

# UMV User Manual

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UNEX Molecular Viewer (UMV) is a program for fast and easy visualization of molecular structures produced by the [UNEX](#) program. Additionally UMV can visualize structures from files in the following formats:

- [Gaussian](#)
- [US GAMESS](#)
- [Firefly](#)
- [Cfour](#)
- [XYZ](#)
- WFN (conventional PROAIM wavefunction) files.
- [MDL Mol](#) [1]

## Installation and running

Copy UMV files to some directory, for example `~/Apps/UMV`, and add this directory to your PATH environment variable. Now UMV can be started from command line just as

```
$ umv structure.xyz
```



Note, UMV uses Qt5 library. The Windows and OSX versions of UMV come already with the required library files. In Linux you have to install Qt5 (including Qt5OpenGL) before using UMV.

## Using the Program

Upon starting UMV reads all available sets of Cartesian coordinates from the input file and shows the structure corresponding to the last set of the coordinates. The structures can be switched by using **Left** and **Right** arrow keys. The graphical style of structures can be changed by using **Up** and **Down** arrow keys. With mouse you can rotate molecules and scale their size. Left mouse clicks mark corresponding atoms. Up to four atoms can be marked at the same time. By right click UMV prints values of geometrical parameters, related to the marked atoms. Depending on the number of marked atoms UMV can print values of interatomic distances, angles, dihedral (torsion) and out-of-plane angles and also centroids of atom triplets.

Functional keys:

- **C** — print Cartesian coordinates for all atoms of the current structure.
- **B** — add or remove bond between two marked atoms.
- **H** — toggle visibility of hydrogen atoms.
- **F3** — change background.
- **F4** — generate large image of the structure and write it to a PNG file in the current directory.

- **F5**— make screenshot of the UMV window.

## Support

If you have questions or comments you can write an e-mail to the main UMV developer, Dr. Yury V. Vishnevskiy: [yu.v.vishnevskiy@gmail.com](mailto:yu.v.vishnevskiy@gmail.com)

## References

[1] A. Dalby *et al.*, “Description of several chemical structure file formats used by computer programs developed at Molecular Design Limited,” *J. Chem. Inf. Comput. Sci.*, vol. 32, no. 3, pp. 244–255, 1992, doi: 10.1021/ci00007a012.