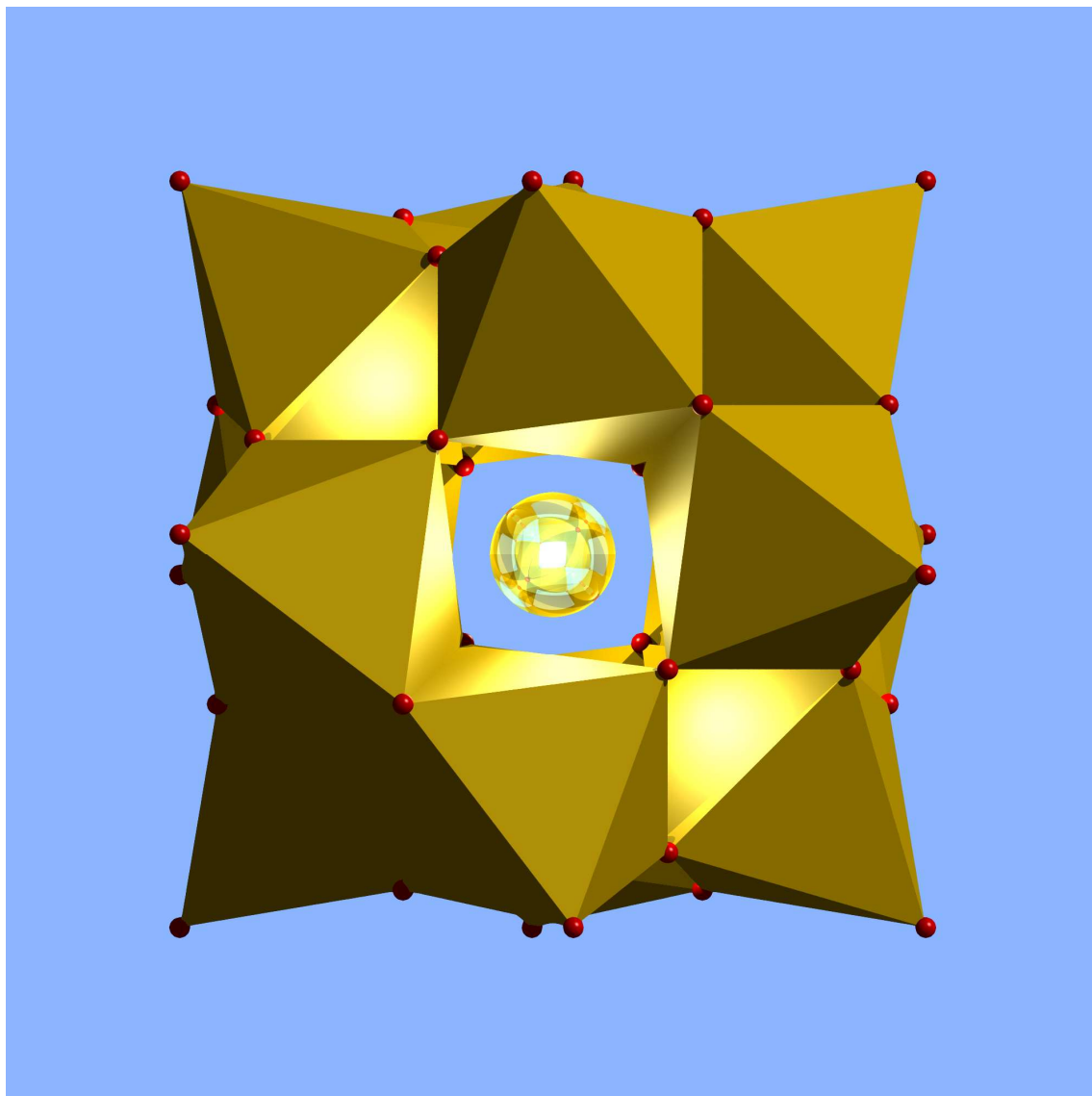




DIAMOND

Crystal and Molecular Structure Visualization



New visions of your crystal structures!



