LOQ 1D ASCII DATA FILE FORMAT

The short example file below was written out by COLETTE, it has been reduced to 6 data points, the third record has been edited by the user so that only points 2 to 4 are to be used when the data is read back in. The IFLAG= 3 at the start of the fifth record shows that Q, I(Q) & error(Q) are expected, using the format shown.

```
LOQ Thu 15-JAN-1998 11:43 SAMPLE: 54331 EMPTY CAN: 54332 used /FLAT
Wav 2.20 > 10.00 Phi -180.0 > 180.0 Rad 53.0 > 750.0 Scaled* 1.000
6 0 0 0 2 4
0 0 0 0
3 (F12.5,2E16.6)
0.00562 1.664269E+01 1.182694E-01
0.00607 1.018861E+01 6.170455E-01
0.00655 4.091472E+00 3.789476E-01
0.00707 4.746222E+00 4.646616E-01
0.00865 6.092464E+00 2.959473E-01
0.00947 8.743887E+00 2.343611E-01
```

The file description was written with "cards" in mind so is tightly formatted. Since <u>the main data format is actually read in</u> (a not widely known feature of FORTRAN) almost any ASCII file from some other source can be read by the addition of five header records (a) to (e):

Record Format Contents
(a) (A80) Title (include a date !)
(b) (A80) second title
(c) (6I5)   NCH number of data points
        NC1 Number of first good data point
        NC2 last good point before beam stop
        NMC centre TIMES TEN (so accurate to 0.1 channel)
        NC3 first good point after beam stop
        NC4 last good point after beam stop
        NOTE: for normal, ascending Q only use NC1=NC2=NMC=0
        NOTE: NCH does not have to equal NC4, "poor" data from the ends of the range may be carried around indefinitely, left in or out as desired by altering the NC's
(d) (4I10) (IC(I),I=1,4) monitor counts
        (Use these four numbers for anything you like, they were originally used for X-ray data monitor counters.)
(e)(I2,1X,A76) IFLAG =1 only C(i=1,NCH) data array to be read; Q(i) are set integers 1 to NCH
        =2 only (Q(i),C(i), i=1,NCH) coordinate and data arrays to be read; E(i) set as sqrt(C(i))
        =3 (Q(i),C(i),E(i), i=1,NCH) coordinate, data and error arrays to be read
        (FMT) character string containing data format
(f) (FMT) using fortran format as read at (e) the actual data.

LOQ 2D ASCII DATA FILE FORMAT

Included below is a small example file with 4 columns x 8 rows of reduced data, immediately followed by a 4x8 block of errors. Note that X, Y and Z axis labels have GENIE-II units "code numbers" associated with them. The second section of the file has a variable number of "nUseRec" user records for further data input to suit other applications. In this example nUseRec=2 and the two lines contain "titles" with information from COLETTE. Thus additional information may be embedded both here and by creative use of the FORTAN data format (as for 1d data).

The third section contains an X array of 5 points and a Y array of 9 points, followed by a 4 x 8 data point array with rescaling of 1.000000, thus the data is in "histogram mode". Since IFLAG=3 before the final data format the 32 DATA values are followed, in a separate block by 32 ERROR values. (Note: IFLAG is now in format I3 not I2 as in the 1d files!) The rescale parameter (actual data = rescale* data following (the opposite of the ILL format !)), may allow smaller files by *careful* choice of a format in COLETTE, e.g. WRITE/SCALE=0.01/FORMAT= "(8f6.1)" W61 FILE.LQA

```
LOQ Fri 16-JAN-1998 16:58 SAMPLE: 55447 EMPTY CAN: 55448
6 Q (Ang-1) X axis label
6 Q (Ang-1) Y axis label
0 Cross section (cm-1) Z axis label
2
LOQ Fri 16-JAN-1998 16:58 SAMPLE: 55447 EMPTY CAN: 55448
Wav 2.20 > 10.00 Phi -90.0 > 90.0 Rad 53.0 > 750.0 Scaled* 1.000
5
-2.000000E-01 -1.000000E-01 0.000000E+00 1.000000E-01 2.000000E-01
9
-2.400000E-01 -1.800000E-01 -1.200000E-01 -6.000000E-02 0.000000E+00
6.000000E
-02 1.200000E-01 1.800000E-01
2.400000E-01
4 8 1.000000000000E+00
3(8E12.4)
2.6871E-01 3.4496E-01 4.0645E-01 2.2671E-01 4.8461E-01 9.7524E-01 9.3726E-01
4.6318E-01
9.3003E-01 2.7835E+00 2.6451E+00 8.6639E-01 1.3917E+00 1.1101E+01 1.1277E+01
1.3427E+00
1.3355E+00 1.1252E+01 1.1217E+01 1.3237E+00 8.3119E-01 2.6887E+00 2.6660E+00
8.4653E-01
4.6725E-01 9.0712E-01 8.9257E-01 4.2111E-01 2.9457E-01 4.6612E-01 4.0653E-01
1.5973E-01
6.8801E-02 7.2672E-02 7.1742E-02 6.7268E-02 1.8736E-02 1.6666E-02 1.6817E-02
1.8134E-02
1.6791E-02 1.2329E-02 1.2287E-02 1.6017E-02 1.8742E-02 1.7109E-02 1.6852E-02
1.7487E-02
1.8954E-02 1.7457E-02 1.7106E-02 1.7632E-02 1.6400E-02 1.2299E-02 1.2408E-02
1.6167E-02
1.9540E-02 1.7533E-02 1.7736E-02 1.9254E-02 6.9760E-02 7.3224E-02 7.3125E-02
6.9384E-02
```