NAME
     AddDrawobj – add line, rectangle or circle

SYNOPSIS
     AddDrawobj (line | rect | circle) (2D | 3D)

DESCRIPTION
     Add a line, rectangle or cirlce for annotation.
     The first argument selects the type of drawing object.

     If the second argument is 2D, the object is placed
     at a default location and can be moved to the desired
     place. It will always keep its screen position and is
     not related to any spectrum.

     If the second argument is 3D, the initial position in
     space is near the center of the selected spectrum.
     The positon relative to this spectrum can be changed
     with the mouse or with the MoveDrawobj command.

EXAMPLES
     AddDrawobj line 3D

SEE ALSO
     SelectSpec, ColorPrim, LinePrim, StyleDrawobj,
     MoveDrawobj, RemovePrim, AddTitle, AddText

DATE
     960912

NAME
     AddText – add 3D text annotation

SYNOPSIS
     AddText expr string

DESCRIPTION
     Add a 3D text annotation. The first argument gives
     the initial size, the second argument the text.

     The initial position in space is at the center of
     the selected spectrum. It can be moved with the
     mouse or with the MovePrim command.

     For an explanation on how to enter greek letters,
     sub– and superscript, see the manual page of the
     EditText command.

EXAMPLES
     AddText 0.15 "Label"

SEE ALSO
     EditText, ColorPrim, LinePrim, MovePrim, SizeText,
     AddTitle, RemovePrim

DATE
     960912

```
NAME
     AddTitle – add 2D text annotation

SYNOPSIS
     AddTitle <coord> expr string

DESCRIPTION
     Add a text annotation at a given screen position.
     The screen position must be entered by a mouse
     click or on the command line. The second argument
     is the size, the third the string to be displayed.

     For an explanation on how to enter greek letters,
     sub- and superscript, see the manual page of the
     EditText command.

EXAMPLES
     AddTitle 0.5 0.3 0.15 "Label"

SEE ALSO
     EditText, ColorPrim, LinePrim, MovePrim, SizeText,
     AddText, RemovePrim

DATE
     960912
```

NAME
     AnglePeak – set angle of line attached to peaks

SYNOPSIS
     AnglePeak expr

DESCRIPTION
     Set the angle of the lines drawn from the center of
     all selected peaks. The angle is given in radians.
     A line is only drawn when the length (LengthPeak) is
     positive, and the style is 'circle'.

EXAMPLES
     AnglePeak 0.5

SEE ALSO
     SelectPeak, StylePeak, LengthPeak

DATE
     960912

NAME
     AttrSpec – list attributes of spectra
     AttrPeak – list attributes of peaks
     AttrPrim – list attributes of primitives

SYNOPSIS
     AttrSpec
     AttrPeak
     AttrPrim

DESCRIPTION
     Lists the values of the attributes of all selected
     spectra, peaks or primitives. All items have to
     share the same set of attributes, an error message
     is issued otherwise.

     Also creates a macro that can be used to set all
     the attributes to these values.

EXAMPLES
     AttrPeak

SEE ALSO
     Select*, Color*, Material*, Texture*, Style*, Line*

DATE
     960912

NAME
     BackColor – change background color

SYNOPSIS
     BackColor expr expr expr

DESCRIPTION
     Set the background color. The color is given by its
     Red, Green and Blue component, all in the range
     between 0.0 and 1.0.

EXAMPLE
     BackColor 1.0 0.2 0.7

DATE
     960912

```
NAME
     ClipPos – set position of clipping planes
     ClipSize – set distance of clipping planes

SYNOPSIS
     ClipPos expr
     ClipSize expr

DESCRIPTION
     Set new values for the distance of the near and
     far clipping planes. By ClipPos, the user sets
     the position of the middle between the two
     planes, by ClipSize the distance:

         near = pos – size / 2
         far  = pos + size / 2

EXAMPLES
     ClipPos 8.0
     ClipSize 5.0

DATE
     950912
```

NAME
      ClusterShape – group similar shapes into clusters

SYNOPSIS
      ClusterShape expr expr expr expr

DESCRIPTION
      Group similar shapes of all selected spectra into
      clusters. This command is executed after Identify
      and before Deconv.

      The first argument gives the direction (domain) of
      the shapes that should be clustered. Domain 0 is
      the detection domain, 1 the evolution domain in
      a 2D spectrum, etc.

      The next argument gives the desired number of
      clusters. This can be given as the expected number
      of chemical shifts, but it is normally given as 1,
      so that the clustering is only stopped when the
      maximum difference given as last argument is
      reached.

      The next argument gives a mimimal difference
      between two clusters, this is only important if
      a desired number of clusters was given in the
      previous argument, otherwise any small number
      will do.

      The last argument gives the maximus difference of
      two shapes to be in the same cluster. This value
      is typically between 1.0 and 2.0.

EXAMPLE
      ClusterShape 0 1 0.2 1.0
      ClusterShape 1 1 0.2 1.0

SEE ALSO
      Identify, SelectSpec, Deconv

DATE
      960913

NAME
    ColorSpec – set color of spectra
    ColorPeak – set color of peaks
    ColorPrim – set color of primitives

SYNOPSIS
    ColorSpec expr expr expr
    ColorPeak expr expr expr
    ColorPrim expr expr expr

DESCRIPTION
    Set the color of all selected spectra, peaks or
    primitives. The color is given by its Red, Green
    and Blue component, all in the range between
    0.0 and 1.0.

EXAMPLES
    ColorPeak 1.0 0.0 0.0

SEE ALSO
    Select*, Material*, Texture*

DATE
    960912

NAME
      Deconv – deconvolute regions to find more peaks

SYNOPSIS
      Deconv expr expr

DESCRIPTION
      Deconvolute all selected regions to find additonal
      peaks that were not found with Identify. The
      Identify and ClusterShape commands must be
      executed before using this command.

      The first argument gives a minimal amplitude for
      peaks identified, as factor of the noise level.
      This is typically between 1.5 and 3.0.

      The second argument defines how large the match
      between a potential peak and the data has to be.
      With a value in the range of 0.5, only very well
      matching peaks are found, a value in the range of
      0.0 will also find rather questionable peaks.
      Typical values are around the middle of these two
      values.

EXAMPLE
      Deconv 1.5 0.2

SEE ALSO
      Segment, Identify, ClusterShape, SelectSpec

DATE
      960913

NAME
     DefPropSpec – define spectrum property
     DefPropPeak – define peak property
     DefPropPrim – define primitive property

SYNOPSIS
     DefPropSpec propertyName expr
     DefPropPeak propertyName expr
     DefPropPrim propertyName expr

DESCRIPTION
     Define a property with the given name by the given
     expression. See SelectSpec for a description of the
     expression syntax. Properties can be used in other
     property definitions or selections. The Select
     commands are actually just special cases of the
     DefProp commands, they defines the property with
     the name "selected". The following properties are
     used internally by the program and should not be
     defined by this command:

          all
          visible

     The value of the "visible" property is maintained
     by the program, it is set for all spectra, peaks
     and primitives that have their attributes (Style*)
     set in a way to make them visible. This is very
     convenient for selecting only visible items.

     The "displayed" property is used by the program to
     decide which items should be displayed. It is not
     recommended to modify it, it is normally better to
     use the Style* commands for changing the visibility.
     It is very useful for spectra, however, but the
     DialSpec command is more convenient for modifying
     it in this case.

