Dimers of quadrupolar chromophores in solution: electrostatic interactions and optical spectra

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Supporting information

Explicit expressions for the electrostatic interactions energies v_i in Table 4.

To simplify notation we define the following distances:

$$a = r$$

$$b = \sqrt{r^2 + l^2}$$

$$c = \sqrt{r^2 + l^2(1 - \cos \phi)^2 + l^2 \sin^2 \phi}$$

$$d = \sqrt{r^2 + l^2 \left(1 - \frac{1}{2} \cos \phi\right)^2 + \frac{l^2}{4} \sin^2 \phi}$$

$$e = \sqrt{r^2 + \frac{l^2}{4}}$$

$$f = \sqrt{r^2 + l^2(1 - \cos \phi)^2 + \frac{l^2}{4} \sin^2 \phi}$$

with these definitions:

$$v_2 = \frac{14.4}{\varepsilon} \left(-\frac{1}{a} - \frac{1}{b} + \frac{1}{d} + \frac{1}{e} \right)$$

$$v_3 = \frac{14.4}{\varepsilon} \left(-\frac{1}{b} - \frac{1}{c} + \frac{1}{d} + \frac{1}{e} \right)$$

$$v_4 = \frac{14.4}{\varepsilon} \left(-\frac{1}{a} - \frac{1}{b} + \frac{2}{d} \right)$$

$$v_5 = \frac{14.4}{\varepsilon} \left(-\frac{1}{a} - \frac{1}{c} + \frac{1}{d} + \frac{1}{e} \right)$$

$$v_6 = \frac{14.4}{\varepsilon} \left(-\frac{1}{b} - \frac{1}{c} + \frac{2}{e} \right)$$

where ε is the solvent dielectric constant, v_i are in eV, and distances in Å.