**Material Composition in the ASAXS functions of XModFit**

A material can be defined in various forms

1. Solid form with known elemental composition using Chemical Formula (Example: Au, Ag, AgNO3..etc)
2. The moles of resonant elements are defined by the parameter ‘Rmoles’ in ‘Multiple Fitting Parameters’
3. In solution form where the material composition will be written in the format of ‘Solute:Solvent’ where both the ‘Solute’ and ‘Solvent’ material described by chemical formula with known elemental compositions (Example: AuCl3:H2O, NaCl:H2O etc)
4. If the resonant element of a material (R) is shared with another element (C), the material should be described as chemical formula as AnABnBCnC\*EnER, where (A, B, C, E) are non-resonant elements with (nA, nB, nC, nE) and R is the resonant element. The number of moles of ‘C’ in the chemical formula will be (nC-Rmoles).
5. The density of the ‘solute’ and ‘solvent’ are provided by parameters ‘Density’ and ‘SolDensity’ in the ‘Multiple Fitting Parameters’. *It is important to note here that If either solute or solvent contains resonant element along with other elements the ‘Density’ or ‘SolDensity’ represents only the density of other elements. The software will calculate the overall density of the material using ‘Rmoles’ of the resonant element. For example, for a solution of RbCl in H2O the material should be described as RbCl:H2O, the ‘Density’ should be the density of the Cl and ‘SolDensity’ should be the density of H2O. If the material is described by a single element and that can be resonant element then the ‘Density’ should be the density of the element itself.*

**Leftover Density of solvent**

Leftover density of resonant element in the solvent

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Combining the above equations, we can write

In terms of the equation in XModFit the constraint for the density of the last layer would be:

(5e-4-3.14159\*norm\*1e-9\*6.023e23\*H\*1e-24\*(\_\_Layers\_R\_000\*\*2\*\_\_Layers\_Density\_000\*\_\_Layers\_Rmoles\_000/16012+((\_\_Layers\_R\_001+\_\_Layers\_R\_000)\*\*2-\_\_Layers\_R\_000\*\*2)\*\_\_Layers\_Density\_001\*\_\_Layers\_Rmoles\_001/159))\*159/1000