

Supporting Information for

Accurate Determination and Modeling of the
Dispersion of the First Hyperpolarizability of an
Efficient Zwitterionic Nonlinear Optical Chromophore
by Tunable Wavelength Hyper-Rayleigh Scattering

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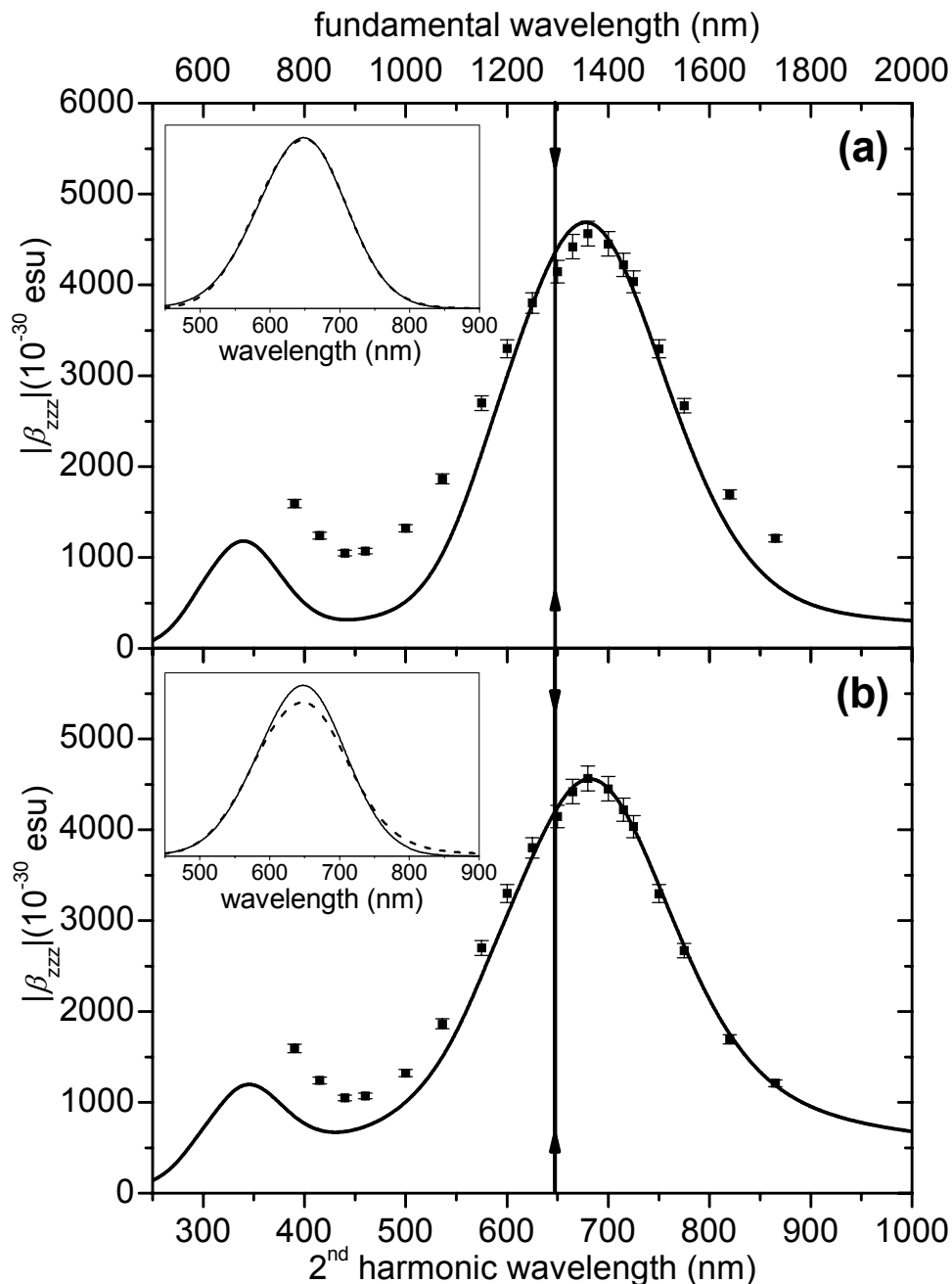


Figure S1. The single-mode vibronic model (curve) fitted to the experimental HRS data in DMF (squares; in DMF- d_7 at the SH wavelengths of 820 and 865 nm), corrected for the β dispersion of the pure solvent. Only the two-photon resonant β values (at SH wavelengths ≥ 600 nm) are taken into account in the fitting procedure. The vertical arrows indicate λ_{max} . In (a) only the amplitude is optimized to fit the data but in (b) also the homogeneous width is used as a fit parameter (yielding $\gamma = 190 \text{ cm}^{-1}$ and $\beta_0 = 323 \times 10^{-30} \text{ esu}$). The insets in both figures show the absorption band calculated using identical parameters as for β (dashed line), compared to the experimental spectrum (solid line), nearly coinciding in (a), while showing an unacceptable deviation in (b).