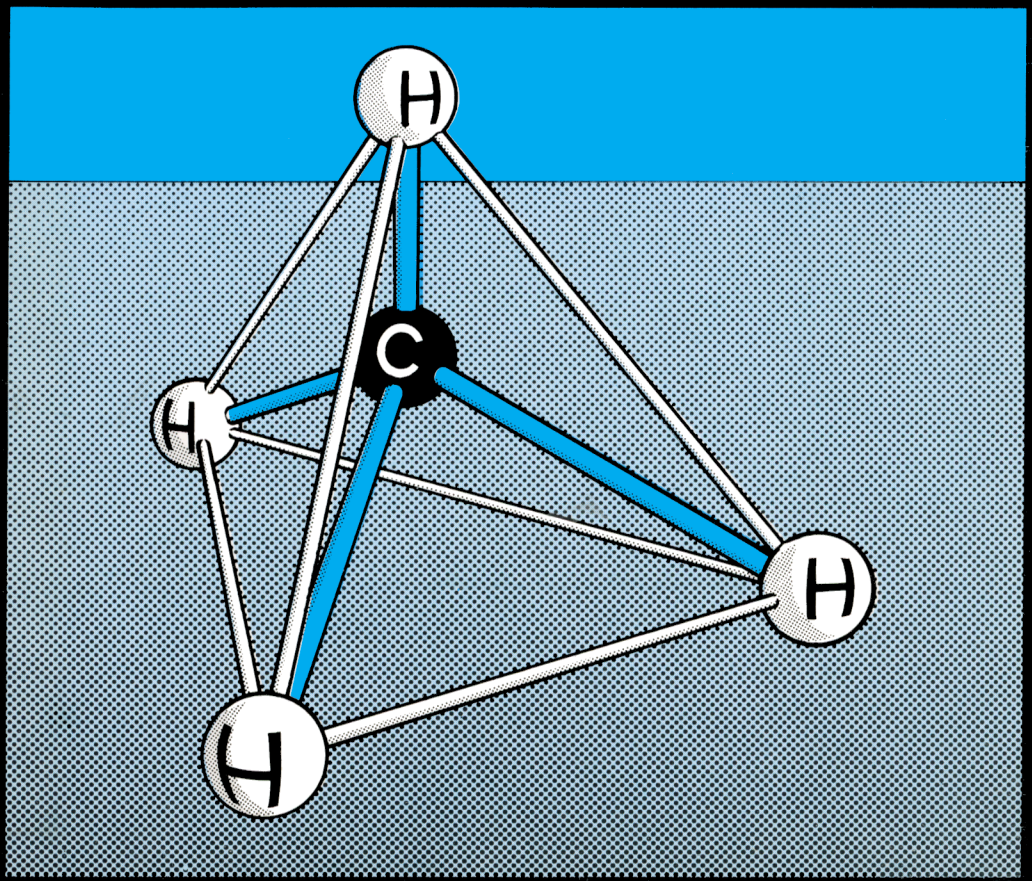
ACORNSOFT EDUCATION

Chemical Structures

for the BBC Microcomputer



ACORNSOFT

Chemical Structures

First published in 1983, by Acornsoft Limited.

FIRST EDITION

Published by:

Acornsoft Limited, 4a Market Hill, Cambridge, CB2 3NJ, England

Contents

Students' Notes are stapled in the centre of this booklet so that they can be pulled out and photocopied.

About the Authors

Charles Duckworth: BONDING

After graduating in Biochemistry from Liverpool University, Charles Duckworth went to Western Ghana to teach physics and chemistry. It was here that he learned an appreciation for simple graphical methods of displaying information to pupils. On return to England he worked as a biochemist at the Royal Alexandra Hospital where he became involved in computing. He is now teaching at Mill Hill School London, where he has the motivation and the facility to develop educational software for use in schools.

Paul Fellows: SHAPE

Paul Fellows obtained his first degree in Chemistry at Cambridge University, and is currently reading for a diploma in Computer Science. Paul worked as a Laboratory Technician in a modern secondary school, and has since taken a strong interest in developing educational software for use in the school curriculum.

