

Supplementary information

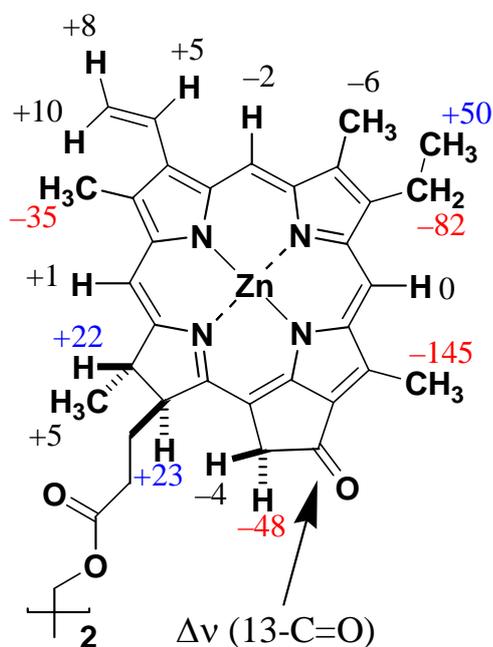
Covalently linked zinc chlorophyll dimers as a model of a chlorophyllous pair in photosynthetic reaction centers

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The difference of chemical shifts δ s in $^1\text{H-NMR}$ and wavenumbers vs in FT-IR spectra between folded **1a**·(MeOH)₂ and randomly orientated **1a**.



The values in each proton were 100-fold $\Delta\delta$.

$$\begin{aligned}\Delta\delta \text{ (ppm)} &= \delta[1\%(\text{v/v})\text{CD}_3\text{OD-CDCl}_3] \\ &\quad - \delta[1\%(\text{v/v})\text{C}_5\text{D}_5\text{N-CDCl}_3]\end{aligned}$$

$$\Delta\nu (13\text{-C=O})$$

$$= 1653 [1\%(\text{v/v})\text{MeOH-CH}_2\text{Cl}_2] - 1682 (\text{CH}_2\text{Cl}_2)$$

$$= -29 \text{ cm}^{-1}$$