Custom *.xyy* Topas output format for *Reel*

The following is a guide to the custom *.xyy* output format intended for *Reel*.

The header is separated in several parts. It starts with a *mandatory* filename on the first line. Then follows a section of *keywords* ending on a colon and followed by a value. There are (currently) three keywords of special significance: "*R_wp:*", "Temperature (K):", and "*Wavelength (Å):*". Any additional keywords will still be read by the program, but no further treatment is implemented yet.
The *keyword* section is terminated by the beginning of the comments section. The comment section is started with *COMMENTS*, and any additional lines will be ignored by the program, until the *END OF HEADER* line.

The data columns start with a column label, followed by the data. *Reel* expects the following *mandatory* columns: "*tth Y_obs Y_calc Y_res Background*". Any additional columns will be plotted with their corresponding label. Although "*Background*" is considered mandatory, it is not actually used in the current version of *Reel*, meaning that any arbitrary placeholder value can be used.

```
File_name
R_wp: 4.702
Temperature (K): 373.500
Wavelength (Å): 2.52098
Counts: 834837.00
COMMENTS
Any additional comments or metadata provided by the user
END_OF_HEADER
```

Mandatory
Special

tth	Y_obs	Y_calc	Y_res	Background	Phase_1	Phase_2	Phase_3	Phase_4
9.970	8039.000	8305.591	-266.591	8287.333	8294.666	8298.258	8287.333	8287.333
10.070	7999.000	8283.805	-284.805	8264.862	8272.764	8275.903	8264.862	8264.862
10.170	8045.000	8262.288	-217.288	8242.581	8251.130	8253.740	8242.581	8242.581
10.270	7960.000	8241.055	-281.055	8220.490	8229.776	8231.768	8220.490	8220.490
10.370	8221.000	8220.122	0.878	8198.587	8208.722	8209.986	8198.587	8198.587
10.470	8110.000	8199.512	-89.512	8176.871	8187.989	8188.394	8176.871	8176.871
10.570	7990.000	8179.257	-189.257	8155.342	8167.607	8166.992	8155.342	8155.342
10.670	8104.000	8159.391	-55.391	8133.999	8147.613	8145.777	8133.999	8133.999
10.770	7990.000	8139.962	-149.962	8112.840	8128.054	8124.748	8112.840	8112.840
10.870	7894.000	8121.036	-227.036	8091.865	8108.997	8103.905	8091.865	8091.865
10.970	8187.000	8102.705	84.295	8071.073	8090.531	8083.246	8071.073	8071.073