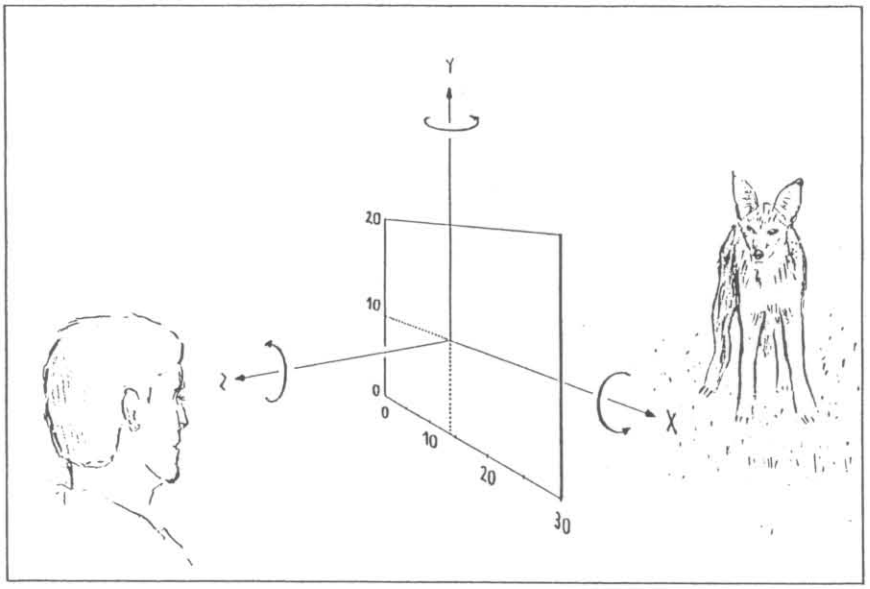
SCHAKAL 99

A computer program for the graphic representation
of molecular and crystallographic models

Tutorial manual and figures



Figures

Note: If viewed with „Acrobat Reader“ , use *double-page* display for this part.

If not stated otherwise, the figures within this manual (except fig. 1) have been generated on an HP LaserJet III. If not stated otherwise, a resolution of 150 dpi (which gives good results on Xeroxing) was used.

Fig. 1: Internal Cartesian Coordinate System and Physical Drawing Area

SCHAKAL's internal atom coordinates refer to the internal Cartesian coordinate system (CCS, –—> 673). The physical drawing area (PDA) is that part of the screen or printer paper onto which something can be drawn.

Dimensions of the PDA are 30 x 20 cm, here. The current origin of the CCS is positioned at X = 14 cm / Y = 9 cm. This has been done

a) automatically by the program (if the model scale factor is not fixed –—> 513)
or
b) by a 'Set Origin 14 9' , a 'Set Origin .47 .45' , or a plain 'Set Origin' command (–—> 57), if the scale factor is fixed presently.

Arrows indicate sense of rotations invoked by 'Rot..' commands (–—> 32), if the rotation angle is given as a positive number.

Fig. 2: Default orientation of the unit cell

Unit cell corners/edges are added automatically to the program's atom/bond lists when a data set is loaded. With respect to drawing they are mostly in a "switched-off" state per default. Switch them on by 'Gen Unit..' (–—> 48).

This drawing demonstrates the usual default orientation of a triclinic unit cell relative to the internal Cartesian coordinates system (CCS, –—> 673). The names of the 8 corners (automatically assigned by the program) are given.

On a colour device, per default, the a edge will be in grey, the b edge will be in red, and the c edge will be in green. All other edges will be blue.

Note: If a "surface model" (see fig. 20) has been generated, the default orientation will be modified by the program after data processing such, that the (hkl) plane in question comes to lie parallel to the drawing plane.

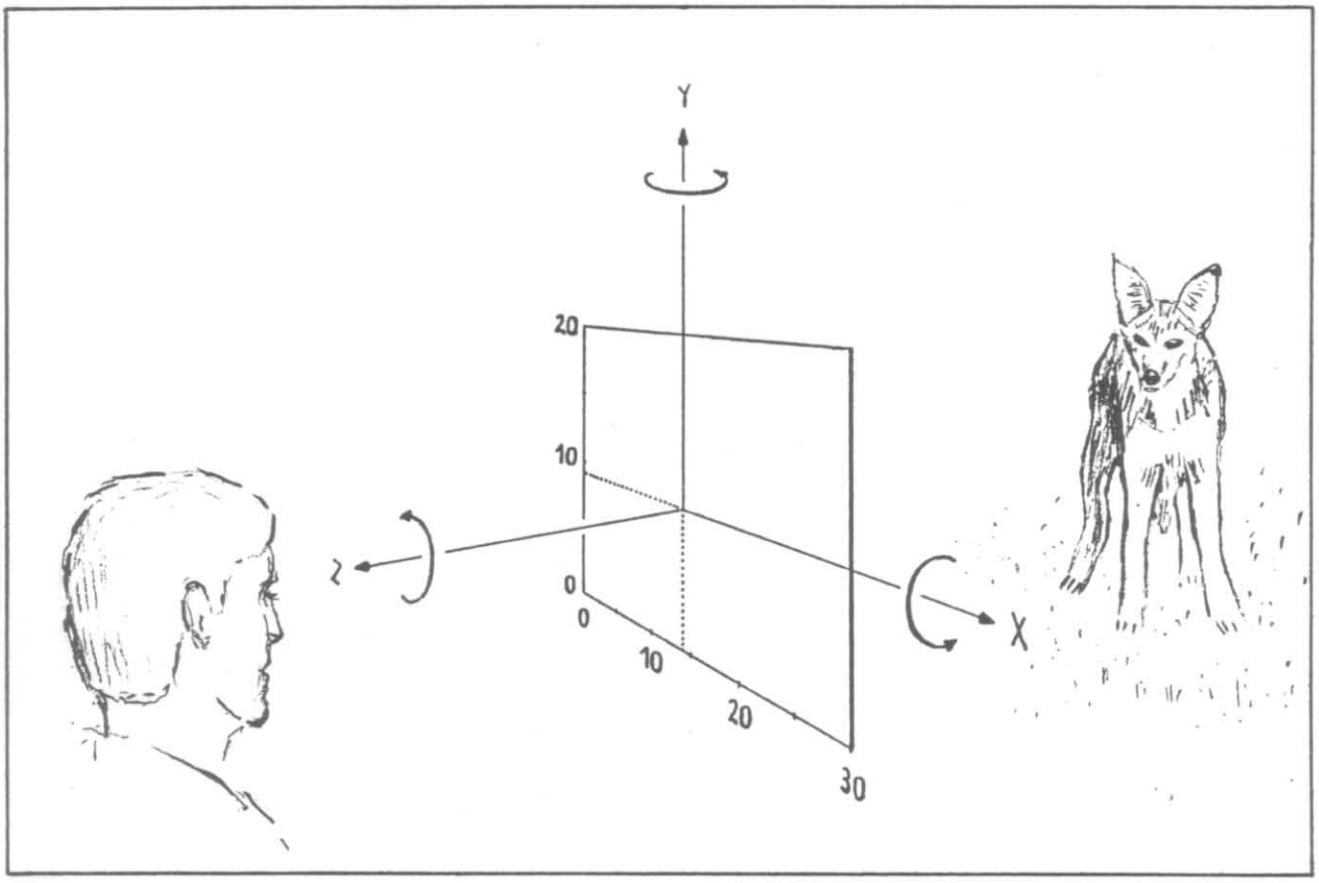


Fig. 1: Internal Cartesian Coordinates System and Physical Drawing Area

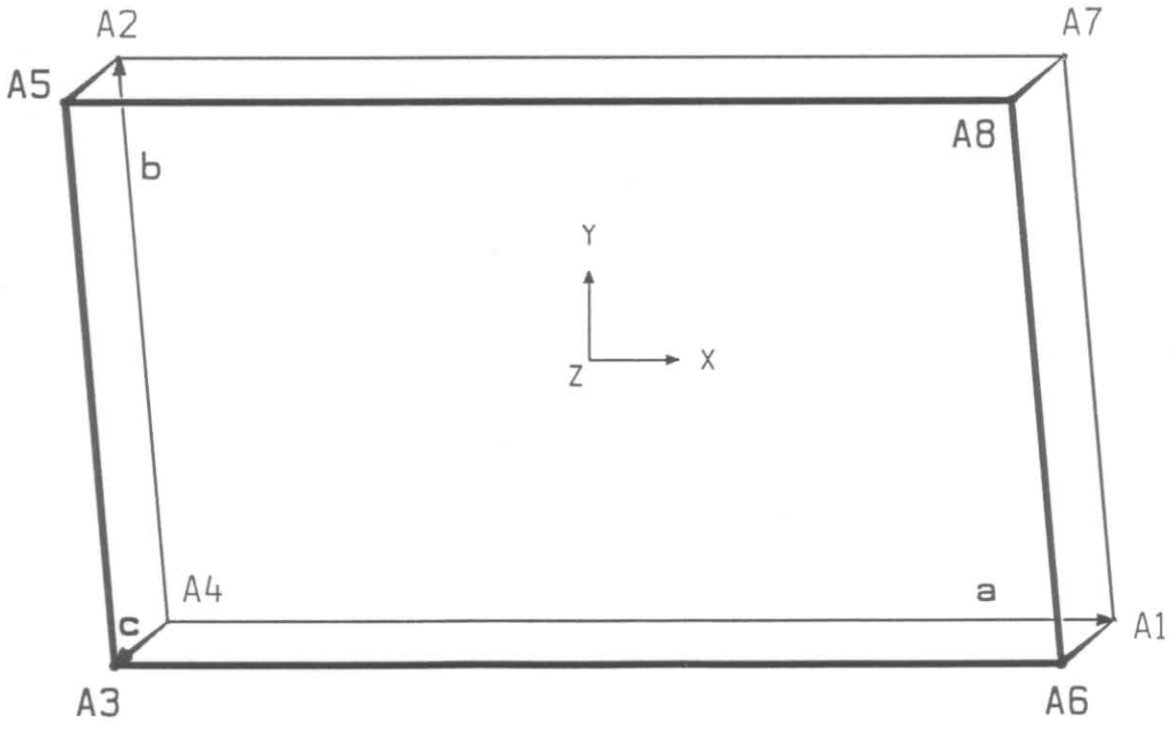


Fig. 2: Default orientation of the unit cell

Fig. 3: Illustration of some terms used in the manuals

The terms illustrated in fig.3 are related to the following commands:

Dashed lines
('Set Dash..', –––> 545)

increased line width
'Brd..', –––> 55)
reduced griddensity
('Set Griddens..', –––> 54)

hatching lines (parallels)

('Gen Hatch..', –––> 444)

north pole

('Set Pole..', –––> 541)

meridians
('Gen Merid..', –––> 445)

foreign shadow
self-made shadow
'Set Shadowl..', –––> 583, 44)

grids
('Gen Grids..', –––> 446)

highlight
('Chge Darkf..', –––> 646,
'Modf Highl..', –––> 527)

fragmentated bond
('Chge Fragm..', –––> 657)

regular dithering

('Set Mode 3n',–––> 453)

broken-off bond

('Trnsf Expnd..', –––> 712)

marginal gap
('Mgn Gaps..', –––> 515)

random dithering
('Set Mode 3n', –––> 453)

group designator
('Wrt All..', –––> 222)

plain colour fill

('Gen Shad -1', –––> 443)

outside labelling

('Set Writopt..', –––> 461)

alternative bond display mode

('Chge Bond..', –––> 658)

inside labelling

('Set Writopt..', –––> 461)

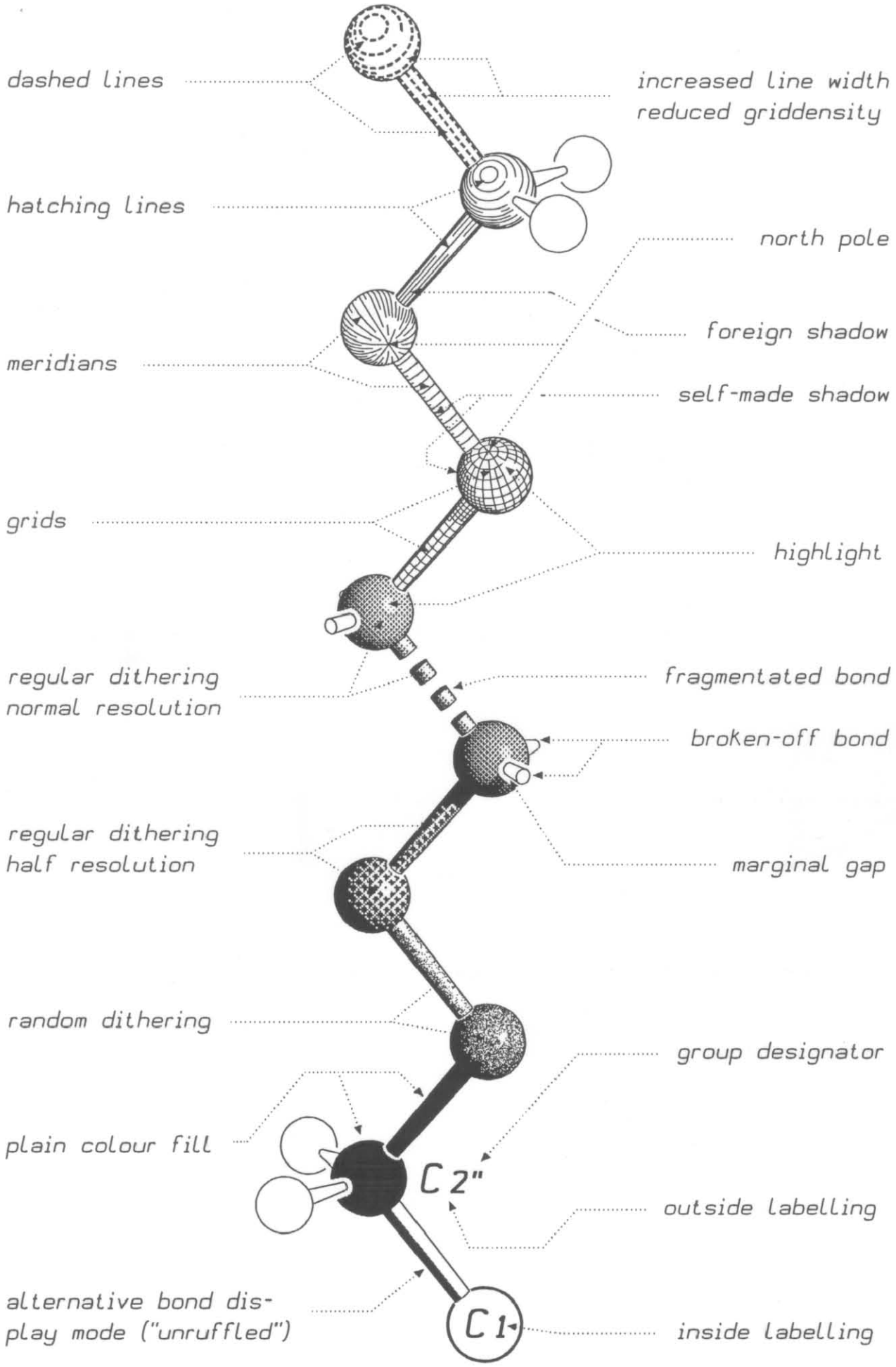


Fig. 3: Illustration of some terms used in the manuals

Fig. 4: Some examples for hatching by parallels, meridians, and grids

This drawing tries to illustrate, how the appearance of hatching patterns invoked by 'Gen Hatch p', 'Gen Merid p', and 'Gen Grids p' (––> 44) is influenced by ...

a) the parameter p
b) 'Set Pole ..' settings ("north pole" position, –––> 541)
c) 'Set Light ..' settings (light source position, –––> 528)

Via 'Set Griddens 4' (–––> 543), a griddensity of 4 lines per cm has been set for this drawing. To draw the sphere in the lower right corner, this griddensity has been reduced by 'Set Griddens *.5' (–––> 544)

The set of commands given under each sphere would not be sufficient to generate the drawing above it: To achieve this, you would have to draw the sphere's outline via 'G O : X' first, then use the specified commands, and finally give another 'X' to invoke drawing of the hatching pattern.

The white spots shown by most of the spheres ("highlights") could have been avoided if a 'Modf Highl 0 0' (–––> 527) would have been given before.

A number of predefined hatching patterns is accessible by the 'Xqt Pattern ..' command (see fig.s 9 and 10).

