

Supporting Information

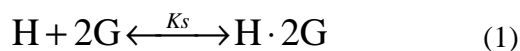
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Spectrophotometric Study of Fluorescence Sensing and Selective Binding of Biochemical Substrates by 2,2'-Bridged Bis(β -cyclodextrin) and Its Water-Soluble Fullerene Conjugate

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Equations to calculate the K_s values for the 1:2 inclusion complexation between host and guest.

After validating the 1:2 complexation stoichiometry between host and guest by the continuous variation method, the inclusion complexation of two guest molecules with a host molecule is expressed by eq 1, and the complex stability constant (K_s) is expressed by eq 2.



$$K_s = \frac{[H \cdot 2G]}{[H][G]^2} \quad (2)$$

where $[H]$, $[G]$, and $[H \cdot 2G]$ represent the equilibrium concentration of the host, the guest, and the formed complex, respectively.

The fluorescence intensity (F) is proportional to the concentration of the fluorophore (c) in dilute solution (eq 3),

$$F = \epsilon_F c \quad (3)$$

From eq 3, we can obtain the following equations. (In this case, the host is nonfluorescent)

$$F_0 = \epsilon_F [G]_0 \quad (4)$$

$$F = \epsilon_F [G] + \epsilon_F' [H \cdot 2G] = \epsilon_F ([G]_0 - 2[H \cdot 2G]) + \epsilon_F' [H \cdot 2G] = \epsilon_F [G]_0 + (\epsilon_F' - 2\epsilon_F) [H \cdot 2G] \quad (5)$$

where $[G]_0$ signifies the initial concentration of the guest, ϵ_F and ϵ_F' represent the molar fluorescence intensity of the free guest and the complex.

Subtracting eq 4 from eq 5, we obtain,

$$\Delta F = F - F_0 = (\epsilon_F' - 2\epsilon_F) [H \cdot 2G] = \Delta\epsilon_F [H \cdot 2G] \quad (6)$$

where ΔF and $\Delta\epsilon_F$ denote the changes in the fluorescence intensity and molar fluorescence intensity of guest molecule upon complexation with host compounds.

We also have the following equations,

$$[H] = [H]_0 - [H \cdot 2G] \quad (7)$$

$$[G] = [G]_0 - 2[H \cdot 2G] \quad (8)$$

By combining eqs 2, 6, 7 and 8, and neglecting the terms of $[H \cdot 2G]^2$ and $[H \cdot 2G]^3$ by similar ways to Tamaki's¹ and Bender's² treatments for spectral changes on complex formation, we can obtain eq 9,

$$\frac{[H]_0 [G]_0^2}{\Delta F} = \frac{1}{\Delta\epsilon_F Ks} + \frac{[G]_0 ([G]_0 + 4[H]_0)}{\Delta\epsilon_F} \quad (9)$$

Using the approximate linear plot $\frac{[H]_0 [G]_0^2}{\Delta F}$ vs $[G]_0 ([G]_0 + 4[H]_0)$, the complex stability constant (Ks) of two guest molecules with a host molecule is obtained.

¹ Tamaki, T.; Kokubu, T.; Ichimura, K. *Tetrahedron* **1987**, 43, 1485-1494.

² VanEtten, R. L.; Sebastian, J. F.; Clowes, G. A.; Bender, M. L. *J. Am. Chem. Soc.*

1967, 89, 3242-3253.