     The "movable" property is used by the program to
     decide which items are moved by rotations etc.
     It only has an influence for spectra, and the
     DialSpec command is more convenient for modifying it.

     Some properties are predefined, they can be seen
     in the file:

          $MOLMOLHOME/setup/PropDef

     or with the HelpProp command.

EXAMPLES
     DefPropPeak 'good' 'qual > 0.4'

SEE ALSO
     DialSelect, SelectSpec, ..., DialSpec, HelpProp

DATE
     960912

```
NAME
     DialColor - switch color dialog on and off

SYNOPSIS
     DialColor ( off | on )

DESCRIPTION
     Switch color dialog on and off. The color dialog
     is a convenient interface to the commands BackColor,
     ColorSpec, ColorPeak and ColorPrim.

EXAMPLE
     DialColor on

SEE ALSO
     BackColor, ColorSpec, ColorPeak, ColorPrim

DATE
     960912
```

NAME
     DialSelect – switch selection dialog on and off

SYNOPSIS
     DialSelect (off | on)

DESCRIPTION
     Switch selection dialog on and off. The selection
     dialog is a convenient interface to the commands
     SelectSpec, SelectPeak and SelectPrim.

EXAMPLE
     DialSelect on

SEE ALSO
     SelectSpec, ..., DefPropSpec, ...

DATE
     960912

NAME
     DialSpec – switch spectrum dialog on and off

SYNOPSIS
     DialSpec (off | on)

DESCRIPTION
     Switch spectrum dialog on and off. The spectrum dialog
     can be used to select spectra and for toggling their
     displayed and movable states. It is a convenient
     interface to the commands SelectSpec and DefPropSpec.

EXAMPLE
     DialSpec on

SEE ALSO
     SelectSpec, DefPropSpec

DATE
     960912

```
NAME
     DialStyle – switch style dialog on and off

SYNOPSIS
     DialStyle ( off | on )

DESCRIPTION
     Switch style dialog on and off. The style dialog
     is a convenient interface to the commands StyleSpec
     and StylePeak.

EXAMPLE
     DialStyle on

SEE ALSO
     SelectSpec, SelectPeak, DialSelect,
     StyleSpec, StylePeak

DATE
     960912
```

```
NAME
     DrawDelay – set drawing delay

SYNOPSIS
     DrawDelay expr

DESCRIPTION
     Set a delay for drawing. The program will pause
     for the given time (in milliseconds) after each
     redraw. This can be useful on machines without
     double buffering, to avoid too much flickering.

EXAMPLE
     DrawDelay 100

DATE
     960912
```

```
NAME
     DrawPrec – set drawing precision

SYNOPSIS
     DrawPrec expr

DESCRIPTION
     Set the precision for certain drawing operations,
     e. g. for the approximation of spheres. Making this
     value larger improves the drawing quality, but makes
     the drawing slower. Reasonable values are in the range
     between 2 (moderate quality) and 4 (good quality).

     The value used for plotting can be set seperately with
     the PlotPar command.

EXAMPLE
     DrawPrec 3

SEE ALSO
     PlotPar

DATE
     960912
```

```
NAME
     DrawSize – set size of drawing area

SYNOPSIS
     DrawSize ( set | save | restore ) [ expr expr ]

DESCRIPTION
     If the fist argument is 'set', set the size of the
     drawing are to the given width and height (in pixels).
     This can be useful in connection with plotting, so
     that the user can enforce a certain aspect ratio for
     the resulting plot.

     With the first argument 'save', the current size is
     saved, this size can be restored by executing the
     command with the first argument 'restore'. The saved
     size is also stored in parameter and dump files.

EXAMPLE
     DrawSize save
     DrawSize set 1000 750
     DrawSize restore

SEE ALSO
     PlotPar

DATE
     960912
```

NAME
     Expand – expand spectrum

SYNOPSIS
     Expand { expr expr }

DESCRIPTION
     Set the currently visible part of all selected
     spectrums. The part is given as a pair of
     coordinates (in points) in each direction. Regions
     will scale together with the spectrum they
     belong to. Calculation commands operating on
     spectra (Noise, Segment) only operate on the
     currently expanded region.

EXAMPLE
     Expand 1024 2047 256 511

SEE ALSO
     Resolution, Level, Scale

DATE
     960913

NAME
     Fog – setup of fog (depth cueing)

SYNOPSIS
     Fog (off | exp | exp2 | linear) expr expr expr

DESCRIPTION
     Set fog mode and parameters. The first argument
     selects the mode (off, exponential, squared
     exponential, linear). The second argument selects the
     density for both kinds of exponential fog. The third
     and fourth argument give the start and end distance
     for linear fog.

     Negative values for any of the numerical arguments
     will leave the value unchanged, this is useful for
     changing only one value if the command is put on a
     slider.

     Not all fog modes are supported on all hardware.

EXAMPLE
     Fog linear 0.1 7.0 13.0

DATE
     960912

NAME
     Fullscreen – switch fullscreen display on and off

SYNOPSIS
     Fullscreen (off | on)

DESCRIPTION
     Switch fullscreen display on and off. Fullscreen
     mode is usefull for making screen photos and it is
     required for stereo display on most machines. Note
     that the menu and the command line are not visible
     in fullscreen mode. If the Fullscreen command is in
     the popup menu (right mouse button), this is the
     easiest way to switch back to normal mode. You can
     also type commands in fullscreen mode, but it is not
     very convenient because there is no feedback.

EXAMPLE
     Fullscreen on

SEE ALSO
     Stereo

DATE
     960912

```
NAME
     HelpApropos - locate commands by keyword

SYNOPSIS
     HelpApropos string

DESCRIPTION
     Show a list of all commands that have the given
     keyword in their one-line description. The menu that
     the command can be found in is given in parentheses.
     The keyword may contain wildcard characters (?, *),
     the search is case insensitive.

EXAMPLE
     HelpApropos "plot"

SEE ALSO
     HelpCmd

DATE
     960912
```

NAME
     HelpButton – show definition of buttons

SYNOPSIS
     HelpButton

DESCRIPTION
     Show the file that contains the definition of the
     buttons.

EXAMPLE
     HelpButton

SEE ALSO
     PathNames

DATE
     960912

```
NAME
     HelpCmd - get help on command

SYNOPSIS
     HelpCmd

DESCRIPTION
     Switch to help mode. The next command that is entered
     on the command line or selected in the menu will not
     be executed, but the according help text will be
     displayed instead.

EXAMPLE
     HelpCmd

DATE
     960912
```

```
NAME
     HelpMouse – show help text about using the mouse

SYNOPSIS
     HelpMouse

DESCRIPTION
     Show a text that explains how to use the mouse.

EXAMPLE
     HelpMouse

DATE
     960912
```

```
NAME
     HelpProp - show definition of standard properties

SYNOPSIS
     HelpProp

DESCRIPTION
     Show the file that contains the definition of the
     standard properties.

EXAMPLE
     HelpProp

SEE ALSO
     PathNames, DefProp*, Select*

DATE
     960912
```

NAME
    Identify – identify simple peaks

SYNOPSIS
    Identify expr { expr } { expr } expr expr

DESCRIPTION
    Find the peaks that can be simply identified in all
    selected regions. The Segment command must be
    executed before using this command.

    The first argument gives a minimal amplitude for
    peaks identified, as factor of the noise level.
    This is typically between 2.0 and 5.0.

