MS5-P1 **Shelxle – a GUI for SHELXL.** Christian B. Hübschle,[a] Birger Dittrich,[a], George M. Sheldrick[a]
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ShelXle[1] is a graphical user interface for SHELXL [2], which is currently the most widely used program for small-molecule structure refinement. Since the first beta release in Februrary 2011 ShelXle has been downloaded more than 10000 times. It combines an editor with syntax highlighting for the SHELXL-associated .ins (input) and .res (output) files with an interactive graphical display for visualization of a three-dimensional structure including the electron density (Fo) and difference density (Fo-Fc) maps. Special features of ShelXle include intuitive atom (re-)naming, a strongly coupled editor, structure visualization in various mono and stereo modes, and a novel way of displaying disorder extending over special positions. ShelXle is completely compatible with all features of SHELXL and is written entirely in C++ using the Qt4 and FFTW libraries. It is available at no cost for Windows, Linux and Mac-OS X and as source code.

[1] Hübschle, C. B., Sheldrick, G. M. and Dittrich, B. (2011). *J. Appl. Cryst.* **44**, 1281-1284.
[2] Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

Keywords: graphical user interface; shelxl; refinement, small molecules

MS5-P2 **Using Partial Observations, Partial Models and Partial Residuals in Least Squares Refinement.**
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The speed of crystal structure refinement makes it appropriate that shortcomings in how least squares refinement is implemented should be discussed and appropriate improvements proposed. The identification of systematic error in structures and the choice of variables for hierarchical model development and comparative refinement requires a better understanding of how information about the various variables and structure components is distributed in diffraction data. Certain features of the standard implementation of least squares methods should be of concern as they are the result of a number of *misconceptions.* Ideas developed using partial observations, partial models and partial residuals suggest how to overcome problems with the way least squares methods are currently implemented. A single crystal study necessarily uses only a fraction $f_{\mathbf{h}}$ of an observation $|\mathbf{Y}(\mathbf{h})|^2$ that is the sum of M components $|F(\mathbf{h})_{\mathrm{m}}|^2$ where $|F(\mathbf{h})_{\mathrm{M}}|^2$ is the background. $\mathbf{Y}(\mathbf{h})$ can be regarded as a vector in an M dimensional space with components $F(\mathbf{h})_{\mathrm{m}}\ \mathbf{i}_{\mathrm{m}}$. The model used to calculate $\mathbf{Y}\mathrm{calc}(\mathbf{h})$ includes the background and the components of $\mathbf{Y}\mathrm{obs}(\mathbf{h})$ are assumed to be in the same ratio as an initial estimate of $\mathbf{Y}\mathrm{calc}(\mathbf{h})$. This needs a reflection file that contains values of a scaled peak-plus-background, its variance, and the scaled background since the background should be an unrefined part of the model of $\mathbf{Y}\mathrm{calc}(\mathbf{h})$ and not a removable component of an observation. This reduces noise associated with weak intensities.

An obsession with not biasing results obtained from diffraction intensities has led to the use of *maximum ignorance statistics*. Ignorance is an appropriate description as available details of the refinement are being ignored.

From an initial estimate of the variance-covariance matrix $\mathbf{M}$ one can evaluate the variance of $\mathbf{Y}\mathrm{calc}(\mathbf{h})$ and the fraction of this variance associated with individual variables and components of $\mathbf{Y}\mathrm{calc}(\mathbf{h})$. This information can be used to individually rescale the elements of the variance covariance matrix **M,** re-estimate the least squares weights, and calculate various statistical functions of the residuals that have been weighted using these fractions. It also allows the evaluation of the overall scale between corresponding components of the $\mathbf{Y}\mathrm{obs}(\mathbf{h})$ and $\mathbf{Y}\mathrm{calc}(\mathbf{h})$ and the effective number of observations associated with a structural feature.

These parameter and component specific functions are capable of indicating where a refinement could be improved, the adequacy of restraints and constraints, and should aid the assessment of problem structures involving twins, disorder, stacking faults, composite structures, commensurate and incommensurate modulation and fraud.

Comparative refinement techniques can be developed to reveal systematic error and to determine which parameters will create the most improvement in an expanded model for refinement. A distinction should be made between a least squares matrix used for model development and one used for the estimation of a variance covariance matrix for both refined and unrefined parameters.

Keywords: least squares refinement; partial observations; error estimation