

## Literatur

### **SHELXL-93**

Sheldrick, G. M.; SHELXL-93; University of Göttingen, 1993.

Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.

### **SHELX-97 (SHELXS-97 + SHELXL-97)**

Sheldrick, G. M.; SHELX-97, Program for refinement of crystal structures, University of Göttingen, 1997.

Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.

### **Absolute structure parameter (Flack parameter)**

Flack, H. D., *Acta Cryst.* *A39* **1983**, 876 – 881.

### **Scalepack**

(a) "Collect" data collection software, Nonius B.V., 1998. (b) "Scalepack" data processing software: Otwinowski, Z.; Minor, W. in *Methods in Enzymology* **1997**, 276 (Macromolecular Crystallography, Part A), 307.

### **Scattering factors**

Cromer, D. T.; Waber, J. T. In *International Tables for X-ray Crystallography*; Ibers, J. A., Hamilton, W. C., Eds.; Kynoch: Birmingham, England, 1974.

## Important Files and Listings

a) **RES-File** (ASCII result file from SHELX refinement programs) => use for ortep plots

(cell constants, space group, molecular formula, internal coordinates of all atoms, isotropic and anisotropic displacement parameters, occupation ratios etc.)

**!!!! Never change the original res-file !!!!**

b) **CIF-File** (Crystallographic Information File)

ASCII-file (with a very special command syntax) generated by all usual structure refinement programs for electronical deposition. and generation of tables for the supplementary material (bond lengths, internal coordinates, R-values etc.).

c) **Listing (= supplementary material) as RTF-Format file (Rich Text Format)**

Can be imported in nearly every word processor. Special characters are now set correctly except the empirical formula

d) Listing in standard Text(ASCII)-Format

**!!!Special characters are not set correctly in ASCII-Format!!!**