the chemical bonding.

In 1869, Dmitri Mendeleev observed that when the elements are arranged in order of increasing atomic mass, certain sets of properties recur periodically. Therefore he arranged and grouped together similar elements on the periodic table.

The rationale behind is that the physical and chemical properties of an element are determined largely by its electron configuration, particularly that of the valence (outermost) electronic shell. Adjacent members of a series of main-group elements in the same period (such as P, S, and Cl) have significantly different properties because they differ in their valence-electron configurations.

Mendeleev periodic table consisted of 8 groups, but most modern periodic tables are arranged in 18 groups of elements. The vertical groups bring together elements with similar properties. The horizontal periods of the table are arranged in order of increasing atomic number from left to right. The groups are numbered at the top, and the periods at the extreme left. The first two groups are the s block and the last six groups the p block together constitute the main-group elements. Because they come between the s block and the p block, the d block elements are known as the transition elements. The f block elements, sometimes called the inner transition elements, would extend the table to a width of 32 members if incorporated in the main body of the table.

The table would generally be too wide to fit on a printed page, and so the f block elements are extracted from the table and placed at the bottom. The 15 elements following barium are called the lanthanides, and the 15 following radon are called the actinides.

Through a color scheme of the periodic table, one evidences that the majority of the elements are metals (orange) and that non-metals (blue) are confined to the right side of the table. The noble gases (purple) are treated as a special group. Metals and nonmetals are often separated by a stairstep diagonal line, and several elements near this line are often called metalloids (green). Metalloids are elements that look like metals and in some ways behave like metals but also have some nonmetallic properties.

2.2 3D-plot of electronegativity

Electronegativity describes an atom's ability to attract the electrons shared with other atoms during the formation of one or more chemical bonds. Many electronegativity scales have been developed in so far, one of the most used in general chemistry textbooks is the [Pauling's scale](#). The values have been transferred in a text file, leaving out those for which the value is not available. The picture of the 3d-trend can be obtained in a very simple manner, employing some of the Octave capabilities.

The `importdata` function has the ability to work with a wide variety of data. In our case the text file 'electronegativity.txt' is loaded into a cell. The text file is imported with the `\n` (new line) option, so as every line becomes now a single cell element. This cell has 94 elements, each consisting in a string of characters, containing the atomic number, atomic symbol, name of the element and finally its electronegativity. (the elements with no value available are omitted). The second step is now to extract the four fields from each element. This is performed by the function `strsplit`; having no option, the space character (ASCII 32) is used as a delimiter.

```
A = importdata("electronegativity.txt","\n");
ln = length(A)
for i=1:ln
    b = strsplit(A{i});
    nAt = str2num(b{1}); eNeg = str2num(b{4});
    .....
endfor
```

As a general rule, electronegativities decrease from top to bottom in a group and increase from left to right in a period of elements, in order to plot this in a 3-D fashion, we must first introduce the function `patch`. This function creates a patch object in the current axes with vertices at locations (x,y,z) and of color defined by `FaceColor` argument. In our case the object is a quadratic [prism](#), whose vertices are numbered according to the figure 2.1.

The function requires two input [matrices](#), one for the vertices ($v2$) and another for the faces ($f2$). The elements in $v2$ are the eight coordinated of vertices, whose connectivity to form faces is described in $f2$ (see fig. 2.1). So as to simplify the script, only the visible faces are created.

```
v2 = [x1 y1 0;x2 y1 0;x2 y2 0;x1 y2 0;x1 y1 h1;x2 y1 h1;x2 y2 h1;x1 y2 h1];
f2 = [3 4 8 7;1 4 8 5;5 6 7 8];
patch('Faces',f2,'Vertices',v2,'FaceColor',[ (h1*0.25) (1-h1*0.25) 0]);view(3);
```

If needed for having a view from every angle, the complete set of faces can be plotted, and now $f2$ becomes :

```
f2 = [3 4 8 7;1 4 8 5;1 2 6 5;2 3 7 6;5 6 7 8];
```

