Format "prf" in Jana2020

As the new Jana2006 allows refinement against different data sets the file can contain several data blocks:

Block1 begin

.....

.....

Block1 end

Block2 begin

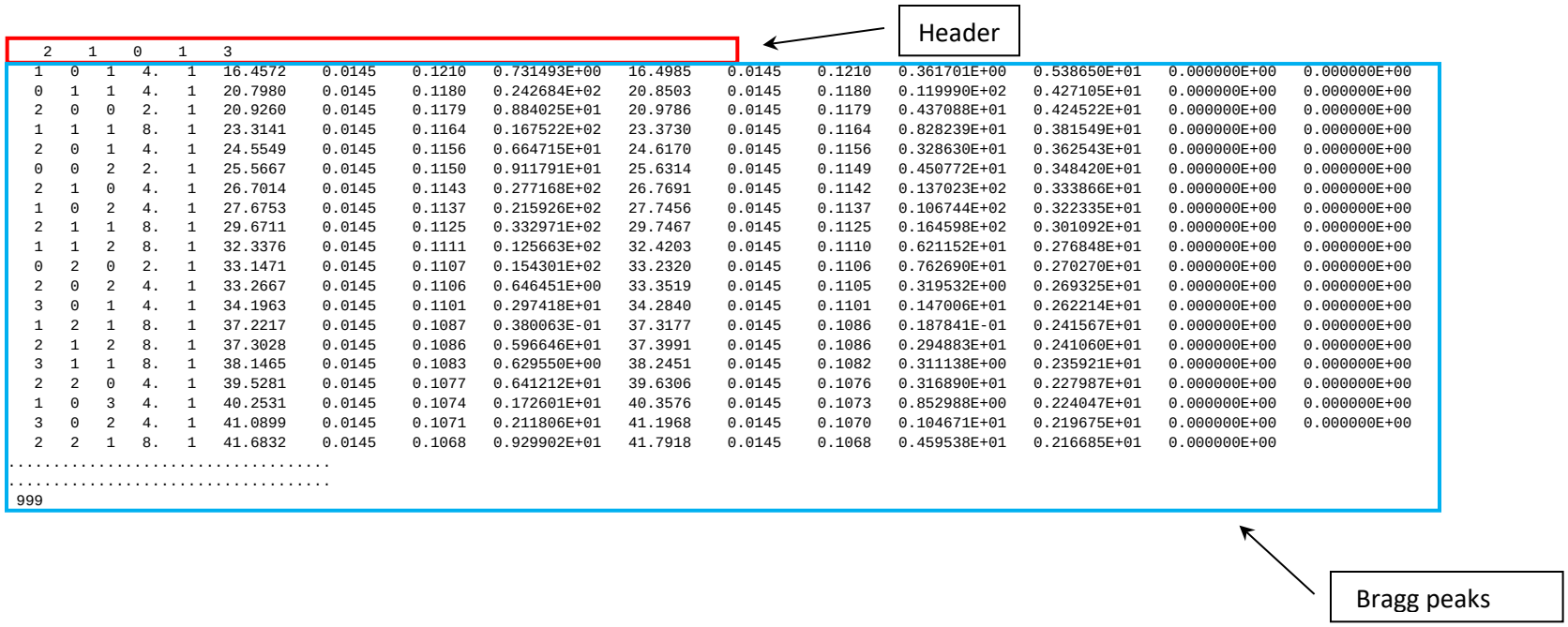
.....

.....

Block2 end

In the case that there is just one data block the labels are avoided.

