NAME

vimol - a powerful molecular viewer and editor with vi-like controls.

SYNOPSIS

vimol [*files*]

DESCRIPTION

vimol is a powerful molecular viewer and editor with vi-like controls. It supports viewing and editing of PDB and XYZ files. Multiple files can be edited simultaneously with convenient navigation between open tabs. Multi-frame file support is implemented for both PDB and XYZ formats.

KEY BINDINGS

The default key bindings are described below. The following notation is used throughout:

S- Shift key.
C- Ctrl key.

Arrow keys are equivalent to [hjkl] keys. Most commands operate on an atom selection, (sel). An explicit atom index can be specified with number keys [0-9] for such commands. See the *SELECTIONS* section for more details.

(sel)a Fill unsatisfied valencies of selected atoms with hydrogen atoms.
S-a Select all hydrogen atoms.
(sel)b Toggle a bond between two selected atoms.
(sel)c Center selection in a window.
(sel)S-c Center and fit selection to a window.
(sel)d or (sel)Delete
Delete selected atoms.
e Clear selection.
[fg] Zoom in/out.
S-[fg] Rotate the camera along the view axis.
[hjkl] Rotate the camera.
S-[hjkl] Move the camera.
i Toggle display of atom indices.
S-i Toggle display of atom names.
(sel)m Measure position, distance, angle, or torsion depending on the number of selected atoms. For example, 123m displays the position of an atom with index 123.
(sel)n Select all atoms which are within the 4 angstrom radius of atoms in the current selection.
o Toggle display of the coordinate system origin and axes.

(sel)S-o	Move selection to the coordinate system origin.
p or C-v	Paste atoms to the current tab.
q	Quit **vimol**.
S-q	Quit **vimol** discarding unsaved changes.
r	Start recording of issued commands. Recordings can be replayed by pressing ‘t’.
123s	Select an atom with index 123.
(sel)S-s	Select all atoms directly connected to the selected atoms.
t	Replay last recording. Period key ‘.’ with count can be used to repeat many times after that.
123u	Unselect an atom with index 123. Unselect last selected atom if no index is specified.
(sel)v	Hide selected atoms. Atoms can be made visible again by pressing ‘z’.
(sel)w	Select whole molecules containing selected atoms. 123w selects the molecule to which atom 123 belongs.
S-w	Select all water molecules.
(sel)x or (sel)C-x	Cut (copy and delete) selected atoms.
(sel)y or (sel)C-c	Copy selected atoms.
z	Show all hidden atoms.
C-a	Select all atoms.
C-[hjklfg]	Rotate selected atoms.
CS-[hjkl]	Move selected atoms.
C-r	Redo last change.
C-z	Undo last change.
123.	Repeat last command 123 times.
=	Invert current selection.
Space	Toggle full screen mode.
‘	Reset the view.
[	Go to the previous frame.
]	Go to the next frame.
{	Go 100 frames backward.
}	Go 100 frames forward.
<	Switch to the previous tab.
>	Switch to the next tab.

SELECTIONS

An atom selection, *sel*, can be specified in various ways.

First, an explicit atom index can be provided using number keys [0-9]. This is useful with key combinations. For example, 123d deletes an atom with index 123.

Atom indices can be explicitly listed on the command line (see the *COMMANDS* section). The indices are separated by a space character. Index ranges can be specified using colon ‘:’. For example, 6:8 specifies atoms with indices 6, 7, 8. Negative indices are used to count backwards starting from the last index, i.e., -1 is the last atom. An asterisk ‘*’ can be used to specify all atoms.

Finally, if no explicit index is specified and no command-line arguments are listed, selected atoms from the current tab are used.

COMMANDS

Below is the list of available commands. Command mode is started by pressing the colon key ‘:’. Most of the commands are bound to a key for convenience (see the *KEY BINDINGS* section). Multiple commands can be separated by a semicolon.

about Display information about **vimol**.

add-hydrogens [*sel*]
Fill unsatisfied valencies of atoms in selection *sel* with hydrogen atoms.

atom [*element* [*x y z*]]
Create an atom with coordinates *x y z*. The default is to create a carbon atom at coordinate origin.

bind *key* [*command*]
Bind key to command. Display current binding if *command* is not specified.

bond [*sel*]
Toggle a bond between two atoms. The selection *sel* must contain exactly two atoms.

chain [*n*]
Create a carbon chain of length *n*. The default *n* is 4.

clo[se] Close current tab.

clo[se]!
Close current tab discarding unsaved changes.

copy [*sel*]
Copy atoms from selection *sel* to a copy-buffer.

delete [*sel*]

Delete atoms in selection *sel*.

first-tab

(alias: **first**)

Switch to the first tab.

frame [*n*]

Go to a specific frame *n*. Count from the end if *n* is negative, i.e., -1 is the last frame.

fullscreen

Toggle full screen mode.

hide-selection [*sel*]

Hide atoms specified by *sel*.

invert-selection

Invert current selection.

last-tab

(alias: **last**)

Switch to the last tab.

measure [*sel*]

Measure position, distance, angle, or torsion depending on the number of atoms in selection.

move-selection *x y z* [*sel*]

Move selection by the specified amount. The displacement *x y z* is relative to the camera coordinate system.

move-selection-to *x y z* [*sel*]

