# SUPPORTING INFORMATION

## Host-Guest Inclusion Complexation of α-Cyclodextrin and Triiodide Examined Using UV-Vis Spectrophotometry

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{NOTE: Figures 1-7 are the Figures from the manuscript, reproduced here for convenience.}

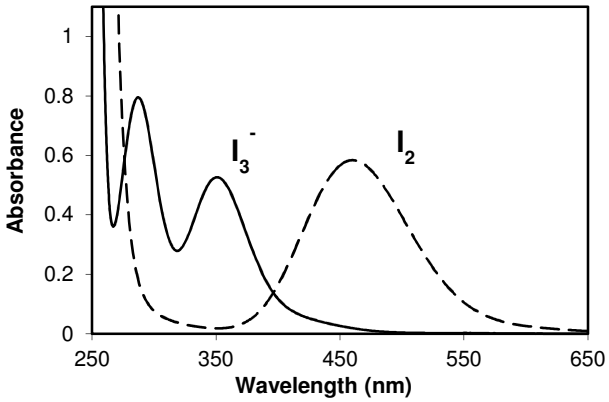


**Figure 1.** Reference UV-Vis spectra for triiodide and iodine in aqueous solutions at room temperature. Solid line: $[I_3^-]$ = 20 μM (made from 20 μM $I_2$ and 20 mM $I^-$); dashed line: $[I_2]$ = 800 μM (with 50 mM $HIO_3$ to force any $I^-$ to $I_2$).

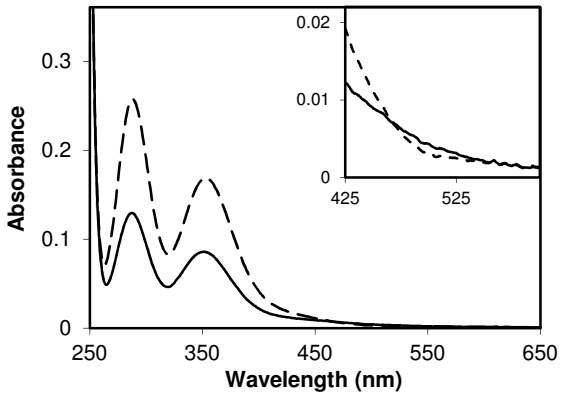


**Figure 2.** Spectra showing the increase in absorbance with the addition α-CD to a solution with triiodide. Solid line: $[I_3^-]$ = 3 μM (made from 8 μM $I_2$ and 800 μM $I^-$; 38% $I_2$ converted to $I_3^-$); dashed line: with the addition of 10 μM α-CD. Inset shows decrease in absorbance due to iodine conversion to triiodide with added α-CD.

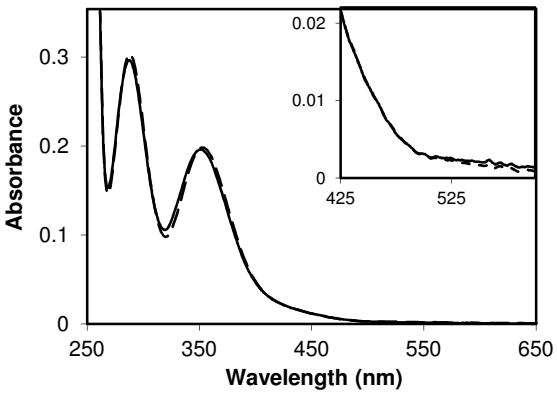


**Figure 3.** Spectra demonstrating the similarity of the molar absorptivities of "free" $I_3^-$ and the complex αCD·$I_3^-$. Solid line: $[I_3^-]$ = 7 μM (made from 8 μM $I_2$ and 8 mM $I^-$; 86% $I_2$ converted to $I_3^-$); dashed line: with the addition of 10 μM α-CD. Inset shows negligible change in absorbance in the iodine region.

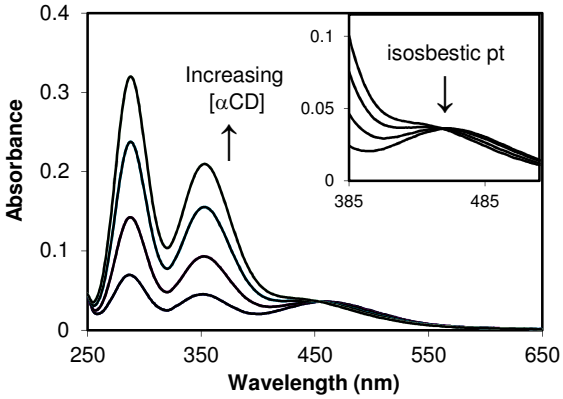


**Figure 4.** Representative spectra at room temperature demonstrating the spectrophotometric approach for determining the complex stoichiometry and binding constant for triiodide and α-CD. $[I_2]_0$ = $[I^-]_0$ = 50 μM; [α-CD] = 5-50 μM. Inset: the isosbestic point indicates the well-behaved conversion of $I_2$ to $I_3^-$ with the addition of α-CD.