Paul is also the Editor for the series of Chemistry programs for schools: Chemical Analysis, Chemical Simulations and Chemical Structures. His other work includes Sphinx Adventure for the BBC Microcomputer and several programs in the above-mentioned chemistry packs.

BONDING:
Teachers' Guide

This program is intended for use with 'O' level pupils. It assumes that compounds are either purely ionic or covalent and will show how they are formed from the constituent atoms. Ionic compounds are shown being formed by donation of electrons from metals to non-metals and covalent ones by electrons being shared between the atoms.

The program starts by displaying the first 18 elements of the periodic table. The metals are shown in red and the non-metals in yellow. A few elements are coloured green, these are the 'semi-metals' i.e. elements like boron and silicon.

Two of the elements shown have to be selected and their symbols typed in, one at a time. The chemical symbols have to be entered correctly e.g. Li for lithium not li or LI. If one is entered wrongly then the computer will not accept it and will ask the user to try again.

Metallic bonding is not dealt with by the program, therefore if two metallic elements are entered an error message is printed and the user is then allowed to type in two others. Similarly, polymers or giant structures cannot be shown. If one of the noble gases is selected then the user is informed that these do not form compounds and again is returned to the input stage.

When two acceptable elements have been chosen the computer decides whether the simplest compound formed by the two is ionic or covalent. It then draws the structure showing the outer shells of electrons. Elements are drawn in different sizes where appropriate, hence showing, for example, that hydrogen atoms are smaller than oxygen atoms etc.

For covalent compounds the bonding is represented by overlapping circles which contain spots representing the electrons. Two different elements will be shown in different colours. This means that the source of the shared electrons can be seen. Double bonds are shown by having two pairs of electrons in the overlap.

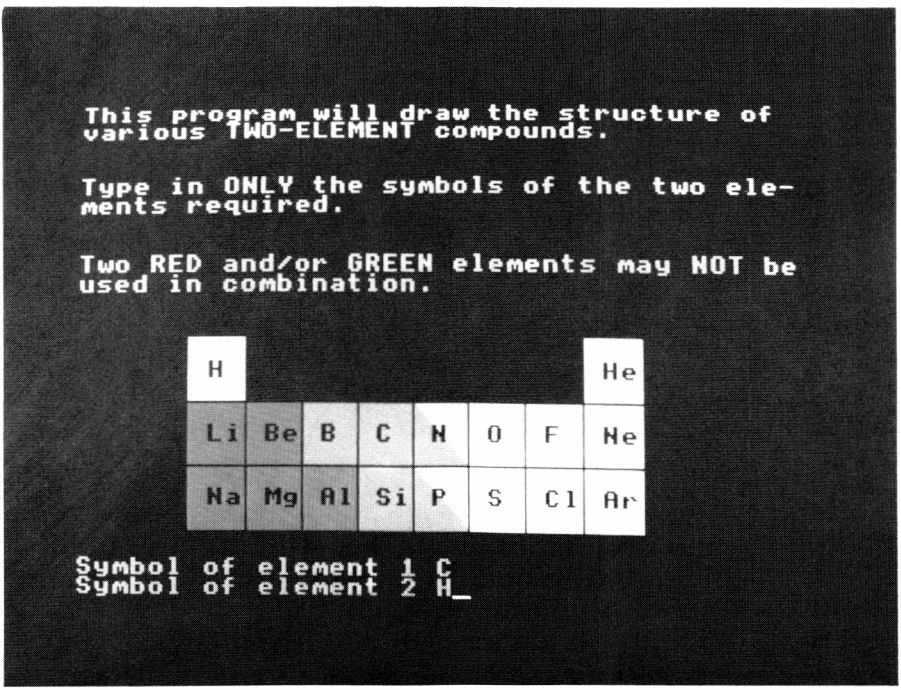
In the case of ionic compounds, the metal and non-metal atoms are drawn separately. Each non-metal atom has its outer electron shell displayed and each metal atom its outer two shells. Ions are formed by

electrons moving across from the metal shells to the non-metal ones. When the outer shell of the metal is empty it disappears. Finally the charges on the ions are added.

