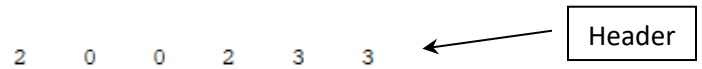
Format "prf" in Jana2020

The Jana2020 program allows refinement across different datasets. If the file contains several data blocks, each block is separated by special labels:

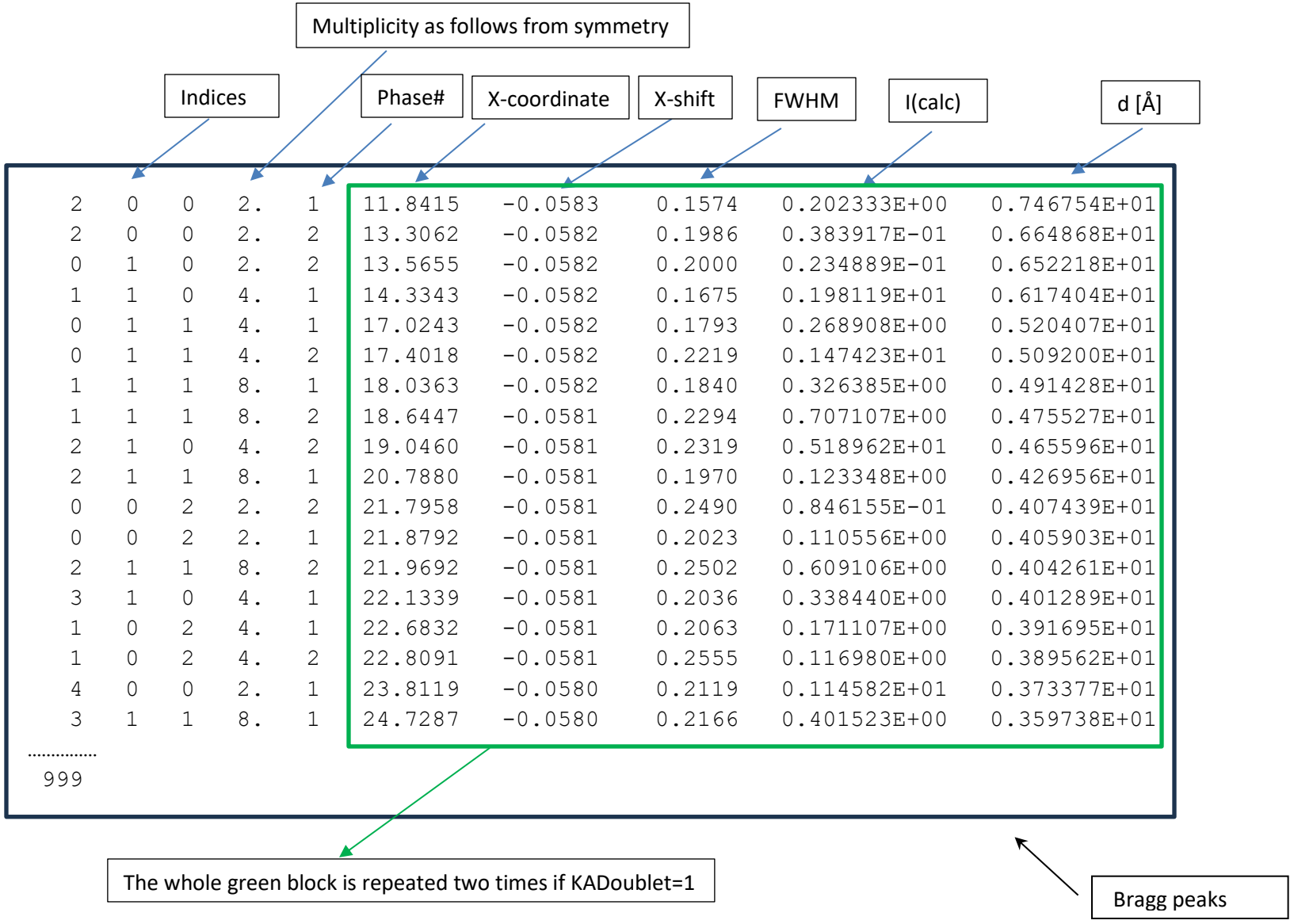
Block1 begin
.....
.....
Block1 end
Block2 begin
.....
.....
Block2 end

When there is only one data block, labels are avoided.