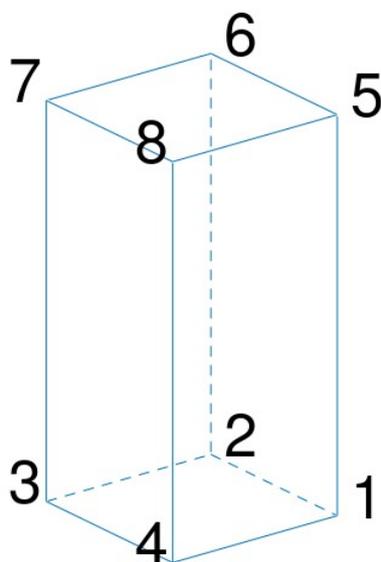


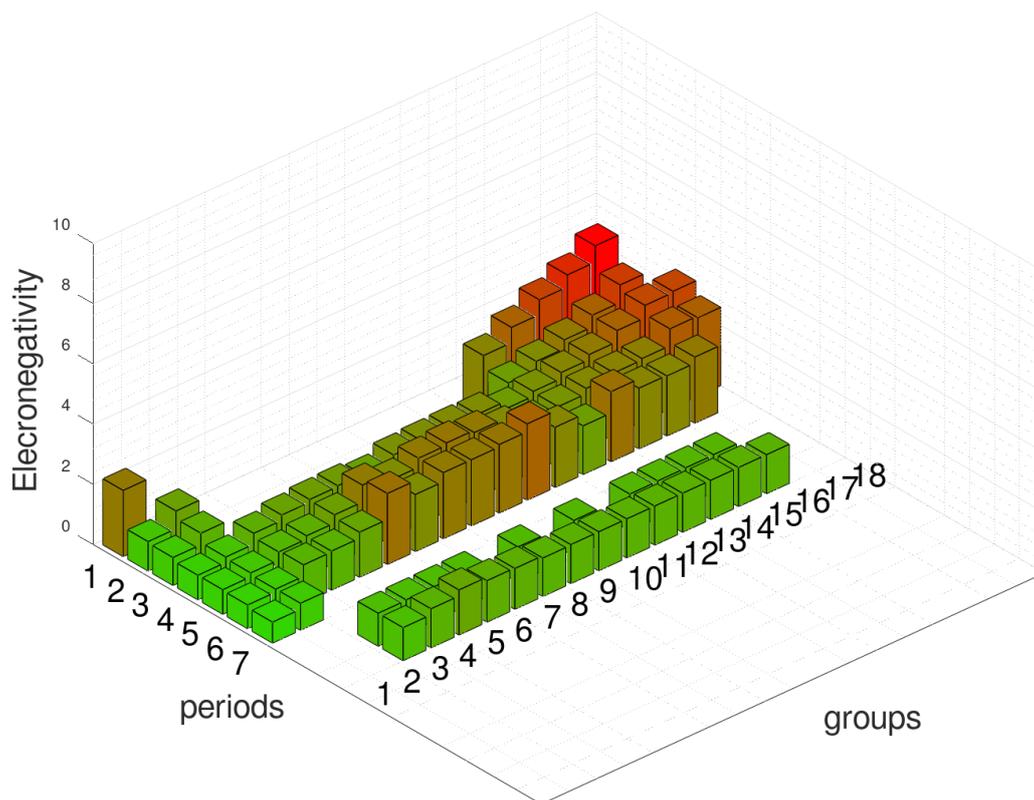
Figure 2.1 Quadratic prims and numbering scheme.

The complete script is listed below, while the auxiliary data (electronegativity.txt) required by the script is to be found in this same web site in text format. It is downloaded by the `'urlwrite'` command into a local file in the octave working directory, to be used immediately by the following program lines. Once the program is run for the first time, the .txt file remains, so as it is unnecessary to reload it. To do this the line beginning with `'urlwrite'` command can be inactivated, transforming it into a remark (adding the octave remark symbol `'%'` in the script)

It is loaded with `'importdata'` function and the `'\n'` option, so as each line is translated a single string. Each single string is then split with `'strsplit'` function and further analysed, in order to extract information about atomic number and electronegativity. Array `'AtNo'` contains the positions of the different prism on to the x,y plane for all the elements, from atomic number 1 ([hydrogen](#)) to atomic number 118 ([oganesson](#)). As not all of the 118 elements have an electronegativity value, the program script only accounts for those listed in the auxiliary data. To the missing elements a blank space is assigned.

