

## The Determination of Quantum Dot Radii in Various Solutions

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### Abstract

Quantum Dots are a real world problem that enables one to better visualize the problem from quantum mechanics of the particle in the box. It has real world applications in biology, chemistry, and the production of light sources. Using fairly simple data collection and analyses techniques, the determination of various Quantum Dot radii is capable.

### Theory

The particle in a box problem solvable in fundamental quantum mechanics is sometimes a very difficult thing to visualize. This is because there is not a good real world example of a particle in a box. However, there is one good example that can now be used: Quantum Dots. Inside small semiconductors that make up microprocessors and flash drives there are small semiconductor particles. These can contain one electron and one “hole” or absence of an electron. These are real world particles in a box because they can never get outside of the semiconductor and by observing the Quantum Dots the effects of changing the size of the box on the energy levels of the system can be observed.<sup>1</sup>

Quantum Dots are used in a whole host of applications in the real world. A primary use of Quantum Dots is in biology. Biologists use fluorescent dyes to help analyze various biological systems. However, organic dyes currently used are not capable of meeting the expectations that are now arising in modern biology. Quantum Dots are being looked at for their use as a replacement to the organic dyes of the past. This is because they 20 times brighter and 100 times more stable than the traditional dyes.<sup>2</sup>

Another use of Quantum Dots could be in replacing LED light sources. Chemists at Vanderbilt University have figured out how to make Quantum Dots emit broad-spectrum white light. If this is developed further it could be used to make almost any surface a light source just by applying paint that contains these Quantum Dots within it.<sup>3</sup>

Austrian physicist Erwin Schrödinger first introduced the wave equation in 1925. The wave equation is used to calculate the probable values of a particle’s position, energy, momentum, etc. The wave equation is normally represented in the following form.

$$\hat{H}\Psi = E\Psi \quad (1)$$

In Equation 1,  $\hat{H}$  is the Hamiltonian operator and  $E$  is the eigenvalues of the wave function,  $\Psi$ . The Hamiltonian operator is also represented in the form below.

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (2)$$

In Equation 2,  $\hbar$  is Planck's constant divided by  $2\pi$ , and  $V(x)$  is the potential energy experienced by the particle as a function of position. The wave equation can be written in a one-dimensional form and this is shown below.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + V(x) = E\Psi(x) \quad (3)$$

Solving the particle in a box problem in one-dimension is relatively straightforward. The potential function can be set to zero since the particle is trapped inside the box, the equation can be rearranged, and doing so allows the differential equation to be solved easily.

$$\frac{\partial^2 \Psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2} \Psi(x) \quad (4)$$

Equation 4 above shows the form of the rearranged equation and this differential equation has a solution of trigonometric functions. Define  $k^2$  as;

$$k^2 = \frac{2mE}{\hbar^2} \quad (5)$$

This yields a solution of the form below.

$$\Psi(x) = A\sin(kx) + B\cos(kx) \quad (6)$$

Boundary conditions need to be identified and applied to the equation.

#### *Boundary Conditions*

1.  $V(x)=0$  for  $0 \leq x \leq L$  ( $L$ =length of box) (7)
2.  $V(x)=\infty$  for  $x$  less than 0 and greater than  $L$

Applying boundary condition 1 when  $x=0$  yields that  $B$  needs to be zero since outside the box the potential goes to infinity. This means the wave function must disappear at the boundaries. Then when  $x=L$  tells one what  $k$  is specifically equal to.

$$k = \frac{n\pi}{L} \quad (8)$$

Equation 8 is valid because at  $x=L$ , the wave function must vanish. In order for that to happen the sine term must disappear. Applying the boundary conditions the wave function becomes,

$$\Psi(x) = A \sin\left(\frac{n\pi}{L}x\right) \quad (9)$$

and E becomes,

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad (10)$$

The value of A can also be found but it is not important for the purposes of this lab. This problem is not the same as the Quantum Dot problem since the box is three-dimensional and spherical in shape for the Quantum Dots. However, the equation for E in the Quantum Dot problem has a similar expression.

$$E = \frac{\hbar^2\pi^2}{2m_e R^2} + \frac{\hbar^2\pi^2}{2m_h R^2} + E_g \quad (11)$$

In Equation 10, the two m's are the mass of the electron and the mass of the hole respectively, and the R is the radius of the Quantum Dot. The  $E_g$  is the energy of the semiconductor bandgap. The values of  $m_e$ ,  $m_h$ , and  $E_g$  are;  $m_e=7.29 \times 10^{-32}$ kg,  $m_h=5.24 \times 10^{-31}$ kg,  $E_g=2.15 \times 10^{-19}$ J.

