ShelXle – A Qt† GUI for SHELXL

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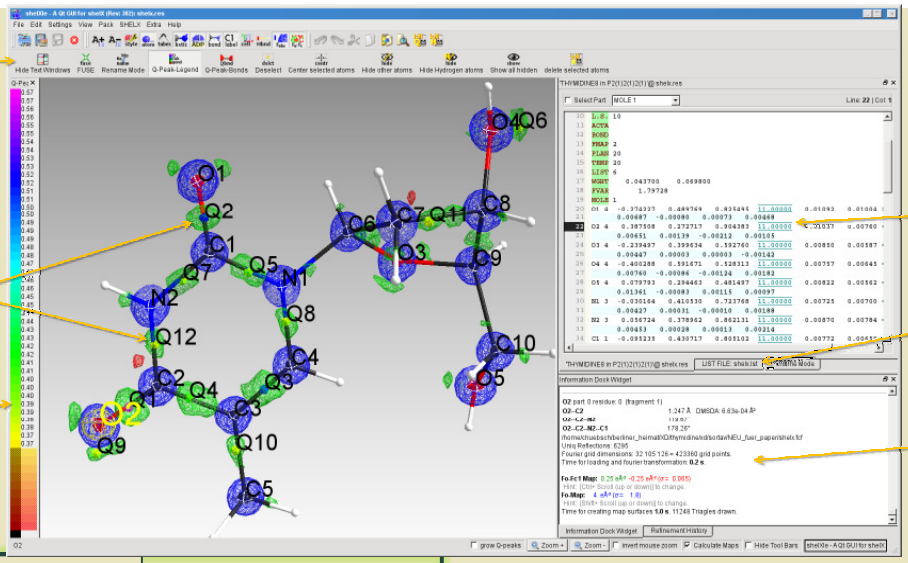
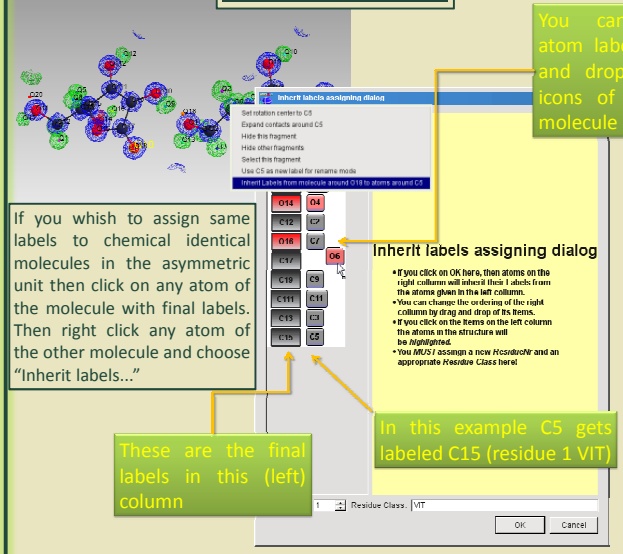
ShelXle is available for **Windows , Linux, MacOs and WeTab.**

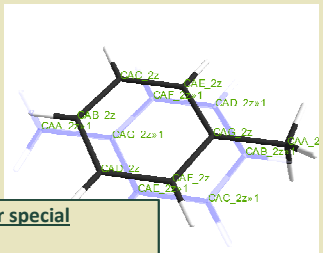


Inherit labels

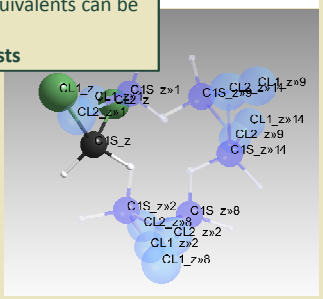


Abstract:

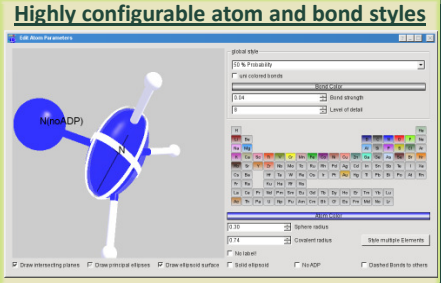
ShelXle is a graphical user interface (GUI) for small-molecule refinements with SHELXL[1]. It is designed like a integrated development environment and combines an editor with syntax highlighting and auto completer with a graphical representation of the three dimensional structure. ShelXle is a tool for expert users of SHELXL giving them the full control over the *.res/*.ins input file. Non expert users can rapidly learn how to appreciate the full capability of SHELXL by exploring the functionality of ShelXle. The electron density and difference electron density maps (F_o and F_o-F_c) can be visualized as wire framed iso-surfaces. A 'rename mode' provides the ability to re-label atoms including residues and/or parts and assigning free variables for occupation constraints. Molecules can be moved so that their centers of gravity lie inside of the unit cell by just one click. Identical molecules in the asymmetric unit can inherit their labels semi- automatically from a previous labeled molecule. The 'auto HFIX' function uses electron density (F_o-F_c) for the placement of Hydrogen atoms with suitable constraints/restraints. For convenience functions to update the number of atoms in the cell (UNIT) and the weighting scheme (WGHT) are build in. A refinement history and a save history allow to go back to previous file versions. The three dimensional representation of the molecule is drawn using OpenGL. Several stereoscopic projection modes are available including one for Zalman Monitors. The ShelXle is written entirely in C++ using the Qt. The program has been thoroughly tested prior this launch. ShelXle is available for Windows (XP/Vista/7), MacOS X (10.5/10.6), Linux (SuSE [11.1-11.4] / Debian) and as source. On all systems it is easy to install. ShelXle is licensed under LGPL(2.1) and can be downloaded free of charge at http://ewald.ac.chemie.uni-goettingen.de/shelx/ .

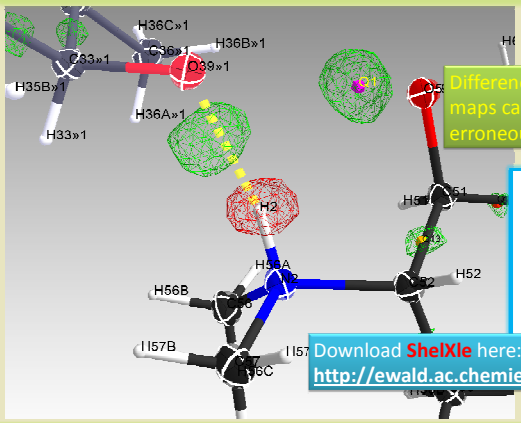


Disorder over special positions:
Symmetry equivalents can be visualized as **PART -N Ghosts**



Highly configurable atom and bond styles





Download **ShelXle** here:
http://ewald.ac.chemie.uni-goettingen.de/shelx/

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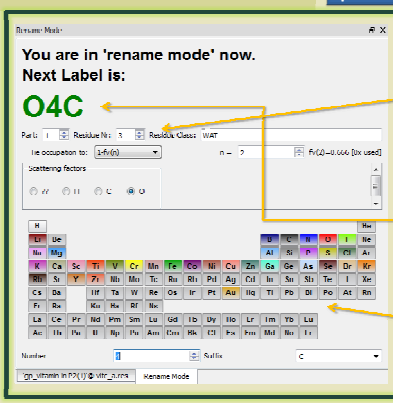
Special thanks to all β-testers!!!



Refinement and Save History