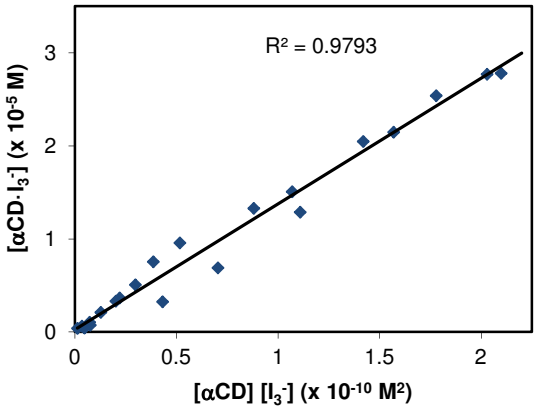


**Figure 5.** Plot of concentrations for determining the complex binding constant at room temperature according to Equation 5. The linearity for the 21 different concentration combinations confirms the 1:1 stoichiometry. The slope is the binding constant (*cf.* $K_{H\text{-}G} = (1.35 \pm 0.05) \times 10^5\ M^{-1}$ at room temperature). The error for each individual measurement is 5%.

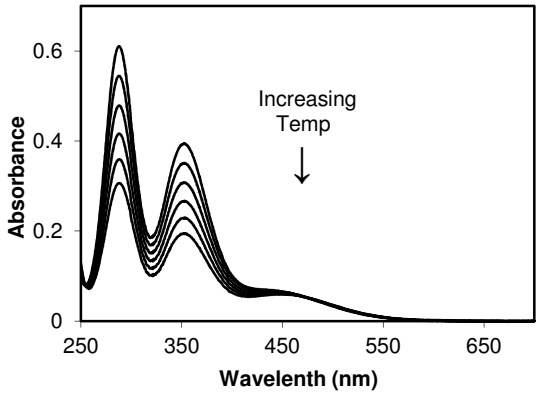


**Figure 6.** Spectra demonstrating the temperature dependence of the complexation of triiodide and α-CD. T = 15-40 ºC; $[I_2]_0 = [I^-]_0 = 50$ μM; [α-CD] = 20 μM.

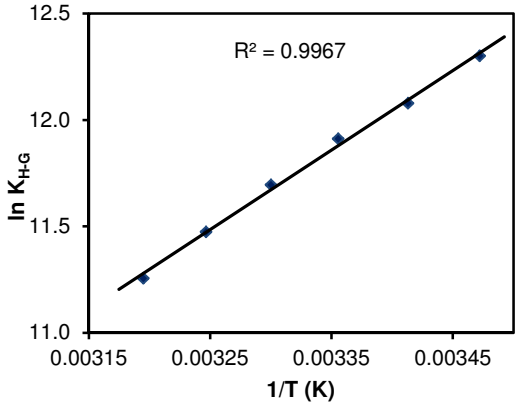


**Figure 7.** van't Hoff plot for the temperature dependence of the complexation of triiodide and α-CD. Each point is the average of four different experimental conditions (*cf.* $[I_2]_0 = [I^-]_0 = 50$ and 100 μM; [α-CD] = 5 and 20 μM). The slope yields the enthalpy of complexation $\Delta H = -31.0 \pm 0.9$ kJ/mol. The error for each individual measurement is 5%.

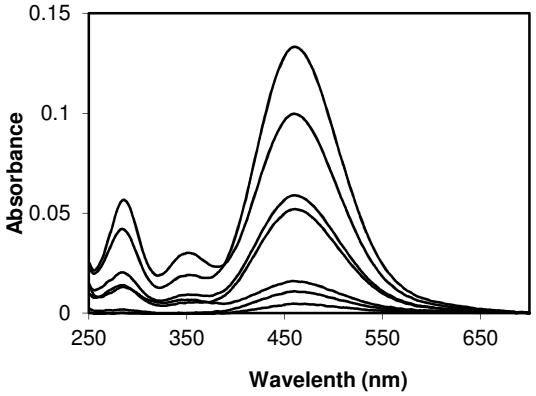


**Figure S1.** Representative UV-Vis spectra of iodine in aqueous solution at room temperature for determining the molar absorptivities. $[I_2]$ = 10-187 μM. At the highest concentration, a small amount of triiodide is present (peak at 350 nm) as an impurity due to reaction of iodine with water (*cf.* this represents only an 0.6% impurity).