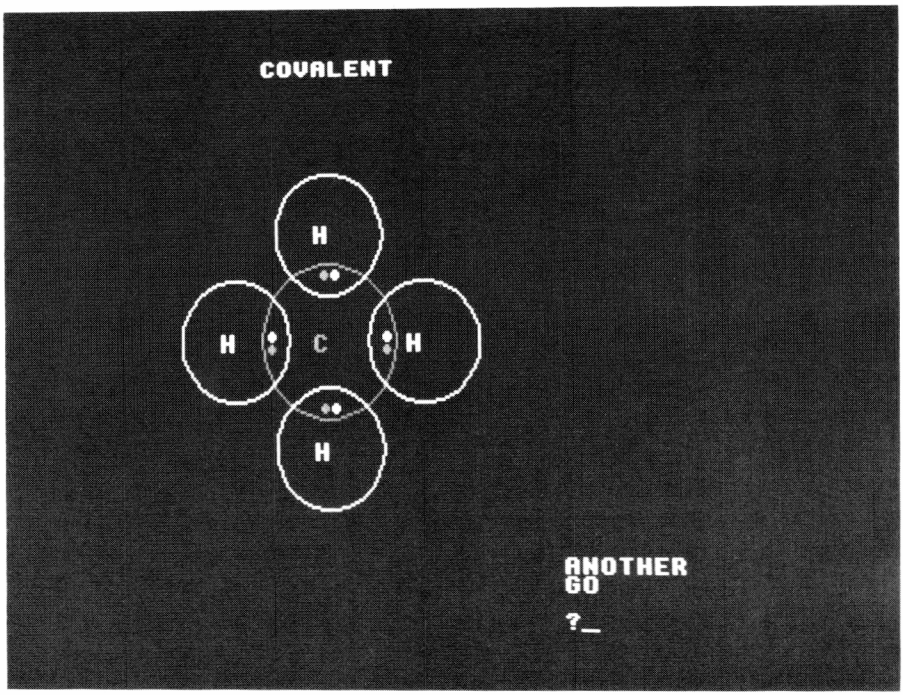
After each compound has been drawn the user is asked whether or not he wants to have another go. To get out of the program 'No' needs to be typed here and then the program will stop.

Sample Run

When the program is run a picture of the periodic table will appear and the computer asks for the symbols of two elements (one at a time).



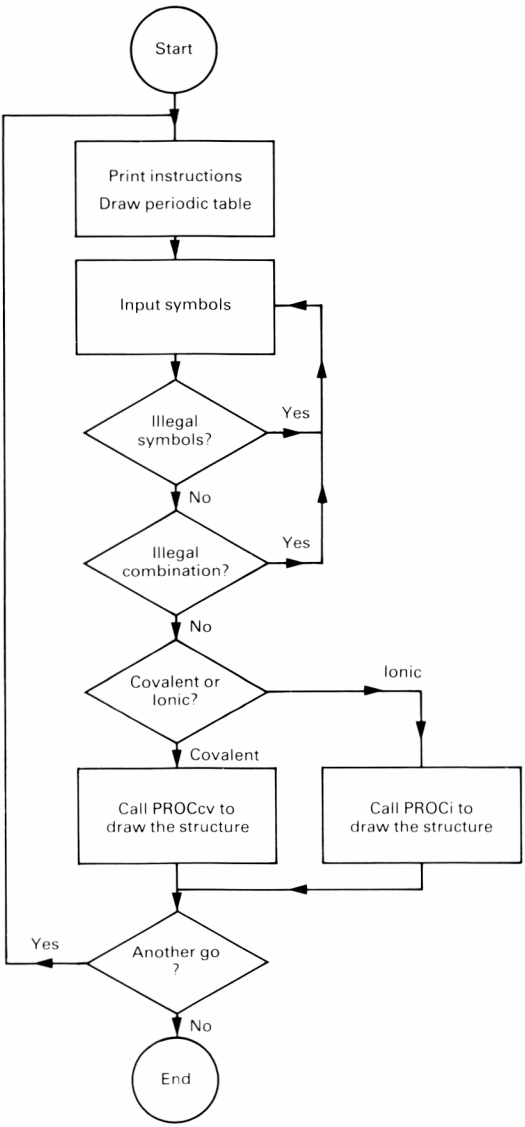
For this example type 'C' for carbon as the first element and then press RETURN. The computer then asks for the second element, 'H' for hydrogen is a good one to try. When you press RETURN, the compound, in this case methane, will be drawn on the screen.