Each block consists of three parts: header, Bragg positions, and profile points:



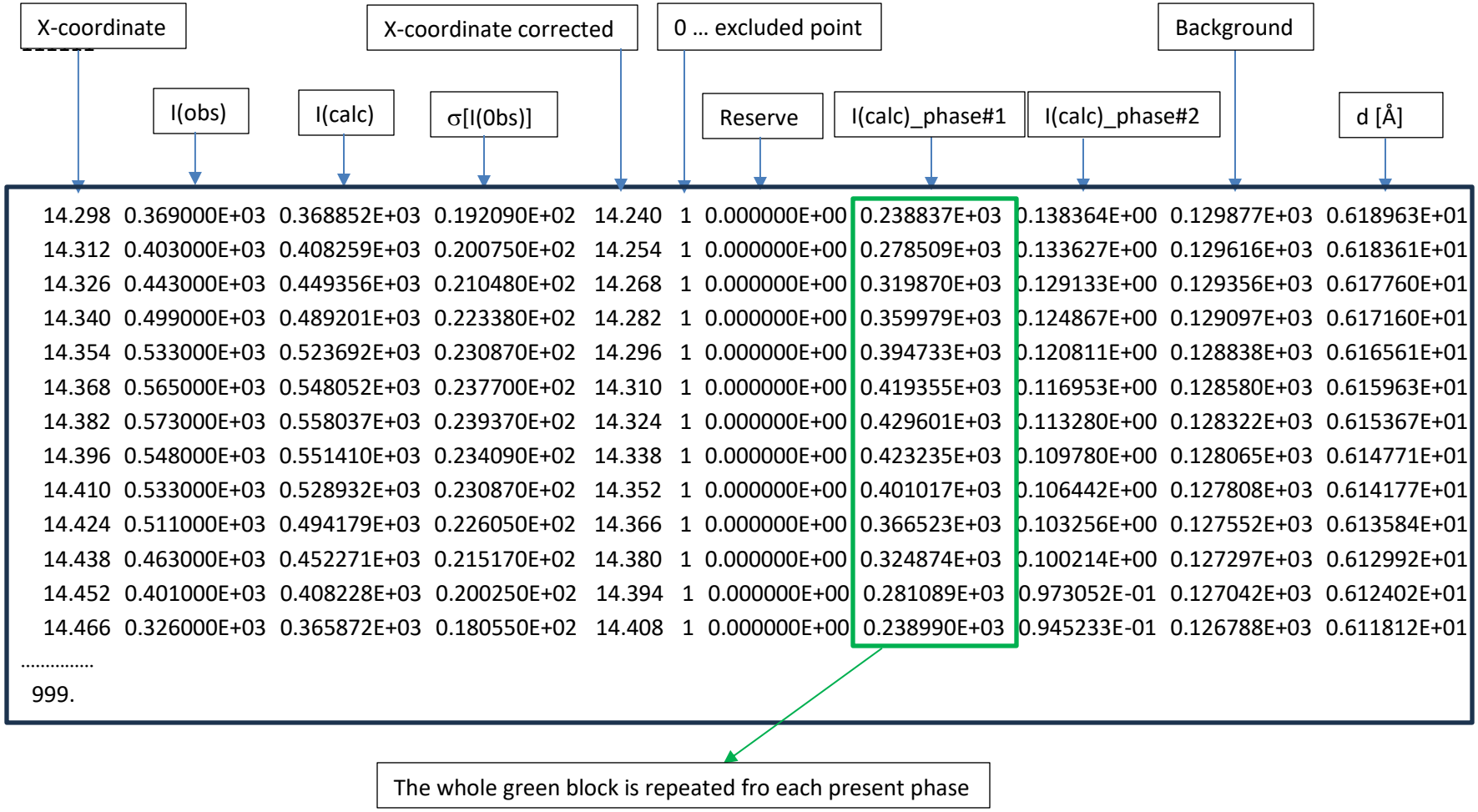
kType	2	for Jana2020
KADoublet	0	data for data measured at one wavelength
	1	for $K\alpha_1$ and $K\alpha_2$
DataType	0	X-ray/neutron CW data
	1	TOF data as a function of time
	2	TOF data in d values
	3	energy dispersive data
NPhases		number of phases
(NDim(I),I=1, NPhases)		number of indices used for each phase



Indices: In the case that some of the present phases are modulated, the number of indices will be equal to the maximal number of indices for all phases. Then, the phases with fewer indices are padded with zeros.

Units: The X-coordinate, X-shift, and FWHM are reported in degrees, microseconds, and μeV for Two-Theta, Time, d, and energy, respectively.

I(calc): intensity as calculated from Rietveld (corrected for multiplicity and preference orientation) or as extracted from the profile by le Bail fit.



The parameters X-coordinate and X-coordinate corrected are in the same units as the Bragg peaks. The corrected values are adjusted for the zero shift from the refinement process.

The following equation holds: I(calc)= I(calc)_phase#1+ I(calc)_phase#2+…+Background

Deconvolution for all phases is performed for both le Bail and Rietveld refinement. However, only Rietveld refinement allows us to obtain reliable volume fractions for individual phases.