Move selection center to the coordinates *x y z*.

next-frame [*n*]

Switch to the next frame. Number of frames to advance, *n*, can optionally be specified. It can be negative.

next-tab

Switch to the next tab.

open [*path*]
(alias: **new**)
Open file in a new tab.

paste Paste atoms from a copy-buffer to the current tab.

prev-tab
Switch to the previous tab.

quit
(alias: **q**)
Quit **vimol**.

quit!
(alias: **q!**)
Quit **vimol** discarding unsaved changes.

record Start recording of issued commands. A recording can be replayed using **replay** command.

redo Redo last change.

rename *name* [*sel*]
Set a new name for all atoms in selection.

replay Replay last recording.

reset-bonds
Reset all bonds.

ring [*n*]
Create a carbon ring of size *n*. The default *n* is 6.

rotate-selection *a b c* [*sel*]
Rotate selected atoms. Rotation angles relative to the camera coordinate system are specified by *a b c*.

select [*sel*]
(alias: **s**)
Add atoms specified by *sel* to the current selection.

select-connected [*sel*]
Select all atoms directly connected to atoms in selection *sel*.

select-element *name* ...
Select all atoms of a particular type. This command takes a list of element names. Atoms of those types will be added to the current selection. For example,

```
select-element H N
```

selects all hydrogen and nitrogen atoms.

select-molecule [*sel*]
For each atom in selection *sel*, select the whole molecule containing the atom.

select-within *radius* [*sel*]
Select all atoms which are within a specified *radius* of atoms in the selection *sel*.

select-water
Select all water molecules.

select-x [*x*]
Select atoms with x coordinate grater than *x*. Invert selection to get the complementary set of atoms. This is useful for making solvation boxes. The default *x* is 0.

select-y [*y*]
Select atoms with y coordinate grater than *y*. Invert selection to get the complementary set of atoms. This is useful for making solvation boxes. The default *y* is 0.

select-z [*z*]
Select atoms with z coordinate grater than *z*. Invert selection to get the complementary set of atoms. This is useful for making solvation boxes. The default *z* is 0.

set *setting* [*value*]
Set the *setting* to a new value. Current value is displayed if the second argument is omitted. See the *SETTINGS* section for the list of available options.

show-all
Show all hidden atoms.

source *path*
Execute commands from a file.

toggle *setting*
Toggle a boolean setting. See the *SETTINGS* section for the list of available options.

undo Undo last change.

unselect [*sel*]
(alias: **u**)
Remove atoms specified by *sel* from the current selection. Unselect last selected atom if the argument is omitted.

view-center-selection [*sel*]
Center selection in a window.

view-fit-selection [*sel*]
Center and fit selection to a window.

view-move *x y z*
Move the camera. Arguments *x y z* specify a displacement.

view-reset
Reset the view.

view-rotate *a b c*
Rotate the camera. Arguments *a b c* specify rotation angles.

view-zoom *factor*
Change zoom. *factor* should be a number close to 1.

write [*path*]
(alias: **w**)
Write changes to a file. Save to the current file if *path* is not specified.

SETTINGS

The following settings control various aspects of **vimol**. They can be changed using the **set** command. Boolean settings can be switched on/off using the **toggle** command. Colors are specified using an RGB value. For example, red is 255 0 0.

atom-size
(type: **float**)
Atom size used for drawing.

atom-visible
(type: **boolean**)
Specifies whether to draw the atoms.

bg-color
(type: **color**)
Background color.

bond-size
(type: **float**)
Bond size used for drawing.

bond-visible
(type: **boolean**)
Specifies whether to draw the bonds.

id-color
(type: **color**)
Color of atom index labels.

id-font
(type: **string**)
Atom index label font.

id-font-size
(type: **float**)
Atom index label font size.

id-visible
(type: **boolean**)
Atom index label visibility.

name-color
(type: **color**)
Color of atom name labels.

name-font
(type: **string**)
Atom name label font.

name-font-size
(type: **float**)
Atom name label font size.

name-visible
(type: **boolean**)
Atom name label visibility.

origin-color
(type: **color**)
Color of coordinate system axes and labels.

origin-font

(type: **string**)

Coordinate system axis labels font.

origin-font-size

(type: **float**)

Coordinate system axis labels font size.

origin-line-width

(type: **float**)

Coordinate system axis line width.

origin-visible

(type: **boolean**)

Specifies whether to draw coordinate system axes and labels.

selection-color

(type: **color**)

Color of atom selection markers.

selection-size

(type: **float**)

Size of atom selection markers.

statusbar-color

(type: **color**)

Status bar background color.

statusbar-error-color

(type: **color**)

Status bar error text color.

statusbar-font

(type: **string**)

Status bar text font.

statusbar-font-size

(type: **float**)

Status bar font size.

statusbar-text-color

(type: **color**)

Status bar text color.

statusbar-visible

(type: **boolean**)

Status bar visibility.

color-x

(type: **color**)

Color of an unknown element. Colors of common elements can be specified using **color-h**, **color-he**, **color-li**, and so on.

FILES

~/.vimolrc

Commands from this file will be executed on each **vimol** start. It can be used to customize various settings, such as background color.

~/.vimolhistory

Stores **vimol** command-line history.

AUTHORS

vimol was developed by Ilya Kaliman