Dear Dr Skoda,

I have considered your spectra and possibility to fit the base line (continuum) by a simple model function. At first I would like to mention that proper model function is, strictly speaking, essential for DLS; i.e. the parameters of the model function and associated uncertainties have both - correct physical and statistical meaning. However, in case that model function is not known, DLS will work fine with any model function which has a shape close to the expected shape of the spectrum base line. Of course meaning of the reported parameters is limited.

Regarding your spectra I supposed that simple, four parameters model function, is good enough to illustrate strength and limitations of the DLS.

I have divided your spectra in two groups:

the first suitable for base line approximation by (the 3th order) polynomials

the second which needs more specific (4 parameters) model function

Also, different spectra have different amount of noise. In some spectra it is clear that noise is caused by data scatter; in some intensity variations are recognized as noise due to inadequately simple model function.

At first I normalized your data to fall both "x" and "y" in the range 0 – 100; the names of these files are extended by "!n" to distinguish it from original files. After that I have fit your data without any sectioning. DLS report contains several files:

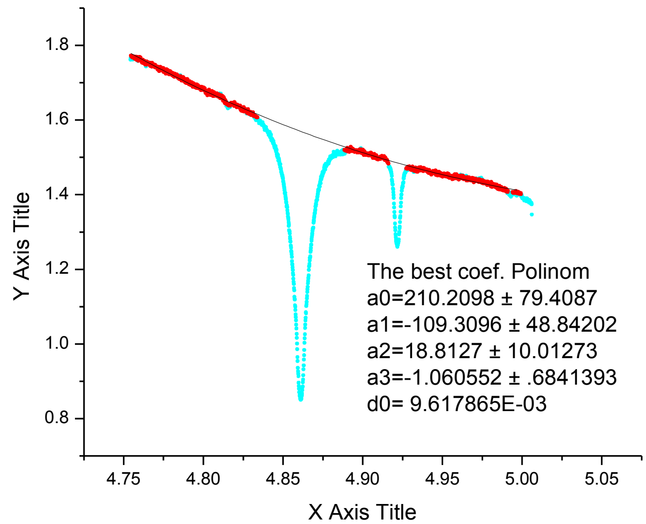
"OriginalName!ncoef.dat"	best coefficients
"OriginalName!ncp.dat"	close points recognized by DLS (i.e. base line)
"OriginalName!ndp.dat"	distant points (spectral lines)
"OriginalName!ndiscr!.dat"	discrimination level (ModelFunction – d0)
"OriginalName!ndiscr.dat"	Discrimination level (ModelFunctio +d0)
"OriginalName!nfit.dat"	Fit function calculated in 100 points within X interval
"OriginalName!nmf.dat"	Merit Function
"OriginalName!nrep.dat"	Report

File with the best coefficients contains d0 value, the width of the nose ditributin; this value is included in the report file also. Note that close and distant points (files "OriginalName!ncp.dat", "OriginalName!ndp.dat") must be plotted as points, not as points connected by lines.

I have included an Origin file for overview of data and appropriate fit.

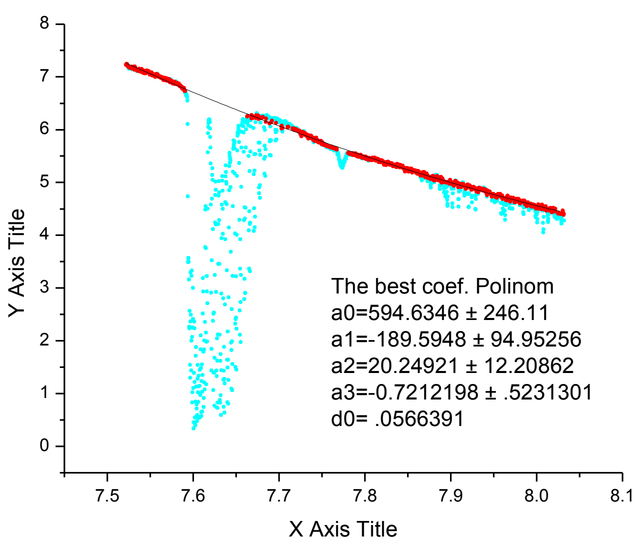
Polynomial fit: y=a0 + a1*x + a2*x^2 + a3*x^3
Initial guess is not necessary