$$E = \frac{hc}{\lambda} \quad (12)$$

Using Equation 12 the E on the left hand side of Equation 11 can be determined and thus the radius of the Quantum Dot can be found using Equation 11.<sup>1</sup>

### Experimental

In this experiment, the radii of four different size quantum dots were determined. The dots were contained within individual vials, each one a different color. The colors of the solutions were green, yellow, red and orange. Vials were contained within a metal rack parallel to one another. A clamp system was set up to hold the rack vertically. Using an XPlorer unit coupled with the Red Tide spectrum analyzer, the wavelength of light emitted from the excited electrons was recorded for each color solution. The solutions were excited using an LED light source of 400 nm that was provided with the experiment kit. Once all the solutions had been excited and the data collected it was analyzed with the help of the program DataStudio.

### Results

Below are the graphs of the excited solutions. On each graph there is a peak at about 400 nm and this is the line for the LED light source used to excite the solution. The other main peak on the graph is that of the wavelength emitted by the excited electrons.

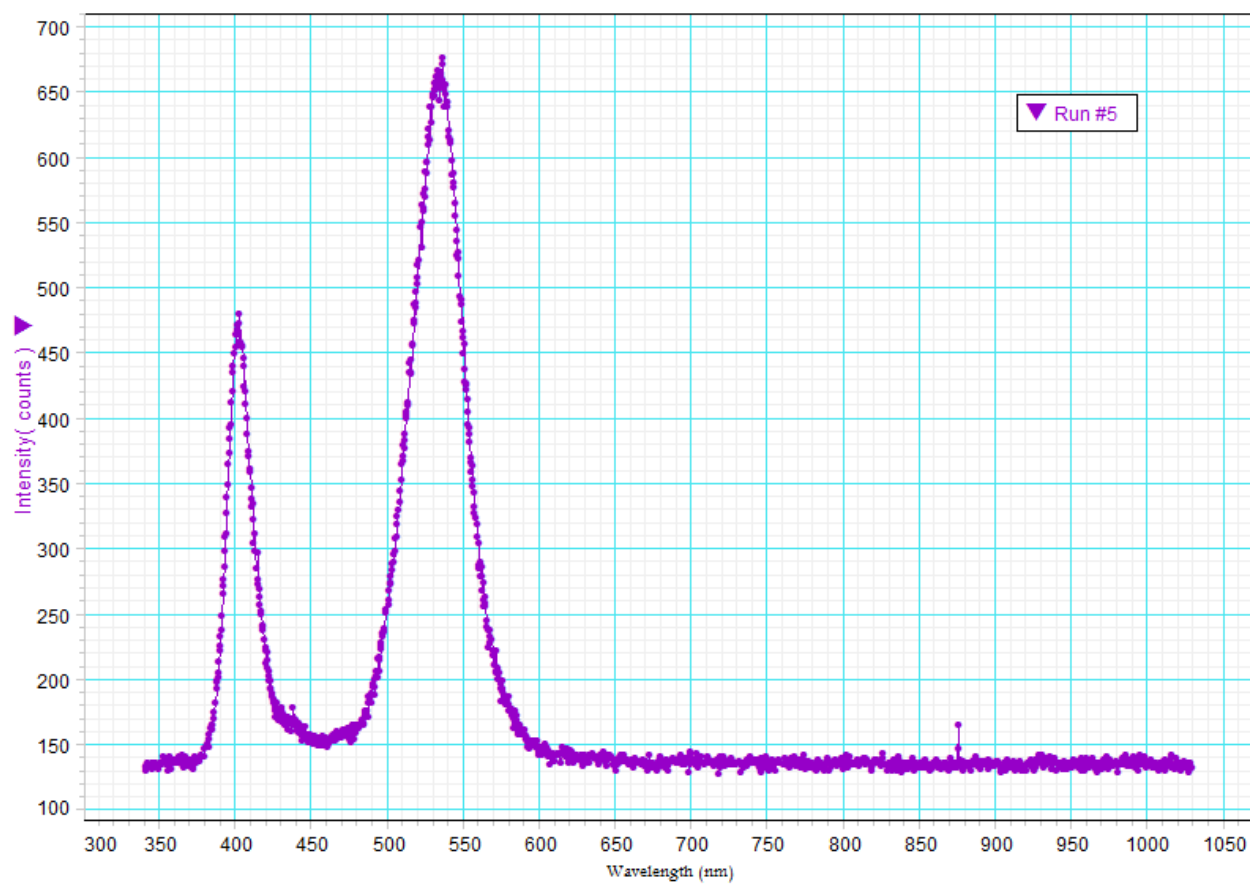


Figure 1 Green Solution

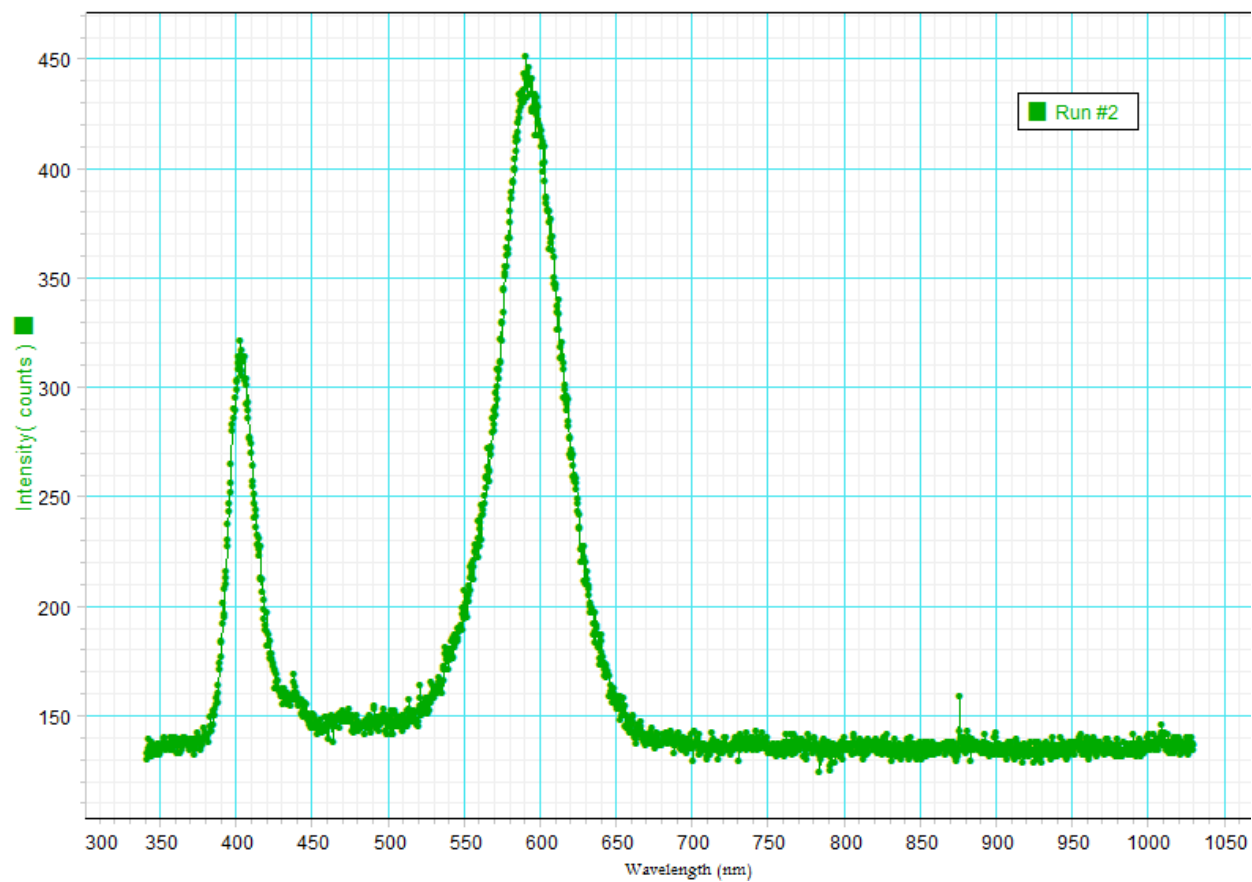


Figure 2 Orange Solution

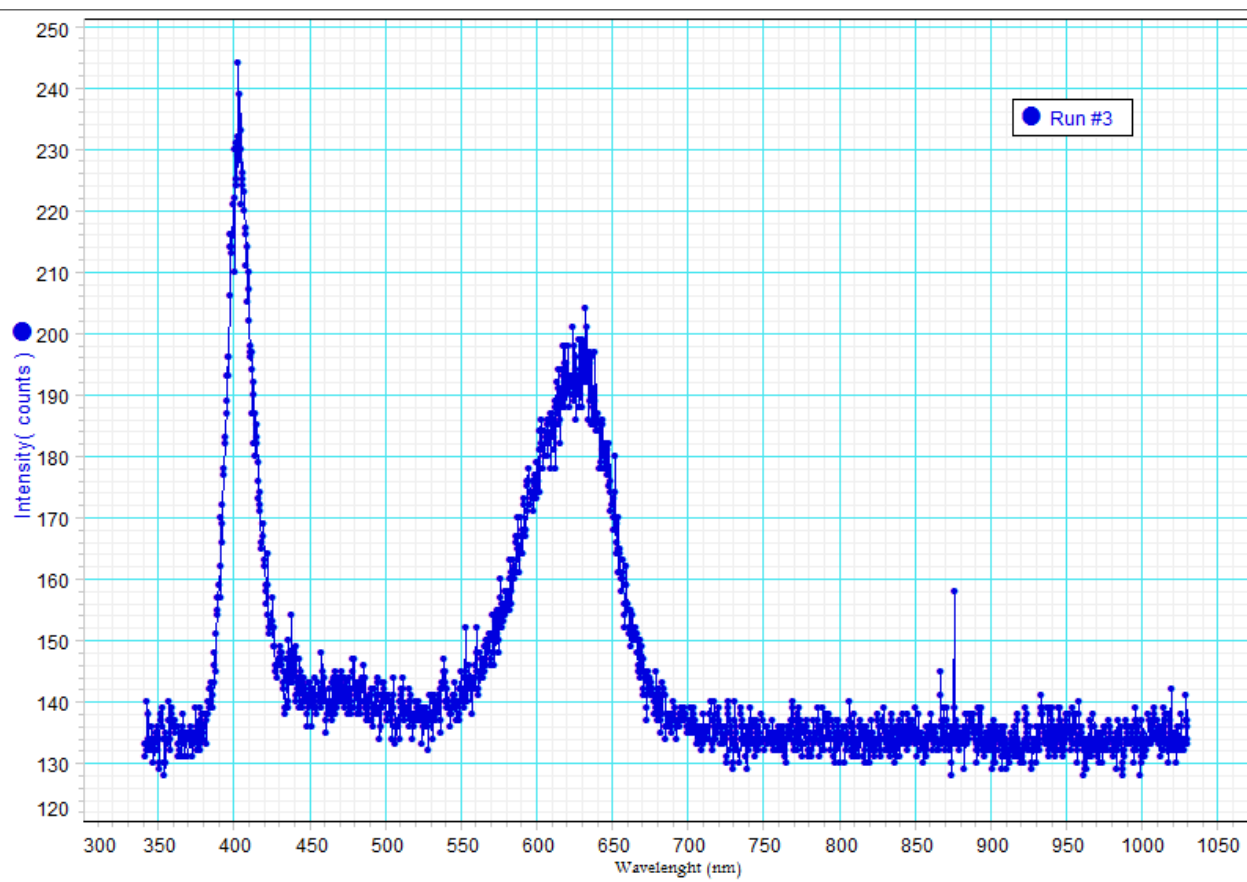


Figure 3 Red Solution

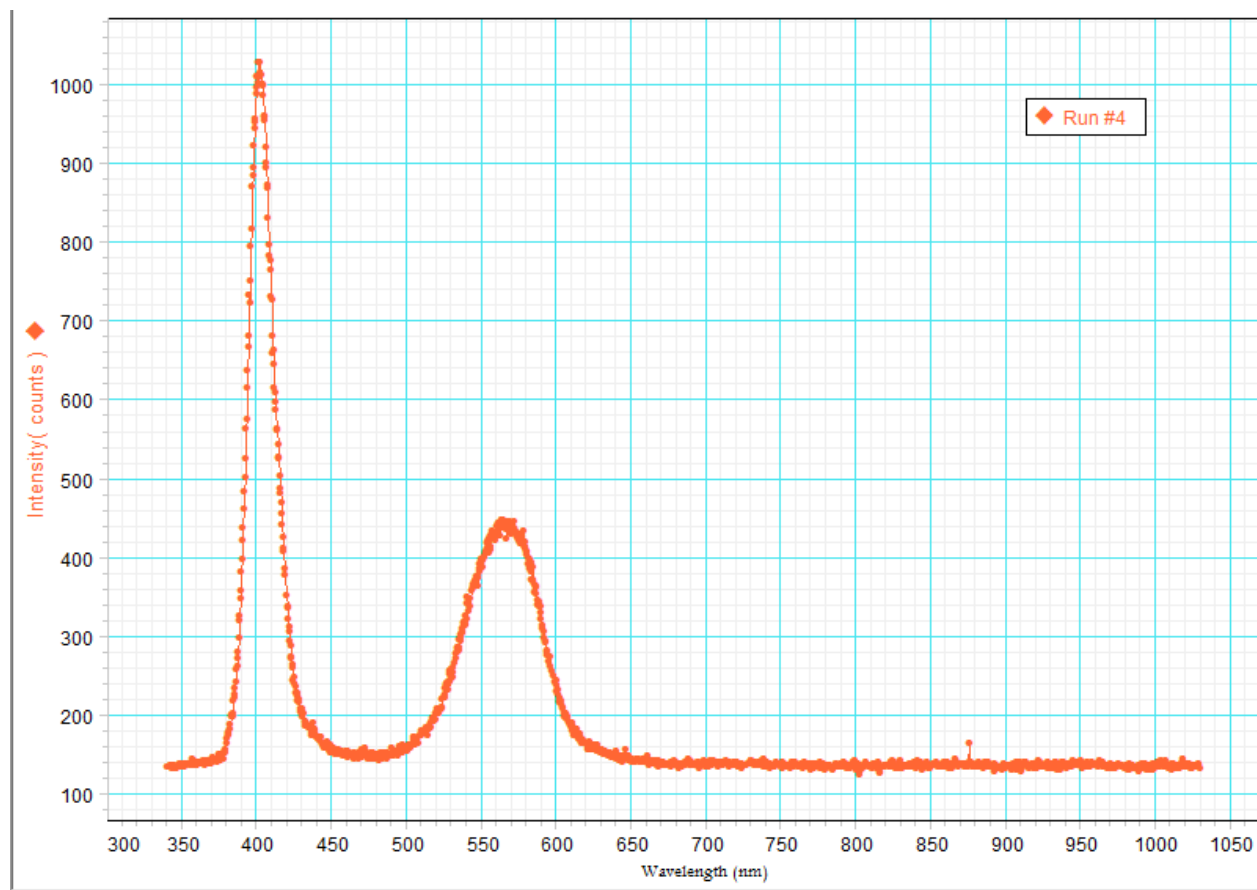


Figure 4 Yellow Solution

Solution	Peak Wavelength (nm)	Energy (J)	Radius of Quantum Dot (nm)
Green	536.77	$3.703 \times 10^{-19}$	2.3425
Orange	590.72	$3.365 \times 10^{-19}$	2.6484
Red	631.9	$3.1458 \times 10^{-19}$	2.9254
Yellow	569.4	$3.491 \times 10^{-19}$	2.5209

Table 1) Wavelength and Experimental radius for each solution.

<b>Solution</b>	<b>Experimental Radius (nm)</b>	<b>Accepted Radius (nm)</b>	<b>Percent Error (%)</b>
Green	2.3425	2.3674	1.05
Orange	2.6484	2.7182	2.57
Red	2.9254	2.9249	.017