The computer then asks you if you want another go. If you press 'Y' or 'y' then the picture of the periodic table should appear again for you to make another choice. If you don't want another go press 'N' or 'n' and the program will stop. You can start it running again by typing RUN and pressing RETURN. If you press ESCAPE at any time, while the program is running, then the program will start again at the beginning.

BONDING:
Technical Documentation

Flowchart



Variables and Arrays

Variables

J,X,I	Used as control variables in loops.
H	The number of the metal atom being dealt with.
ZY	Indicates the direction of vertical movement.
R,S	The radii of the metal and non-metal respectively.
P,Q	The number of electrons in the outer shell of the metal and non-metal respectively.
G	The number of metal atoms in the compound.
U	Represents the charge on the metal ions.
A$	Holds the symbol of element 1 of a covalent compound.
B$	Holds the symbol of element 2 of a covalent compound.
C	The distance of the electrons from the central atom.
N	Controls the shape to be drawn. (see PROCcr for details.)
O	Controls the colour of circle drawing.
W	The number of electrons in a shell.
V	Set to 1 if a covalent compound is too difficult to draw.

Arrays

E$(2)	Used to hold the symbols of the two elements typed in.
K(2)	The number of electron shells in elements 1 and 2.
M(2)	The number of electrons in the outer shell of elements 1 and 2.
C(3)	The X-coordinates of the metal's electrons in the diagram.
D(3)	The Y-coordinates of the non-metal's electrons in the diagram.
E(3)	The X-coordinates of the non-metal's electrons.
F(3)	The Y-coordinates of the non-metal's electrons.

The Program

60-120 Draw the beginning of the periodic table.

130-150 Input the symbols of the elements.

150-210 Decide whether the compound is ionic or covalent.

Procedures

PROCe ends or re-runs the program. Also it prints a message if the structure is not available, indicated by V being set to 1.

PROCT calls PROC_C to draw the non-metal atoms. Then it puts in the correct number of electrons in the outer shell.

PROCi sets up the parameters of both the metal and the non-metal atoms. F$ is set to the symbol of the metal, G$ is set to the symbol of the non-metal. R is set to the radius of the metal and S to the radius of the non-metal. P is the number of electrons in the outer shell of the metal, Q is the number in the non-metal.

On lines 300-390 PROCr is called to draw the non-metal atoms. Lines 400-600 draw out the metal atom, transfer the electrons and delete the outer shells of the cations by calling PROC_C. Lines 610-690 print the charges on the ions. G is the number of metal ions, U relates to the charge on each ion. C(1. . .X3), D(1. . .Y3) hold the positions of the metal's electrons which are to be transferred. E(1. . .X4), F(1. . .Y4) hold the positions on the non-metal atoms that the electrons are to be transferred to. H is the number of the metal atom being dealt with. Zy indicates the vertical direction of electron movement.

PROCcv deals with covalent compounds. First it decides whether it can be drawn or not by looking it up in the data. The pair of elements are sorted to get them into a standard order. F$, G$, R, S and C are set up, C being the distance from the central atom where the electrons are to be drawn. Then PROC_C is called to draw the atoms. The value of N is set to control the shape of the drawing as follows.

N=0	Linear diatomic species	HCl
N=1	V-shaped	H_2O
N=2	Triangular	BF_3
N=3	Linear triatomic species	CO_2

N=4	Trigonal pyramidal species	NH_3
N=5	Tetrahedral species	CH_4
N=6	A2B3-structure	B_2O_3

PROC_C chooses the colour to draw circles for the atom. For metal atoms O=0 so I=1 and they are drawn in red. If O=8 the circle is in black for deletion of the outer shells of ions. Then it prints the symbols for the elements in the centre of the circle. If N=8 then the outer shell of a metal atom has just been drawn and the electrons will be put in by lines 440-460. If N=7 then the inner shells of a metal atom have just been drawn. W is then the number of electrons in a shell, their positions are given by data in lines 1000,1010.

