

Supporting Information

for

Molecular solubilization of fullerene C₆₀ in water by

γ-cyclodextrin thioethers

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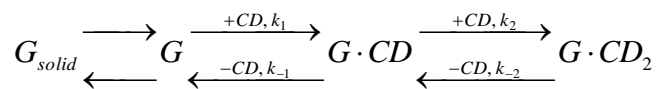
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Detailed dissolution kinetics

2-step model



Approximations:

concentrations: $[G] = \text{const} = [G]_0$, $[CD] = \text{const} = [CD]_0$

stationarity of $G \cdot CD$: $[G \cdot CD_2] \gg [G \cdot CD] \approx \text{const}$

rate determining steps: $k_1[G]_0[CD]_0 \ll k_2[G \cdot CD][CD]_0$, $k_2[G \cdot CD_2] \ll k_{-1}[G \cdot CD]$

rate equation: $\frac{d[G \cdot CD_2]}{dt} = k_1[CD]_0[G]_0 - k_{-2}[G \cdot CD_2]$

equilibrium state: $k_1[CD]_0[G]_0 \equiv k_{-2}[G \cdot CD_2]_{equ}$

equilibrium constant: $K' = \frac{k_1}{k_{-2}} = \frac{[G \cdot CD_2]_{equ}}{[G][CD]} \approx \frac{[G \cdot CD_2]_{equ}}{[G]_0[CD]_0}$

rate equation of complexation:

$$\frac{d[G \cdot CD_2]}{dt} = k_1[G]_0[CD]_0 - k_{-2}[G \cdot CD_2] = k_1[G]_0[CD]_0(1 - c'[G \cdot CD_2])$$

$$\text{with } c' = \frac{1}{[G]_0[CD]_0 K'} = \frac{1}{[G \cdot CD_2]_{equ}}$$

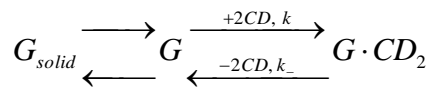
integrated form: $\frac{\ln(1 - c'[G \cdot CD_2])}{c'} = -k_1[G]_0[CD]_0 t$

kinetics of complexation: $[G \cdot CD_2] = (1 - \exp(-k_1 c'[G]_0[CD]_0 t)) / c'$

$$[G \cdot CD_2] = [G \cdot CD_2]_{equ} (1 - \exp(-k_{-2} t))$$

initial slope: $\left(\frac{d[G \cdot CD_2]}{dt} \right)_{t=0} = [G \cdot CD_2]_{equ} k_{-2} = k_1[G]_0[CD]_0$

1-step model



Approximations:

concentrations: $[G] = \text{const} = [G]_0$, $[CD] = \text{const} = [CD]_0$

rate equation: $\frac{d[G \cdot CD_2]}{dt} = k[CD]_0^2[G]_0 - k_{-}[G \cdot CD_2]$

equilibrium state: $k[CD]_0^2[G]_0 \equiv k_{-}[G \cdot CD_2]_{equ}$

equilibrium constant: $K = \frac{k}{k_{-}} = \frac{[G \cdot CD_2]_{equ}}{[G][CD]^2} \cong \frac{[G \cdot CD_2]_{equ}}{[G]_0[CD]_0^2}$

Rate equation of complexation:

$$\frac{d[G \cdot CD_2]}{dt} = k[G]_0[CD]_0^2 - k_{-}[G \cdot CD_2] = k[G]_0[CD]_0^2(1 - c[G \cdot CD_2])$$

$$\text{with } c = \frac{1}{[G]_0[CD]_0^2 K} = \frac{1}{[G \cdot CD_2]_{equ}}$$

integrated form: $\frac{\ln(1 - cx)}{c} = -k[CD]_0^2[G]_0 t$

Kinetics of complexation: $[G \cdot CD_2] = (1 - \exp(-kc[G]_0[CD]_0^2 t)) / c$

$$[G \cdot CD_2] = [G \cdot CD_2]_{equ} (1 - \exp(-k_{-}t))$$

Initial slope: $\left(\frac{d[G \cdot CD_2]}{dt} \right)_{t=0} = [G \cdot CD_2]_{equ} k_{-} = k[G]_0[CD]_0^2$