    The next arguments give a mimimal size (in data
    points) for each direction used for doing the
    necessary calculations of symmetry etc. This is
    typically chosen the same or somewhat less than
    the minimal size given for segmentation.

    The next arguments give a maximal splitting of
    peaks (in data points) for each direction.
    A value of 1.0 should be given if no splitting
    is expected.

    The next argument gives the allowed relative
    difference of amplitudes for split peaks. This
    is typically a very small value.

    The last argument is the maximum allowed symmetry
    error of a peak relative to its amplitude. If the
    error is larger than this value, it is considered
    to be consisting of multiple peaks. Typical
    values are between 0.1 and 0.5.

EXAMPLE
    Identify 3.0 3 2 5.0 1.0 0.02 0.5

SEE ALSO
    Segment, SelectSpec, ClusterShape

DATE
    960913

NAME
    InitAll – delete and initialize everything

SYNOPSIS
    InitAll (yes | no)

DESCRIPTION
    Delete all data and initialize the program. This can
    be used before starting with something new. It is
    also needed after changing certain parameters (see
    PathNames) to make sure that they take effect.

    The command asks for a confirmation.

EXAMPLE
    InitAll yes

SEE ALSO
    PathNames, RemoveSpec

DATE
    960912

```
NAME
     LabelPeak – set format of peak label

SYNOPSIS
     LabelAtom string

DESCRIPTION
     Set the format of the label of all selected peaks.
     If the character 'N' appears in the string, it is
     replaced by the peak number. 'A' is replace by the
     amplitude, 'S' by the symmetriy error, 'U' by the
     uniformity error, and 'Q' by the quality. All other
     characters are displayed in the label unchanged.

EXAMPLE
     LabelPeak "Q"

SEE ALSO
     SelectPeak

DATE
     960912
```

NAME
      LengthPeak – set length of line attached to peaks

SYNOPSIS
      LengthPeak expr

DESCRIPTION
      Set the length of the lines drawn from the center of
      all selected peaks. A line is only drawn when the
      style is 'circle'.

EXAMPLES
      LengthPeak 0.5

SEE ALSO
      SelectPeak, StylePeak, AnglePeak

DATE
      960912

NAME
     Level – set contouring level of spectra

SYNOPSIS
     Level expr

DESCRIPTION
     Set the minimal level of all selected spectra as
     fraction of the maximal value. For regions, the given
     value is automatically clamped at the segmentation
     level, so that a very small value can be given for
     displaying the whole region.

EXAMPLE
     Level 0.001

SEE ALSO
     Resolution, Expand, Scale, StyleSpec

DATE
     960913

```
NAME
     Light - setup of light source

SYNOPSIS
     Light ( off | point | infinite ) expr expr expr

DESCRIPTION
     The first argument selects between no light source,
     a point light source or a light source at infinity.
     The coordinates are used as position if a point light
     source was chosen as point, or only as direction for
     an infinite light source. Point light sources might
     not be supported on all hardware, or they may be
     slower than infinite light sources.

EXAMPLE
     Light point 0 5 5

DATE
     960912
```

NAME
     LineSpec – set style and width of spectrum lines
     LinePeak – set style and width of peak lines
     LinePrim – set style and width of primitive lines

SYNOPSIS
     LineSpec (solid | dashed) expr
     LinePeak (solid | dashed) expr
     LinePrim (solid | dashed) expr

DESCRIPTION
     Set the style and width of the lines used for
     drawing all selected spectra, peaks or primitives.
     The default width of 0 is the minimal width that
     can be drawn, it is also the one that can be
     drawn fastest.

EXAMPLE
     LinePrim solid 3

SEE ALSO
     Select*, Color*

DATE
     960912

NAME
     ListPropSpec – list all spectrum properties
     ListPropPeak – list all peak properties
     ListPropPrim – list all primitive properties

SYNOPSIS
     ListPropSpec
     ListPropPeak
     ListPropPrim

DESCRIPTION
     Lists the set properties of all selected spectra,
     peaks or primitives. All items have to share the
     same set of properties, an error message is
     issued otherwise.

EXAMPLES
     ListPropPeak

SEE ALSO
     DefProp*, Select*

DATE
     960912

NAME
     MaterialSpec – set material properties of spectra
     MaterialPeak – set material properties of peaks
     MaterialPrim – set material properties of primitives

SYNOPSIS
     MaterialSpec expr expr expr expr expr expr expr
     MaterialPeak expr expr expr expr expr expr expr
     MaterialPrim expr expr expr expr expr expr expr

DESCRIPTION
     Set the material properties of all selected spectra,
     peaks primitives. The first three paramters give the
     coefficients for ambient, diffuse and specular
     reflection. For good results, the ambient and
     diffuse terms should sum up to around 1.

     The fourth parameter gives the shininess, it only
     has an effect if the specular coefficient is not zero.
     Higher values for the shininess result in smaller
     specular highlights. Values can be from 1.0 (very
     dull) to 200 and more (highly polished metal).

     The fifth parameter gives the reflection. 1.0 results
     in a complete reflection of other objects in the scene
     (mirror), 0.0 in no reflection.

     The sixth parameter gives the opacity. 1.0 results
     in a completely opaque material, 0.0 in complete
     transparency.

     The seventh parameter gives the index of refraction,
     it only has an influence for (partly) transparent
     materials. 1.0 gives no refraction, 1.5 is the value
     for glass, 2.4 for diamond.

     Transparency is not supported on most hardware, and
     only to a limited amount on machines with high-end
     graphics. It is mainly useful for preparing files
     for ray tracing (PlotPOV). Reflection is not supported
     on screen, it is only used for ray tracing.

     Giving a value less than 0.0 for any value will not
     change it, this is useful for changing only part of
     the parameters.

EXAMPLES
     MaterialSpec 0.3 0.7 0.4 30 0.0 1.0 1.0

SEE ALSO
     Select*, Texture*, PlotPov

DATE
     960912

```
NAME
      Memory – set memory buffer size for spectrum input

SYNOPSIS
      Memory expr

DESCRIPTION
      Set the size of the memory buffer for input of
      spectra. The size is given in MBytes, the default
      value is 4. Making the value larger makes the reading
      of spectra faster, but requires more memory.

EXAMPLE
      Memory 16

SEE ALSO
      OpenBruker, OpenEasy

DATE
      960912
```

```
NAME
     MoveDrawobj - move draw object

SYNOPSIS
     MoveDrawobj expr expr expr expr

DESCRIPTION
     Move all selected draw objects (like lines or
     rectangles) by the given amount. The first argument
     gives the index of the control point (starting at 0)
     to be moved, the rest of the arguments give the
     amount of movement in each direction.

     Moving the control points of drawing objects is
     normally done interactively by using the middle
     mouse button.

EXAMPLE
     MoveDrawObj 0 0.3 0.1 0.2

SEE ALSO
     AddDrawobj, SelectPrim

DATE
     960912
```

```
NAME
     MovePrim – move primitive

SYNOPSIS
     MovePrim expr expr expr

DESCRIPTION
     Move all selected primitives by the given amount.
     Only circles, cylinders and texts can currently be
     moved. Moving texts is normally done interactively
     by using the middle mouse button.

EXAMPLE
     MovePrim 0.3 0.1 0.2

SEE ALSO
     SizeText, RadiusPrim

DATE
     960912
```

NAME
     MoveX – move spectra in X direction

SYNOPSIS
     MoveX expr

DESCRIPTION
     Move all movable (set with DialSpec) molecules by the
     given amount in X direction. Moving is normally done
     interactively by pressing the middle mouse button.
     This command is useful for being used in macros or
     for setting up the slider box.