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



```
    10.000   0.179000E+03   0.963079E+02   0.133791E+02    10.014    1   0.000000E+00   0.000000E+00   0.963079E+02   0.884546E+01
    10.026   0.147000E+03   0.963155E+02   0.121244E+02    10.040    1   0.000000E+00   0.000000E+00   0.963155E+02   0.882258E+01
    10.052   0.167000E+03   0.963231E+02   0.129228E+02    10.066    1   0.000000E+00   0.000000E+00   0.963231E+02   0.879982E+01
    10.078   0.170000E+03   0.963308E+02   0.130384E+02    10.092    1   0.000000E+00   0.000000E+00   0.963308E+02   0.877718E+01
    10.104   0.151000E+03   0.963384E+02   0.122882E+02    10.118    1   0.000000E+00   0.000000E+00   0.963384E+02   0.875465E+01
    10.130   0.164000E+03   0.963461E+02   0.128062E+02    10.144    1   0.000000E+00   0.000000E+00   0.963461E+02   0.873224E+01
    10.156   0.151000E+03   0.963537E+02   0.122882E+02    10.170    1   0.000000E+00   0.000000E+00   0.963537E+02   0.870994E+01
    10.182   0.153000E+03   0.963614E+02   0.123693E+02    10.196    1   0.000000E+00   0.000000E+00   0.963614E+02   0.868776E+01
    10.208   0.133000E+03   0.963691E+02   0.115326E+02    10.222    1   0.000000E+00   0.000000E+00   0.963691E+02   0.866569E+01
    10.234   0.155000E+03   0.963767E+02   0.124499E+02    10.248    1   0.000000E+00   0.000000E+00   0.963767E+02   0.864373E+01
    10.260   0.167000E+03   0.963844E+02   0.129228E+02    10.274    1   0.000000E+00   0.000000E+00   0.963844E+02   0.862189E+01
    10.286   0.149000E+03   0.963921E+02   0.122066E+02    10.300    1   0.000000E+00   0.000000E+00   0.963921E+02   0.860015E+01
    10.312   0.138000E+03   0.963998E+02   0.117473E+02    10.326    1   0.000000E+00   0.000000E+00   0.963998E+02   0.857853E+01
    10.338   0.158000E+03   0.964075E+02   0.125698E+02    10.352    1   0.000000E+00   0.000000E+00   0.964075E+02   0.855701E+01
    10.364   0.158000E+03   0.964152E+02   0.125698E+02    10.378    1   0.000000E+00   0.000000E+00   0.964152E+02   0.853560E+01
    10.390   0.146000E+03   0.964229E+02   0.120830E+02    10.404    1   0.000000E+00   0.000000E+00   0.964229E+02   0.851430E+01
    10.416   0.156000E+03   0.964306E+02   0.124900E+02    10.430    1   0.000000E+00   0.000000E+00   0.964306E+02   0.849310E+01
    10.442   0.145000E+03   0.964384E+02   0.120416E+02    10.456    1   0.000000E+00   0.000000E+00   0.964384E+02   0.847202E+01
    10.468   0.160000E+03   0.964461E+02   0.126491E+02    10.482    1   0.000000E+00   0.000000E+00   0.964461E+02   0.845103E+01
    10.494   0.160000E+03   0.964538E+02   0.126491E+02    10.508    1   0.000000E+00   0.000000E+00   0.964538E+02   0.843015E+01
    10.520   0.133000E+03   0.964616E+02   0.115326E+02    10.534    1   0.000000E+00   0.000000E+00   0.964616E+02   0.840937E+01
    10.546   0.143000E+03   0.964693E+02   0.119583E+02    10.560    1   0.000000E+00   0.000000E+00   0.964693E+02   0.838870E+01
    10.572   0.132000E+03   0.964771E+02   0.114891E+02    10.586    1   0.000000E+00   0.000000E+00   0.964771E+02   0.836813E+01
    10.598   0.139000E+03   0.964848E+02   0.117898E+02    10.612    1   0.000000E+00   0.000000E+00   0.964848E+02   0.834766E+01
    10.624   0.147000E+03   0.964926E+02   0.121244E+02    10.638    1   0.000000E+00   0.000000E+00   0.964926E+02   0.832729E+01
    10.650   0.155000E+03   0.965004E+02   0.124499E+02    10.664    1   0.000000E+00   0.000000E+00   0.965004E+02   0.830702E+01
    10.676   0.148000E+03   0.965082E+02   0.121655E+02    10.690    1   0.000000E+00   0.000000E+00   0.965082E+02   0.828684E+01
    10.702   0.140000E+03   0.965160E+02   0.118322E+02    10.716    1   0.000000E+00   0.000000E+00   0.965160E+02   0.826677E+01
    10.728   0.137000E+03   0.965237E+02   0.117047E+02    10.742    1   0.000000E+00   0.000000E+00   0.965237E+02   0.824679E+01
    10.754   0.128000E+03   0.965315E+02   0.113137E+02    10.768    1   0.000000E+00   0.000000E+00   0.965315E+02   0.822691E+01
    10.780   0.150000E+03   0.965394E+02   0.122474E+02    10.794    1   0.000000E+00   0.000000E+00   0.965394E+02   0.820713E+01
    10.806   0.139000E+03   0.965472E+02   0.117898E+02    10.820    1   0.000000E+00   0.000000E+00   0.965472E+02   0.818744E+01
    10.832   0.114000E+03   0.965550E+02   0.106771E+02    10.846    1   0.000000E+00   0.000000E+00   0.965550E+02   0.816785E+01
.............
.............
999.
```

Header:

kType	2	for Jana2020
KADoublet	0	data for data measured with 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 phases

Bragg peaks:

h,k,l,... n diffraction indices, where n = max(NDim(1), …, NDim(NPhases)). For phases having the dimension smaller than n the indices are completed by zeros.

Multiplicity multiplicity of the reflection following from the symmetry

KPhase defines the phase which the reflection belongs to

The following four items are repeated twice if KADoublet=1. Then the first block corresponds to $K\alpha_1$

TwoTheta/Time/d/energy
angular position/time for TOF/d value/energy of the peak as calculated from cell parameters and modulation vectors

Shift the angular shift of the peak position due to a zero shift, sycos and sysin (it need not be constant for all reflections). The actual of reflections with respected to the profile should be calculated as: [TwoTheta/Time/d/energy] -Shift

FWHM in the same units are previous values

Icalc(h,k,l) intensity as calculated from Rietveld (corrected for multiplicity and preference orientation) or as extracted from the profile by le Bail fit.

d for of Bragg peak

\+ additional reserve items for internal use of the program

The list of Bragg peaks ends with the integer 999 at the position of the h index.

Profile points:

TwoTheta/Time/d/energy

diffraction angle/time for TOF/d value/energy of the profile point

Iobs observed intensity

Icalc calculated intensity

sig(Iobs) standard uncertainty of Iobs

TwoTheta-corr/Time-corr/d-corr/energy-corr

diffraction angle/time for TOF/d value/energy of the profile point corrected for zero shift, sysin and sycos

Skip flag 0 if the profile point was used in the refinement

1 if the profile point belongs to one of excluded regions

Icalc(1) calculated intensity of the first phase

. . . .

Icalc(NPhases) calculated intensity of the last phase

Ib background intensity

d d value

The list of profile points ends with the real number “999.”.