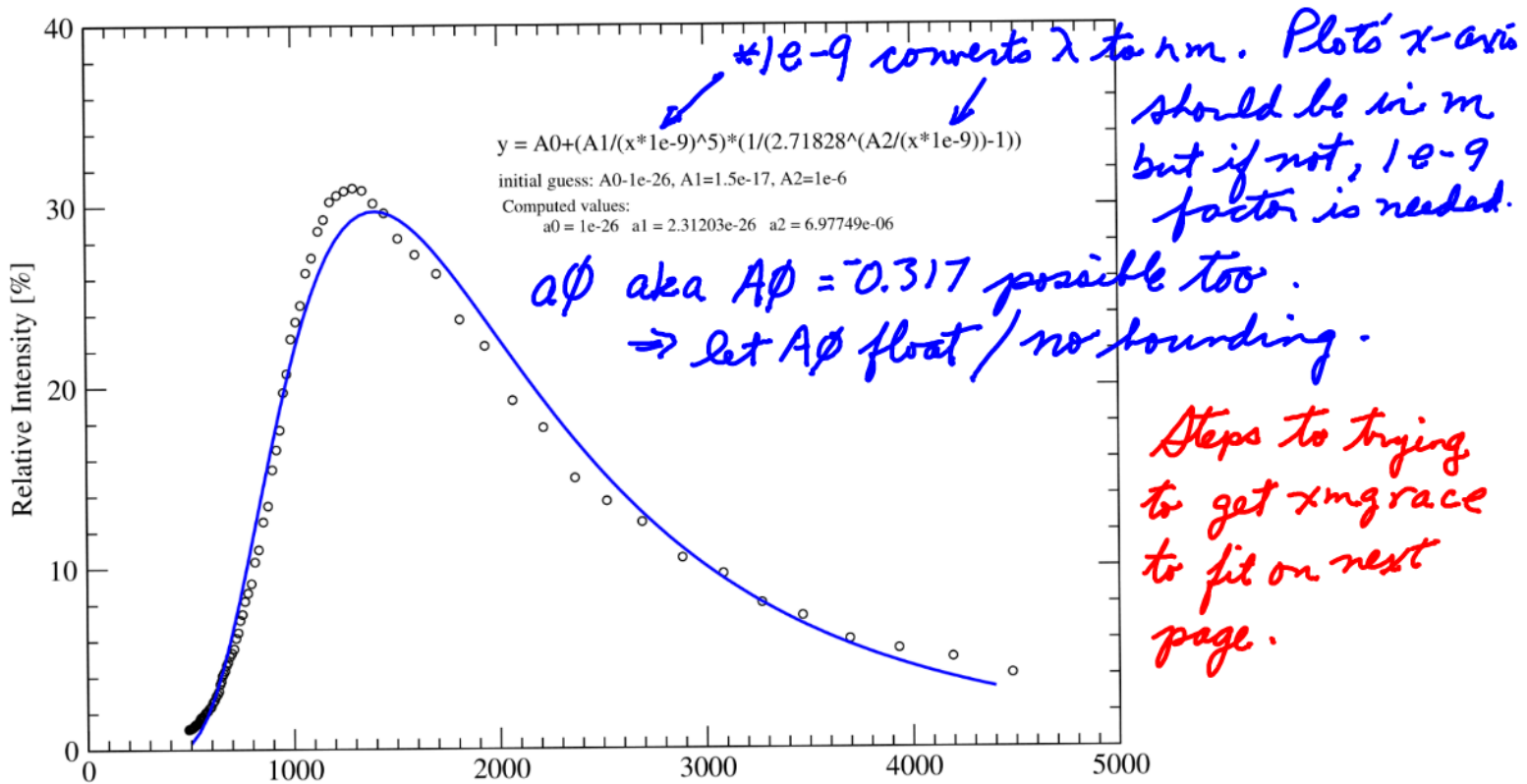


Test fit



The fitting process of the BB data can be challenging

- ① More exploration reveals that bounding $A\phi$ (the vertical offset if the equation is entered as shown in the graph above) is generally problematic.
- ② Bounding of A_1 & A_2 is beneficial: so far achieving a fit w/o bounding A_1 + A_2 has eluded me.
- ③ "Tight" bounding of A_1 + A_2 seems advisable: that is a range of 10^4 to 10^6 . This is a suggestion not a solid requirement. If A_1 & A_2 are unbounded, the algorithm fails to fit in at least two ways:
 - 1) a horizontal line @ the average intensity ($\sim 10\%$)
 - 2) "Free is orthogonal to blah, blah" error.

Suggested bounding for A1 + A2:

$$1e-28 < A_1 < 1e-25$$

$$1e-8 < A_2 < 1e-4$$

Initial guess for A_1 : $1e-26$

A_2 : $1e-6$

Initial guess for $A\emptyset$: \emptyset

no
guarantee
these will
work. test.agr
has slightly different
values quoted

Fit to Test Data Steps:

- ① Open test.agr file in xmgrace. This data is already truncated, the far IR region has been removed.
- ② Click on: Data, Transformations, Non-linear curve fitting...
- ③ Set parameters to 3
- ④ Formula field needs:

← on "Main" page of
non-linear curve fitting
dialog

$$Y = A\emptyset + (A_1 / (x * 1e-9)^{15}) * (1 / (2.71828^{(A_2 / (x * 1e-9))} - 1))$$

This assumes x-axis is in [nm] which is true for test.agr. Your data may be different.

$A\emptyset$ bounds not active

A_1 bounds active

A_2 bounds active

$$1e-28 < A_1 < 1e-25$$

$$1e-8 < A_2 < 1e-4$$

On "Advanced" tab of Non-linear curve fitting dialog

① Source Data filtering + Weighting: leave as defaults.

② Load Options:

Load: Function \leftarrow change to Function

Start Load At: Stop Load At:

(500nm + 4400nm)

of points

* Source Set needs to be selected: GØ. SØ ≠

Destination Set: leave unselected initially, but
if the fit fails, just keep overwriting the S1 set
 \Rightarrow not SØ, that is the input data ;

Finally: click "Apply"