Supporting Information

For

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 continous 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.

$$\mathrm{H} + 2\mathrm{G} \xleftrightarrow{Ks} \mathrm{H}\cdot 2\mathrm{G} \qquad (1)$$

$$Ks = \frac{[H\cdot 2G]}{[H][G]^2} \qquad (2)$$

where [*H*], [*G*], and [*H*·2*G*] 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),

$$F = \varepsilon_F c \qquad (3)$$

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

$$F_0 = \varepsilon_F[G]_0 \qquad (4)$$

$$F = \varepsilon_F[G] + \varepsilon_F'[H{\cdot}2G] = \varepsilon_F([G]_0 - 2[H{\cdot}2G]) + \varepsilon_F'[H{\cdot}2G] = \varepsilon_F[G]_0 + (\varepsilon_F'-2\varepsilon_F)[H{\cdot}2G] \qquad (5)$$

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,

$$\Delta F = F - F_0 = (\varepsilon_F - 2\varepsilon_F')[H{\cdot}2G] = \Delta\varepsilon_F[H{\cdot}2G] \qquad (6)$$

where ΔF and $\Delta\varepsilon_F$ 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,

$$[H] = [H]_0 - [H{\cdot}2G] \qquad (7)$$

$$[G] = [G]_0 - 2[H{\cdot}2G] \qquad (8)$$

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's[1] and Bender's[2] treatments for spectral changes on complex formation, we can obtain eq 9,

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

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 (*K*s) of two guest molecules with a host molecule is obtained.

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[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.