# DIAMOND 

Crystal and Molecular Structure Visualization



## New Features

- The new POV-Ray interface lets you prepare photorealistic graphics containing sky spheres, multiple light sources, textures and shadows.
- Best or hkl planes and lines are available for both display and evaluation of geometric information like distances or angles between planes, lines and points.
- Vectors can be assigned to atoms e.g. to indicate a magnetic moment.
- Powder diffraction data can be calculated and displayed in both table and diagram, with automatic update when structural parameters change.
- Video sequences can be recorded to create e.g. AVI files.
- An optional assistant helps you to create a (new) structure picture. A variant of this assistant, the AutoBuilder, can create pictures automatically or according to a user-defined strategy. This is helpful when you frequently change the structural parameters or browse through data sets from crystal structure databases.
- A Diamond 3 document may contain multiple structural parameter sets and multiple pictures for every structure in a document. You can copy or shift structures or pictures between different documents. (Diamond 2 format is of course automatically supported during opening or saving of DSF files.)
- Pictures associated to a structure or all pictures of a document can now be surveyed in thumbnail view.
- Online update (automatic or manual)


## System Requirements

- MS Windows 98, ME, 2000, XP, Vista (NT 4 on request)
- Microsoft Internet Explorer 5.01 (or higher)
- 64 MB of RAM (or more)
- 100 megabytes of free disc space (or more)
- Graphics resolution: $1024 \times 768$, high color

Diamond, the well-known and wide-spread program for the visualization and exploration of crystal structures, has entered its third round!
Many of the functions of version 2 have been enhanced and improved, and a lot of new features have been added.
Please find the lists of improvements and new features below. Visit our Diamond web pages for more detailed information:
http://www.crystalimpact.com/diamond

## Download the free-of-charge trial version from

 the Diamond web page:http://www.crystalimpact.com/diamond

## Enhanced Functions

- Structures with no cell and symmetry given are now supported directly. These can be converted into crystal structures and vice versa.
- Additional molecular file formats and an optional data import assistant to confirm the (automatically detected) file format.
- The models ball-and-stick, wire, space-filling, and ellipsoid can now be assigned to individual atoms or groups of atoms rather than defined globally, which allows to mix different models within one structure picture.
- ORTEP-like styles, such as open octants, are not more limited to flat mode but also available in rendering mode.
- Improved layout mode for printout pages, new layout format for fixed-sized bitmaps. Improved automatic adjustment and placement of objects in the window or on the page, rsp.
- Distances and angles table now provide histograms and statistics.
- Walk-through mode and several more enhancements for movements. New spin option to accelerate motion in tracking mode.
- The Object Info window has been enhanced to a new Property window and shows information in context with the current situation, e.g. properties of the selected atom, distances and angles between the selected atoms, and many more.

Prices*

|  | non-profit org. profit.org. |  |
| :--- | :---: | :---: |
| Single licence: | $599 €$ | $1,198 €$ |
| Site licence ${ }^{* *}:$ | $1,198 €$ | $2,396 €$ |
| Campus licence $^{* * *}:$ | $2,396 €$ | $4,792 €$ |

* Prices do not include V.A.T., which may be due.
** Unlimited number of installations within one institute/dept.
*** Unlimited number of installations within one university/company
Prices for version updates and licence upgrades on request.

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