EXAMPLE
     MoveX 10

SEE ALSO
     DialSpec, MoveY, MoveZ

DATE
     960912

NAME
      MoveY – move spectra in Y direction

SYNOPSIS
      MoveY expr

DESCRIPTION
      Move all movable (set with DialSpec) spectra by the
      given amount in Y direction. Moving is normally done
      interactively by pressing the middle mouse button.
      This command is useful for being used in macros or
      for setting up the slider box.

EXAMPLE
      MoveY 10

SEE ALSO
      DialSpec, MoveX, MoveZ

DATE
      960912

```
NAME
     MoveZ - move spectra in Z direction

SYNOPSIS
     MoveZ expr

DESCRIPTION
     Move all movable (set with DialSpec) spectra by the
     given amount in Z direction. Moving in Z direction is
     very similar to zooming, which is normally done
     interactively by pressing the left and the middle mouse
     buttons simultanously. The effect is somewhat different
     if a perspective projection is chosen, and also the
     clipping planes work differently.

EXAMPLE
     MoveZ 10

SEE ALSO
     DialSpec, MoveX, MoveY, Zoom*,
     ClipPos, ClipSize, Projection

DATE
     960912
```

```
NAME
      Noise – calculate noise values

SYNOPSIS
      Noise

DESCRIPTION
      Calculate noise values for all selected spectra.
      This must be done before using the Segment command.

      The program handles the noise as spectrum. By
      default it is invisible, but this can be changed
      with StyleSpec.

EXAMPLE
      Noise

SEE ALSO
      OpenBruker, OpenEasy, SelectSpec, Segment

DATE
      960913
```

```
NAME
      OpenBruker – open BRUKER file

SYNOPSIS
      OpenBruker fileName

DESCRIPTION
      Open a file in BRUKER format. The name given must be
      the name of a processed data file, e. g. 2rr, the
      parameter files will automatically be read from the
      same directory.

      2D spectra will be displayed as contours by default,
      spectra with more dimension will not be displayed
      until their style is changed with StyleSpec.

EXAMPLE
      OpenBruker /home/joe/data/foo/1/pdata/1/2rr

SEE ALSO
      OpenEasy, StyleSpec

DATE
      960913
```

```
NAME
     OpenEasy – open EASY file

SYNOPSIS
     OpenEasy fileName

DESCRIPTION
     Open a file in EASY format. The name given must be
     the name of a parameter file, the corresponding data
     file will automatically be read from the same
     directory.

     2D spectra will be displayed as contours by default,
     spectra with more dimension will not be displayed
     until their style is changed with StyleSpec.

EXAMPLE
     OpenEasy /home/joe/data/foo.param

SEE ALSO
     OpenBruker, StyleSpec

DATE
     960913
```

NAME
     PathNames – set path names

SYNOPSIS
     PathNames string string string

DESCRIPTION
     Set path names for some configuration files.
     Normally the program reads these file from the
     directory $MOLMOLHOME/setup.

     The following is a list of all configuration files:

          PropDef: Contains definitons of standard
             properties.

          MenuDir: Directory that contains menu definition
             files (MenuBar, *.menu, Popup, Valuator).

          ColorList: List of colors used for DialColor.

     Generally the configuration files are read when
     they are used the first time, and the contents is
     kept in memory. This means that changing the path
     only has an effect after leaving the program and
     starting it again. This is always true for MenuDir.
     It is also necessary for ColorList if the color
     dialog (DialColor) was opened and for PropDef as
     soon as a spectrum was loaded.

     If the file with the given path name cannot be
     openend, the program will silently fall back to the
     default file.

     The special name "0" can be given for path names,
     in this case an empty file will be taken for the
     corresponding configuration file.

EXAMPLE
     PathNames "myprop" "" ""

SEE ALSO
     DialColor, InitAll, DefProp*

DATE
     960913

```
NAME
     PlotCps - make a color PostScript plot

SYNOPSIS
     PlotCps fileName

DESCRIPTION
     Make a color PostScript plot of the current screen
     contents. If a nice plot of a schematic drawing is
     desired (shading, hidden surface elimination), this
     has to be selected with the command Rendering first.
     Hidden surface elimination of complex scenes can
     take a long time.

EXAMPLE
     PlotCps /home/joe/MyPlot.ps

SEE ALSO
     Rendering, Stereo, PlotPs

DATE
     960912
```

```
NAME
      PlotFm3 – make a FrameMaker 3 plot
      PlotFm4 – make a FrameMaker 4 plot

SYNOPSIS
      PlotFm3 fileName
      PlotFm4 fileName

DESCRIPTION
      Make a plot of the current screen contents in MIF
      format. This can be imported into FrameMaker.

      PlotFm3 produces a file that can be read by
      FrameMaker 3 or later. This only supports 8
      different colors.

      PlotFm4 makes use of color possibilities introduced
      in FrameMaker 4, these files cannot be read by
      earlier versions. They are also larger.

EXAMPLE
      PlotFm4 /home/joe/MyPlot.fm

SEE ALSO
      Rendering, PlotCps, PlotPs

DATE
      960912
```

```
NAME
     PlotJpeg - make a JPEG plot

SYNOPSIS
     PlotJpeg fileName

DESCRIPTION
     Save the current screen contents as JPEG File. The
     horizontal resolution can be set with the PlotPar
     command, the vertical resolution is calculated to
     maintain the aspect ratio of the screen.

     Note that that JPEG uses a lossy compression scheme,
     the quality factor can be adjusted with the PlotPar
     command.

     This command is not supported on all machines and
     with all graphics systems. It will give an appropriate
     error message if it is not supported.

     The freely available JPEG library written by the
     Independent JPEG Group is used for writing the JPEG
     file.

EXAMPLE
     PlotJpeg /home/joe/MyPlot.jpg

SEE ALSO
     PlotPar, PlotTiff, PlotPng,
     PlotFm3, PlotFm4, PlotCps, PlotPs

DATE
     960912
```

NAME
     PlotPar – set plot parameters

SYNOPSIS
     PlotPar expr expr expr expr expr
         (0 | 1) (0 | 1) (0 | 1) (0 | 1)
           expr expr expr

DESCRIPTION
     Set size and options for plots. The first argument
     gives the width of the paper, the second one the
     height. The third argument gives the width of the
     plot, the fourth one the height. If one of the plot
     sizes is 0, it is calculated to correspond to the
     dimensions (aspect ratio) of the window. The plot
     is centered on the paper.

     The current unit for these sizes is shown in the
     prompt, it can be changed with the PlotUnit command.
     The default paper size also depends on the current
     unit.

     The fifth argument selects the horizontal resolution
     used for saving image (TIFF, JPEG, PNG) files.

     The first option switches stereo plotting on or off.

     The second option switches shading and hidden surface
     elimination for the plot. The third only has an
     influence if shading is switched on. If it is
     selected, a full hidden surface elimination is done.
     This can take a few minutes for complex plots, but it
     is necessary to produce perfect results as soon as the
     scene contains spheres, cylinders or primitives. If it
     is not selected, a simple depth sorting is used, which
     is much faster, but the result can contain slight
     errors. For important plots (publications), this
     option must always be switched on.