File: **kk160075!n.dat**



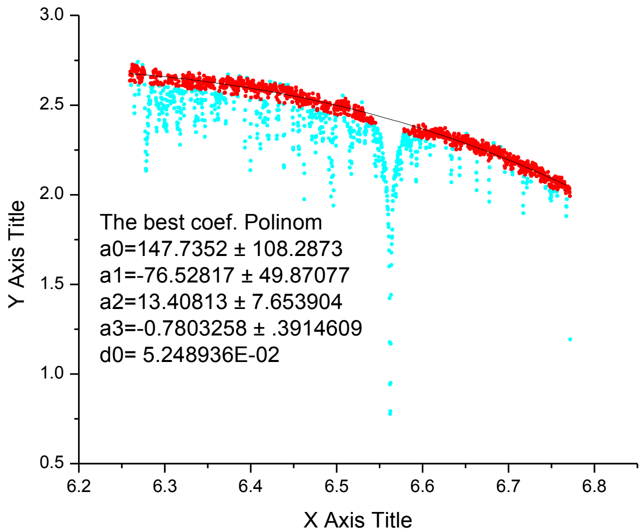
Red color – close points; cyan – distant points, spectral lines; black - the best fit function. This is nice fit with small amount of noise. The width of the noise distribution is d0=9.6e-3

File: **la220068!n.dat**



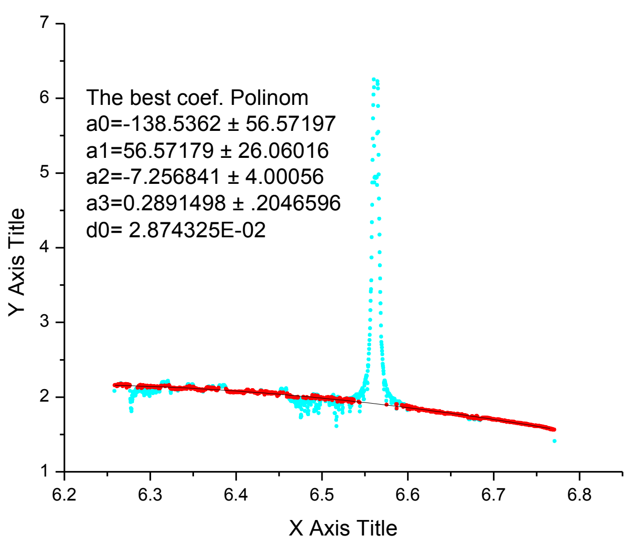
It seems that model function around x=7.65 is not adequate. Number of spectral features around x=7.65 are sorted out as a single object.

File: **lb010023!n.dat**



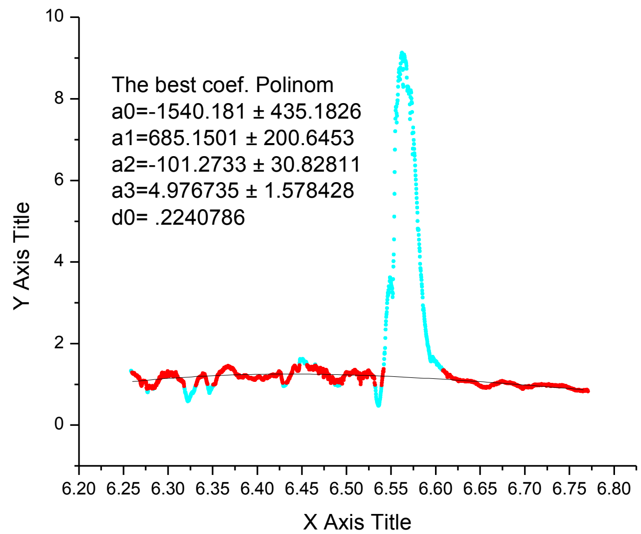
More noise here. There is a small deviation in the flow around x=6.3 which I can notice by eye. Due to noise, there is no improvement in the fit if the higher degree polynomials are applied.

