Supplementary material for “On the space group dispute of stibnite”, Sørensen and Lundegaard.

Table 1: UMWEG98 input file used for reflection 530

```
Renninger pattern of the forbidden 5 3 0 - reflection
530.ps
11.2783  3.8216  11.1966  90. 90.  90.
Mo
0.10  0.10  76.  2.00 0.01
-70. 40. 50. 0  .05 0.
62  5 2
Sb                     1
S                      1
1  0.5  0.029290     0.250     0.674267
0.00564  0.00378  0.00609  0.0    0.00051   0.0
1  0.5  0.350512     0.250     0.464675
0.00540  0.00638  0.00955  0.0    0.00187   0.0
2  0.5  0.049922     0.250     0.122635
0.00564  0.00472  0.00665  0.0   -0.00054   0.0
2  0.5  0.374715     0.250     0.061241
0.00685  0.00449  0.00584  0.0   -0.00076   0.0
2  0.5  0.207609     0.250     0.808635
0.00573  0.00546  0.00570  0.0   -0.00021   0.0
5  3  0   0.  0.  0.  0.
0. 1. 1.
4. 0. 0.
0. 0. 0.
```

Figure 1: Ψ-scan of reflection 10 6 0

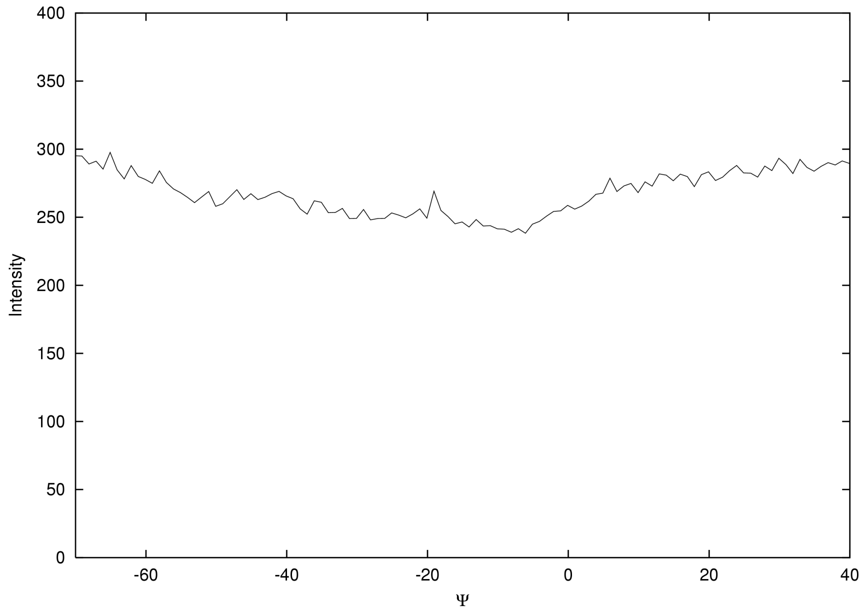


Figure 2: Ψ-scan of reflection 020

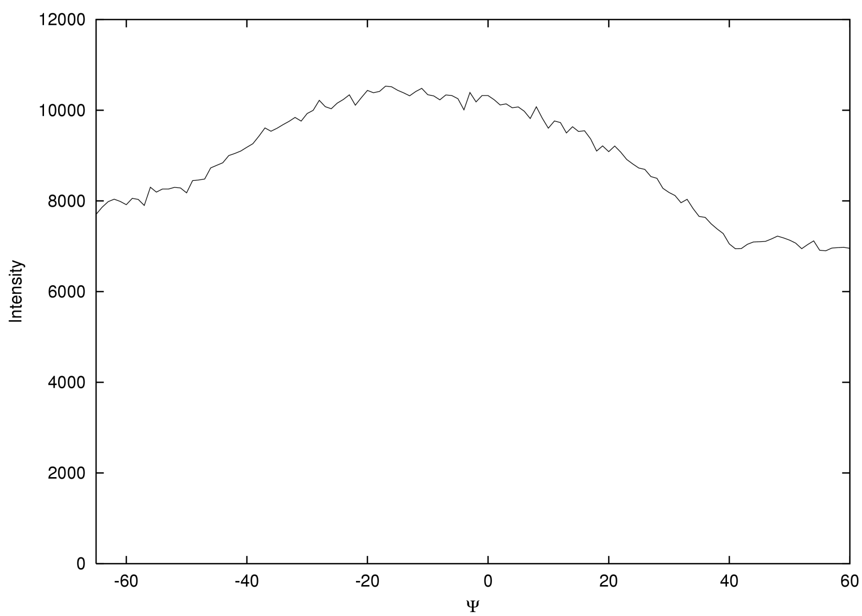


Figure 3: Ψ-profiles for the systematic absent 012 reflection. (a) experimentally determined and (b) calculated by UMWEG98 [2].

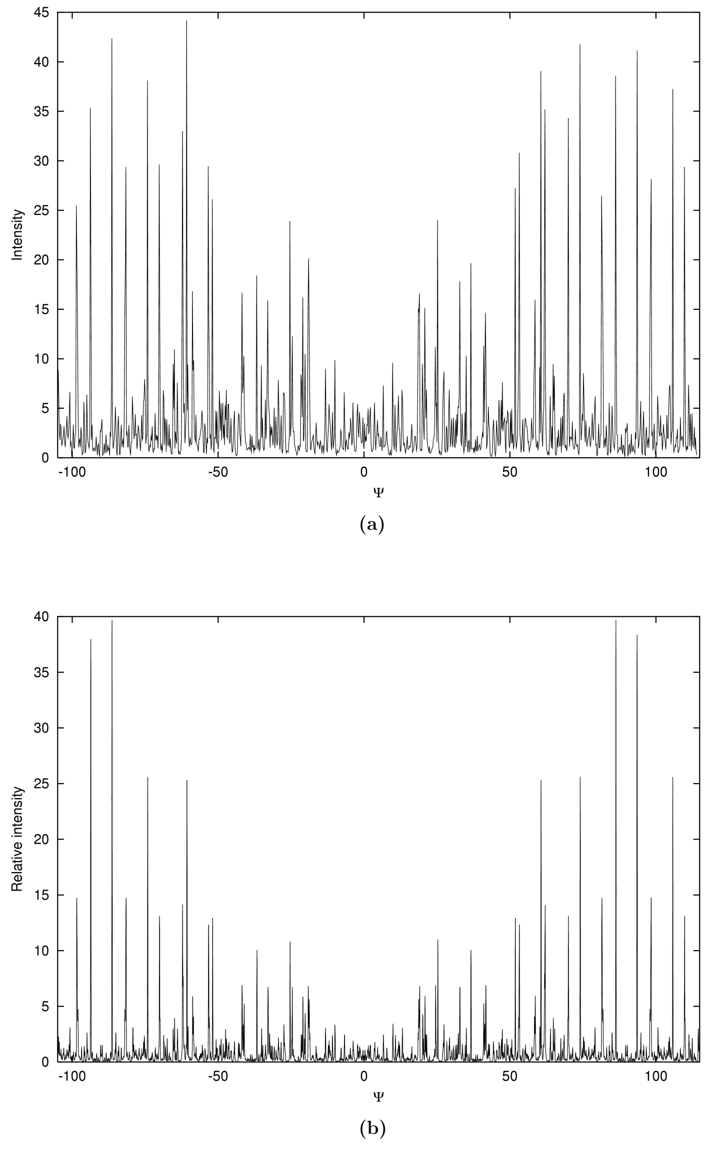


Figure 4: Ψ-scan of reflection 024. The mirror symmetry is lost due to the step size in Ψ being large than the width of the peaks. The $180°$ rotational symmetry is maintained, since the used step size ($\Delta\Psi = 1°$) is a modulus of $180°$.