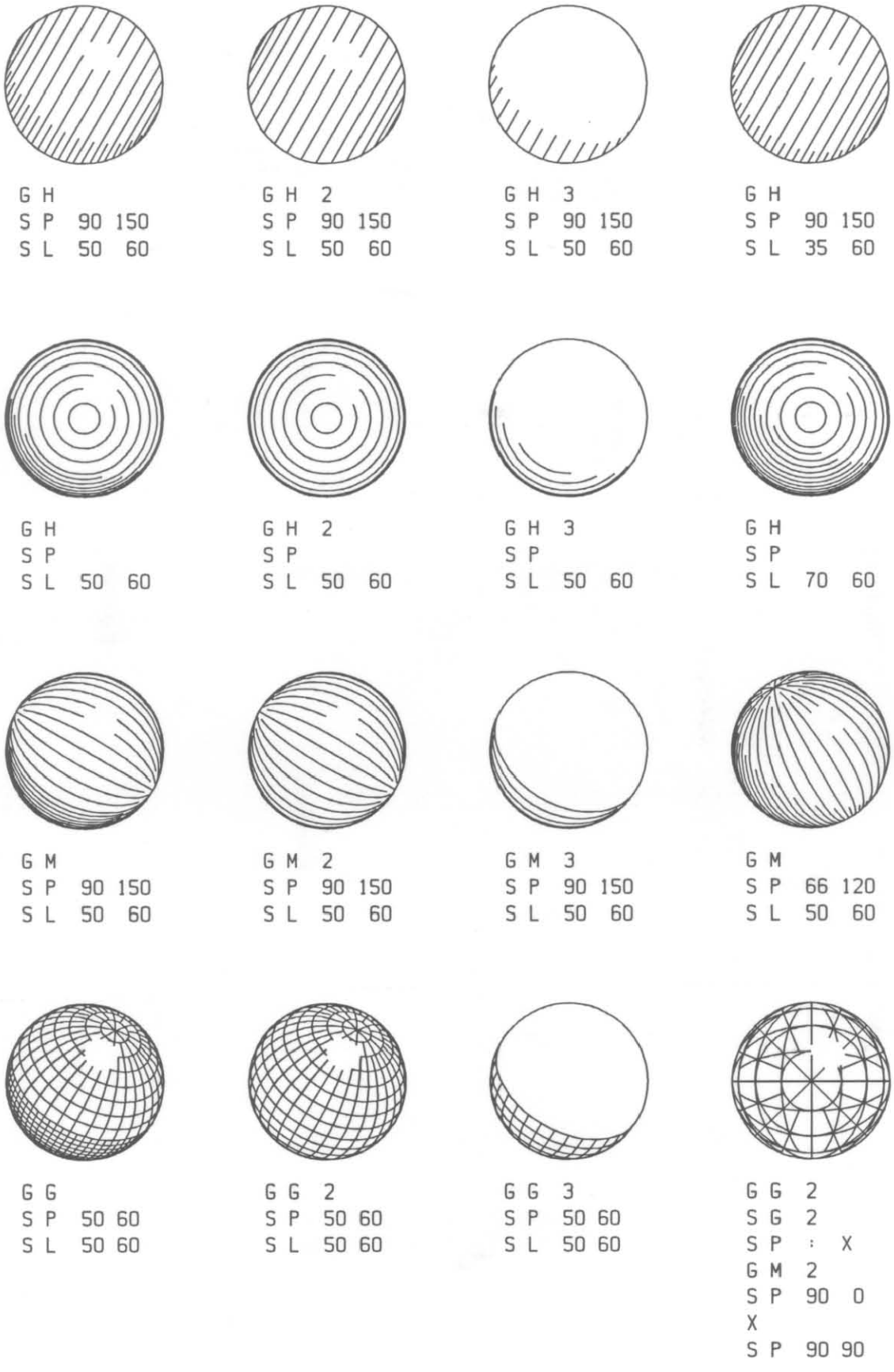


Fig. 4: Some examples for hatching by parallels, meridians, and grids

Fig. 5: Darkening functions

This drawing illustrates the 30 basic darkening functions (to be selected with 'Chge Darkf n ir', –––> 646) and the corresponding numbers n ("darkening function number", DFN).The drawing has been generated using shading mode 33 ('Set Mode 33', –––> 453).

The function with n = 11 (reserved for edges and 3D lines) is not shown.

Instead of the n = 130 function (which hardly differs from that one with n = 70), the special n = 12 function is included.

Set i = 1 or 2 to weaken or eliminate the highlight (this adds 20 or 40 to the DFN)

Set r = 1 or 2 to make the surface rougher (this adds 240 or 480 to the DFN). This will not affect shading by dots (–––> 451).

Per default, the following DFNs are assigned to the following selected types of atoms:

Metals	generally DFN = 1 (with some exceptions). DFN 1 should be used in connection with low-saturated colours (–––> 538.2) on a multi-colour device (screen).
C	DFN 26 (= 6 + 1 * 20; i.e., 6 with weakened highlight)
H	DFN 122
O, N	DFN 5
bond sticks	DFN 4

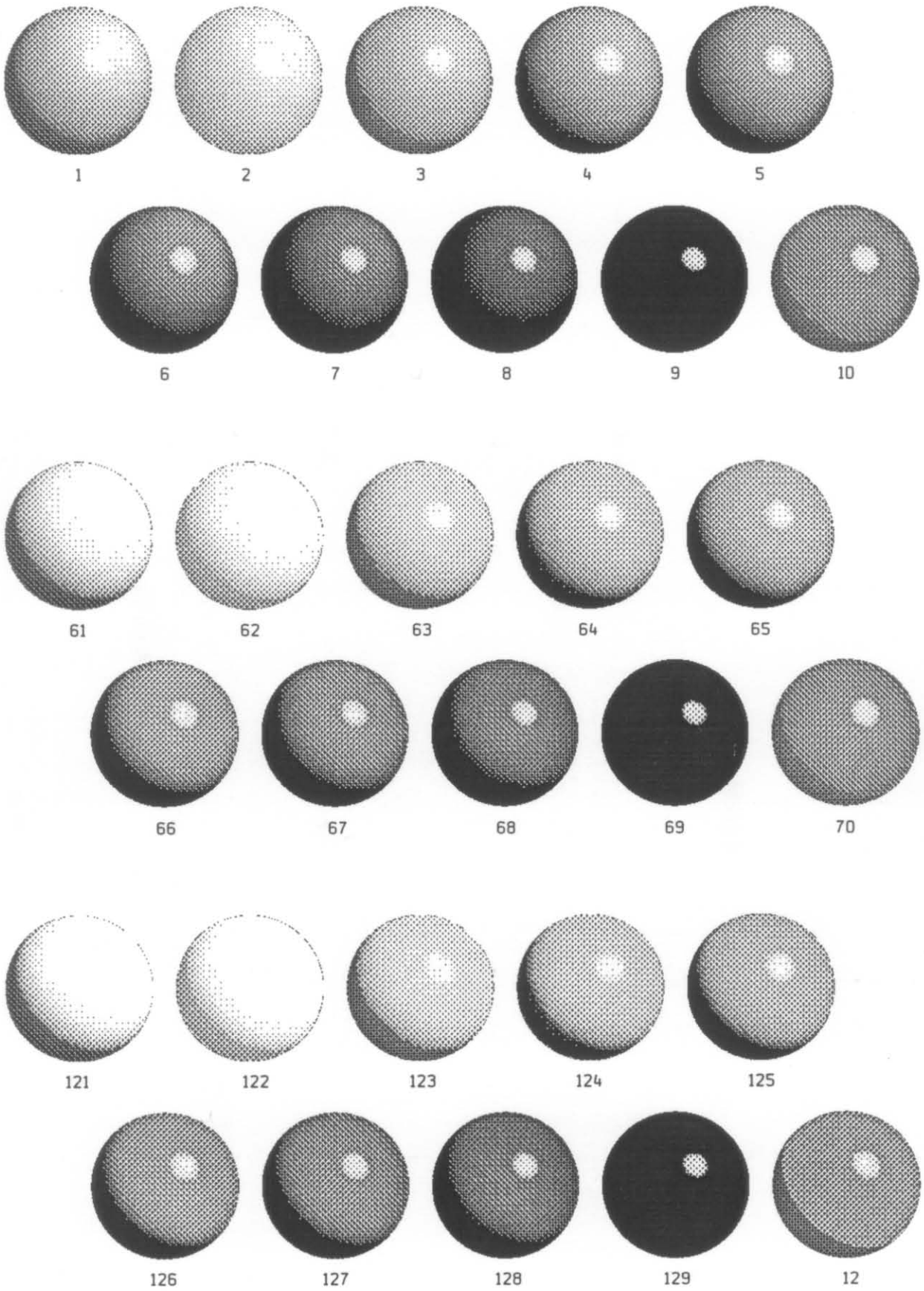


Fig. 5: Darkening functions

Fig. 6: Some shading modes

This drawing illustrates some of the shading modes which may be controlled via 'Set Mode mn' or 'Set Mode m n' (–—> 45). The 'Set Mode 1n' modes (dots/colour steps) which affect drawings on multi-colour devices only, are not illustrated, here. The 'Set Mode 2n' modes (bond shading) which affect the geometrical way in which bonds are shaded, are also not illustrated, here.

The 'Set Mode 3n' modes affect the way in which darkness variations are visualized by dots or colour steps ("dithering"). Modes 30 and 31 are called "random dithering", modes 32 - 34 are called "regular dithering (normal resolution)", and modes 35 - 37 are called "regular dithering (half resolution)". Mode 32 is not very appropriate for use on a laser printer (but see below). The corresponding sphere would look better, though, if a decreased darkness would have been selected before (e.g., by 'Modf Darkn .7').

If a multi-colour device is switched on, the meanings of the 3n modes (n > 0) differ partially from the meanings illustrated here, if shading by colour steps is switched on (which is the default for a multi-colour device).

The 'Set Mode 4n' modes control calculation of darkness. Mode 40 tries to calculate "realistic" darkness variations; modes 41 and 42 calculate purely depth-dependent darkness (the latter dependent on the 'Set Zlim..' setting (–—> 578)).

The 'Set Mode 5n' modes control shading of the peripheral region of an object, i.e, n is a measure for the width of outlines which are added to the darkening function.

The three spheres in the last row have not been drawn by means of a laser printer but by means of an HP7475A plotter (device no. 3), using shading mode 32. On a pen plotter, mode 32 is the only one which should be used for regular dithering. A DFN of 5 (see fig. 5) was assigned to the atom, here (instead of 1, above).

For the first sphere, default (= "theoretical") settings of resolution were used. The pen had already been used several times, i.e., its tip was broadened slightly. Therefore, single dots are not or hardly resolved.

For the other two spheres, the default value of 13 plotter coordinate units per pen width was increased to 15 or 17 by the command written underneath. Single dots are better resolved, in these cases. The corresponding modifications could also have been achieved by the command 'Gen Device ! 303 .033 n' (n = 15 or 17). Given in the initializing Command file *sch97.ini* , this command would make the modification permanent.

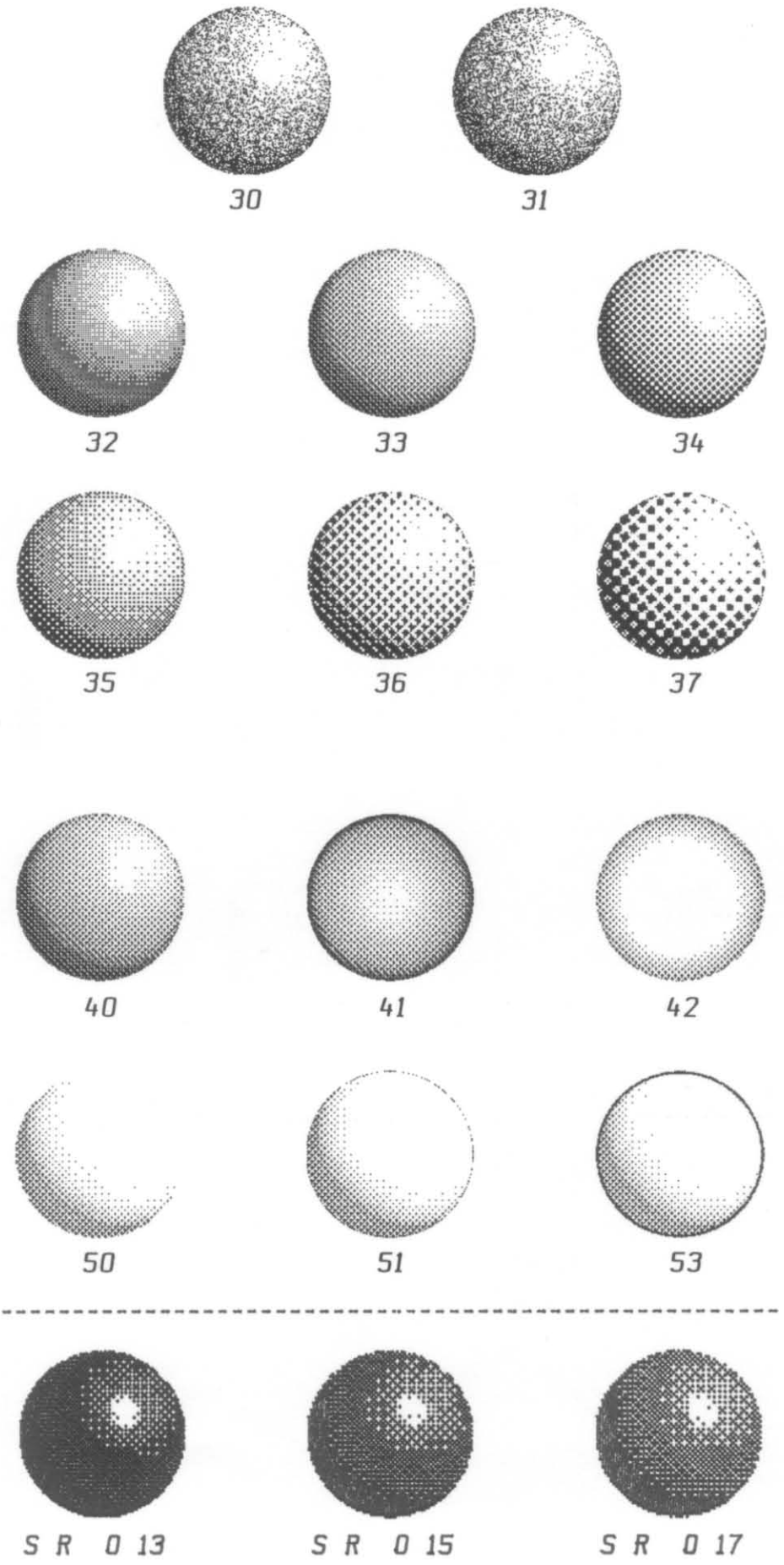


Fig. 6: Some shading modes

Fig. 7: Lines, arrows, and polygons

This drawing illustrates most of SCHAKAL's (poor) extra graphic facilities, where "extra" means: "besides the facilities to draw structure models".

The commands which have been used to generate the different parts of the drawing are given on the left side. Some commands appear in square brackets either because they reset default conditions, or because they appear already in a previous line.

The following table gives the commands in un-abbreviated form as well as the manual index and the group to wich the commands belong in the graphical user interface (GUI):

Command	Manual	GUI
Broaden Lines	(–> 556)	{ MGN }
Set Dashing	(–> 545)	{ SET }
Xqt Line	(–> 251)	{ XQT }
Xqt Arrow	(–> 254)	{ XQT }
Set Mode	(–> 45)	{ G/S }
Modify Pellucidity	(–> 523)	{ MGN }
Xqt Region	(–> 26)	{ XQT }

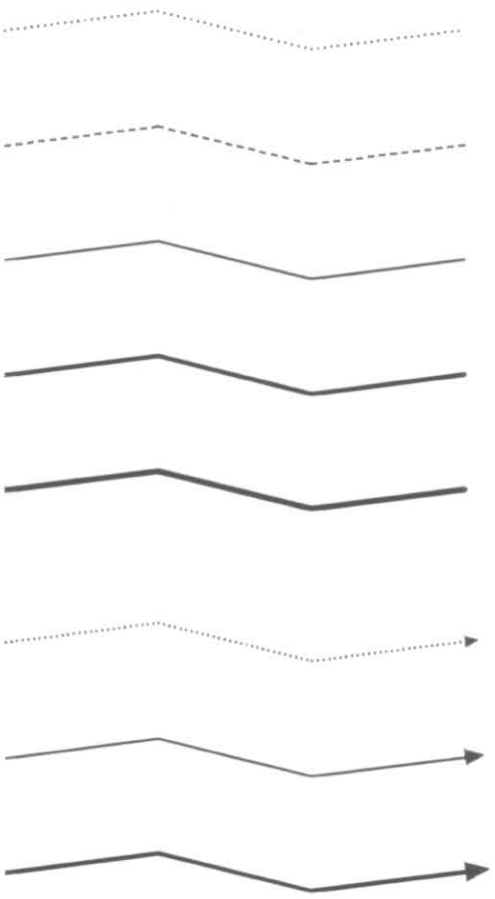
Note: In some cases, arrow tips are a d d e d to a line, such that they prolongate the line. For more info, see –> 254.

Note: When trying to generate a slightly shaded polygon for a high-resolution printer, it may happen, that no shading is to be seen on the monitoring screen becaue of a disadvantageous interference of dot drawing with the pixel pattern of the screen.