File: **mg150041!n.dat**



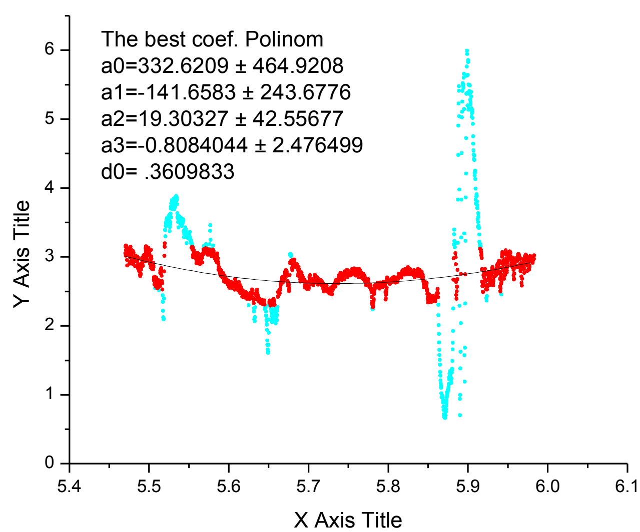
It looks OK.

File: **mi180019!n.dat**



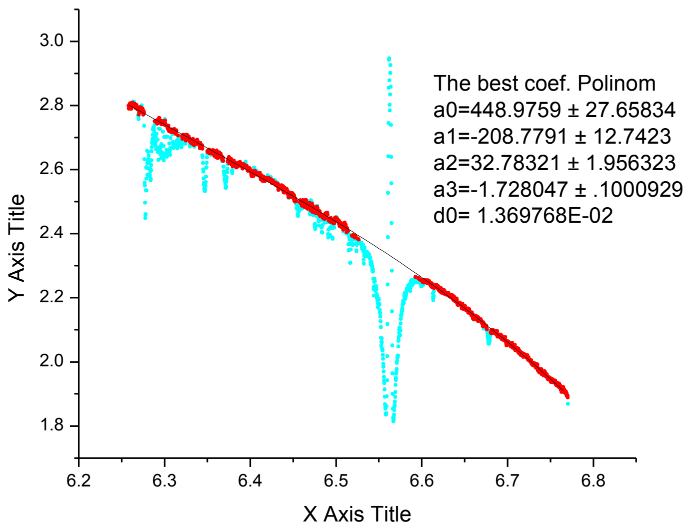
If the spectrum base line is expected to be smooth then there is just one feature around x=6.55, the rest is recognized as noise.

File: **mi180027!n.dat**



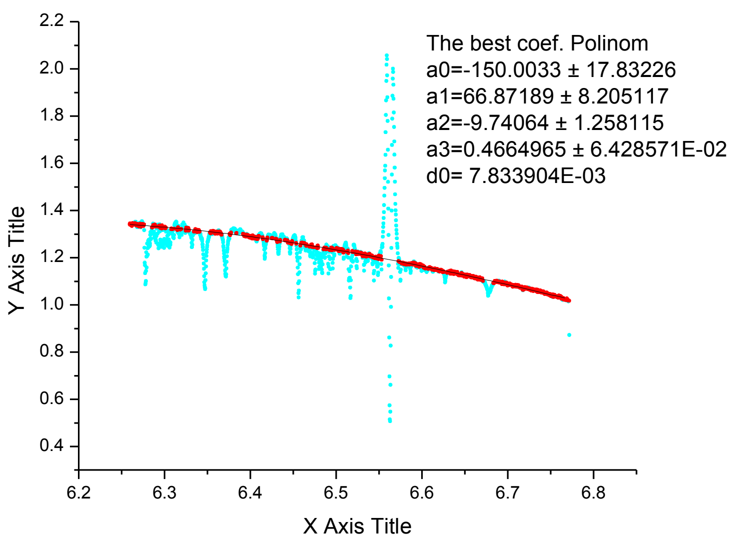
It seems to me that more detailed model function is to be applied here.