     The fourth option selects whether the plot is
     rotated by 90 degrees to produce a landscape plot.
     Note that the size of the plot (arguments 3 and 4)
     is still given in the original orientation of the
     plot, before rotation. The size of the paper is
     given in the orientation used by the printer, which
     is normally portrait. So e. g. good size for a
     landscape plot on A3 format are 29.7 42 0 26.

     The third but last parameter select the precision
     (resolution) of the plot. See DrawPrec for an
     explanation of this parameter.

     The second but last parameter selects a gamma correction
     parameter. 1.0 will leave the colors unchanged, values
     less than 1.0 will make the colors brighter, values
     greater than 1.0 will make the colors darker. Note

that the "correct" gamma value depends on the output
device used, so using gamma correction when producing
the file is in principal not the right thing to do.
We offer this possibilty for convenience sake, it is
often difficult to do decent gamma correction on the
output file (e. g. for PostScript) with other
possibilities.

The last parameter selects the quality for JPEG plots.
Recommended values are between 50 (strong compression
with reasonable quality) and 95 (excellent quality).

EXAMPLES
    PlotPar 21 29.7 18 0 1000 0 0 1 0 3 1.0 75
    PlotPar 21 29.7 0 18 2000 0 1 1 1 3 0.7 60
    PlotPar 29.7 42 0 26 1500 0 1 1 1 4 0.5 90

SEE ALSO
    PlotUnit, PlotCps, PlotPs, PlotFm*,
    PlotTiff, PlotJpeg, PlotPng, DrawPrec

DATE
    960912

NAME
    PlotPng - make a PNG plot   - 52 -

SYNOPSIS
    PlotPng fileName

DESCRIPTION
    Save the current screen contents as PNG File. The
    horizontal resolution can be set with the PlotPar
    command, the vertical resolution is calculated to
    maintain the aspect ratio of the screen.

    This command is not supported on all machines and
    with all graphics systems. It will give an appropriate
    error message if it is not supported.

    The freely available PNG library written by
    Guy Eric Schalnat, Group 42, Inc., is used for writing
    the PNG file.

EXAMPLE
    PlotPng /home/joe/MyPlot.png

SEE ALSO
    PlotPar, PlotTiff, PlotJpeg,
    PlotFm3, PlotFm4, PlotCps, PlotPs

DATE
    960912

```
NAME
     PlotPov – make a POV-Ray plot

SYNOPSIS
     PlotPov fileName

DESCRIPTION
     Make a plot of the current screen contents in POV-Ray
     format. This can be used as input file for the ray
     tracing package POV-Ray (Persistence of Vision Ray
     Tracer) to produce high quality pictures.

     The POV-Ray software is available free of charge by
     anonymous ftp from ftp.povray.org, directory
     /pub/povray/Official. See the accompanying files for
     copyright conditions and instructions on installation
     and use of the program. The output files were tested
     with version 2.2 of POV-Ray.

EXAMPLE
     PlotPov /home/joe/MyPlot.pov

SEE ALSO
     PlotFm*, PlotCps, PlotPs

DATE
     960912
```

```
NAME
     PlotPs – make a black and white PostScript plot

SYNOPSIS
     PlotPs fileName

DESCRIPTION
     Make a black and white PostScript plot of the current
     screen contents.

EXAMPLE
     PlotPs /home/joe/MyPlot.ps

SEE ALSO
     Rendering, Stereo, PlotCps

DATE
     960912
```

```
NAME
     PlotTiff - make a TIFF plot

SYNOPSIS
     PlotTiff fileName

DESCRIPTION
     Save the current screen contents as TIFF File. The
     horizontal resolution can be set with the PlotPar
     command, the vertical resolution is calculated to
     maintain the aspect ratio of the screen.

     This command is not supported on all machines and
     with all graphics systems. It will give an appropriate
     error message if it is not supported.

     The freely available TIFF library written by
     Sam Leffler, Copyright (c) 1988-1995 Sam Leffler and
     Silicon Graphics, is used for writing the TIFF file.

EXAMPLE
     PlotTiff /home/joe/MyPlot.tif

SEE ALSO
     PlotPar, PlotJpeg, PlotPng,
     PlotFm3, PlotFm4, PlotCps, PlotPs

DATE
     960912
```

```
NAME
     PlotUnit – set unit of plot parameters

SYNOPSIS
     PlotUnit ( cm | mm | inch )

DESCRIPTION
     Set the unit used for paper and plot sizes in the
     PlotPar command. Changing the unit will also reset
     the paper size to the default associated with the
     unit, which is A4 for cm and mm and US Letter for
     inch.

EXAMPLE
     PlotUnit cm

SEE ALSO
     PlotPar

DATE
     960912
```

```
NAME
     PlotVrml – make a VRML plot              - 57 -

SYNOPSIS
     PlotVrml fileName

DESCRIPTION
     Make a plot of the current screen contents in VRML
     (Virtual Reality Modeling Language) format. VRML is
     the standard format for transferring and displaying
     three-dimensional geometry on the World Wide Web.
     The created files follow version 1.0 of the VRML
     specifications and can be displayed by any VRML
     browser.

EXAMPLE
     PlotVrml /home/joe/MyPlot.wrl

SEE ALSO
     PlotFm*, PlotCps, PlotPs, PlotPov

DATE
     960912
```

```
NAME
     Projection – choose projection

SYNOPSIS
     Projection ( orthogonal | perspective )

DESCRIPTION
     Choose between orthogonal and perspective projection.

EXAMPLE
     Projection orthogonal

SEE ALSO
     ClipPos, ClipSize, ViewAngle

DATE
     960912
```

```
NAME
     Quit - quit the program          - 59 -

SYNOPSIS
     Quit

DESCRIPTION
     Quit the program.

EXAMPLE
     Quit

DATE
     960913
```

```
NAME
     RadiusPeak - set radius of peaks

SYNOPSIS
     RadiusPeak expr

DESCRIPTION
     Set the radius of all selected peaks.

EXAMPLES
     RadiusPeak 0.1

SEE ALSO
     SelectPeak, StylePeak, LengthPeak, AnglePeak

DATE
     960912
```

```
NAME
     RecordMac – open macro recorder

SYNOPSIS
     RecordMac

DESCRIPTION
     Open a macro recorder. The text area shows the macro
     recorded so far, it can also be edited manually.
     The 'Add' button adds the most recently executed
     commands, the number of commands is given in the
     text field. If 'automatic' is switched on, each
     executed command is recorded automatically.

     The 'Test' button executes the recorded macro, the
     'Save' button stores it with the given file name.

EXAMPLE
     RecordMac

SEE ALSO
     XMacUser

DATE
     960912
```

NAME
     Register – register as AUTOPSY user

SYNOPSIS
     Register string string string string [string]

DESCRIPTION
     Send an E-mail to register as AUTOPSY user. The first
     argument gives your name, the second argument the name
     of the organisation (university/company) where you
     work, the third argument the S-mail address, the
     fourth argument the E-mail address. The fifth argument
     is the program name and release, just leave the value
     that is automatically filled in.

     Getting registered is strongly recommended, so that we
     can inform you of new releases and send you other
     useful information.