Diamond, the well-known program for the visualization and exploration of crystal structures, has been improved again: Version 4 contains a lot of new features, in addition to many functions of earlier versions that have been enhanced significantly (like the definition of connectivity or the exploration of the structure).

Below the screenshot, you will find a list of some of the most outstanding improvements and new features. Visit our Diamond 4 web pages for more detailed information:

<http://www.crystalimpact.com/diamond/Default.htm>

The screenshot displays the Diamond software interface. At the top, a menu bar includes File, Edit, View, Structure, Picture, Build, Objects, Move, Tools, Window, and Help. Below the menu is a toolbar with various icons. The main window is divided into several panes:

- Auto Picture Creator:** A docked pane on the left with sections for 'Picture building' (Scheme, Basics, Molecules, Create cell edges, Fill spheres around, Create polyhedra around, Complete fragments, Automatic centering) and 'Picture design' (Scheme, Layout, Model etc., Format, Avoid duplicate atom main colors, Picture viewing).
- Data Table:** A table listing crystal structures with columns for No., Title, Pics, Code, Formula sum, HM symbol, SGR no., and Cell parameters.
- Structure View:** A central 3D ball-and-stick model of a crystal structure. A tooltip shows coordinates: $x(1) = (4i, m)$ and $x/a, y/b, z/c = 0.2964(3), 0, 0.7249(7)$.
- Data Sheet:** A pane on the right showing general information (Origin, Formula), bibliographic data (Author(s), Publication title, Citation), phase data (Space-group, Cell), and atomic parameters.
- Thumbnail Strip:** A row of small thumbnail images at the bottom of the main window.

The status bar at the bottom indicates: Success: 188 atoms created. | Auto Picture | 0.44897 | 6 perms | 114 atoms | 122 bonds | polymeric | 0 polyh.

New and Enhanced Features

- "Auto Picture Creator" docking pane automatically applies changes in building options, picture design and viewing direction directly to the structure picture.
- "Grab mode": New mode for more intuitive rotation, shifting or zooming during exploration of a crystal or molecular structure.
- Intuitive structure exploration: preview neighbouring atoms and molecules e.g. using the mouse wheel.
- Improved evaluation of bonding spheres (connectivity), including non-bonding contacts, improved handling of H-bonds, and determination of atom site environments using Dirichlet domains (Voronoi polyhedra).
- Easy application of user-defined design schemes.
- New options to create a packing diagram: cell range, sphere, slab, or slice of molecules.
- Creation of Voronoi polyhedra
- Improved functions to complete molecular fragments, generate symmetry-equivalent molecules, and search for non-bonding contacts.
- Expand or reduce coordination spheres around selected atoms, clusters of molecules, molecular fragments or polymers.
- Full screen view of structure picture.
- Access to the crystal structure database COD ("Crystallography Open Database").
- Improved searching of Diamond documents and structure files on your hard disk.
- Undo/Redo now with multiple steps together, assisted by thumbnail pictures of the previous conditions.

System Requirements

- Windows XP, Vista, Windows 7, 8/8.1 or 10
- Microsoft Internet Explorer 8 (or higher)
- 1 GB of RAM (or more)
- 3.8 GB of free disc space (or more)
- DVD drive (for installation from DVD)
- Graphics resolution: 1024 x 768, high color

Prices

	non-profit org.	profit org.
Single licence	599 € (299 €)**	1,198 € (599 €)
Site licence***	1,198 € (599 €)	2,396 € (1,198 €)
Campus licence****	2,396 € (1,198 €)	4,792 € (2,396 €)

* Prices do not include taxes which may be due.

** Prices in brackets are update prices from version 3.

*** Unlimited number of installations within one institute/dept.

**** Unlimited number of installations within one university/company.



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