File: **mj180022!n.dat**

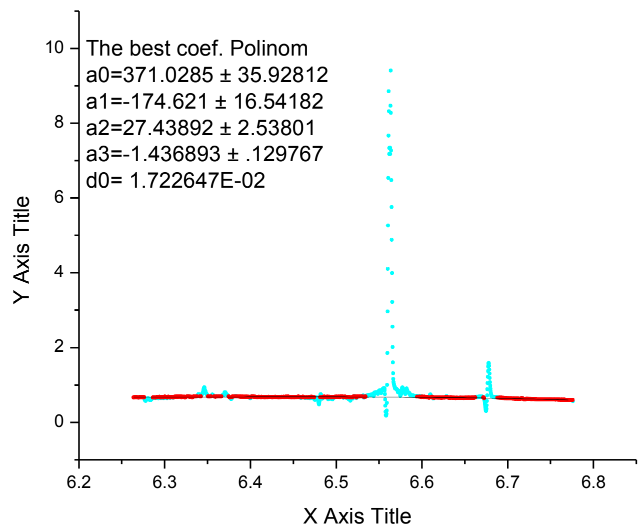


OK

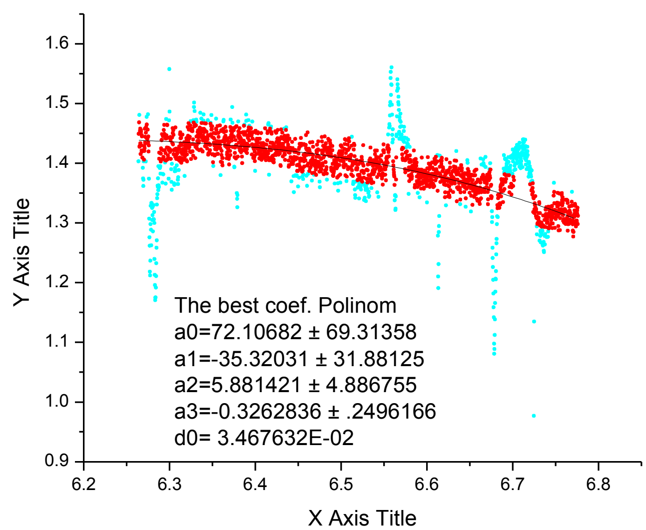
File: **nc170040!n.dat**



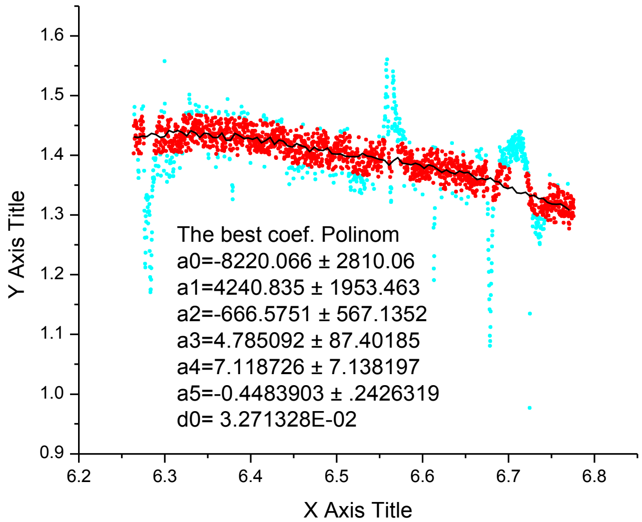
File: **nh100009!n.dat**



File: **nk240013!n.dat**



Lot of noise. By eye I would expect more straight line as a base line. The curvature is caused (probably) by the feature at x~6.257. There are two ways to fix it: to apply straight line or to apply higher order polynomial. The 5th order polynomial, however, does not provide any better fit, see below.