Note: Lines, arrows and regions may be defined by coordinates, by mouse clicks, or by atom positions.

```
B L 1 : S D 6 1 : X L
B L 1 : S D 10 5 : X L
B L 1 :  [ S D : ]  X L
B L 3 : X L
B L 5 : X L

B L 1 6 : S D 5 1 : X A
B L 1 10 :  [ S D : ]  X A
B L 3 10 : X A
```



```
B L 1 : S M 34 : M P 14 : X R
[ S M 34 : ]  M P 12 : X R
[ S M 34 : ]  M P  8 : X R
[ S M 34 : ]  M P  4 : X R
[ M P : ]  X R
```

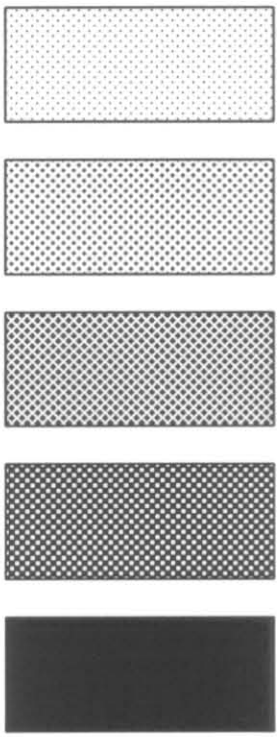


Fig. 7: Lines, arrows, and polygons

Fig. 8: Graphic text

The text in the upper part has been produced by executing an older version of the distributed Writing file *ex.txt* via the command 'Use Writingfile' (––> 16):

```
Use Writingfile
ex
```

The first text line was positioned by means of the mouse. Then, writing of the residual text was invoked by pressing <ESC>.

Note: Graphical text may be positioned by coordinates, by mouse clicks, or relative to atom positions.

Text in the lower part has been generated via 'Wrt Text..' (––> 241). It demonstrates the effect of the commands 'Mgn Text..' (––> 564), 'Brd Text..' (––> 557), and 'Set Inscr..' (–––> 466). These commands belong to the { EDT } group in the GUI.

Note, that the 'S I mn' commands (which could have also been written as 'S I m n') refer to the case where you would generate the corresponding text on the screen (which displays a "landscape" format, usually). To generate the drawing on the laser printer (in "portrait" format), the value of 1 had to be added to m , actually (cf. section 4.4.).

0123456789 -+*/=.,;:-'" !? %#$ <>()[]{}
ABCDEFGHIJKLMNOPQRSTUVWXYZ ÄÖÜ
abcdefghijklmnopqrstuvwxyz äöüß
αβχδεφγηιψκλμνωπθρσστξυζ ΔΓΛΠΣΩΞ
ÅÄåäáàâãëéèěêîíìñšÿýÓóò ¥Ø≠≡Ççı

$Fe_4(CO)_{12}[\eta^6\text{-}NC\text{-}C_6H_5]$ $(\bar{2}\ 0\ \bar{3})$

MT 1 : BT 1 : SI

MT2 MT21 MT12

BT4 **BT41** **BT14**

SI3 *SI6* *SI9*

SI10 OZIS SI30

MT 1.25 : BT 64 : SI 4

Fig. 8: Graphic text

Fig. 9: Predefined 3D patterns

This drawing illustrates the 30 predefined "3D patterns" which are contained in the distributed command file *patt.scf* .

The number underneath a sphere is the corresponding pattern number (i.e., the partition label of the corresponding labelled partition of file *patt.scf*).

Patterns are activated by means of the 'Xqt Pattern' command (–—> 217). For example,

```
Xqt Pattern  21  N          (alternative syntax: 'Xqt Pattern 0 21 N')
```

applies pattern 21 to all Nitrogen atoms.
Bonds can also be shaded or hatched with this command. An illustration is not given for this case, however.

Predefined patterns generally don't show "foreign" shadows (see fig. 3). This is, because the commands in file *patt.scf* have been designed accordingly.

Patterns with hatching lines may be modified by the following commands:

```
Set Griddens  *p          (controls density of hatching lines, –—> 544)
Brdn All  p [q [n]]       (controls the line width used for outlines and
                           hatching lines, –—> 554;  fig.15)
Modf Highl  p q           (q controls the size of highlights, –—> 527)
```

Patterns with dot shading use shading modes 33 or 34 (–—> 453). They may be modified by the following commands (–—> 52):

```
Modf Darkn  ..            (modifies the overall darkness)
Modf Shadows  s           (modifies the darkness of the shadow area)
Modf Highl  p q           (modifies intensity and size of highlights)
```

See also last section of text discussing fig. 10 .

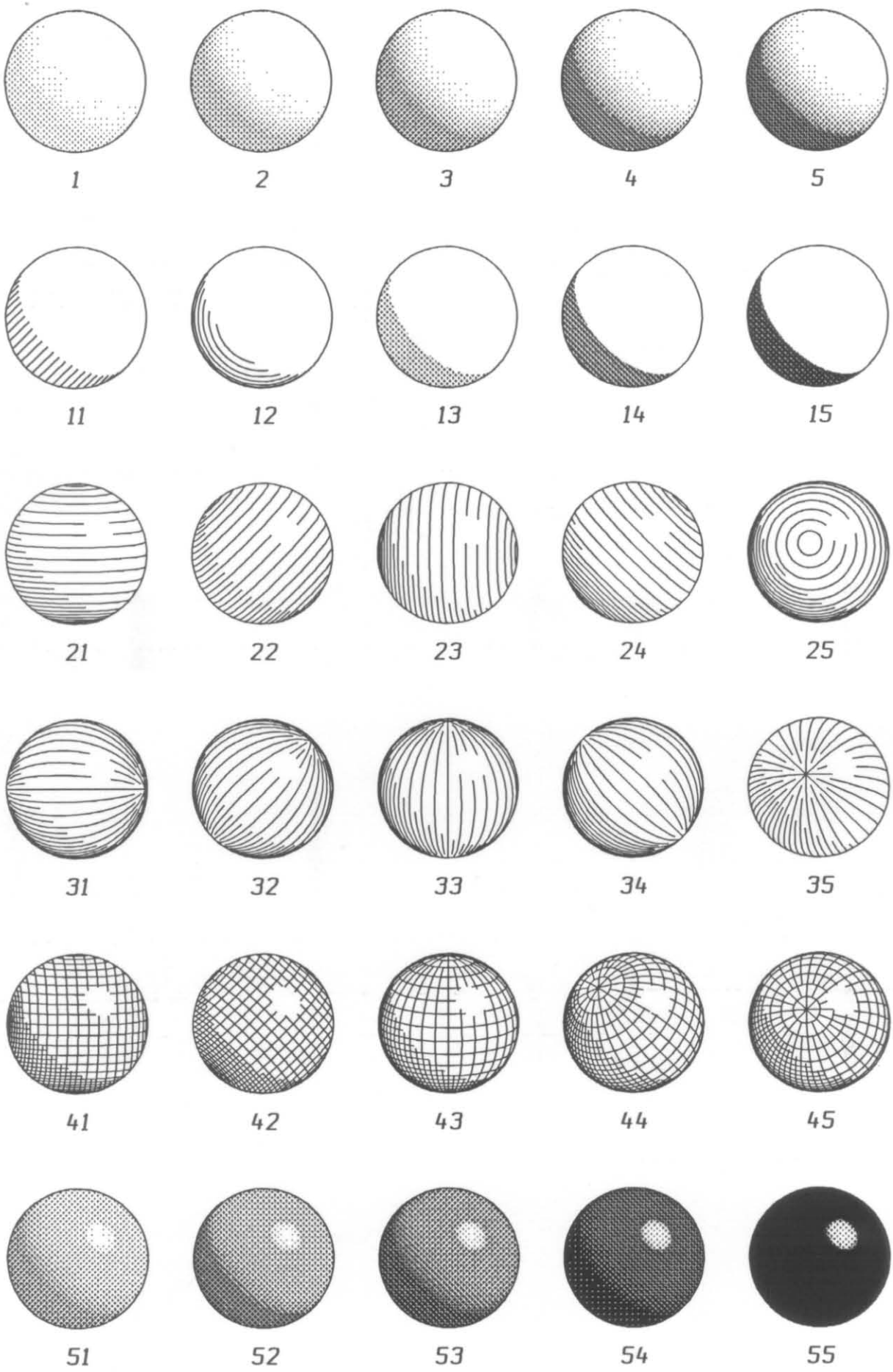


Fig. 9: Predefined 3D patterns

Fig. 10: Predefined 2D patterns

This drawing illustrates the 30 "2D patterns" contained in the distributed command file *patt.scf* . Generally, 2D pattern no. 1nm resembles closely the corresponding 3D pattern no. nm (see fig. 9). However, 2D patterns show neither a highlight nor a "self-made" shadow. A 2D pattern can be selected either with 'Xqt Pattern 1mn' or with 'Xqt Pattern 1 mn' .

Patterns with hatching lines may be modified by the following commands:

`Set Griddens *p`	(controls the density of hatching lines, –—> 544)
`Brdn All p [q [n]]`	(controls the line width used for outlines and hatching lines (–—> 554; fig.15)

Patterns with dot shading use shading modes 33 or 34 (–—> 453). They may be modified by the following command (–—> 521):

`Modf Darkn ..`	(modifies the overall darkness)

Note: Patterns with dot shading are not appropriate for a pen plotter (because of the large relative size of a single dot). Here, you should use pattern 2mn instead of pattern 1mn , as patterns 2mn base on shading mode 32 instead of 33 or 34 (see text describing fig. 6).

Note: If the atom circles are rather small (for example, because the structure contains a large number of atoms), patterns may look rather different as compared to fig. 10 (or 9), simply, because only a small number of lines or dots fit into the circle (or stick) area. On a laser printer, you may use a higher resolution (300 dpi instead of 150 dpi) in this case.

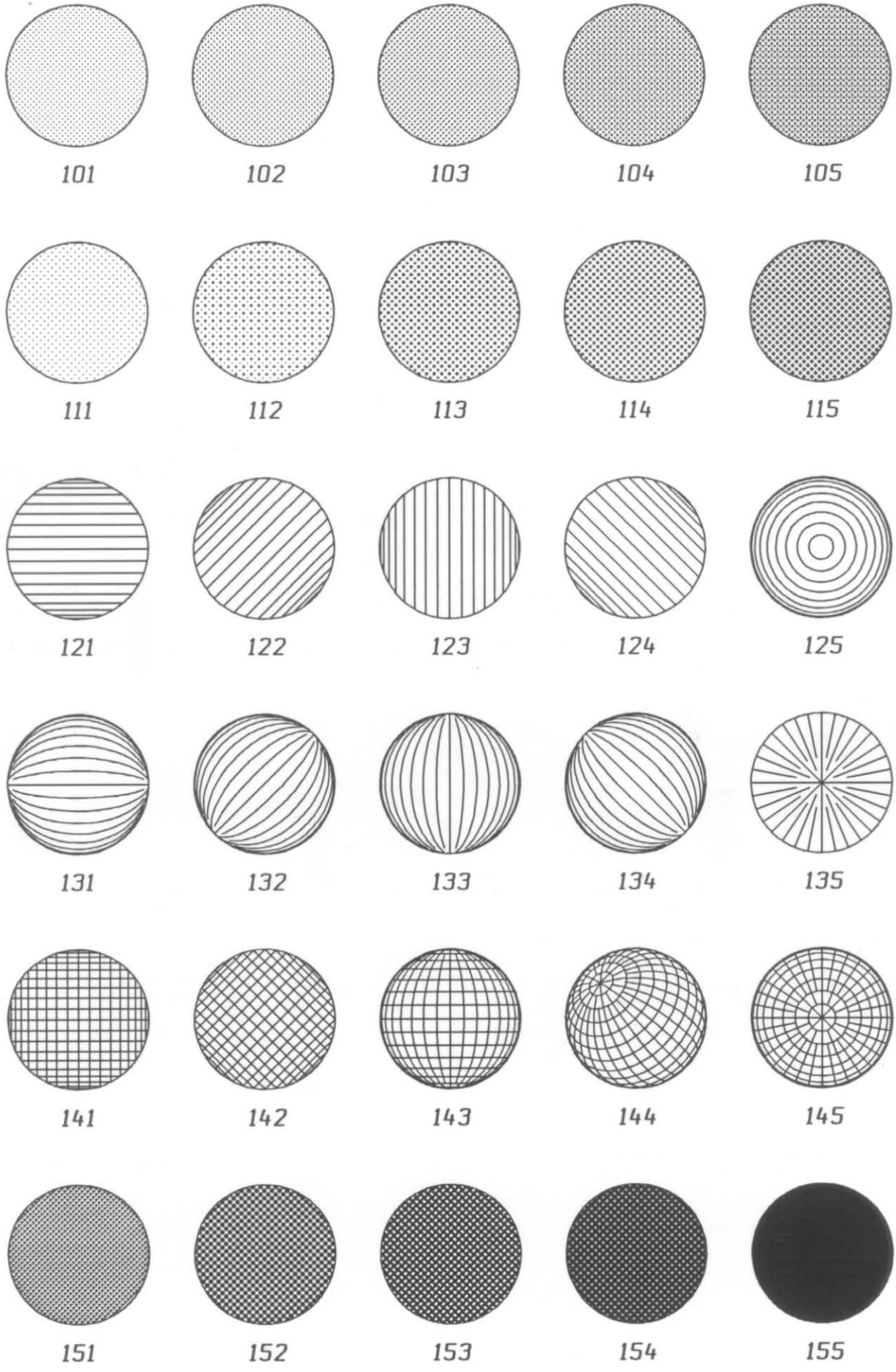


Fig. 10: Predefined 2D patterns

Fig. 11: The Penicillin molecule

This drawing of the ball-and-stick model of the penicillin molecule may serve as a demonstration for the use of 3D and 2D patterns (see fig.s 9, 10). After adjusting the orientation of the model, the drawing has been generated by the following commands:

```
Chge Thickn  *.5 H=nn          (multiply thickness of all bonds to or
                                from H atoms by 0.5, –-> 652)
Chge Thickn  *1.5 nn=nn        (multiply all stick thicknesses by 1.5)
Defn $  N1 C2 C3 S C6 C7 C8    (define group $ by atoms of bicyclic
                                ring system –-> 664)
Defn $  $  C11-C16 (H          (add phenyl C atoms to group $ )
Genr Outl : Xqt                (draw outlines)

Xqt Pattn 11 H S               (use pattern no. 11 for H and S atoms)
Xqt Pattn 41 C                 (etc.)
Xqt Pattn 21 O
Xqt Pattn 33 N
Xqt Pattn 52 nn=nn (h=nn $=$   (use pattern no. 52 for all bonds ex-
                                cept those ones between the $ atoms
                                and those ones to or from H atoms)
Xqt Pattn 155  $=$             (etc.)
Xqt Pattn  21  h=nn
```

To label the atoms, the molecule has been divided into four regions (separated by the dotted lines). For each region, an individual set of 'Set Writeopt..' / 'Set Inscription..' commands (–-> 46) has been used. The 4 different sets of commands are shown within the four different regions:

The second parameter of the 'Set Writeopt' command controls the arrangement of element symbols and numbers (horizontal/vertical) and the use of parentheses/ brackets.

'Set Inscr' controls the slantedness of the characters. As was explained for fig. 8, a value of 1 was added to the 'S I' parameter m , actually, to generate the drawing in "portrait" format.