EXAMPLE
     Register "Joe User" "Useless Univ."
         "Street 42, Nowhere, USA" "joe@useless.edu"

DATE
     960912

```
NAME
     RemovePrim – remove primitive

SYNOPSIS
     RemovePrim

DESCRIPTION
     Remove all selected primitives (texts, etc.).

EXAMPLE
     RemovePrim

SEE ALSO
     AddTitle, AddText, AddDrawobj, SelectPrim

DATE
     960912
```

```
NAME
     RemoveSpec - remove spectra

SYNOPSIS
     RemoveSpec

DESCRIPTION
     Remove all selected spectra.

EXAMPLE
     RemoveSpec

SEE ALSO
     DialSpec

DATE
     960912
```

NAME
     Rendering – set rendering options

SYNOPSIS
     Rendering (0 | 1) (0 | 1) (0 | 1)
         (0 | 1) (0 | 1) (0 | 1) (0 | 1) (0 | 1)

DESCRIPTION
     Set some rendering options. Depending on the output
     device, some options may always be enabled, no
     matter whether they are switched on or off by this
     command. Some of these options (like two-sided
     lighting) are also used to generate plots, so the
     appropriate options have to be set before giving the
     plotting command.

     The following options are supported:

         Anti Aliasing: Draw smooth lines. This may not
             be supported on all hardware.

         Transparency: Use transparent drawing for objects
             that are not completely opaque. This may not
             be supported on all hardware.

         Fast Spheres Drawing: Instead of approximating
             spheres with many polygons, they are drawn
             as circles. This makes shading impossible,
             but can make the display much faster.

         Backface Elimination: Eliminate polygons that
             face away from the viewpoint at an early
             display step. This has normally no visual
             effect on the display, but can make it
             faster.

         Shading: Color polygons depending on the angle
             from the light source and the view point.
             This is also necessary for the support of
             depth cueing on most devices, e. g. for
             plotting.

         Two-sided Lighting: Normally lighting calculations
             are only done for the "outside" of an object.
             This triggers lighting calculation to be done
             for both sides. The effect is visible if
             objects are cut, mostly by the front clipping
             plane. It is not switched on by default on
             most devices because it can make all rendering
             slower.

         Depth Sorting: Sort all display elements by depth
             before drawing. This gives a quick, but
             sometimes unexact, method for hidden surface
             elimination.

Hidden Surface Elimination: Eliminate display
elements that are hidden by other elements
closer to the viewpoint. If the hardware
supports this feature, it is enabled by
default. If it has to be emulated by the
program, the display can get very slow.

EXAMPLE
    Rendering 0 0 0 1 1 0 1 0

SEE ALSO
    PlotPar PlotCps, PlotPs, PlotFm*, Fog

DATE
    960913

NAME
     Resolution – set display resolution

SYNOPSIS
     Resolution { expr }

DESCRIPTION
     Set the current display resolution (in number of
     points) for all selected spectra. The resolution
     is given with one integer value for each direction.

EXAMPLE
     Resolution 256 256

SEE ALSO
     Expand, Level, Scale

DATE
     960913

```
NAME
      RotateInit - undo all rotations

SYNOPSIS
      RotateInit

DESCRIPTION
      Bring all movable (set with DialSpec) spectra back
      to their original orientation.

EXAMPLE
      RotateInit

SEE ALSO
      DialSpec, RotateX, RotateY, RotateZ

DATE
      960912
```

NAME
     RotateX – rotate spectra around X axis

SYNOPSIS
     RotateX expr

DESCRIPTION
     Rotate all movable (set with DialSpec) molecules by
     the given angle around the X axis. Rotation is
     normally done interactively by pressing the left
     mouse button. This command is useful for being used
     in macros or for setting up the slider box.

EXAMPLE
     RotateX 90

SEE ALSO
     DialSpec, RotateY, RotateZ

DATE
     960913

NAME
      RotateY – rotate spectra around Y axis

SYNOPSIS
      RotateY expr

DESCRIPTION
      Rotate all movable (set with DialSpec) molecules by
      the given angle around the Y axis. Rotation is
      normally done interactively by pressing the left
      mouse button. This command is useful for being used
      in macros or for setting up the slider box.

EXAMPLE
      RotateY 90

SEE ALSO
      DialSpec, RotateX, RotateZ

DATE
      960913

```
NAME
      RotateZ – rotate spectra around Z axis

SYNOPSIS
      RotateZ expr

DESCRIPTION
      Rotate all movable (set with DialSpec) spectra by
      the given angle around the Z axis. Rotation is
      normally done interactively by pressing the left
      mouse button. This command is useful for being used
      in macros or for setting up the slider box.

EXAMPLE
      RotateZ 90

SEE ALSO
      DialSpec, RotateX, RotateY

DATE
      960913
```

```
NAME
     Scale - set contouring level of spectra

SYNOPSIS
     Scale expr

DESCRIPTION
     For all selected 2D spectra, set their scaling factor
     for amplitudes when they are displayed as surface.

EXAMPLE
     Scale 10.0

SEE ALSO
     Resolution, Expand, Level, StyleSpec

DATE
     960913
```

NAME
     Segment – spectrum segmentation

SYNOPSIS
     Segment expr expr expr expr (0 | 1) { expr }

DESCRIPTION
     Do a segmentation of all currently selected
     spectra. The Noise command must be executed before
     using this command.

     The first argument gives the level for segmentation,
     as factor of the noise level. This is normally
     around 1.0.

     The next argument gives a minimal level (also as
     factor of the noise level) for at least one of the
     points within a region. This is typically taken
     around 1.5 for high quality spectra, somewhat higher
     for spectra that are less well processed.

     The next two arguments select which/if the diagonal
     should be excluded. This is done by giving the two
     domains between which the diagonal should be
     excluded, this will normally be 0 and 1. If no
     diagonal exclusion is desired, 0 should be given
     for both domains.

     The next argument selects whether regions connected
     to the border of the spectrum should be excluded.
     In many spectra, the first/last rows are not
     properly baseline corrected, in this case this
     option should be selected.

     The remaining arguments give a minimal size (in data
     points) for each direction.

     The program handles the created regions as spectra.
     By default they are drawn as contours in 2D, and are
     invisible for more dimensions. This can be changed
     with StyleSpec.

EXAMPLE
     Segment 1.0 1.5 0 1 1 3 2

SEE ALSO
     OpenBruker, OpenEasy, SelectSpec, Noise, StyleSpec

DATE
     961004

NAME
     SelectSpec – select spectra
     SelectPeak – select peaks
     SelectPrim – select primitives

SYNOPSIS
     SelectSpec expr
     SelectPeak expr
     SelectPrim expr

DESCRIPTION
     Select spectra, peaks or primitives that satisfy a
     conditions specified by an expression. The expression
     must give a result of type boolean (truth value).

     There are two special values not covered by the
     expression syntax below. If an empty string is given
     as expression, everything is selected. If the value
     "0" is given, nothing is selected (i. e. everything
     deselected).

