

# 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:

$$a = r$$

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

$$c = \sqrt{r^2 + 4l^2(1 - \cos\varphi)^2 + 4l^2 \sin^2\varphi}$$

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

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

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

with these definitions:

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

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

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

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

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

where  $\varepsilon$  is the solvent dielectric constant,  $v_i$  are in eV, and distances in Å.