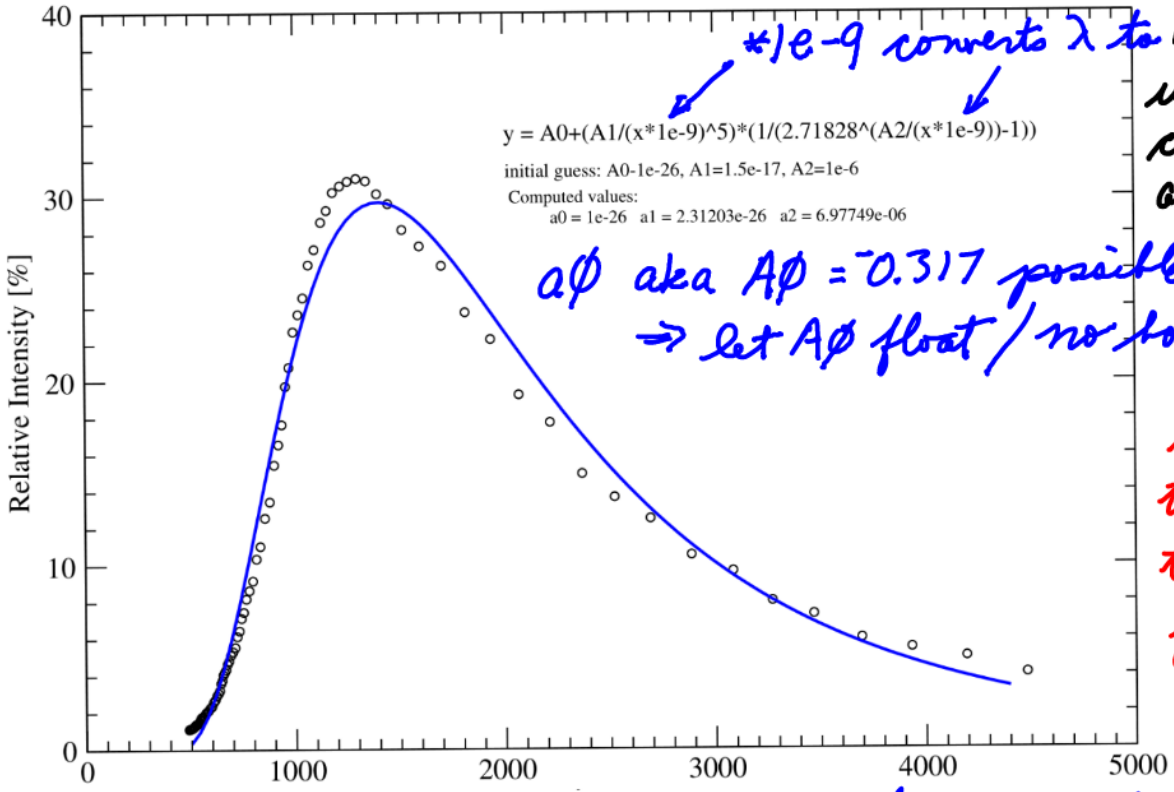
2020 changes in black Test fit



*1e-9 converts λ to meters Plot x-axis usually in nm, constants/values are SI units.

aØ aka AØ = 0.317 possible too.
⇒ let AØ float / no bounding.

Steps to trying to get xmgrace to fit on next page.

The fitting process of the BB data can be challenging

① Owing to a little too much data been deleted on the blue end of the spectrum allowing the offset parameter A0 to actually go -ve (-25 to -30) is likely necessary to get the curve to fit the peak better. Putting some short λ data back may be beneficial

② Bounding of A_1 & A_2 is advised.

③ Bounding on constants A1 + A2 seems advisable: A_1 between 1e-28 to 1e-24 or tighter and A_2 between 1e-8 and 1e-4 approximately.
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 (~10%)
2) "Free is orthogonal to blah, blah" error.

Suggested bounding for A1 & A2:

$1e-28 < A_1 < 1e-24$

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

Initial guess for A_1: $1e-26$

A_2: $1e-6$

Initial guess for $A\emptyset$: $\emptyset$

} no guarantee these will work.

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

④ Formula field needs:

$$Y = A\emptyset + (A_1/(X*1e-9)\wedge 5)*\left(1/\left(2.71828\wedge\left(A2/(X*1e-9)\right)-1\right)\right)$$

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

A$\emptyset$	$\emptyset$	bounds active	-40 to 10 initially.
A1	1e-26	bounds active	$1e-28 < A1 < 1e-24$
A2	1e-6	bounds active	$1e-8 < A2 < 1e-4$

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

① Source Data filtering + Weighting: leave as defaults.

② Load Options:

Load: Function ⇐ change to Generation

Start Load at: [500] Stop Load at: [2500]

which is 500 nm to 2500 nm # of points [100]

* Source Set needs to be selected: G0.S0 *

Destination Set: leave unselected initially, but if the fit fails, just keep overwriting the S1 set ⇒ not S0, that is the input data ;)

Finally: Click "Apply"