# Diagnosis output files

If setup in read\_in\_parameters.h two diagnosis files of the program can be returned: “uncorrelated\_peaks.asc” and “peak\_ignored.asc”. “peak\_ignored.asc” contains a list of the reflections in the input file that have been ignored by the program. Reflections are added to “peak\_ignored.asc” when

1. the Monte Carlo integration method does not achieve a reduction in the uncertainty below the ‘tolerance’ parameter (see section “Advanced parameter file” for explanation of ‘tolerance’). The reflections in the input file taking part in such integrals are added to peak\_ignored.asc.

2. In some cases I have experienced that the correlation matrix elements in the input data file have been partially corrupted due to some rounding errors introduced when generating these. Therefore, the correlation matrix elements are scanned to see if each block satisfies the condition that the corresponding correlation block matrix is positive definite. If this is not satisfied the reflections in such blocks are added to the list of ignored reflections in “peak\_ignored.asc”.

A number of the reflections in the input data file are categorized as uncorrelated. A number of these will be known to be present in the powder pattern irrespective of the extinction symbol of the Laue class. “uncorrelated\_peaks.asc” provides a list of all these reflections. It is the arithmetic mean of the intensity values of these reflections which is used to provide an estimate of the (prior) mean value of a present intensity in the spectrum, see Markvardsen *et al*. (2001) Sec 6, where (prior) mean value = *μ*. If the number of these uncorrelated reflections is less than 5, *μ* is calculated as the arithmetic mean of all the intensities in the input data file.