Using UV-VIS as a tool to determine size and concentration of Spherical Gold Nanoparticles (SGNPs) from 5 to 100 nm

In this technical note, we describe the use of a UV-VIS as a QA/QC instrument for sizing and concentration determination of spherical gold nanoparticles (SGNPs). Up until now, Transmission Electron Microscopy (TEM) has been used. However, electron microscopy does not lend itself to being a good QA/QC instrument due to its limitations in sample size, invitation to the potential increase in operator error, and low throughput.

**Calculating SGNP size from SPR Peak location**

Two equations were provided from the reference. One equation applied to nanoparticles greater than 35 nm in diameter, the other for gold nanoparticles 5 to 30 nm in diameter. The different equation for the smaller gold nanoparticles can be attributed to a pronounced increase of the ratio of surface atoms to bulk atoms. From his publication, for nanoparticles 35-100 nm in size, Haiss uses:

\[
d = \frac{\ln\left(\frac{\lambda_{spr} - \lambda_0}{L_1}\right)}{L_2}
\]

where \( d \) is the diameter of the SGNP, \( \lambda_{spr} \) is the wavelength at the peak of the surface plasmon resonance (SPR), \( \lambda_0 = 512, L_1 = 6.53, \) and \( L_2 = 0.0216. \) Utilizing over 50 data points in his paper, Haiss finds an absolute error of 3%. Applying the equation to our

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gold nanoparticles determined by TEM, we find an error of 4%.

To calculate the diameter of our SGNPs for sizes 5 to 30 nm, we use another Haiss equation:

\[
d = \left( \frac{A_{\text{spr}} (5.89 \times 10^{-6})}{c_{\text{Au}} \exp(C_1)} \right)^{\frac{1}{C_2}}
\]  

(2)

Where \(A_{\text{spr}}\) is the absorption (AU) at the peak SPR, \(c_{\text{Au}}\) (moles/L) is the amount of gold used in the synthesis, \(C_1 = -4.75\), and \(C_2 = 0.314\). The error calculated by Haiss is \(\sim 6\%\).

**Calculating SGNP concentration**

Concentration is determined by using the diameter of the gold nanoparticles calculated in (1) and (2) with the known absorption at 450 nm. This equation is given by:

\[
N = \frac{A_{450} \times 10^{14}}{d^2 \left[ -0.295 + 1.36 \exp\left( \frac{d - 96.8}{78.2} \right)^2 \right]}
\]

(3)

where \(N\) is the number density of SGNPs in nps/ml, \(A_{450}\) is the absorption (AU) at 450 nm, and \(d\) is the diameter of the SGNP. Haiss finds this equation to be accurate to \(\sim 6\%\).

From this equation, we can find a host of other concentration measurements. This includes Wt. conc., Wt. %, ppm, molarity, and molar extinction.

\[
Wt.\text{conc}\left(\frac{\mu g}{ml}\right) = \frac{4 \pi r^3 c m^3 x 19.28 \times 10^{-3} g}{nps} \times \frac{10^6 \mu g}{g}
\]

(4)

where \(r\) is the radius of the gold nanoparticle, and \(nps\) refers to the number of particles.

\[
Wt.\% = Wt.\text{conc.} \times 10^{-6}
\]

(5)

\[
ppm = \text{wt. conc.}
\]

(6)
molarity (pM) = nps/ml x 1.67x10^{-9} \hspace{1cm} (7)

Molar Ext. (M^{-1}cm^{-1}) = OD x 10^{12}/molarity \hspace{1cm} (8)

To determine the percentage attributed to absorption and scattering of the total extinction, we use Jain et. al\textsuperscript{2} where we curve fit their data points for sizes 20-80 nm with the equation:

\[
\% \text{ scattering} = 0.0001d^2 - 0.0054d + 0.0589 \hspace{1cm} (9)
\]

\[
\% \text{ absorption} = 1 - \% \text{ scattering} \hspace{1cm} (10)
\]

where \(d\) is the diameter of the gold nanoparticle.