The resulting picture is shown in fig 2.2

Electronegativity , Pauling scale



```

Clear all;clc;format short;format compact;
d = 0.18; % clearance

figure(1,'position',[100 100 1000 800]);
axis([0 18 0 18 0 10]);axis on;grid on;grid minor on;xticks(20);yticks(20);

AtNo = [0 18;17 18;0 17;1 17;12 17;13 17;14 17;15 17;16 17;17 17;... % x(i),y(i)
0 16;1 16;12 16;13 16;14 16;15 16;16 16;17 16;...
0 15;1 15;2 15;3 15;4 15;5 15;6 15;7 15;8 15;9 15;10 15;11 15;12 15;13 15;14 15;15 15;16 15;17 15;...
0 14;1 14;2 14;3 14;4 14;5 14;6 14;7 14;8 14;9 14;10 14;11 14;12 14;13 14;14 14;15 14;16 14;17 14;...
0 13;1 13;2 10;3 10;4 10;5 10;6 10;7 10;8 10;9 10;10 10;11 10;12 10;13 10;14 10;15 10;...
2 13;3 13;4 13;5 13;6 13;7 13;8 13;9 13;10 13;11 13;12 13;13 13;14 13;15 13;16 13;17 13;...
0 12;1 12;2 9;3 9;4 9;5 9;6 9;7 9;8 9;9 9;10 9;11 9;12 9;13 9;14 9;15 9;...
2 12;3 12;4 12;5 12;6 12;7 12;8 12;9 12;10 12;11 12;12 12;13 12;14 12;15 12;16 12;17 12];

% The following line is to be used once. When the file id downloaded, inactivate the line by adding % (remark
symbol)
f = urlwrite('www.molecularmodels.eu/electronegativity.txt','electronegativity.txt');

A = importdata("electronegativity.txt","\n");
ln = length(A)
for i=1:ln
    b = strsplit(A{i});
    nAt = str2num(b{1});eNeg = str2num(b{4});h1 = eNeg;
    x1 = AtNo(nAt,1) + d;y1 = AtNo(nAt,2) - d;x2 = x1 + 1 - d;y2 = y1 - 1 + d;
    v2 = [x1 y1 0;x2 y1 0;x2 y2 0;x1 y2 0;x1 y1 h1;x2 y1 h1;x2 y2 h1;x1 y2 h1];
    f2 = [3 4 8 7;1 4 8 5;5 6 7 8];
    patch('Faces',f2,'Vertices',v2,'FaceColor',[ (h1*0.25) (1-h1*0.25) 0]);view(3);
endfor

xlabel("groups",'FontSize',20);ylabel("periods",'FontSize',20);zlabel("Electronegativity",'FontSize',20);
title("Electronegativity , Pauling scale",'FontSize',20);

for i=0.5:17.5
    text(i,7,num2str(i+0.5),'FontSize',20);
endfor
for i=18:-1:12
    text(-1.3,i-1,num2str(19-i),'FontSize',20);
endfor

```

Fig. 2.2 Tridimensional periodic table of electronegativity

2.3 Tridimensional plot of atomic radius

The [atomic radius](#) of a chemical element is a measure of the size of its atoms, usually the mean or typical distance from the center of the nucleus to the boundary of the surrounding shells of electrons. Since the boundary is not a well-defined physical entity, there are various non-equivalent definitions of atomic radius. Four widely used definitions of atomic radius are: Van der Waals radius, ionic radius, metallic radius and covalent radius. Typically, because of the difficulty to isolate atoms in order to measure their radii separately, atomic radius is measured in a chemically bonded state; however theoretical calculations are of course simpler when considering atoms in isolation.

Again, the auxiliary data (atomicRadius.txt) required by the script is to be found in this same web site in text format. It is downloaded by the '[urlwrite](#)' command into a local file in the octave working directory, to be used immediately by the following program lines. Once the program is run for the first time, the .txt file remains, so as it is unnecessary to reload it. To do this the line beginning with 'urlwrite' command can be inactivated, transforming it into a remark (adding the octave remark symbol '%' in the script). The listing of the atomic radii is computed from theoretical models, as published by Enrico Clementi and others in 1967. The values are in picometres (pm). The octave script is very similar to the preceding one, so it isn't listed here but in [appendix](#).