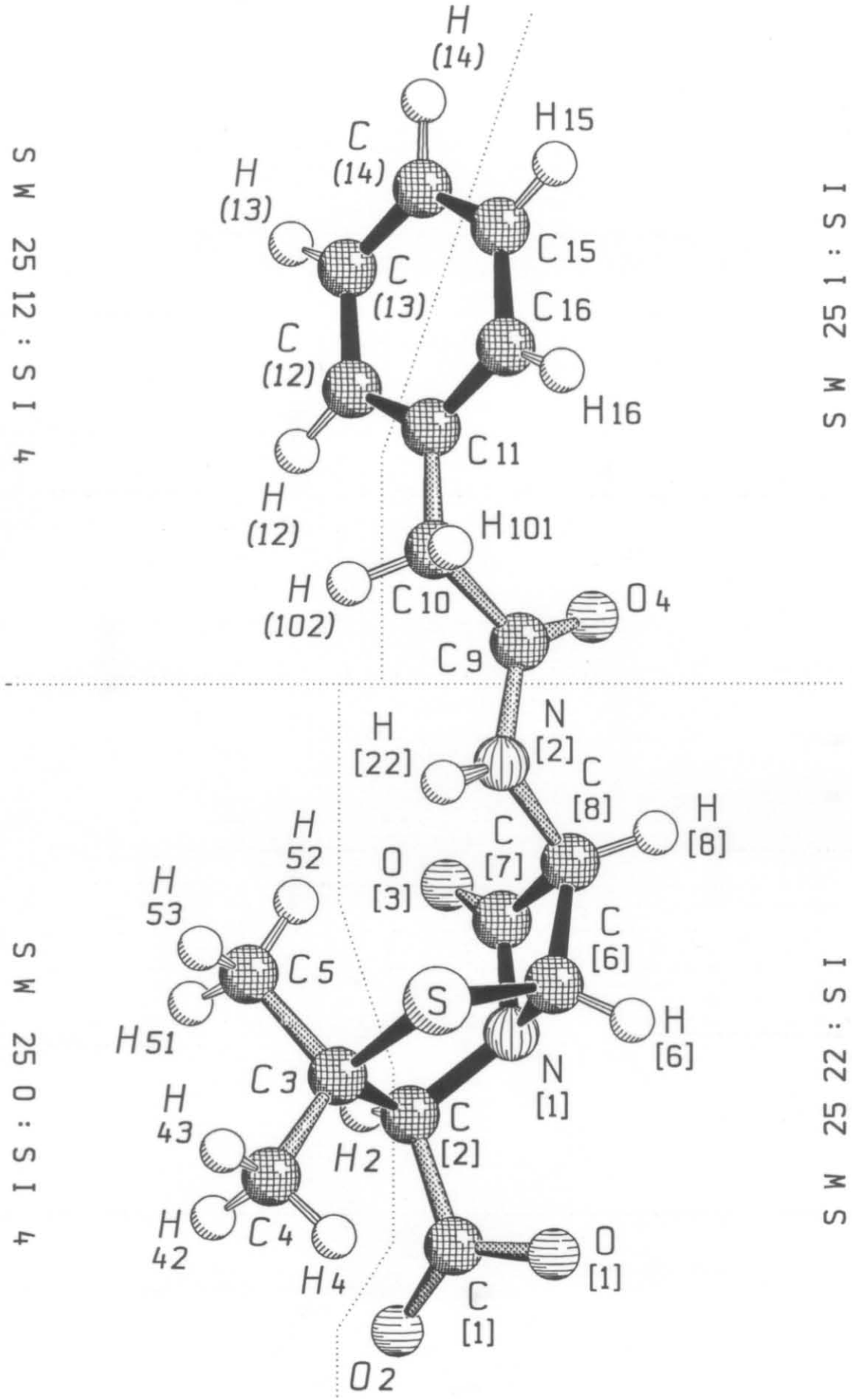


Fig. 11: The Penicillin molecule

Fig. 12: The ($C_{20}H_{24}$) Zr Cl_2 complex (I)

The drawing of this organometallic catalyst may serve as an example for several measures to make the drawing of a molecule more comprehensible (furthermore, it demonstrates labelling with names including "group designators" (––> 222)):

a) Reducing the radius of H atoms and the thickness of the bond sticks connecting them with other atoms (e.g., by 'Chge Size *.7 H H=nn') generally leads to more transparency and clarity.

b) It is recommended to generally enhance the bonds of ring systems either by colour or by thickness or by other graphic means (see also fig. 11) . Here, the 10 "aromatic" bonds within the two 5-membered rings have been made thicker via the following procedure:

```
Def $     C1 C2 C3 C7a          (group $ is defined by all 10 ring atoms, –––> 664)
Chg Thickn  *1.5  $=$           (multiply stick thicknesses by 1.5, –––> 652)
```

c) The large number of bonds generated per default between metal atoms and the atoms of organic π-bonded rings should be replaced by single "pseudo-bonds".This can be done with the DCF *pilig.scf* , wich is available on the GUI from { other^{L} } / { pi-lig } . This DCF asks you first to click a "central atom" and then to click all the π-bonded atoms of one π-ligand bonded to it.

A labelling procedure was started by 'Wrt All..' (–––> 222) and then stopped via <ESC>. This let the program know that any 'W #..' command contained in the Command file *p.scf* (below) was to be replaced by a 'W A..' command ('W A..' labels atoms with names plus group indicators).

Originally, all atoms belonged (per default) to the numerical group 1. However, atoms in the upper half of the drawing have been assigned to the numerical group 2 (to have an apostrophe added to the name as a group designator) by the following commands:

```
Filt Y   0.2 100          (Set a filter for internal Y coordinates, –––> 683)
Def Group   2 nn          (assign all atoms in the upper half to group no. 2, –––> 668)
Filt                      (switch filter off)
```

The drawing of fig. 12a was then generated with the help of the following commands:

```
Set View  30              (perspective distortion, –––> 476)
Set Inscr ! 1 4           (rotate model and establish a vertical writing direction to
                           have drawing in portrait format)
Use Commandf              (execute Command file p.scf incl. ´Wrt All..' labelling for
pattn  s92+w               non-Hydrogen atoms)
Trl Inscr  C1 C7a (gg1    (move two unsatisfyingly positioned labels, –––> 229)
```

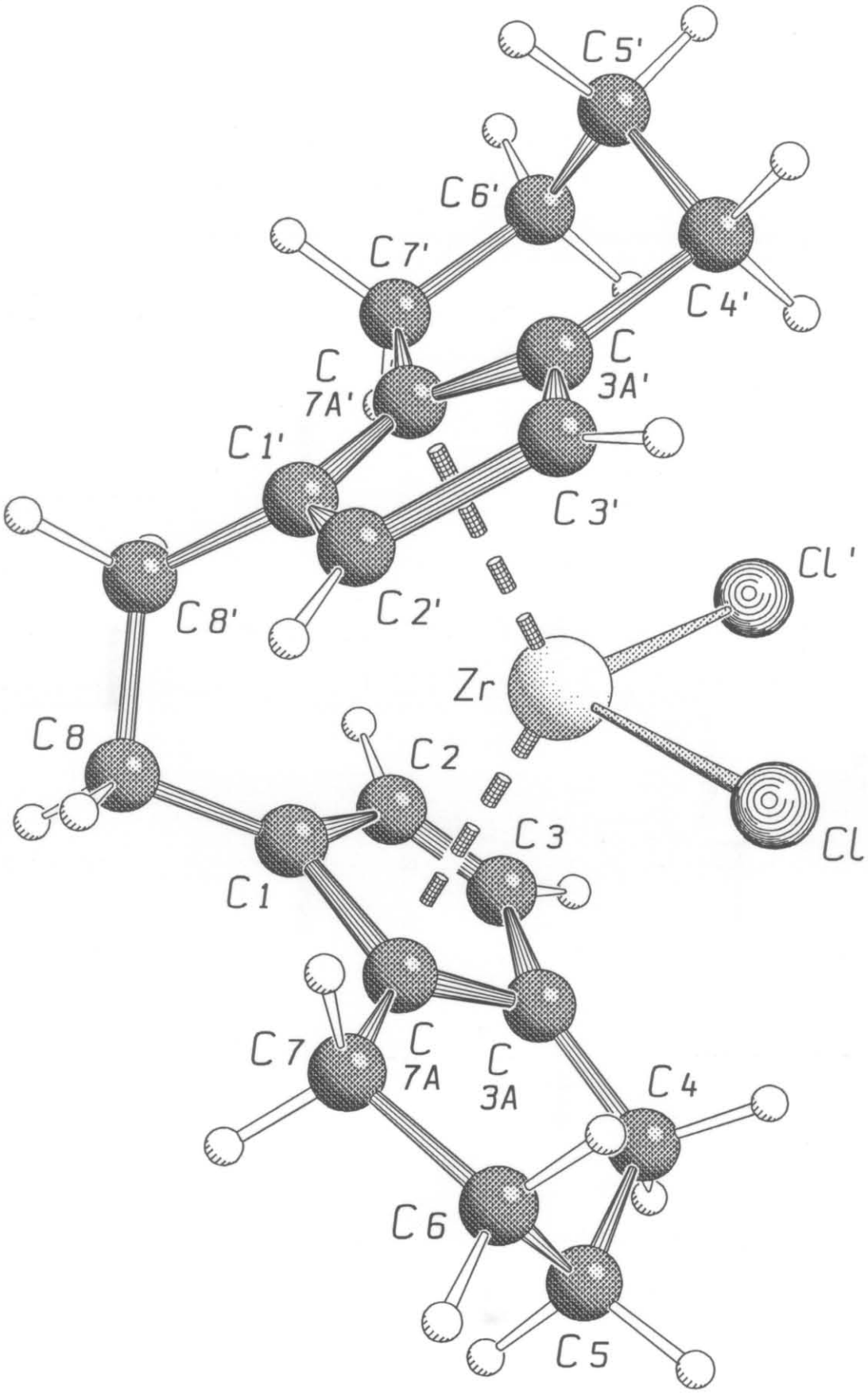


Fig. 12: The $(C_{20}H_{24})$ Zr Cl_2 complex (I)

Fig. 13: The $(C_{20}H_{24})$ Zr Cl_2 complex (II)

Fig. 13 was generated right after fig. 12 (same program run). First, the darkening function numbers assigned to several atoms/bonds (–—> 646) were modified by the following commands (for meaning of $, see fig.12, section b):

```
Chge Darkn  3 Cl,  5 C,  9 $
Chge Darkn  7 nn=nn (H=nn Zr=nn
Chge Darkn  1 $=$
```

Then the drawing was generated by the following commands

`Set Tapering  .5`	(less exaggerated tapering of bond sticks, –—> 581)
`Use Commandfile shade`	(execute command file *s.scf* without labelling)
`Mgnf Inscr  -1.5`	(increased size of characters, –—> 561)
`Brdn Inscr  3`	(increased boldness, –—> 551)
`Wrte Symbols Zr Cl`	(label selected atoms with chemical element symbols, –—> 223)

Note: Command file *s.scf* (as well as some other distributed Command files) increases the contrast between different darkening functions when used for the laser printer.

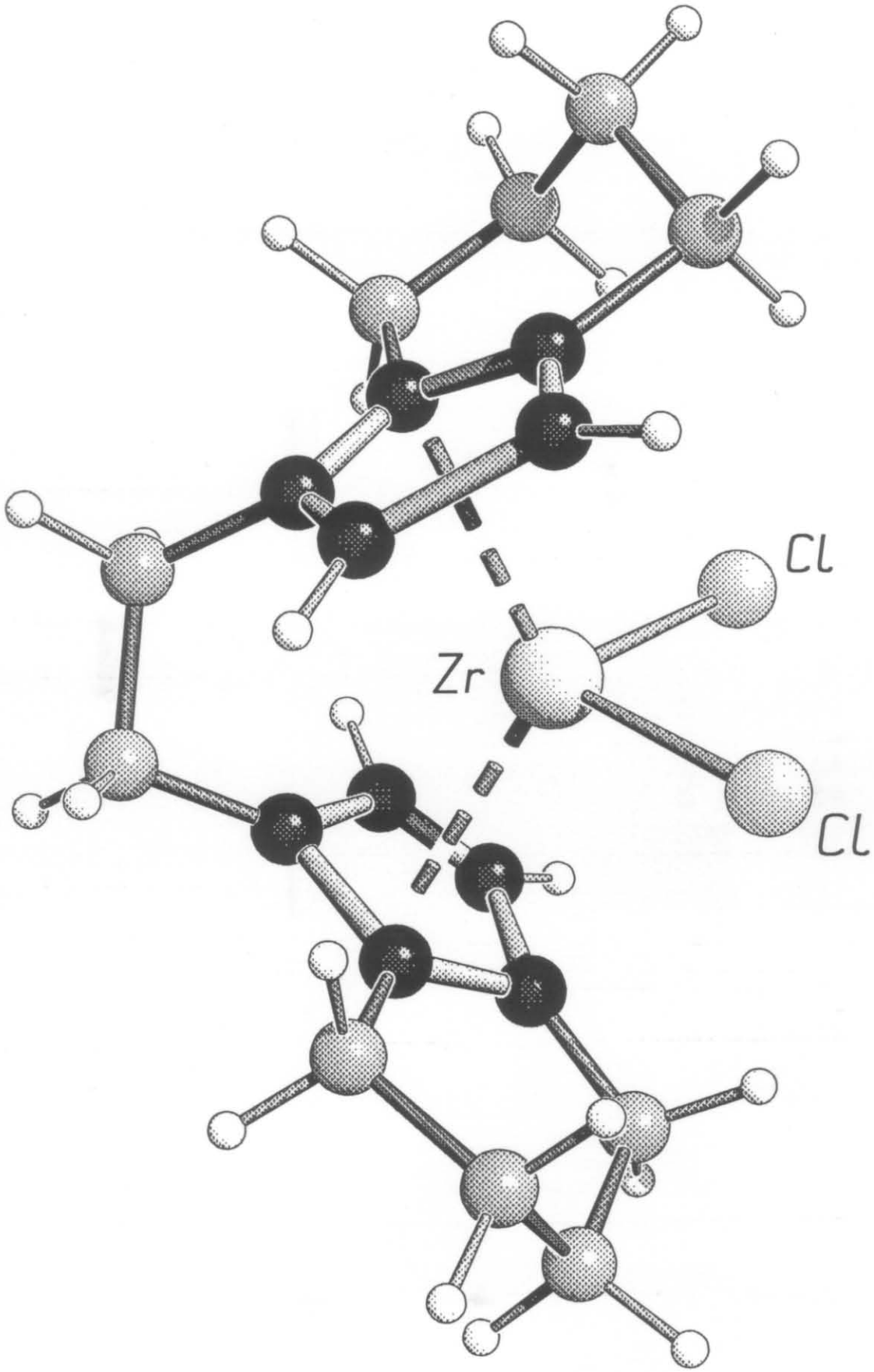


Fig. 13: The $(C_{20}H_{24})$ Zr Cl_2 complex (II)

Fig. 14: The ($C_{20}H_{24}$) Zr Cl_2 complex (III): stereo labelling

This drawing has been generated by means of the DCFs { lines / lstreo } [*ls.scf ;* upper part] and { shade / lstreo } [*las.scf* ; lower part]. Both parts are stereo drawings.

The drawings were generated by the following commands:

{ }$_{3,1.5}$	(switch a n y erasing of drawings off, –––> 724. This is to have two Command file drawings generated on the same sheet)
`Set Inscr 0 4`	(use slanted characters [actually, to have the drawing in portrait format, 'S I ! 1 4' was used; see fig. 8)
`Mgnf Inscr 1.5`	(use positive inscription size parameter !, –––> 561)
`Set Griddens *.8`	(slightly decreased line density for hatching –––> 544)
`[Mgnf Model]`	(switch to variable model scale factor [default], –––> 512)
`Set Xlim 0 .45`	(set X drawing limits to first half of drawing area, –––> 577; note that at the time, when the drawing was generated, it was actually rotated by 90 degrees on the screen. Therefore the X axis was parallel to a line which is now vertical when you look at this drawing)
`Defn $`	(group $ is defined by all atoms (–––> 664), i.e., all atoms will be labelled by *ls.scf* and *las.scf* , below *)*
{ lines^{L} }$_{2,4}$ { lstreo }$_{14,2}$	(execute Command file *ls.scf*)
`Set Xlim .45 .9`	(set X drawing limits to the second half of the drawing area)
{ shade^{L} }$_{3,5}$ { lstreo }$_{21,2}$	(execute Command file *las.scf*)
{ K }$_{3,1.5}$	(switch back to automatic screen erasing, –––> 722)

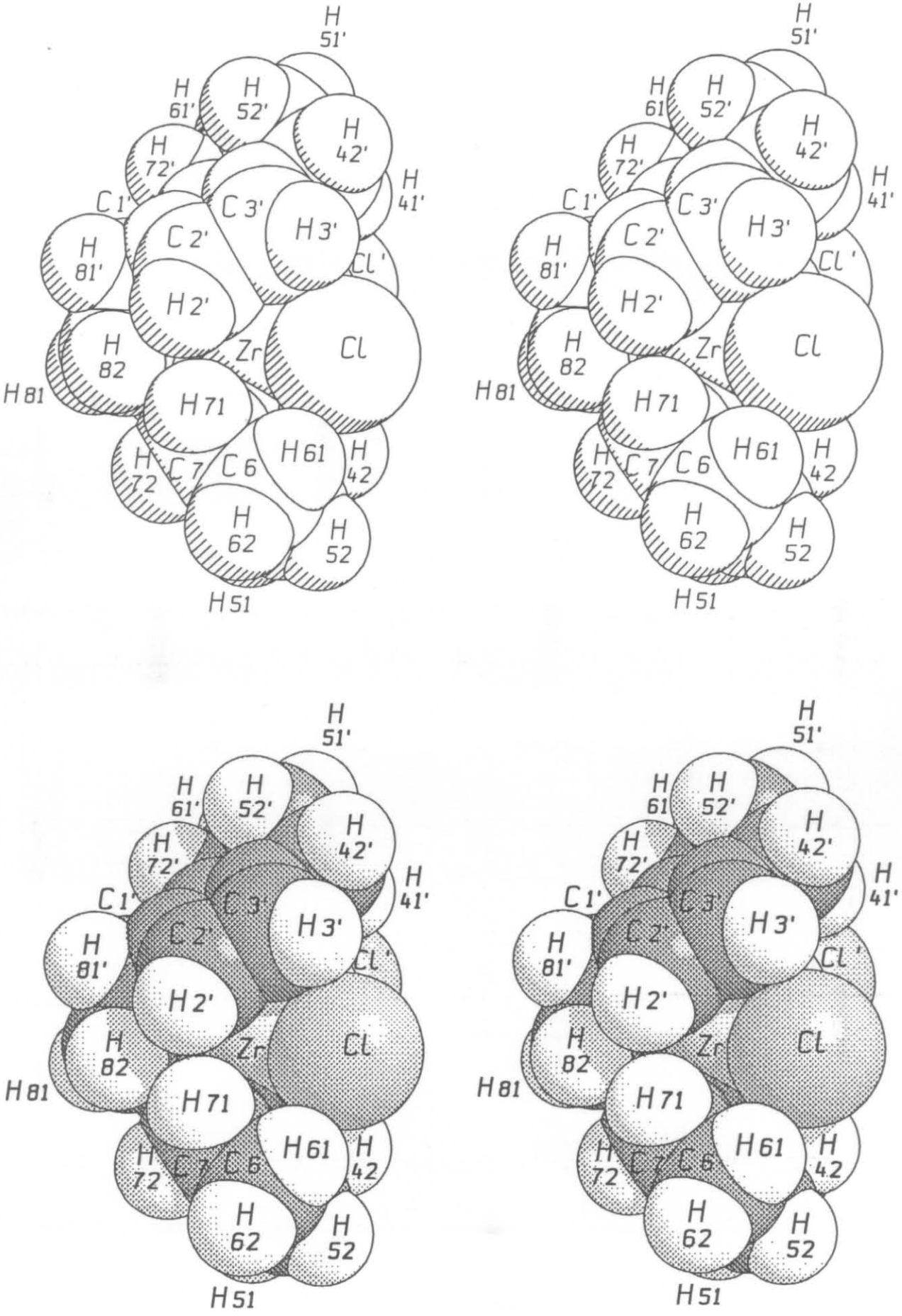


Fig. 14: The $(C_{20}H_{24})$ Zr Cl_2 complex (III): stereo labelling

Fig. 15: The $AgGaS_2$ structure

This drawing demonstrates how to generate an arbitrary section of a crystal structure with boundary walls parallel to the unit cell walls (BOx, –—> 841), and how to add the corners of more than one unit cell to the atom list (ADd, –—> 863).

