



Appendix

8.1 The PDH file format

The PDH file format is a column and line specific file type to store data of linear detectors:

Line 1 ASCII string up to 80 characters (Format (A80)). Used for problem description

Line 2 Keywords KW_1 - KW_{16} (Format (16(A4,1X))), sequence of characters to define the type of experiment.

Line 3 Integer Constants I_1 - I_8 (Format (8(I9,1X))). I_1 : Number of points in this file. All other constants are unused and free for your special use

Line 4 Real Constants R_1 - R_5 (Format (10(E14.6,1X))). R_4 : Normalisation factor. Default is 1.0. Never use 0.0!

Line 5 Real Constants R_6 - R_{10} (Format (10(E14.6,1X)))

Line 6-Line I_1+5 Data lines x , y and σ (Format (3(E14.6,1X))). x : x -value, y : y -value $y(x)$, σ : $\sigma(x)$ standard deviation of $y(x)$ (if unknown or for exact functions use $\sigma(x) = -1.0$)

e.g.:

Example for a simple PDH file of 5 points

```
SAXS
      5      0      0      0      0      0      0
0.000000E+00 0.000000E+00 0.000000E+00 0.100000E+01 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.120000E-01 0.210900E+04 0.104720E+03
0.140000E-01 0.192190E+04 0.100940E+03
0.160000E-01 0.202430E+04 0.969290E+02
0.180000E-01 0.201880E+04 0.927930E+02
0.200000E-01 0.173250E+04 0.886280E+02
```