

Supplementary material

Observed and calculated intensities as well as differences $I_{\text{obs}} - I_{\text{calc}}$ are provided as data files in 'NIPL' format and as Postscript files. The calculated intensities are obtained from the fittest individual in the final generation of the reference refinement.

To obtain the files download `sh0158sup1.tgz` and uncompress and untar the files in the current directory using the following commands:

```
gunzip sh0158sup1.tgz
tar xfv sh0158sup1.tar
```

File names are encoded as explained in the following example:

The file '6.8kl.b2.obs.ni' is a section from the **6.8kl**-layer. It is described as layer **b2** in Table 1 and contains **observed** intensities in **NIPL**-format.

Table 1:

layer	h	k	l	nh	nk	nl
A2	5-10	0 - 3	2	51	31	1
B2	2 - 5	7 - 11	2	31	41	1
A3	5-10	0 - 3	3	51	31	1
B3	2 - 5	7 - 11	3	31	41	1
a2	6.5	0 - 2	1.8 - 2.2	1	21	21
b2	6.8	0 - 2	1.8 - 2.2	1	21	21
c2	7.2	0 - 2	1.8 - 2.2	1	21	21
d2	7.5	0 - 2	1.8 - 2.2	1	21	21
e2	2.5	7 - 11	1.8 - 2.2	1	41	21
f2	3.5	7 - 11	1.8 - 2.2	1	41	21
a3	6.5	0 - 2	2.8 - 3.16	1	21	19
b3	6.8	0 - 2	2.8 - 3.16	1	21	19
c3	7.2	0 - 2	2.8 - 3.16	1	21	19
d3	7.5	0 - 2	2.8 - 3.16	1	21	19
e3	2.5	7 - 11	2.8 - 3.16	1	41	19
f3	3.5	7 - 11	2.8 - 3.16	1	41	19

NIPL files are ASCII text files, which are easy to read:

“The NIPL format ('ni') is defined as follows:

```
1  nx ny
2  xmin xmax ymin ymax
3ff z z z z ...
```

The first line contains the number of data points in x- and in y-direction. The next line gives the x- and y-limits of the plot area. All following lines contain the z-values row by row starting in the lower left corner. The z-values are real numbers and not restricted in any way. However, the value -9999.0 is reserved for excluded regions.” (Proffen & Neder, 1999, p.18)

NIPL-files can be read with the program KUPLOT (Proffen & Neder, 1999), which may be obtained under:

<http://www.uni-wuerzburg.de/mineralogie/crystal/discus/kuplot.html>

KUPLOT macros ‘hk.mac’ and ‘kl.mac’, which are included in the supplementary material, may help to plot the NIPL-files:

```
run KUPLOT
```

```
type  @hk <filename>           to plot the hk*.ni file <filename>
```

```
or    @kl <filename>           to plot the *kl*.ni file <filename>
```

(Macros were provided by one of the referees)

Reference:

Proffen, Th. & Neder, R.B. (1999) *User Guide KUPLOT Version 4.0*. Department for Physics and Astronomy, Michigan State University, East Lansing, USA.