Lines 1140-1470 select the data statements for the compound. Note that the data for the compounds overlaps in places.

Lines 1480-1630 print the electrons allowing for double and triple bonds, M is a variable determining the distance of the electrons from the central atom.

PROCt draws the transfer of the electrons in ionic compounds.

X1,Y1	The starting position.
X2,Y2	The final position.
ZX	The horizontal increment.
ZY	Indicates the direction of vertical movement.

SHAPE:
Teachers' Guide

This program could be used with either 'O' or 'A' level pupils. It will draw the shape of simple molecules containing one or two different elements. The geometrical shape the molecule is based on is given, as are the actual bond angles in the molecule and any lone pairs it contains. Three views, at different angles, are shown for each structure which is helpful for visualising some of the larger structures.

Initially a periodic table is drawn containing the first 18 elements. Metals are shown in red, non-metals in yellow and 'semi-metals' e.g. boron and silicon, in white. Two elements have to be chosen from these by typing in their symbols. These have to be entered separately with RETURN being pressed after each one. The chemical symbols have to be typed properly e.g. Cl for chlorine not CL or cl.

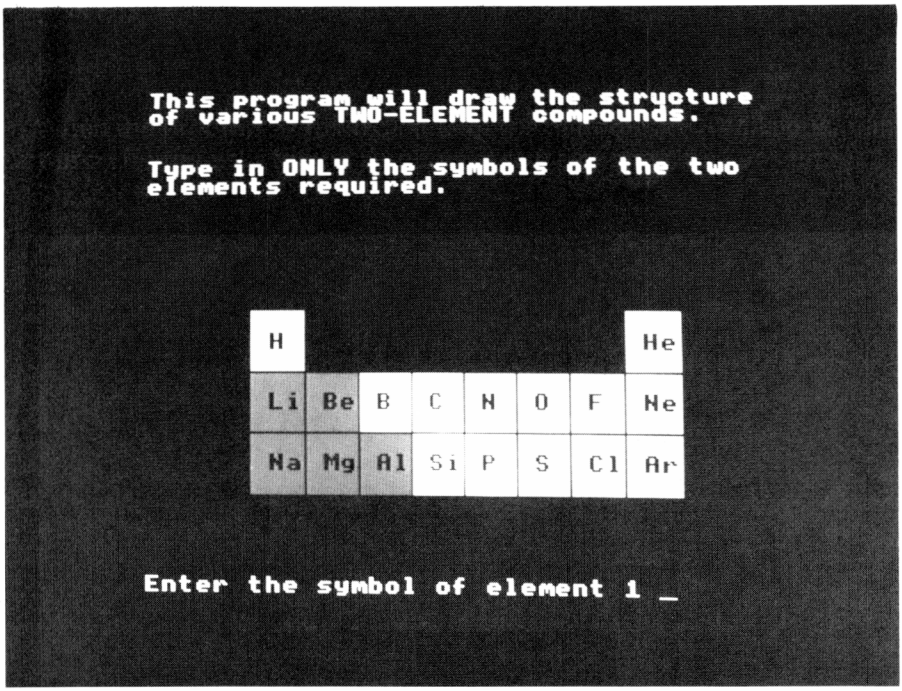
Only molecular structures can be shown and therefore metals, which give ionic lattices cannot be used. Also some giant structures are not allowed e.g. compounds consisting of boron and hydrogen atoms are not dealt with. In some cases a choice will be given when more than one different compound can be formed by the two chosen elements e.g. for P and Cl the user is asked whether he wants PCl_3 or PCl_5 shown.

