



DIAMOND

Crystal and Molecular Structure Visualization

The screenshot shows the 'Exploration Controller' window on the left and a 3D molecular structure on the right. The controller includes a histogram of contact spheres, a table of atom pairs with their distances and types, and a legend for atom types (N, O, H, C). The 3D view shows a complex molecular structure with atoms represented by spheres and bonds by sticks. A tooltip for an oxygen atom is visible, showing its coordinates and contact information.

| Atom 1 | Atom 2 | d 1,2 | d-vdW | Type | File |
|--------|----------------------------|---------|------------|--------------|------|
| "O2" | "C1" | 1.22245 | 1.99736 | Bond | |
| "O2" | "H1" (-1+x, 1/2-y, -1/2+z) | 2.00797 | 0.62328 | A..H_inter | |
| "O2" | "H11" | 2.34311 | 0.72786 | O..A_intra-2 | |
| "O2" | "C2" | 2.54472 | 0.87530 | Cnt_intra-2 | |
| "O2" | "H3A" (-1+x, y, z) | 2.59816 | -0.0118426 | Cnt_inter | |
| "O2" | "O3" (-1+x, 1/2-y, -1/2+z) | 2.81626 | -0.223743 | A..D_inter | |
| "O2" | "H16B" | 2.91901 | 0.30901 | Cnt_intra-4 | |
| "O2" | "H8" | 2.95375 | 0.34375 | Cnt_intra-3 | |
| "O2" | "H21" (-x, -y, 1-z) | 2.97772 | 0.367723 | Cnt_inter | |
| "O2" | "H7" | 3.03392 | 0.423919 | Cnt_intra-4 | |
| "O2" | "H19" (x, 1/2-y, -1/2-z) | 3.12189 | 0.511895 | Cnt_intra-3 | |
| "O2" | "C16" | 3.14332 | -0.0766771 | Cnt_intra-3 | |

Version 5 Preview

The upcoming Diamond version 5 will contain several new features:

The most outstanding new feature is the **Exploration View**, which enables to study (strong) bonds as well as H-bonds and non-bonding contacts when checking for neighbouring atoms and molecules. A bond (or contact or H-bond, resp.) can be added or removed by clicking the checkmark in the distance table or shifting the boundary in the histogram or by clicking on the bond/contact in the structure picture graphics (see screenshot above).

The commands *Take Picture* and *Continue With New Picture* offer an improved workflow when creating multiple pictures for a structure data set.

The *More Pictures* docking window and the *Caption Bar* give a simplified overview of structure pictures.

Settings can be imported from version 4.

A newer version of Crystallography Open Database (COD; www.crystallography.net) is available.

More outstanding functions:

- ✓ Import with automatic format recognition
- ✓ Build up structure pictures automatically or manually
- ✓ Schemes (style sheets) for building and design
- ✓ Structure type database
- ✓ Ellipsoids, disorder, mixed sites
- ✓ Molecules, packing diagrams
- ✓ Polymers and molecule clusters
- ✓ Fragmentated and broken-off bonds
- ✓ H-bonds and non-bonding contacts
- ✓ Preview of neighbouring atoms and -molecules
- ✓ Atomic environments from Dirichlet domains
- ✓ Coordination and Voronoi polyhedra
- ✓ Atom vectors, labels, and free text
- ✓ Reflection parameters and diffraction diagrams
- ✓ Distances, angles, and torsion angles
- ✓ hkl- and L.S.-planes and lines
- ✓ 3D export to POV-Ray, OBJ, and STL
- ✓ Video sequences and animations

With Diamond version 5 we will switch over to the **Update Permission Time model**:
<https://www.crystalimpact.de/subscription.htm>.

Diamond version 5 will be released in the second half of 2022. The **update from Diamond 4 to 5** will be **free-of-charge**.

<https://www.crystalimpact.de/diamond/v5preview.htm>

| Price* for new License | academic | regular |
|-------------------------------|----------|---------|
| Semiannual license (6 months) | 149,50 € | 299 € |
| Annual license (12 months) | 299 € | 598 € |
| Single license (permanent) | 599 € | 1.198 € |
| Site license (permanent) | 1.198 € | 2.396 € |
| Campus license (permanent) | 2.396 € | 4.792 € |

* Prices do not include taxes which may be due.



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