     The following is a formal sytax description of
     expressions in EBNF notation. Typical examples are
     shown in the next section.

```
     expr       = andExpr { "|" andExpr } .
     andExpr    = relExpr { "&" relExpr } .
     relExpr    = simpleExpr [ relOp setExpr ] .
     relOp      = "=" | "!=" | "<=" |
                  "<" | ">=" | ">" .
     setExpr    = rangeExpr { "," rangeExpr } .
     rangeExpr  = simpeExpr [ ".." simpleExpr ] .
     simpleExpr = term { addOp term } .
     addOp      = "+" | "-" .
     term       = factor { mulOp factor } .
     mulOp      = "*" | "/" | "%" .
     factor     = [ "-" | "sqrt" | "log" | "!" ] primary .
     primary    = constant | designator | "(" expr ")" .
     constant   = string | int | float .
     designator = [ qual "." ] field [ "[" int "]" ] .
     qual       = "spec" | "peak" | "prim"
     field      = "num" | "number" | "name" | "attr" |
                  "amp" | "symm" | "unif" | "qual" |
                  "shift0" | "shift1" |
                  "shift2" | "shift3" |
                  "width0" | "width1" |
                  "width2" | "width3" |
                  propertyName .
```

     For selecting items by their number or name,
     there is a shorter notation of the form:

```
     expr     = exprPart { exprPart } .
     exprPart = [ "#" set ] .
     set      = sel { "," sel } .
     sel      = string | range .
```

- 74 -

```
        range     = int ".." int | int "-" int .
```

Strings are not quoted in this notation.

The full and the short notation can be mixed, in
this case a part written in the short notation
behaves like a primary with a boolean value.

EXAMPLES
```
    SelectSpec 'num > 2'
        # all spectra but the first two
    SelectPeak 'qual > 0.3 & width0 > 4.0 & width1 > 1.0'
        # all peaks with minimal quality of 0.3 and
        # minimal line widths 4.0 and 1.0
```

SEE ALSO
    DialSelect, DefPropMol,... , DialMol

DATE
    960913

```
NAME
     ShadePeak – set shading of peaks

SYNOPSIS
     ShadePeak ( none | flat | gouraud | phong |
        dots | lines )

DESCRIPTION
     Set the shading method for peaks if they are
     displayed as spheres.

        none:     no shading
        flat:     polygons shaded in uniform color
        gouraud:  color interpolated between vertices
        phong:    normals interpolated, highest quality
        dots:     draw surface using dots
        lines:    draw surface using lines

     Not all graphics devices support all shading methods.

EXAMPLE
     ShadePeak phong

SEE ALSO
     SelectPeak, StylePeak, ColorPeak

DATE
     960913
```

NAME
     ShadePrim – set shading of primitives

SYNOPSIS
     ShadePrim (none | flat | gouraud | phong |
         dots | lines)

DESCRIPTION
     Set the shading method for primitives.

         none: no shading
         flat: polygons shaded in uniform color
         gouraud: color interpolated between vertices
         phong: normals interpolated, highest quality
         dots: draw surface using dots
         lines: draw surface using lines

     Not all graphics devices support all shading methods.

EXAMPLE
     ShadePrim phong

SEE ALSO
     SelectPrim, ColorPrim

DATE
     960913

```
NAME
     ShadeSpec – set shading of spectra

SYNOPSIS
     ShadeSpec ( none | flat | gouraud | phong |
         dots | lines )

DESCRIPTION
     Set the shading method for spectra if they are
     displayed as surfaces.

         none:    no shading
         flat:    polygons shaded in uniform color
         gouraud: color interpolated between vertices
         phong:   normals interpolated, highest quality
         dots:    draw surface using dots
         lines:   draw surface using lines

     Not all graphics devices support all shading methods.

EXAMPLE
     ShadeSpec phong

SEE ALSO
     SelectSpec, StyleSpec, ColorSpec

DATE
     960913
```

```
NAME
     SizeText – resize text

SYNOPSIS
     SizeText ( abs | rel ) expr

DESCRIPTION
     Resize all selected text primitives. If the first
     argument is 'abs', all sizes are set to the given
     value. If it is 'rel', the given value is added to
     the current size.

     Resizing texts is normally done interactively by
     using the middle mouse button.

EXAMPLE
     SizeText abs 0.15

SEE ALSO
     MovePrim

DATE
     960913
```

```
NAME
     StartAnim – start animation

SYNOPSIS
     StartAnim ( once | cycle ) int

DESCRIPTION
     Start an animation. This can be used for displaying
     series of spectra. If the first argument is "once",
     every selected spectrum will be displayed once. If
     it is "cycle", the program will loop through all
     selected spectra until the StopAnim command is
     executed.  The second argument is the minimal delay
     in milliseconds between displaying spectra.

     It is possible to execute the command while an
     animation is running, e. g. for changing the delay.

EXAMPLE
     StartAnim cycle 50

SEE ALSO
     SelectSpec, DialMol, StopAnim

DATE
     960913
```

```
NAME
     StartRock – start rock

SYNOPSIS
     StartRock ( once | cycle ) int

DESCRIPTION
     Start to rotate spectra automatically. There
     are parameters for two phases, so that it is
     possible to rotate back and forth. If the first
     argument is "once", the movement will only happen
     once. If it is "cycle", the program will repeat it
     until the StopRock command is executed.
     The second argument is the minimal delay in
     milliseconds between rotations. The rest of the
     arguments are rotation angles for all three axis
     and number of steps.
     It is possible to execute the command while
     rocking is running, e. g. for changing the delay.

EXAMPLE
     StartRock cycle 50 0 10 0 18 0 –10 0 18

SEE ALSO
     StopRock

DATE
     960913
```

NAME
      Stereo – set stereo mode

SYNOPSIS
      Stereo (off | left | right | side_by_side |
          cross_eye | hardware)

DESCRIPTION
      Set stereo mode. Hardware stereo is not supported by
      all hardware. If it is supported, it normally works
      only in fullscreen mode (see command Fullscreen).

      Hardware stereo is also supported for certain plot
      devices. E. g. generating a PostScript plot in
      hardware stereo mode will produce a side by side
      stereo image with the correct eye distance, while
      the distance between the images will very likely
      be wrong when plotting in side_by_side mode.

EXAMPLE
      Stereo side_by_side

SEE ALSO
      Fullscreen

DATE
      960913

```
NAME
     StopAnim – stop animation

SYNOPSIS
     StopAnim

DESCRIPTION
     Stop an animation started with StartAnim.

EXAMPLE
     StopAnim

SEE ALSO
     StartAnim

DATE
     960913
```

```
NAME
     StopRock - stop rock

SYNOPSIS
     StopRock

DESCRIPTION
     Stop automatic rotation started with StartRock.

EXAMPLE
     StopRock

SEE ALSO
     StartRock

DATE
     960913
```

```
NAME
     StyleDrawobj – set display style of draw objects

SYNOPSIS
     StyleDrawobj ( invisible | line | cylinder | neon )

DESCRIPTION
     Set the display style of all selected draw objects
     (lines etc.). The style cylinder draws the object as
     a cylinder with flat ends, neon draws it as cylinder
     with round ends.  Not all display styles are supported
     for all draw objects types.

EXAMPLE
     StyleDrawobj cylinder

SEE ALSO
     SelectPrim, AddDrawobj, ColorPrim

DATE
     960913
```

```
NAME
     StylePeak - set display style of peaks

SYNOPSIS
     StylePeak ( invisible | circle | cross )

DESCRIPTION
     Set the display style of all selected peaks.
     The style 'circle' is drawn as sphere for 3D
     display, 'cross' as tetrahedron.

EXAMPLE
     StylePeak sphere

SEE ALSO
     SelectPeak

DATE
     960913
```

```
NAME
     StyleSpec – set display style of spectra

SYNOPSIS
     StyleSpec ( invisible | grid | surface | contour )

DESCRIPTION
     Set the display style of all selected spectra.

EXAMPLE
     StyleSpec contour

SEE ALSO
     SelectSpec

DATE
     960913
```

NAME
    Symmetrize – symmetrize peak list

SYNOPSIS
    Symmetrize expr expr expr

DESCRIPTION
    Modify the quality setting of the peaks of all
    selected spectra depending on the symmetry of
    the peak list.