Furthermore, this drawing illustrates different modes of interpolation for depth-dependent features like darkness ('M D..', –—> 522), pellucidity ('M P..',–—> 523) and line width ('B A.',–—> 554). The following data set was used to generate the model:

```
TITL AgGaS_2_  space group I4&-2d
CELL  5.750    5.750   10.290
ASSM  Ionic
ATOM   Ag      0         0         0
ATOM   Ga      0         0        1/2
ATOM   S      .2908     1/4       1/8
SPGR   I -4 2 d
```

When loading the data set, the following additional data cards were added "by hand":

```
ADD
BOX  0 2  0 1  0 1
END
```

After adjusting radii and stick thicknesses and performing the necessary rotations, the following commands were given:

`Mgnf Model 1`	(scale factor 1 cm / A)
`Mgnf Gaps -2`	(fixed size of marginal gaps, –—> 515)
`Set Tapering .5`	(reduced bond stick tapering, –—> 581)
`Set View 150`	(perspective distortion, –—> 476)
`Set Inscr ! 1 0`	(generate "portrait" format, –—> 466)

The following 'Broaden All' commands were then used to establish different depth-dependence of the line width (–—> 554) for the four different drawings (differences between the two upper drawings are only small):

upper left: `Brdn All  4 1` upper right: `Brdn All  4 1 3`

lower left: `Brdn All  4 1 4` lower right: `Brdn All  4 1 5`

Each of the fhe four drawings was then generated by the following commands:

`S O ...`	(select position for the center of the drawing, –—> 57)
`G O : X`	(draw the outlines)
`X P  41 Ag`	(use pattern 41 for Ag)
`X P  33 Ga`	(use pattern 33 for Ga)

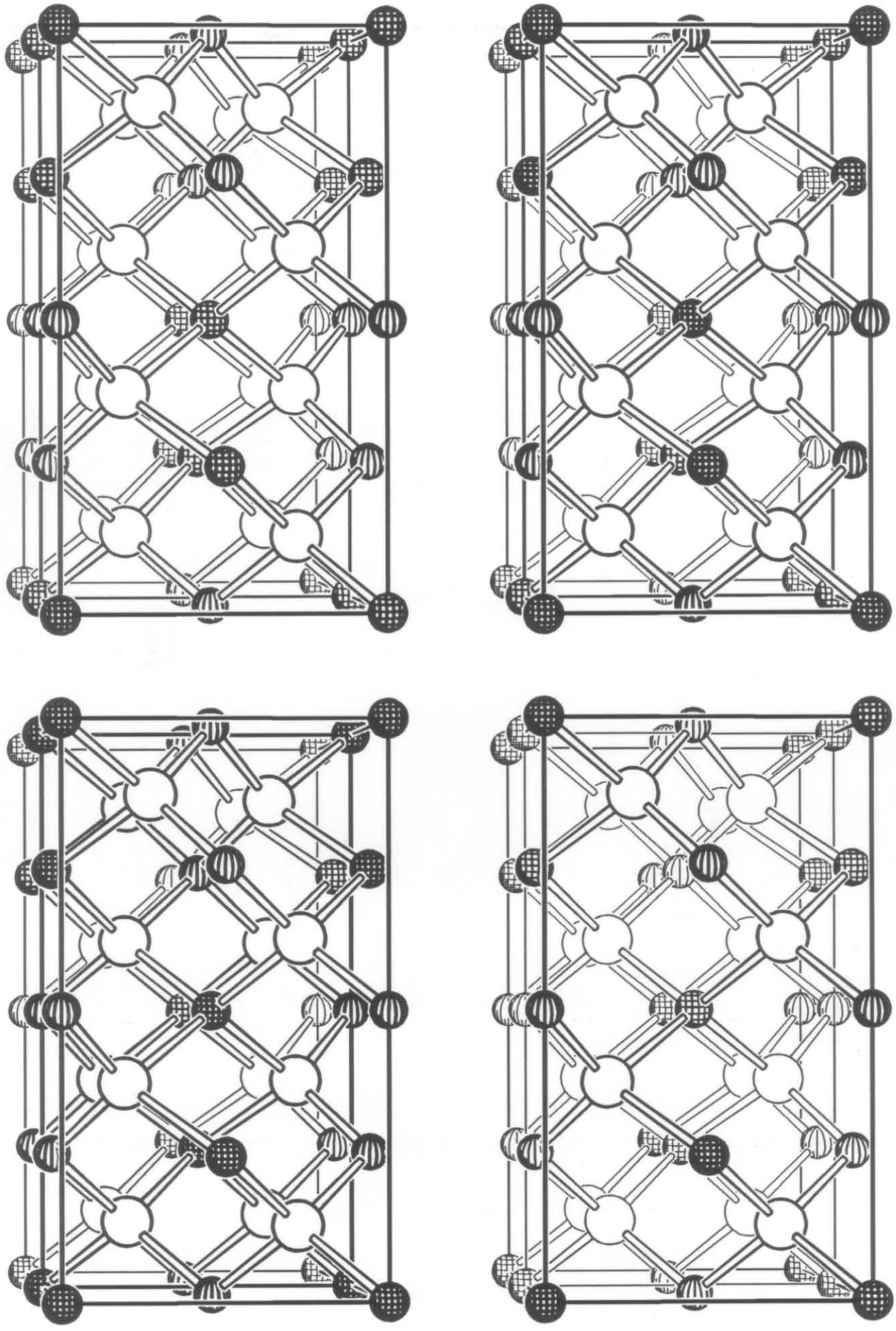


Fig. 15: The $AgGaS_2$ structure

Fig. 16: The (fluoranthene)$_2$ PF_6 structure

This drawing of the crystal structure of (fluoranthene)$_2$ PF_6 illustrates different facilities to generate drawings of crystal structures containing individual building blocks ("molecules"). First, the data set *fluor.dat* (see box, below) was transferred via { cryst^L } / { bld+p } into the data set *fluor_p.dat* (cf. section 5.6. of this manual):

```
TITL Fa_2_PF_6_
CELL   6.610  12.570  14.770  104
ATOM   P     .0000   .0000    .0000
.
.
ATOM   H5    .3830  -.0890    .8340
SPGR A 2/m
```

To both data sets (*fluor.dat* and *fluor_p.dat*) , the following lines were added (for convenience). The commands in the last four lines are executed whenever the data set is loaded.

```
ASSM Comm
STOP
A D 1 0 0                 (align the direction [100] perpend. to drawing plane)
S L 45 45                 (position the light source)
S V 80                    (set perspective)
S M 33                    (set regular dithering mode for shading)
```

To generate the different drawings, the following files were loaded and the following additional input was given "by hand":

upper drawing: *fluor.dat*

add.l data for left part:

```
END
```

add.l data for right part:

```
EXPAND  2
END

Transf Expandr 1
```

lower drawing: *fluor_p.dat*

additional data:

```
END
```

Then, the following additional commands (plus a few others) were given:

upper drawing:

```
Gen Outl : Xqt Xqt  tt

Gen Shading 1
Set Zlim  0 7.5
Mdf Darkn  .9 .2 -2
Xqt Xqt  tt
Set Zlim
Brd All 3 1
Xqt Unitcell
```

lower drawing:

```
Set Zlim 0 7.5
Gen Outl : Xqt Xqt tt
Set Zlim
Gen Shading 1

Mdf Darkn .9 .1 3
Xqt Xqt  tt

Brd All 3 1
Xqt Unitcell
```

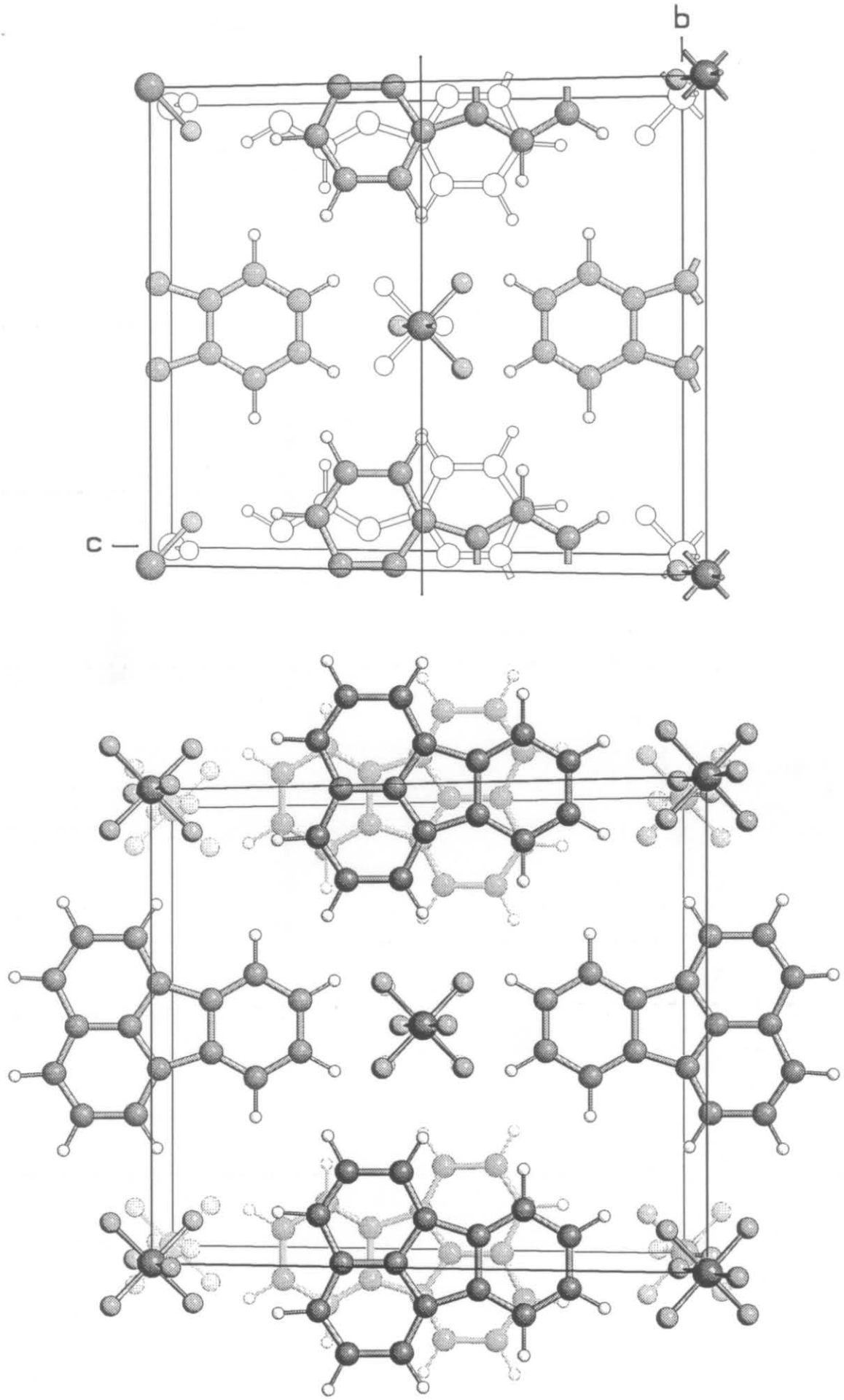


Fig. 16: The $(fluoranthene)_2\ PF_6$ structure

Fig. 17: The $YBa_2Cu_3O_7$ structure

These drawings demonstrate how addition of an EXpand region (–––> 845) to a BOx section (–––> 841) can be used to shape the boundary regions of a solid-state model. All four drawings have been generated by using the following data set, which adds an EXpand region of thickness 3.5 Angstrom to the BOx section (which is simply the unit cell, here):

```
TI  YBa 2 Cu 3 O 7
CE 3.821 3.886 11.668 AS I
AT Cu1 0 0 0
.
.
AT O4  0 .5 0
SGrp P m m m
EXpa 3.5
ASsm C
END                          (a plain BOx card is added by the program)
C D  9 Y, 122 O              (use non-default darkening functions)
C T / 3 Y=nn Ba=nn           (modify thicknesses of some bond sticks)
C R * 1.25 Y Ba Cu           (increase some radii)
R X -90; Y 10; X 10          (rotate the model)
S V 100; L 45 45; M 33       (set perspective, light position, and shading mode)
```

The data set has been made "ready-to-use" by inserting an ENd card (i.e., there is no request for input of more data cards when the data set is loaded). Furthermore, some commands have been added to the data set (cf. fig. 16).