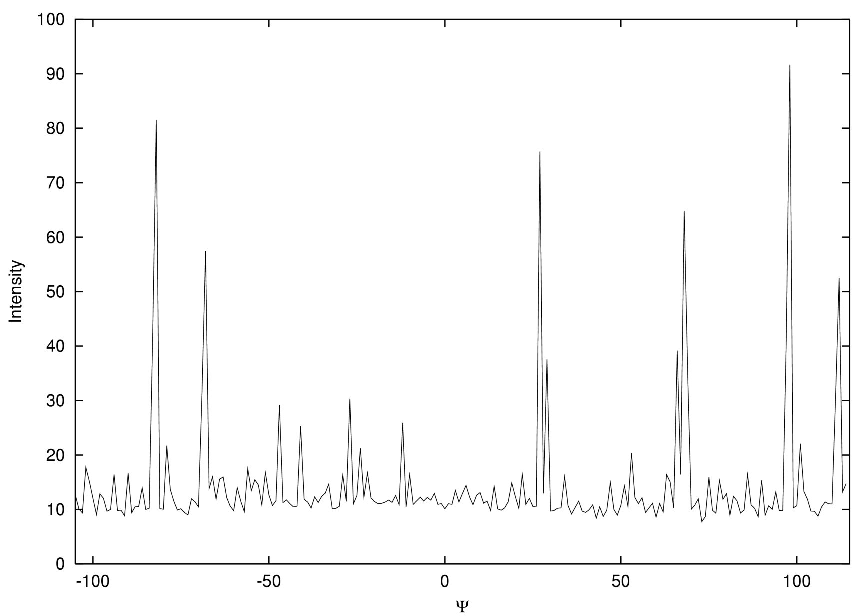
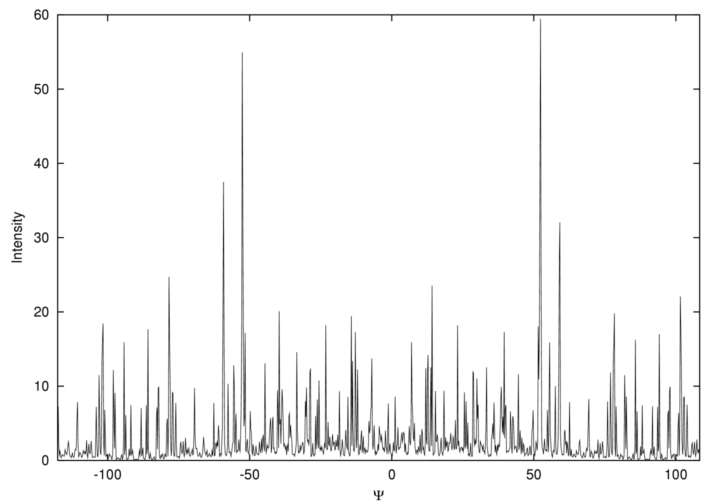
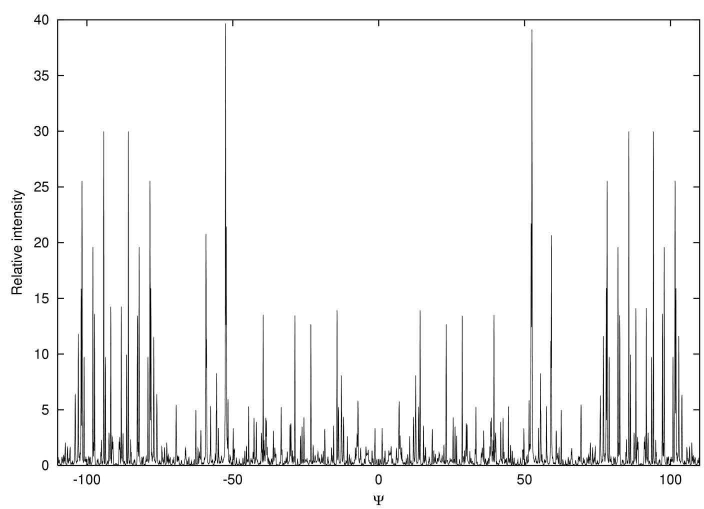


Figure 5: Ψ-profiles for the systematic absent 003 reflection. (a) experimentally determined and (b) calculated by UMWEG98 [2]. The hight of the measured profile in the range -110 to -80° (and 80 to 110°) is lower than the calculated profile. This is in good accordance with the absorption profile, which is similar to the profile of the 006 reflection (Fig 6).