Yellow	2.5209	2.5339	.513

Table 2) Experimental and Accepted Radii compared and Percent Error

### Discussion

The purpose of this lab was to determine the size of quantum dots in four different solutions. It can be seen in Table 1 that as the wavelength of light emitted from the excited electrons increased, the radius of the dot also increased. Also observed in Table 1 is that the radius of the dot decreased as the energy of the emitted photons increased. All of this makes sense when looking at Equation 13 shown below.

$$R = (9.2314 \times 10^{-19}) \sqrt{\left(\frac{1}{E - E_g}\right)} \quad (13)$$

In Equation 13, the constant in front of the square root consists of fundamental constants associated with the problem. From Equation 13 it can be seen that as the energy of the emitted photons increases, larger and larger numbers will be divided into one. This will result in smaller numbers being produced for overall radius of the Quantum Dot. So it now makes sense that the red solution has the largest radius of the Quantum Dots but the lowest energy, and the green has the smallest radius but the largest energy.

This experiment works fairly well however there was some noise in the spectrum data. This was most likely caused from reflections off of the surfaces in the room that was worked in or from light coming in from other rooms. This noise in the data would compensate for the very small percent errors attained in the lab. In an ideally dark room with non-reflective surfaces the percent error would all but disappear.



## References

1. Experiment Guide, Operating Instructions: 1751-18 CENCO Quantum Dots, Nanosys.
2. Walling, Maureen A.; Novak, Jennifer A.; Shepard, Jason R. E. 2009. "Quantum Dots for Live Cell and *In Vivo* Imaging." *Int. J. Mol. Sci.* 10, no. 2: 441-491.
3. [http://www.vanderbilt.edu/exploration/resources/quantumdotled\\_print.pdf](http://www.vanderbilt.edu/exploration/resources/quantumdotled_print.pdf), Vanderbilt University