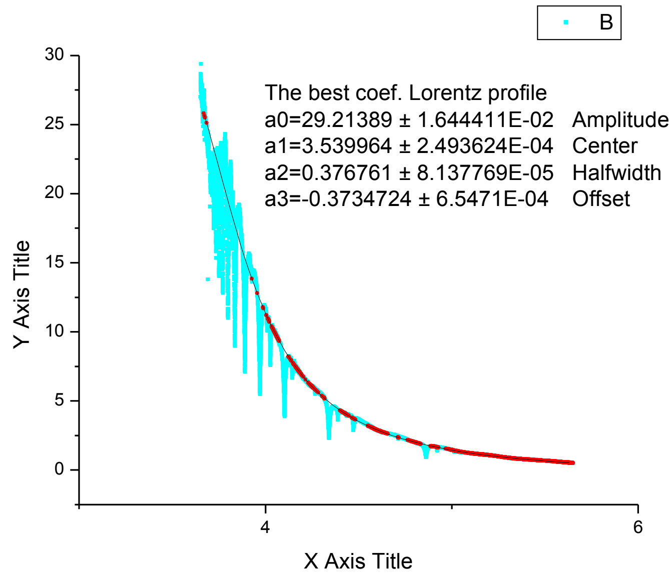


The fit line is zigzag due to insufficient accuracy in calculating polynomial values for plot. Otherwise the fit is correct I suppose.

Non polynomial fit
Initial guess is necessary

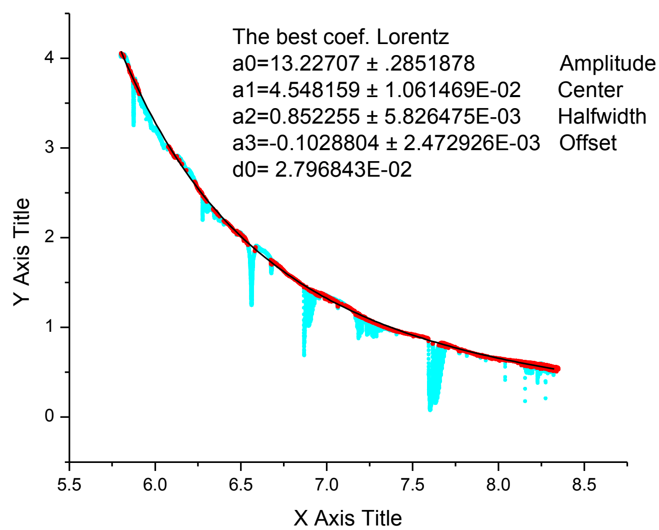
For files: **bxn5267!n.dat** and **rxn5612!n.dat** the polynomial fit is not suitable. It seems that my knowledge is insufficient (I am physicist, not astrophysicist) to recognize behavior of **bxn5267!n.dat** around x=3.75. For both files an exponential function seems to be a reasonable choice. However, I have employed Lorentz function (the initial guess estimation is easy, it is 4 parameters function, it has more complex curvature in respect to the exponential model, finally I have already implemented this function).

File: **bxn5267!n.dat**



Around x=3.75 the fit fails to be correct. I suppose that adequate model function should be more detailed, with a priory knowledge taken into account.

File: **rxn5612!n.dat**



On the original scale 4 parameters function produces reasonable fit. However, file contains large number of data and for fine scale details (around 7, for example) the four parameters function is not adequate.