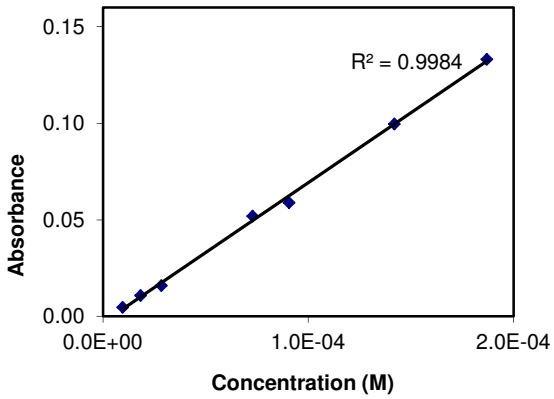


**Figure S2.** Representative Beer's Law plot for iodine using the peak at 459 nm. The slope yields $\varepsilon_{459nm}$ = 725 ± 13 $M^{-1}cm^{-1}$.

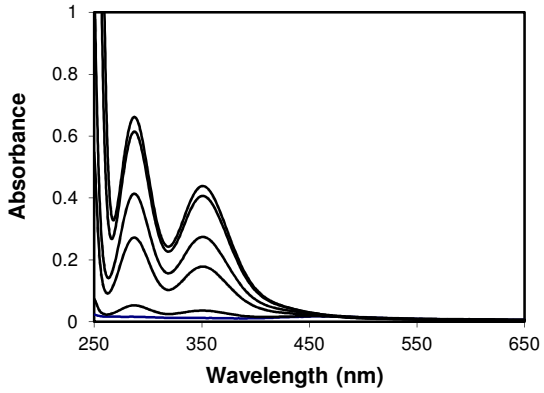


**Figure S3.** Representative UV-Vis spectra of triiodide in aqueous solution at room temperature for determining the molar absorptivities. $[I_3^-]$ = 1-19 μM, with $[I^-]_0 = 1000x[I_2]_0$.

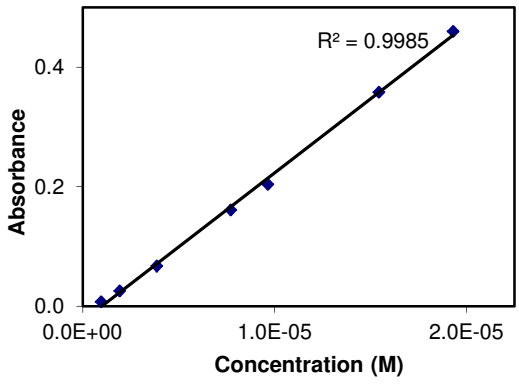


**Figure S4.** Representative Beer's Law plot for triiodide using the peak at 352 nm. The slope yields $\varepsilon_{352nm}$ = 24800 ± 400 $M^{-1}cm^{-1}$.

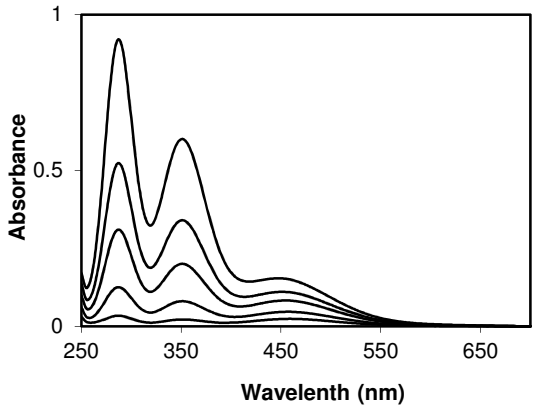


**Figure S5.** Representative UV-Vis spectra of a mixture of iodine and triiodide at room temperature for determining the equilibrium constant for Reaction 1. $[I^-]_0 = [I_2]_0 = 40\text{-}200$ μM.