After processing of the data set, the following 'Trnsf Expandregion..' commands (–––> 712) have been used to modify the model (note: the spheres with the smallest radii represent Cu atoms; note: "normal" atoms are those within the section defined by BOx):

upper left: `T E  Cu`

(all EXpand region atoms are deleted except those ones bonded to normal Cu atoms)

upper right: `T E Cu : T C  Cu`

(as upper left; additionally, the coordination polyhedra of the Cu atoms have been modelled by bonds)

lower left: `T E  1`

(all EXpand region atoms are deleted except those ones bonded to any normal atom. The remaining EXpand region atoms are converted into pseudo atoms at half bond distance, thus forming broken-off bond sticks)

lower right: `T E  1 Cu`

(all EXpand region atoms are deleted except those ones bonded to any normal Cu atom. Remaining EXpand region atoms are converted into pseudo atoms at half bond distance, thus forming broken-off bond sticks)

Then the drawings were generated using the commands

```
Gen Outlines :  Xqt
Gen Shadg : Xqt Xqt tt
```

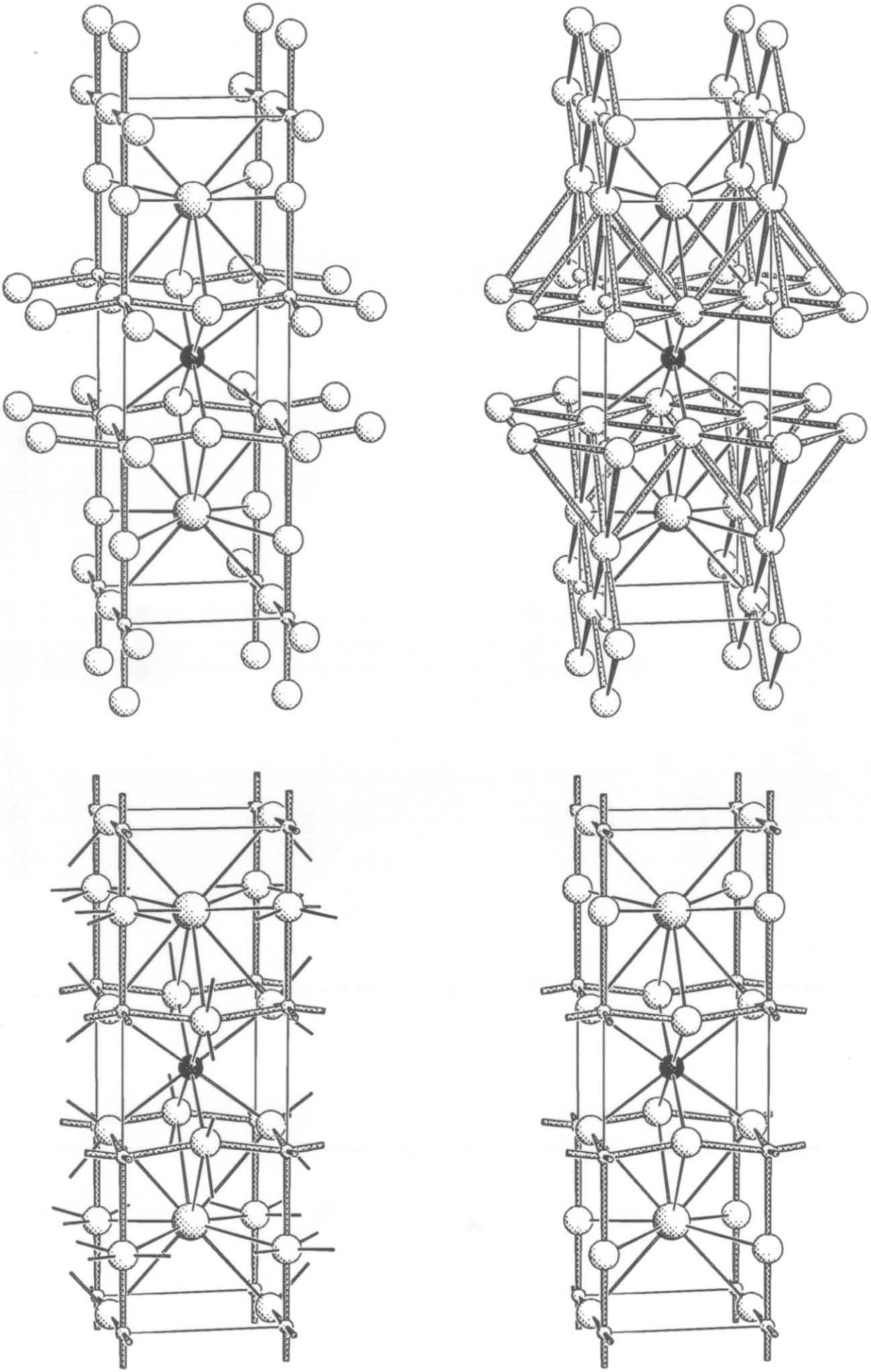


Fig. 17: The $YBa_2Cu_3O_7$ structure

Fig. 18: The ß-Bi_5O_7I structure

This drawing demonstrates the use of 'FAce h k l' cards (–> 853) to define a non-parallelepipedal section of a crystal structure. The following data set was used to generate this model:

```
CELL           18.319   4.245  13.221     108.30
ASSM  Ionic
ATOM   BI1      .2055   .0000   .3656
.
.
ATOM   O7       .5968   .0000   .5210
SPGR C 2 / m
DIST Bi I 4.2
FACE  1 0 0  2.5 2.5
FACE  0 1 0
FACE  0 0 1  2.5 2.5
FACE -2 0 1  2 2
ASSM Comm
END
Aln Dir 0 1 0
```

Instead of defining the desired crystal section by a suitable BOx card, a non-parallelepipedal section was generated here, using FAce cards (–> 853). This allowed (via the last FAce card) to cut off the two corners on top and on bottom which would have been included otherwise [*].

The syntax used for the FAce cards, here, refers to the "default position" of the corresponding planes. This is the position a plane (hkl) would have if it would be shifted from outside towards the unit cell until it touches the cell at a corner, edge, or face. The default distance of the plane to the **center** of the unit cell is multiplied by the parameter on the FAce card to achieve the final position. If two parameters are specified, the second parameter refers to the plane (-h -k -l).

The drawing was generated using the following commands (plus a few others, omitted here):

`Chge Darkn 122 I`	(assign non-default darkening functions, –> 646)
`Chge Darkn  61 Bi, 5 O`	
`Chge Radii *5`	(use non-reduced radii for ball-and-stick model, –> 642)
`Set Light 45 45`	(set the light source, –> 528)
`Set Inscr ! 1 0`	(drawing in portrait format, –> 466)
`Filt U -2  .5`	(use a filter for crystallographic x coordinates, –> 684; here, the x axis is running vertically from top to bottom)
`Defn $ nn`	(define group $ by all atoms [with x < 0.5], –> 664)
`Filt`	(switch filter off)
`Defn $  $ Bi I`	(add the remaining Bi and I atoms to group $)
{ imptt^R }$_{2,6}$	(use Command file *i.scf* to have "unimportant" atoms [i.e., those ones not belonging to group $, i.e., in this case, the O atoms of the upper half] drawn pseudo-transparently)

[*] Another method would have been to generate a normal parallelepipedal box section and cut off the corners with 'Xqt Lines' and 'Kill Atoms rg', cf. end of section 1.6.

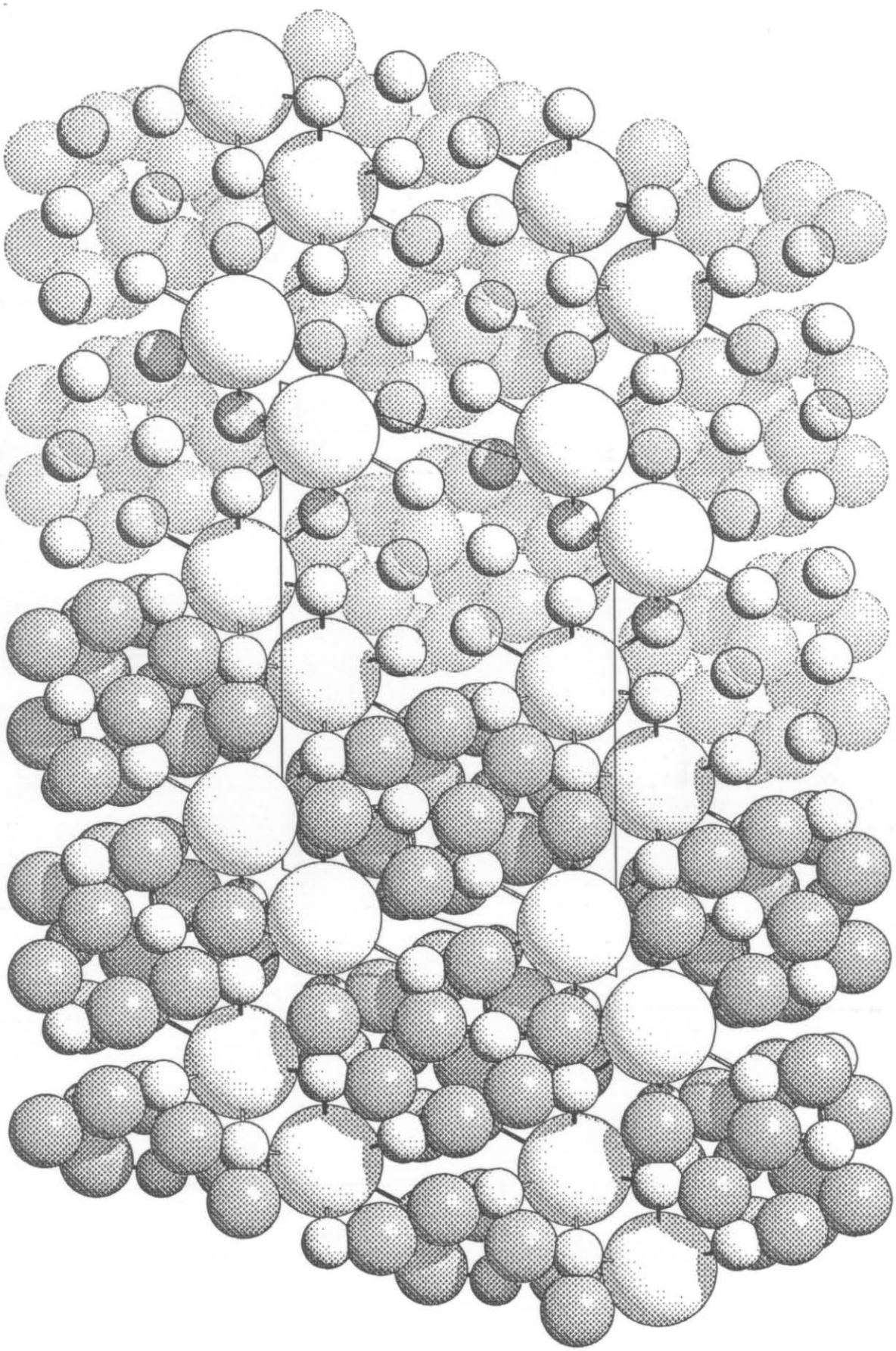


Fig. 18: The ß-Bi_5O_7I structure

Fig. 19: The $KCd_4Ga_5S_{12}$ structure

This drawing demonstrates the use of FAce cards (–—> 583; different syntax as compared to fig. 18) together with EXpand (–—> 845). The following data set has been used to define this model:

```
TITL  KCd 4 Ga 5 S 12
CELL  13.782  13.782   9.330   120
ATOM  M1      .3589   .1014   .0799
.
.
ATOM  S4      .0757   .2994  -.0021
SPGR R 3
FACE H 1.25
FACE 0 0 1 *.85 *.15
EXPA 2.5
BOX
ATOM A101  1.25  0    0
ATOM A102  1.25  1.25 0
.
.
ATOM A107  1.25  0    0
ASSM C
END
F W  -1 -.15 : K A  nn        (delete atoms with cryst. z < -.15)
F W  0.85 2  : K A  nn        (delete atoms with cryst. z > .85)
T E  1                        (generate broken bonds to the EXpand region)
F U  -.25  2 : D $  nn        (define group $ by all atoms with  -.25 < x < 2,
F V  -.25  2 : D $  $          -.25 < y < 2,   and
F W   .15  1 : D $  $ : F      +.15 < z < 1  )
D F  nn ($                    (define a fragment with all atoms except $ atoms)
C S  *1.5 tt (M               (change some radii and stick thicknesses)
```

The first FAce card specifies a hexagonal prism, default distance of planes to unit cell **origin** multiplied by 1.25 (note: with respect to this, 'FAce H..' behaves different from other 'FAce N..' cards, –—> 856).

Within the second FAce card, "*.85" selects, as a boundary plane, a version of the (001) plane which has a distance of $d_{(001)}$ * 0.85 to the unit cell **origin** (different syntax as compared to the FAce cards of fig. 18 !). "*.15" selects, as a second boundary plane, a version of the (00-1) plane which has a distance of $d_{(00\text{-}1)}$ * 0.15 to the unit cell **origin** (note: the lattice plane distance $d_{(001)}$ is equal to the height h of the unit cell in **c** direction which is equal to c itself, here, because the vector **c** is perpendicular to (001)).

The A10n atoms are used to define the dashed hexagon. It visualizes the region addressed by the 'FAce H 1.25' card.

The structure can be seen as consisting of layers parallel to (001). All EXpand atoms with z < -0.15 or z > 0.85 are deleted (to have no broken-off bond sticks above the surface, when the EXpand region is shaped with 'Trnsf EXpnd 1', –—> 713). In a certain region (see upper right part of upper drawing), two layers are removed reversibly to reveal the structure of a single layer (see commands between 'F U ..' and 'D F..').

The upper drawing displays a plan view, the lower one a side-view of the model.

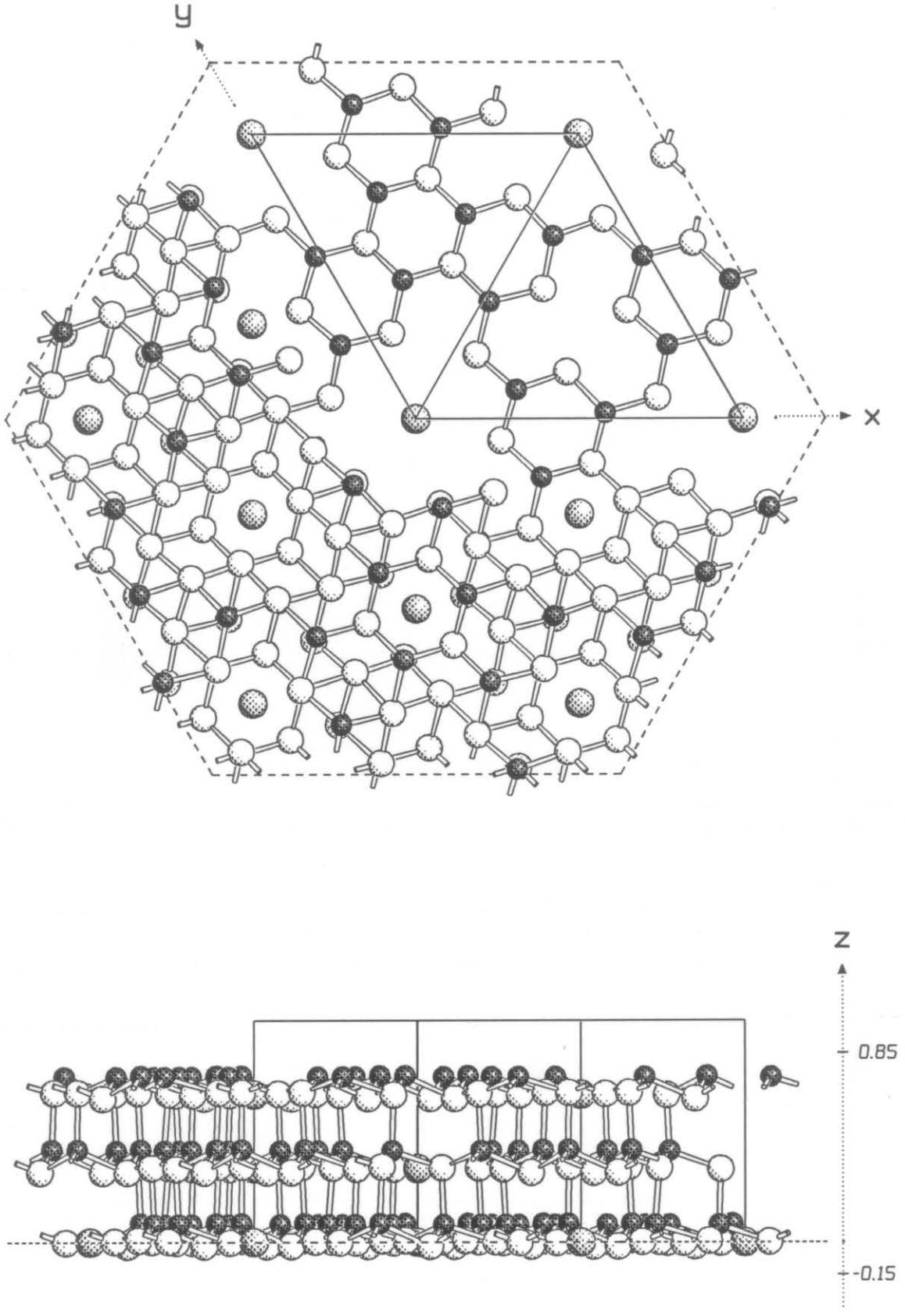


Fig. 19: The $KCd_4Ga_5S_{12}$ structure

Fig. 20: A (111) surface model of the $Pb_3(PS_4)_2$ structure (I)

While the models of fig.s 18 and 19 could be seen to be "surface models" of the (0 1 0) or (0 0 1) planes, they actually aren't surface models (but "polyhedral models") in the sense of the SCHAKAL manuals (–-> 851). Here, a model is called a "surface model", if the corresponding data set contains only **one** normal 'FAce h k l' card (note that 'FAce H 1.25' of fig. 19 replaces three normal 'FAce h k l' cards !).

The different models of fig. 20 a)-c) have been generated by the data set *ex2_p.dat* [DOS/Win16:

```
TITL  Pb 3 (PS 4 ) 2   Cubic SpGr P2 1  3
CELL   10.9394   10.9394   10.9394  90.0000  90.0000   90.0000
ASSM   P
ATOM   P1         .5743     .5743     .5743
.
.
MOL
ATOM   P2         .8498     .8498     .8498
.
.
MOL
ASSM   I
ATOM   Pb1        .4758     .2570     .6376
SPGR  P213
STOP
```

p_ex2.dat] which had been obtained from *ex2.dat* by means of { crystL } / { bld+p } (see 5.6.). For the model of fig. 20a, the following data cards have been added "by hand":

```
FACE  1 1 1
END
```

This demonstrates the "first-choice" way to generate a surface model. The FAce card contains the h,k,l values only. Size information may be given on a BOx card. As no BOx card is given, the program adds one with no parameters, i.e., just the contents of one "alternative cell" are generated (note that an additional 'BOx 0 1 0 1 0 1' would have led to the same results).

The alternative cell is composed of the plane's 2D unit cell [defined by the two unit vectors "vector 1" ($\mathbf{v_1}$) and "vector 2" ($\mathbf{v_2}$)] and the vector $\mathbf{d}_{(111)}$, –-> 851.2 . Because of the latter fact, the thickness of the generated layer is $d_{(111)} * 1$.