    The first two arguments give the two domains
    that are used for calculating the symmetric
    position of a peak, these are normally 0 and 1.

    The last argument gives the maximal distance
    allowed from the perfectly symmetric position
    for a pair of peaks to be considered symmetric.

EXAMPLE
    Symmetrize 0 1 0.01

SEE ALSO
    SelectSpec, Identify, Deconv

DATE
    960913

```
NAME
     System – execute operating system command

SYNOPSIS
     System string

DESCRIPTION
     Pass the command given as argument for execution
     by the operating system. Since MOLMOL is currently
     only running on UNIX, this will generally be a
     UNIX command.

EXAMPLE
     System 'lp tt.ps'

DATE
     960913
```

NAME
      TextureSpec – set texture of spectra
      TexturePeak – set texture of peaks
      TexturePrim – set texture of primitives

SYNOPSIS
      TextureSpec string expr expr expr
      TexturePeak string expr expr expr
      TexturePrim string expr expr expr

DESCRIPTION
      Set the texture mapping parameters of all selected
      spectra, peaks or primitives. The first parameter
      gives the name of a texture, the second paramter
      its scaling factor.

      The third parameter determines the amount of
      bumpiness of the surface. 0.0 results in a smooth
      surface, 1.0 in a very bumpy surface. The fourth
      paramter is a scaling factor for the bump pattern,
      a larger scaling factor will result in wider bumps.

      Texture mapping is not supported on screen, these
      parameters are used for preparing files for
      ray-tracing (PlotPov).

      The texture name must appear in the texture definition
      file of POV-Ray (textures.inc). If a texture is
      selected, the attributes of this texture will override
      the colors and material properties selected otherwise.
      If the name has the extension ".gif", it is assumed to
      be the name of a GIF file which is used as image map.

      Giving a value of 'as is' for the texture name or
      less than 0.0 for any numerical argument will not
      change it, this is useful for changing only part of
      the parameters.

EXAMPLES
      TextureSpec 'Blood_Marble' 0.5 0.0 1.0
      TexturePeak '' 1.0 0.5 1.0

SEE ALSO
      Select*, Color*, Material*, PlotPov

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```
NAME
     UndefProp – undefine property

SYNOPSIS
     UndefProp propertyName

DESCRIPTION
     Undefine the property with the given name everywhere.
     This command is rarely used. The program cannot detect
     if a property is not used anymore. Executing this
     command with unused properties can help to avoid
     problems (like unnecessarily large dump files or
     overflow of internal tables), especially when a lot
     of different properties are used.

EXAMPLES
     UndefProp good

SEE ALSO
     DefProp*

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```

```
NAME
     UserInterface – switch elements of user interface

SYNOPSIS
     UserInterface ( 0 │ 1 ) ( 0 │ 1 ) ( 0 │ 1 )
          ( 0 │ 1 ) ( 0 │ 1 ) ( 0 │ 1 )

DESCRIPTION
     Switch various parts of the user interface on or
     off. The following elements can be switched:

          Valuator Box
          Log Window
          Buttons
          Command Line
          Status Line
          Menubar

     The program makes sure that Command Line and
     Menubar are not switched off at the same time,
     because this would make it impossible to enter
     any more commands.

EXAMPLE
     UserInterface 0 0 1 1 1 1

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```

```
NAME
     ViewAngle – set view angle

SYNOPSIS
     ViewAngle expr

DESCRIPTION
     Set the view angle. For orthogonal projection, this
     influences only the size (zooming factor) of the
     display, for perspective projection, a larger view
     angle leads to a stronger perspective. The value
     is given in radians.

EXAMPLE
     ViewAngle 0.5

SEE ALSO
     Projection, ClipPos, ClipSize

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```

```
NAME
     WritePeak – write peak list

SYNOPSIS
     WritePeak fileName

DESCRIPTION
     Write all currently selected peaks to a peak
     list. The format corresponds to the one used by
     the latest version of XEASY.

EXAMPLE
     WritePeak /home/joe/easy/autopsy.peaks

SEE ALSO
     SelectPeak

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```

```
NAME
     WriteRotation – write current rotation

SYNOPSIS
     WriteRotation fileName

DESCRIPTION
     Write the current rotation of the first selected
     spectrum to a macro file. Executing this macro
     with XMacUser will restore the orientation. At
     least one spectrum must be selected.

EXAMPLE
     WriteRotation /home/joe/macros/rotate.mac

SEE ALSO
     XMacUser, RotateInit, RotateX, RotateY, RotateZ

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```

NAME
     XMacStand – execute standard macro
     XMacUser – execute user macro

SYNOPSIS
     XMacStand fileName
     XMacUser fileName

DESCRIPTION
     Execute a macro file. A macro file is a sequence of
     commands like they are entered on the command line.
     A history of all executed commands of each session
     is maintained in the file molmol/history in the
     users home directory. It can be used as macro.

     The two commands only differ in their search path.
     XMacStand by default searches in $MOLMOLHOME/macros,
     while XMacUser uses the current directory as
     default search path.

     Additonally to regular commands, macros can also
     contain command definitons. Once a macro with a
     command definiton is read in, this command can be used
     like a builtin MOLMOL command. A command definition
     has the syntax:

          define CommandName
          help one-line-help
          $arg1 = default1 prompt1
          ..
          $argN = defaultN promptN
          Command1
          ..
          CommandN
          end

     The help line is optional. The command can have any
     number of arguments (including zero). If no default
     value is given, the empty string is assumed the first
     time the command is executed, the previous value from
     there on. If the prompt is missing, the name of the
     argument is taken. If default values or prompts
     contain blanks or other special characters, they have
     to be written in single or double quotes.

     At least one command must be present in the body.
     Empty lines and comments (staring with #) are allowed,
     the lines can be indented for better readability.

     In the body, the arguments can be referenced by
     $arg or ${arg}. Any command can be used.

     Example:

          define ZoomRotate
            help zoom and rotate in one step

```
        $Zoom = 1.5
        $rotY = 90 "Rotate Y"

        ZoomRel $Zoom
        RotateY $rotY
     end
```

EXAMPLE
      XMacUser /home/joe/macros/my_favorite.mac

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```
NAME
      ZoomAbs - zoom absolute
      ZoomRel - zoom relative

SYNOPSIS
      ZoomAbs expr
      ZoomRel expr

DESCRIPTION
      Enlarge/reduce the size of the display. ZoomRel
      changes the size by a given factor, relative to the
      current size.  Factors greater than 1 make the
      display larger, factors less than 1 make it smaller.
      ZoomAbs sets the zoom factor to an absolute value.

      ZoomAbs, in conjunction with PlotPar, can be used to
      produce different plots with the same scale. If the
      zoom factor and the plot size are set to the same
      values, the scales will be identical.

      Zooming is normally done interactively by pressing
      the left and the middle mouse button.

EXAMPLES
      ZoomAbs 0.2
      ZoomRel 1.4

SEE ALSO
      PlotPar

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```