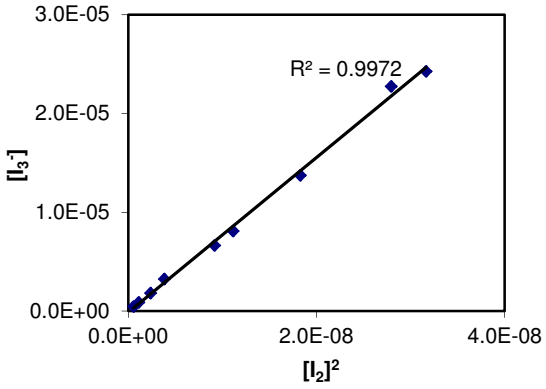


**Figure S6.** Plot of $[I_3^-]$ and $[I_2]$ according to Equation 3 for determining $K_{eq}$ at room temperature (total of nine concentration combinations). The slope yields $K_{eq} = 783 \pm 16$ $M^{-1}$.

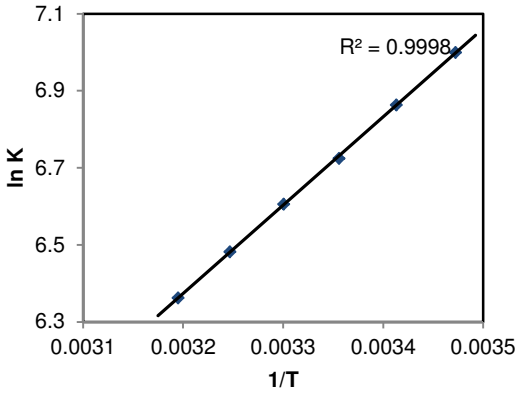


**Figure S7.** van't Hoff plot for the temperature dependence of $K_{eq}$. The slope yields $\Delta H = -19.1 \pm 0.1$ kJ/mol.

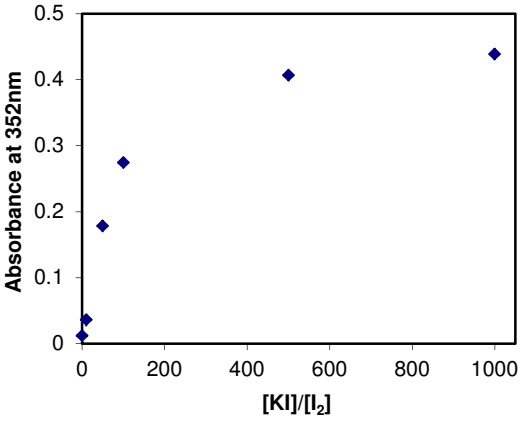


**Figure S8.** Saturation plot for the conversion of iodine to triiodide with increasing amounts of iodide at room temperature. $[I_2]_0 = 20$ μM.

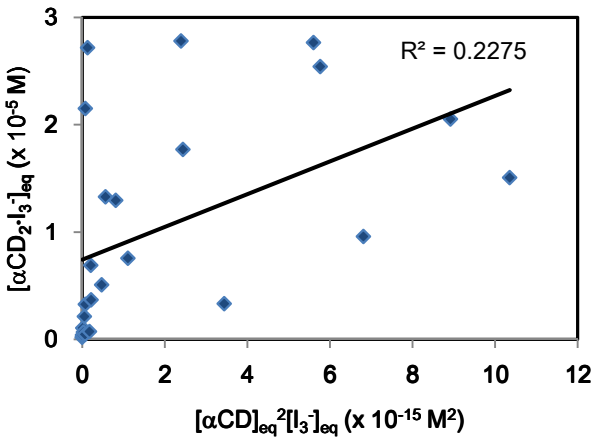


**Figure S9.** Plot of concentrations for determining the complex binding constant at room temperature for 2:1 stoichiometry. The non-linearity for the 21 different concentration combinations confirms the 1:1 stoichiometry according to Figure 5 (above).

**Table S1. Molar Absorptivities** (determined at room temperature in aqueous solutions)

| *Species* | *Wavelength (nm)* | *Molar Absorptivity ($M^{-1}cm^{-1}$)* *This Study* | *Literature* | *Reference* |
|---|---|---|---|---|
| **Iodine** | 459 | 725 ± 13 | 746 | 8 |
| | 500 | 491 ± 11 | - - - | |
| **Triiodide** | 352 | 24800 ± 400 | 25900-26400 | 8, 9 |
| | 500 | 225 ± 5 | - - - | |

***Note:*** *Because of the spectral overlap of iodine and triiodide at 459 nm (cf. the absorbance peak for iodine), the concentration of iodine was determined using the absorbance at 500 nm after accounting for the absorbance of triiodide at 500 nm (i.e. based upon the determination of the concentration of triiodide as determined from the absorbance at 352 nm).*