For the model of fig. 20b, the following data cards were added "by hand":

```
FACE  1 1 1
BOX  -1 2  -.5 1.5  0 1
END
```

Again a layer of thickness $d_{(111)}$ is generated. The lateral boundary walls, however, are now located at $-1 * v_1$, $2 * v_1$, and $-0.5 * v_2$, $1.5 * v_2$.

Note that a side-view of fig. 20b would look very similar to the lower part of fig. 21.

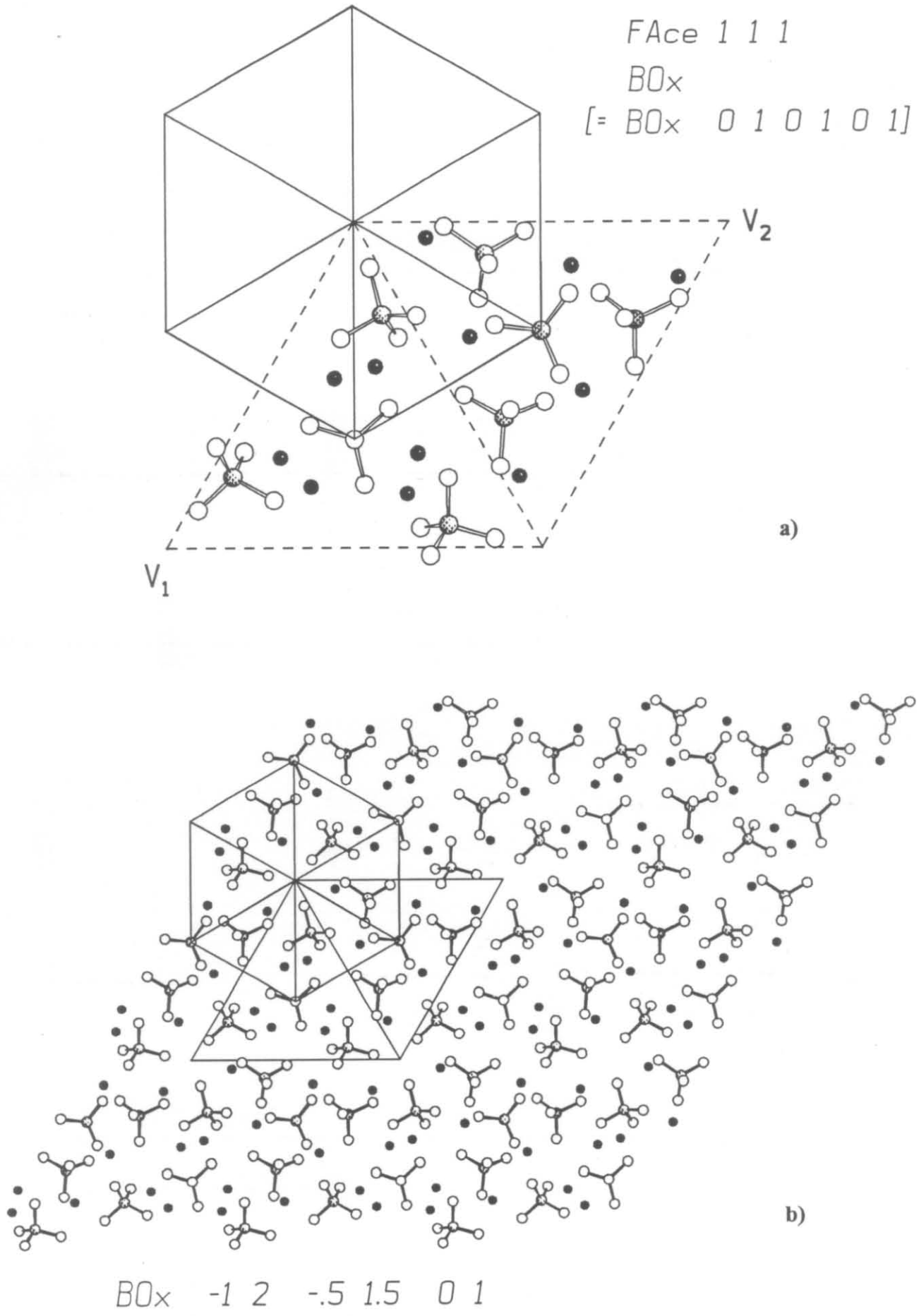


Fig. 20: A (111) surface model of the $Pb_3(PS_4)_2$ structure (I)

Fig. 21: A (111) surface model of the $Pb_3(PS_4)_2$ structure (II)

The same data set, *ex2_p.dat* as described for fig. 20 was used. For the model of fig. 21, the following data cards were added "by hand":

```
FACE  1 1 1 *1 *0
RADI  24
END
```

This is the so-called "alternative" way, to generate a surface model:

The FAce syntax is one of those which have been designed for polyhedral models, originally (see fig. 19). Correspondingly, a (111) plane with distance $d_{(111)}$ * 1 and a (-1-1-1) plane with distance $d_{(111)}$ * 0 to the unit cell origin are established.

The "RAdius 24" card excludes all molecules for which the center of gravity has a distance of more than 24 Angstrom to the unit cell origin.

While the upper drawing displays a plan view of the model, the lower drawing gives a side-view of the same model. Dotted lines are the traces of the (111) lattice planes.

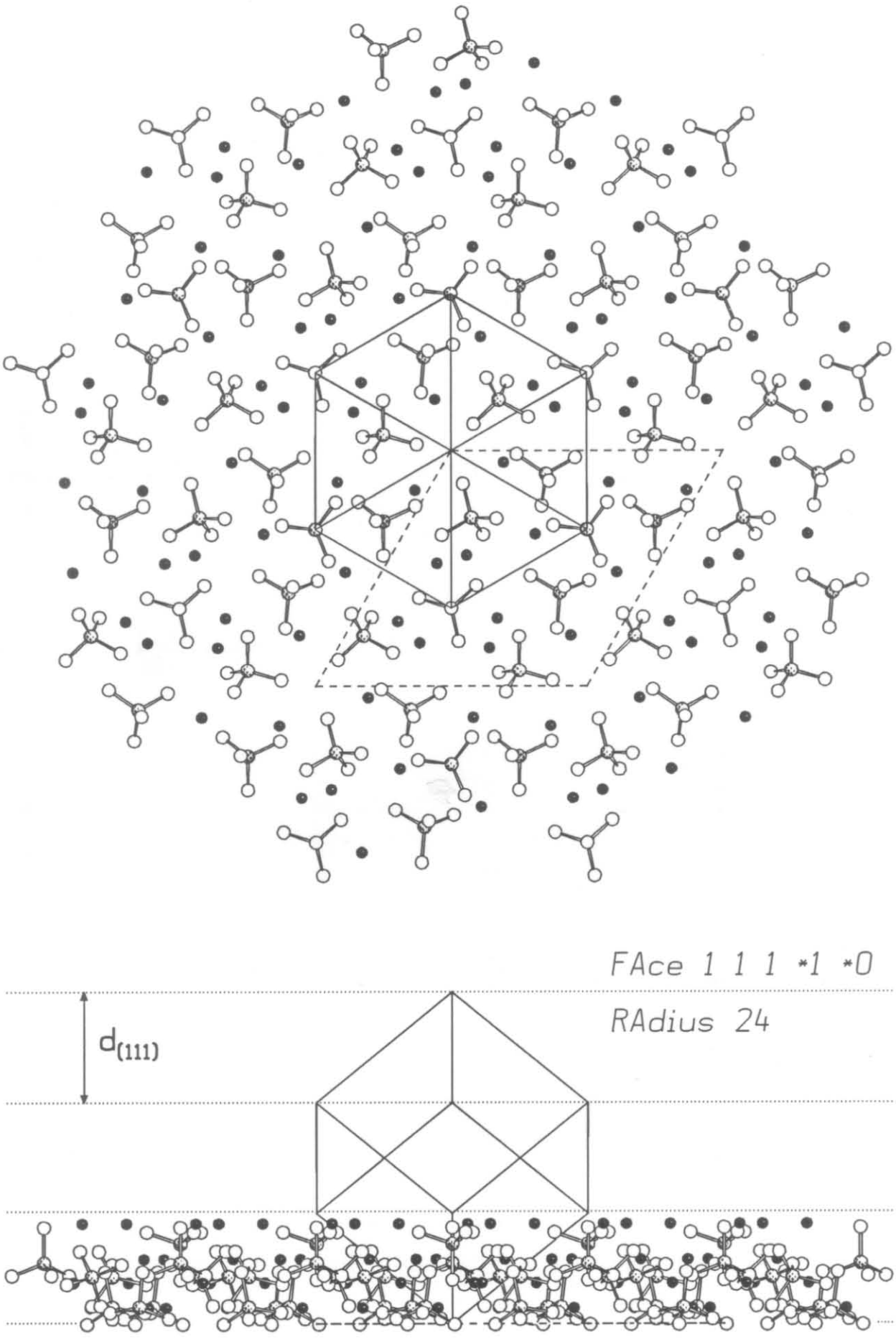


Fig. 21: A (111) surface model of the $Pb_3(PS_4)_2$ structure (II)

Fig. 22: A (230) surface model of the $Pb_3(PS_4)_2$ structure (I)

The data set described with fig. 20 has also been used for the drawings of fig. 22. Here, the following data cards were added "by hand":

```
FAce  2 3 0
BOx   0 1 0 1 z1 z2
```

with different values for z1,z2 in the three different cases. Note that the **range** defined by BOx always **must contain the unit cell origin (**only in connection with FAce !). A comparison of fig.s 22a and 22b demonstrates, how a layer of constant thickness can be "moved" parallel to the plane normal.

If you compare fig. 22a with the side view given in fig. 21 (which would not differ significantly from a side-view of fig. 20, lower part) you will notice that $d_{(230)}$ is much smaller than $d_{(111)}$ [which is due to the general rule, that $d_{(hkl)}$ is the smaller, the larger the absolute values of h, k, and l]. As a compensation, the 2D unit cell of the (230) plane is correspondingly larger than the 2D unit cell of the (111) plane (compare fig. 23 to fig. 20).

Dashed lines are the traces of the (230) lattice planes. If you are not very familiar with Miller indices, you may read the following section:

The Miller index of a set of lattice planes can be determined by the following simple method:

Look at the plane which is the first neighbour to the plane which contains the coordinates system origin (i.e., the unit cell origin). In drawing a), the trace of this first-neighbour-plane is the one which is the upper borderline of the shaded bar. This plane intersects the **a** axis at 1/*2* **a**, the **b** axis at 1/*3* **b**, and the **c** axis (which is parallel to the plane) at infinite = 1/*0* **c**. This corresponds to a Miller index of *2 3 0* .

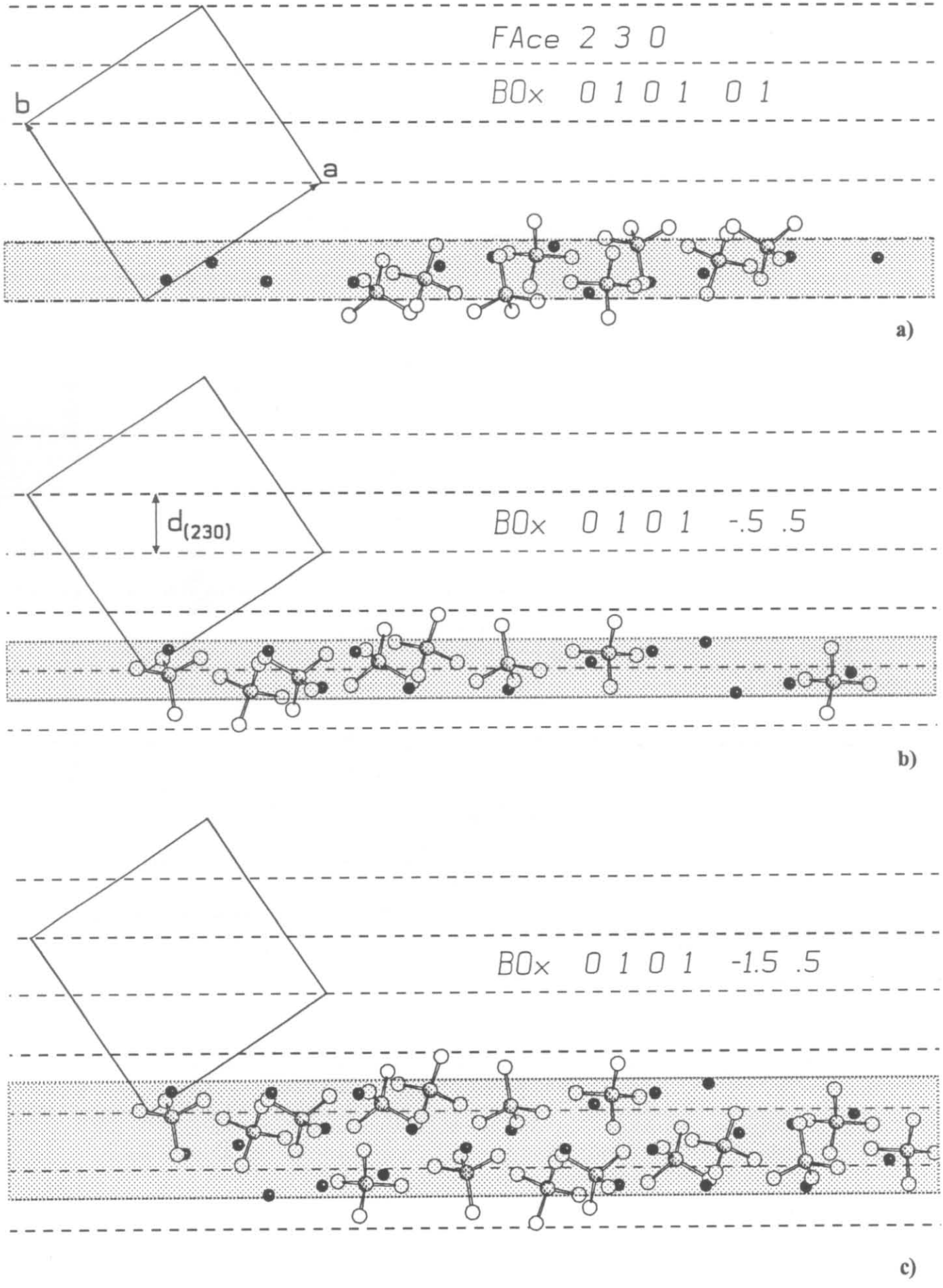


Fig. 22: A (230) surface model of the $Pb_3(PS_4)_2$ structure (I)

Fig. 23: A (230) surface model of the $Pb_3(PS_4)_2$ structure (II)

Fig. 23a gives a side-view of the model*) displayed in fig. 22a;
Fig. 23b gives a side-view of the model*) displayed in fig. 22c.
(*) a slightly modified BOx card [first two parameters] was used for the drawings of fig. 23).

Edges of the structure's unit cell have been omitted, here. However, the edges of the 2D unit cell of the (230) plane (dashed lines, –> 545) have been switched on exclusively by a 'Gen Unitcl 5 -1' command (–> 486).

If you look at fig. 23a, you will see, that this surface model looks rather strange: there are zones where no PS_4 ions are present at all. This is because the thickness of this layer (= $d_{(230)}$) is too small (cf. fig. 22a).

You will have to generate a thicker layer in this case to obtain a reasonable model of the surface. This has been done with the model shown in fig.s 22c/23b which correspond to a layer thickness of $d_{(230)} * 2$.

Generally, you will have to generate thicker layers (in terms of $d_{(hkl)}$) for larger h,k,l values to get a reasonable surface model.

There is a tiny problem, however: a surface model's "alternative cell" (with $v_3 = d_{(hkl)}$) contains just as many atoms as the structure's unit cell itself. Therefore, a model with a layer thickness of $d_{(hkl)} * 2$ will contain at least 2 times the atoms contained in the normal unit cell (provided that at least one complete 2D cell is enclosed between the lateral faces). Thus, you may exceed the program's atom capacity if you continue to increase the layer thickness of your model (but see fig. 24, 7th parameter on BOx card).