When two acceptable elements have been entered the computer will draw out the atoms in the molecule as white circles with their symbols marked on them. The geometrical shape on which the molecule is based is drawn using white lines and the bonds between the atoms are drawn in red. Pressing the Space Bar will lead to the bond angles being printed and any lone pairs being indicated on the diagram. Two more orientations will be drawn then the user is returned to the periodic table to start again.

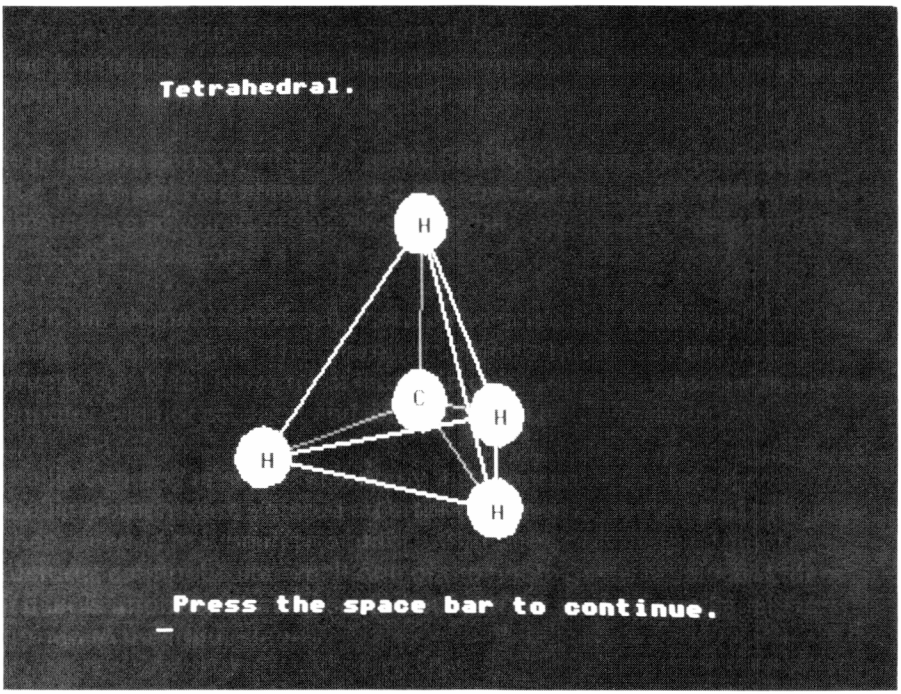
To leave the program ESCAPE can be pressed at any time. This will give the user the choice of pressing 'Q' to quit or any other key to continue.

Sample Run

The periodic table will appear and you can select a pair of elements, a good example is 'C' and 'H'. These are typed in as element 1 and 2 pressing RETURN after each.



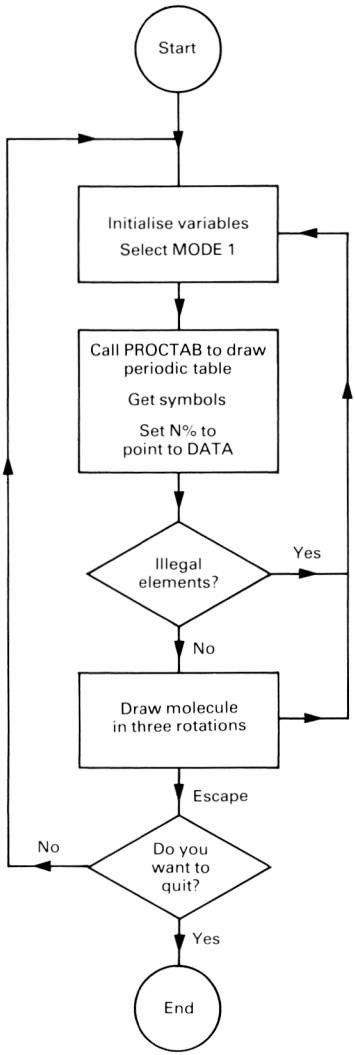
The computer will then display the 3-D structure of the molecule. Pressing the Space Bar will reveal the bond angles and lone pairs and then move you on to the next view.



After the third view, pressing the Space Bar takes you back to the periodic table.