(a)



(b)

Figure 6: Ψ-scan of reflection 006

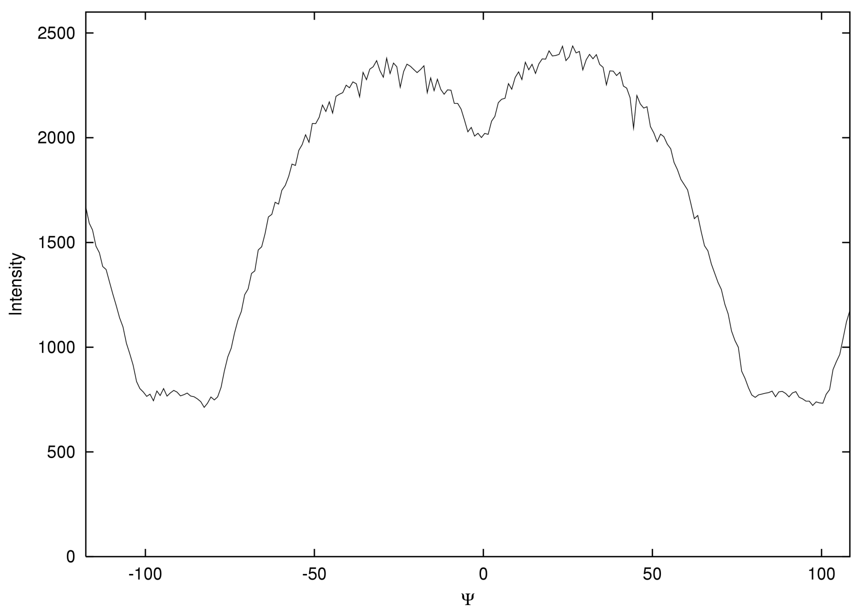
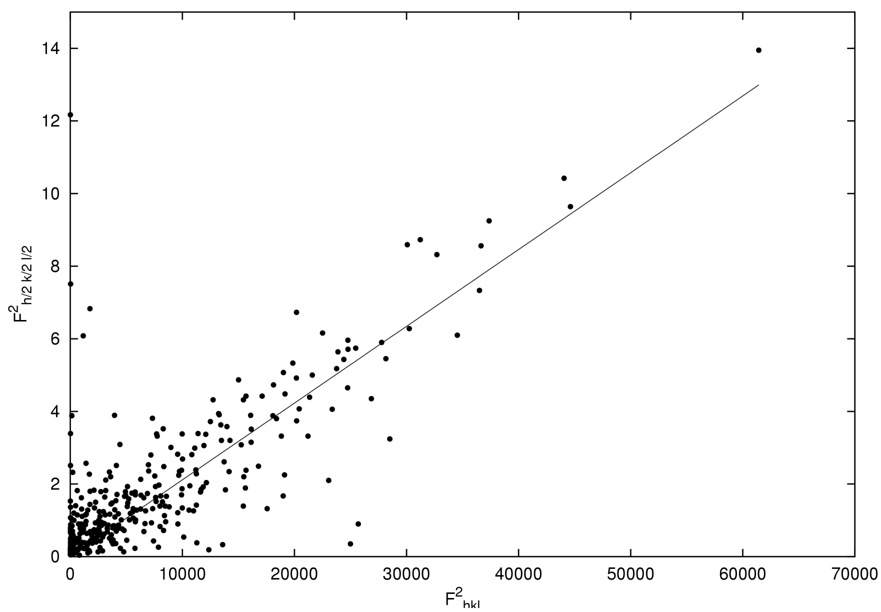


Figure 7: Plot of F^2 of the reflections $h/2\ k/2\ l/2$ as a function of F^2 of the hkl reflections with at least one of the miller indices odd from the 110 K data set [1]. Observed diffraction for the $h/2\ k/2\ l/2$ reflections will therefore be purely from $\lambda/2$ radiation. The linear regression line has a slope of 0.00021(2).



References

[1] L. F. Lundegaard, H. O. Sørensen, T. Balić-Žunić, and E. Makovicky. Unpublished results, 2003.

[2] E. Rossmanith. UMWEG-98: a program for calculation and graphical representation of multiple diffraction patterns. *J. Appl. Cryst.*, 32:355–361, 1999.