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Electronic Supplementary Information (ESI)

Second Harmonic Generation in Laterally Azo-Bridged H-Shaped Ferroelectric Dimesogens†

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1. Estimation of the hyperpolarizability of DR-1 chromophore at 1.6 μm

It was reported that the β value of DR-1 chromophore at 1.9 μm is $\beta(1.9) = 49 \times 10^{-30}$ esu. According to the two-level model, the β value of DR-1 chromophore at 1.6 μm is estimated by the following equation:

$$\frac{\beta(\lambda')}{\beta(\lambda)} = \frac{\left[1-\left(\frac{2\lambda_0}{\lambda}\right)^2\right]\left[1-\left(\frac{\lambda_0}{\lambda}\right)^2\right]}{\left[1-\left(\frac{2\lambda_0}{\lambda'}\right)^2\right]\left[1-\left(\frac{\lambda_0}{\lambda'}\right)^2\right]}, \qquad \text{(a)}$$

where λ_0 is the resonator wavelength. In this specific case, λ' = 1.6 μm, λ = 1.9 μm, and λ_0 = 0.53 μm (the maximum absorption wavelength of compound **2**). The β value at 1.6 μm is obtained, $\beta(1.6) = 62 \times 10^{-30}$ esu.

2. The origin of Eq. (4)

The equation (4) is obtained by the transformation of a third rank tensor when the reference frame is rotated by an angle θ (i.e., the tilt angle) about the y-axis (see the

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transformation in Fig. S1). In general the transformation of the third rank tensor is expressed as

$$\beta^{(d)}_{I,J,K} = \sum_{i,j,k} A_{Ii} A_{Jj} A_{Kk} \beta^{(d)}_{i,j,k} \quad \text{(b)}$$

where all indices go from 1 to 3.

In the particular case the rotation matrix is

$$A = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} \quad \text{(c)}$$

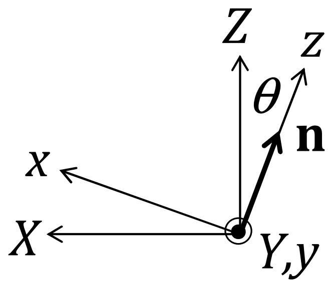

Fig. S1. The transformation from the molecular *xyz* reference system to the laboratory *XYZ* reference system involves the counter-clockwise rotation by an angle θ (i.e., the tilt angle) about the y-axis.

Take $\beta^{(d)}_{YZZ} = \beta^{(d)}_{233}$ as an example. $\beta^{(d)}_{233}$ is expressed as

$$\beta^{(d)}_{233} = \sum_{ijk} A_{2i} A_{3j} A_{3k} \beta^{(d)}_{ijk} = \sum_{jk} A_{3j} A_{3k} \beta^{(d)}_{2jk} = A_{31} A_{31} \beta^{(d)}_{211} + A_{31} A_{33} \beta^{(d)}_{213} + A_{33} A_{31} \beta^{(d)}_{213} + A_{33} A_{33} \beta^{(d)}_{233}$$
$$= A_{31} A_{31} \beta^{(d)}_{yxx} + A_{33} A_{33} \beta^{(d)}_{yzz} = \sin^2\theta \beta^{(d)}_{yxx} + \cos^2\theta \beta^{(d)}_{yzz} \quad \text{(d)}$$

Then the d_{23} (i.e., d_{233} in three-indices notation) coefficient is

$$d_{23} = Nf^3 \beta^{(d)}_{YZZ} = Nf^3 (\beta^{(d)}_{yxx} \sin^2\theta + \beta^{(d)}_{yzz} \cos^2\theta) \,. \quad \text{(e)}$$

The other three **d** tensor components, d_{22}, d_{21}, and d_{14} are obtained as shown in eq. (4) by following the same operation as shown above.