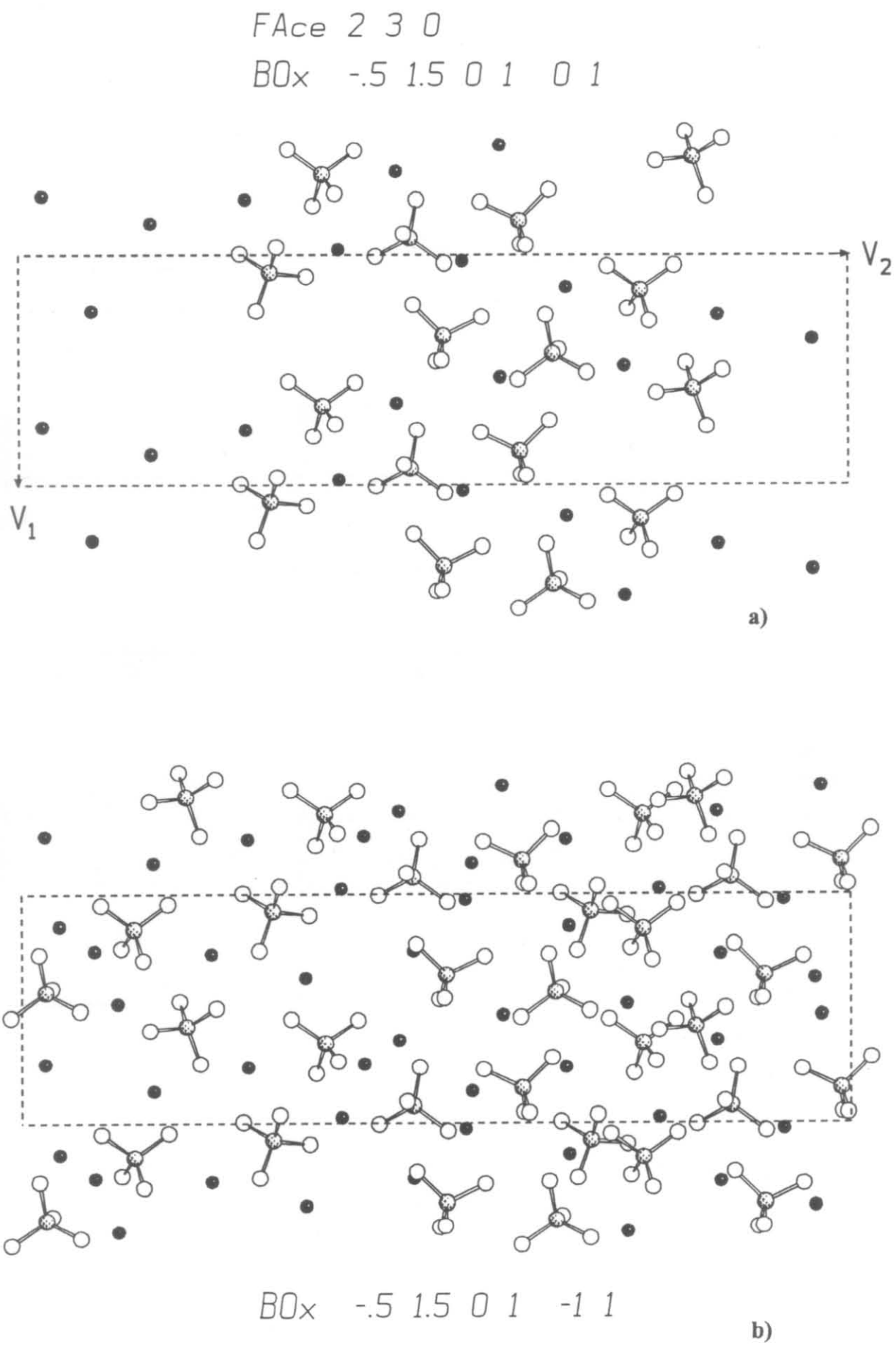


Fig. 23: A (230) surface model of the $Pb_3(PS_4)_2$ structure (II)

Fig 24: A (011) surface model of the (fluoranthene)$_2$ PF_6 structure

The data set to generate the (011) surface model of the (fluoranthene)$_2$ PF_6 was identical to the one for the lower part of of fig. 16 (*fluor_p.dat*):

```
TITL Fa 2 PF 6
CELL   6.610  12.570  14.770   90.00  104.00   90.00
ASSM   P
ATOM   P     .0000   .0000    .0000
.
.
ATOM   F2   -.0977   .0881   -.0731
MOL
ATOM   C1    .2252   .0000    .4489
.
.
ATOM   H5    .3830  -.0890    .8340
SPGR A 2/m
```

The following data cards were added "by hand":

```
FAce 0 1 1
BOx -2 3  -1.5 2.5  0 1  .5
END
```

With the last parameter on the PAck card, it was achieved that the more distant half of the atoms (when seen from the surface itself) was not included in the model (thus saving memory space to increase the lateral width of the model but retaining an intact surface).

To have the uppermost layer contain fluoranthene molecules instead of PF_6 ions, the following BOx card would have to be given:

```
BOx -2 3  -1.5 2.5  -.5 .5  0.01
```

The drawing was then generated with the following commands:

`Genr Unitc  5 -1`	(edges of the plane's 2D unit cell are switched on, exclusively, –> 486)
`Mgnf Model  1`	(fix the model scale factor, –> 511)
{ varyZ }$_{3,6}$ { uni }$_{19,2}$	(use Command file *f.scf*)
`Unlk Model`	(unlock the model for geometry modifications, –> 36)
`Trsl Z  20 A91-A94`	(shift the corners of the 2D unit cell "upwards", –> 851.3)
`Xqt Unitc`	(draw 2D unit cell edges, –> 218)

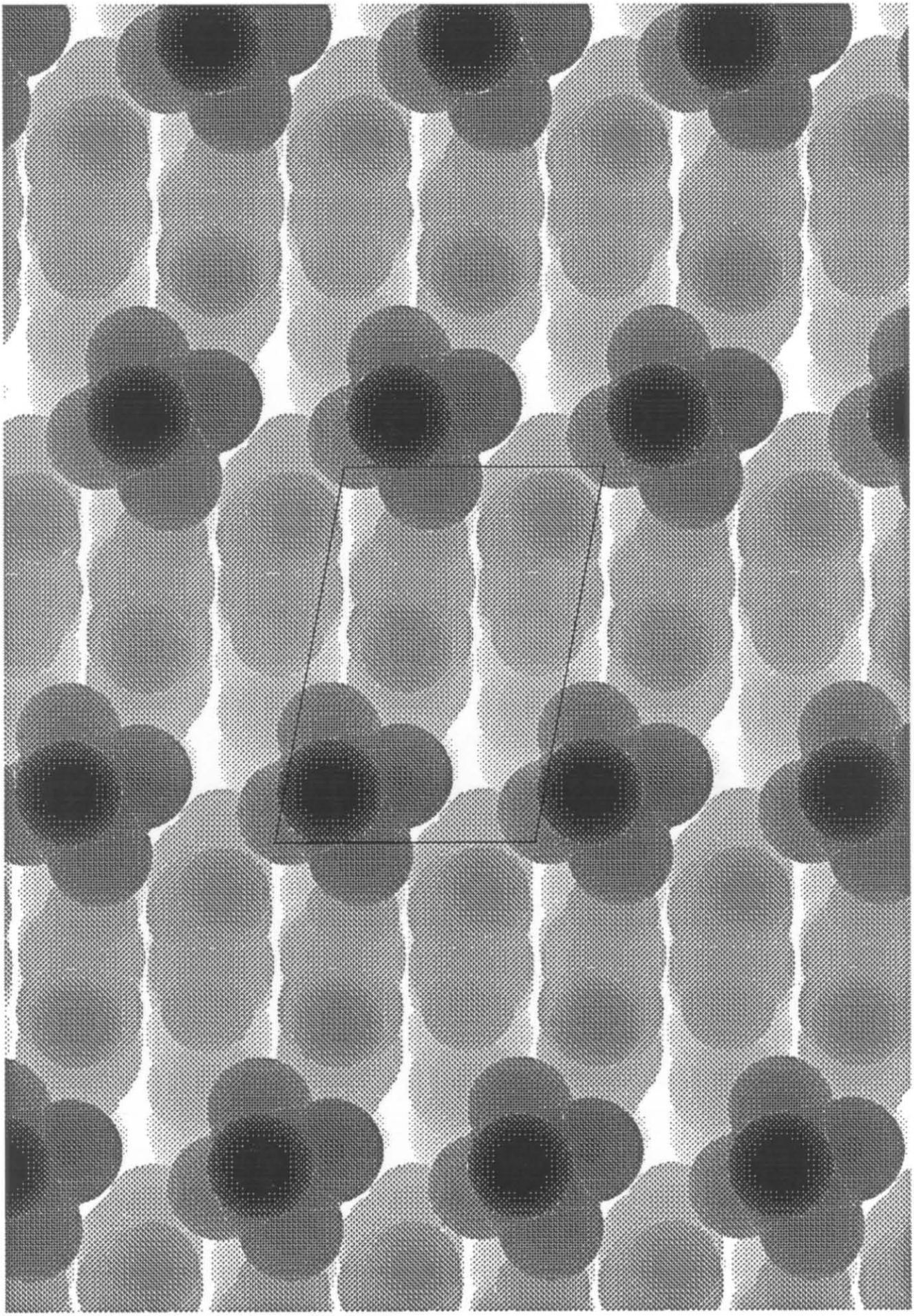


Fig. 24: A (011) surface model of the $(fluoranthene)_2PF_6$ structure

Fig 25: The Graphical User Interface (GUI)

#	***Explanation***	–––>
A	the "1st row" allows to select a group of commands or execute certain commands	931
B	the 10 "coloured control fields" launch some certain, frequently used commands.	933
C	header of the "command column"; [almost] all commands beneath start with 'Use...'.	932
D	control field (CF) for the 'Use Xtaldat' command (light blue part)	932
E	CF for the 'Use Xtaldat' command (yellow part); immediate execution when clicked	932
F	a "command line control field"; may be removed or replaced by another one	774
G	a "green star", indicating that this command is accessible from the 1st row directly.	931
H	"green star" referring to the one labelled "G".	931
I	clears the GUI; use it to remove "parameter boxes", "colour boxes", etc.	933
J	works like <RETURN>, i.e., may be used to send a command to the program	932.2
K	these two CFs may be used to access the hierarchical on-line manual	936
L	opens a directory of "distributed command files" (DCF)	934
M	executes a DCF (namely the "default DCF" of this directory)	934
N	the text "window" which is frameless and of variable size	73
O	the "graphics area" (or "drawing area"), where something can be drawn	2
P	may be used to store a screen drawing as a TIFF file or to print a printer drawing	171, 153
Q	these CFs may contain atom codes (e.g. chemical element symbols)	935
R	may contain numbers or a short message	935
S	may be used to emulate <BACKSPACE>	936
T	same as "J"	932.2
a	toggles between M(ouse), A(rrow_keys) and - possibly - S(ave) mode	311.3
b	toggles between R(otation), F(lip), and - possibly - T(ranslation) mode	311.2
c	makes motion faster (i.e., increases step width)	311.2
d	one of the six CFs to control motion (e.g. rotation, while in R mode)	311
e	may be used to stop motion	
f	these two CFs control the labelling of atoms	311.5
g	fixes the scale factor [sc. f.] and reduces it stepwise	311.6
h	visualizes the current value of the sc. f.; click somewhere to select a new (fixed) one	311.6
i	fixes the sc. f. and increases it stepwise	311.6
j	displays the current value of the sc. f.	311.6
k	sets a special value of the sc. f. : sc.f. = zero (i.e., sc. f. = non-fixed, variable)	311.6
l	switches the unit cell edges on and off	311.7
m	toggles between ball-and-stick and space-filling model	311.7
n	may be used to leave on-screen rotations mode	311
o	undoes rotations and translations	311.5
p	switches to wire model with or without small atom spheres	311.4
q	switches to 'Xqt Quick' drawing	311.4
r	switches to outline drawing	311.4
s	switches to standard shaded drawing	311.4
t	makes motion slower (i.e., reduces step width)	311.2
u	switches to drawing produced by the last active command file	311.4
v	toggles between current line width and line width 1 (fastest)	311.5
w	switches stereo mode on and off	311.7
x	may be used to leave on-screen rotations mode	

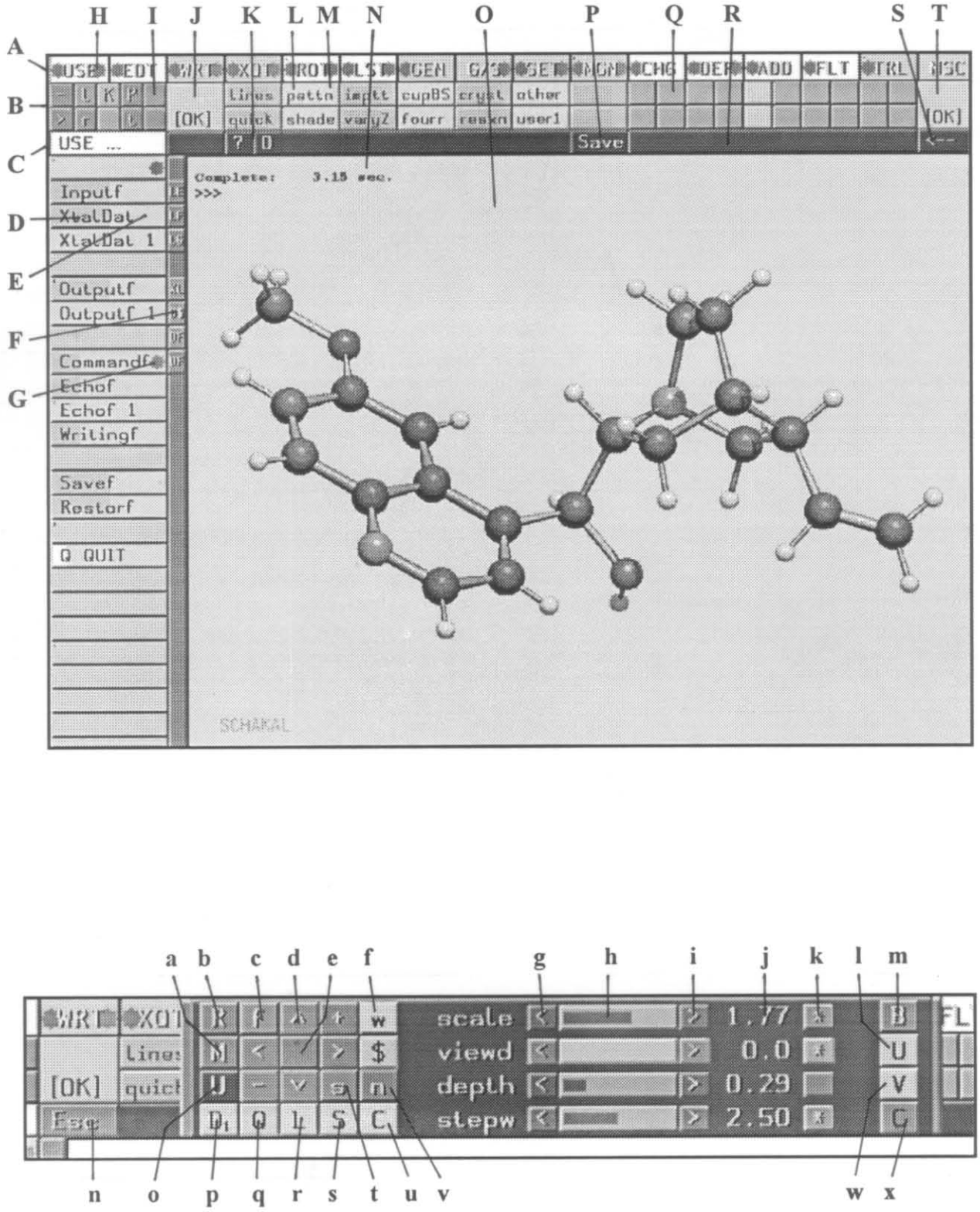


Fig. 25: The Graphical User Interface (GUI)
top: default state; bottom: on-screen rotations box

References

The structures stored in the files *ex*.dat* and those ones mentioned within this manual were taken from the following sources:

$Fe_4(CO)_{12}(NC\text{-}C_6H_5)$ (file *ex1.dat*)
E. Keller & D. Wolters
Chem Ber. **117** (1984), 157
Remark: some atom names and molecular geometry in *ex1.dat* differ from those ones in the publication

$Pb_3(PS_4)_2$ (file *ex2.dat* and figs. 20-23):
E. Post & V. Krämer
Mat. Res. Bulletin **19** (1984), 160

Quinine (file *ex3.dat* and fig. 25)
S. Kashino & M. Haisa
Acta Cryst. **C39** (1983), 310

Penicillin (file *ex4.dat* and fig. 11):
D. Crowfoot, C.W. Bunn, B.W. Rogers-Law & A. Turner-Jones
in "The Chemistry of Penicillin", edited by *H.T. Clarke, J.R. Johnson & R. Robinson,*
1949, pp. 310, Princeton University Press
Remark: original conformation of the molecule has been modified to generate fig. 11

Glycyl-glycyl-glycine (β form) (file *ex5.dat*)
T. Srikrishnan, N. Winiewicz & R. Parthasarathy
Intern. J. of Peptide and Protein Res. **19** (1982), 103

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J. Organomet. Chem. **288** (1985), 63
Remark: some atom names are different from those ones in the publication

$AgGaS_2$ (fig. 15):
S.C. Abrahams & J.L. Bernstein
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$KCd_4Ga_5S_{12}$ (fig. 19):
H. Schwer, E. Keller & V. Krämer
Z. Kristallogr. **204** (1993), 203