SHAPE:
Technical Documentation

Flowchart



Variables and Arrays

N%,S	Point to the data for a shape.
Y%	Controls the rotation of viewing angle.
E1$,E2$	The symbols for the elements for input.
A1$,A2$	The symbols for the elements inside PROCPLOT.
PX,PY	Give the origin of shape drawing.
C	Gives the colour option for PROCPLOT.
ANG	The initial viewing angle.
SC	The scale factor for drawing.
RX,RY,RZ	The X,Y and Z rotations for the shape.
SX,SY,SZ	The sines of the rotations.
CX,CY,CZ	The cosines of the rotations.
OX,OY,OZ	The old coordinates.
A$	The draw-symbol/no-symbol flag and the end-of-data marker.
PLO	Selects MOVE or DRAW options in the PLOT statements.
TX,TY,TZ	The screen position of the point. TZ is not used!
C1	Selects the GCOL mode. OR-ing is used to do hidden line removal.
R%	The radii of the circles.
T	The control variable for circle drawing.
E$	Used to print messages and to draw the periodic table.
I	A control variable used to draw the periodic table.
X,Y	Used as coordinates for drawing the table.

The Program

The data is encoded in lines 41 to 222. The format is a string controlling the printing of chemical symbols, three numbers indicating the coordinates to go to, the colour of the line and then the plot option (4=MOVE 5=DRAW).

Lines 240 to 330 form the main loop which can only be exited by pressing ESCAPE.

261: PROCTAB is called to draw the periodic table and get the symbols of the two elements. N% is set to point to the DATA statement for the structure. If N%=0 the pair of elements was not found in the list. If n%=–1 then one of the elements was a noble gas.

300-310: three views of the structure are presented by calling PROCPLOT. The rotation is controlled by Y%*10.

330: loop round for another structure.

Procedures

PROCPLOT draws the structure specified by its first argument S. PX and PY control the position of the central atom. A1$ and A2$ are the symbols for the two elements. Y% controls the rotation of the drawing. ANG is the initial viewing angle.

SC,RX,RY,RZ are read in from the data pointed to by S. RY is incremented by the rotation Y%. Then the angles are converted to radians and their sines and cosines are calculated. (SX,SY,SZ,CX,CY,CZ)

The old positions of the shape are initialised to zero. (OX,OY,OZ)

The cursor is set to the position of the central atom and the loop to draw the structure is entered. Graphics information is read in as A$,X,Y,Z,COL and PLO. A$ controls the printing of symbols and is used to indicate the end of data. The coordinates are scaled by multipliction by SC. The translation to screen coordinates is then performed to yield TX,TY,TZ. TZ is not used!

The graphics colour and GCOL mode are selected, C1=1 indicates that lines are OR-ed in to the picture to achieve some hidden line removal.

COL determines the colour to be used. The DRAW or MOVE is then performed according to the value of PLO in the PLOT statement. The circles and chemical symbols are then added if PLO and A$ indicate they should be.The old coordinates are then updated.

Control loops around drawing the peripheral atoms until A$='X' indicates the end of data. Then the central atom is drawn in.

After the Space Bar has been pressed the lone pairs are marked in and the bond angles are printed.

PROCCIRCLE uses triangle filling to draw a solid circle of radius R% at PX+TX,PY+TY.

PROCW waits for the Space Bar.

PROCLP draws the lone pairs and prints the bond angle data.

PROCTAB draws the periodic table. Then it inputs the symbols of the elements, rejecting illegal ones, and sets N% to point to the data for the shape by calling FNSHAPE.

FNCL deals with the choice between C I F and ClF_3.

FNPF deals with the choice between PF_3 and PF_5.

FNN selects NO_2.

FNC deals with the choice between CO_2 and CO.

FNELEM checks its argument, Z$, to see if it is a valid chemical symbol from the list of those which are included.

FNSHAPE returns the pointer to the data for the pair of elements chosen. It also puts the elements into a standard order. ANG is set to the initial viewing angle for the shape.

Line 4000 provides the ESCAPE trap allowing restart and quit options.

Chemical Structures

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