



ShelXle – A Qt[†] GUI for SHELXL

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Qt
© 2011 Nokia Corporation and/or its subsidiaries. Qt is the library ShelXle is using. Qt is spoken like the word 'cute'.

The 'selection toolbar' shows possible actions.

Q-Peaks are visualized as colored icosahedra. Each color refers to an electron-density peak height.

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

The text cursor of the editor jumps immediately to the clicked atom.

Sub-windows can be gathered together in tabs.

The Information Window



Abstract:
ShelXle is a graphical user interface (GUI) for small-molecule refinements with SHELXL^[1]. It is designed like an 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