Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Electronic Information for

Charge-transfer state and state mixing in tetracyanoquinodimethane probed using electroabsorption spectroscopy

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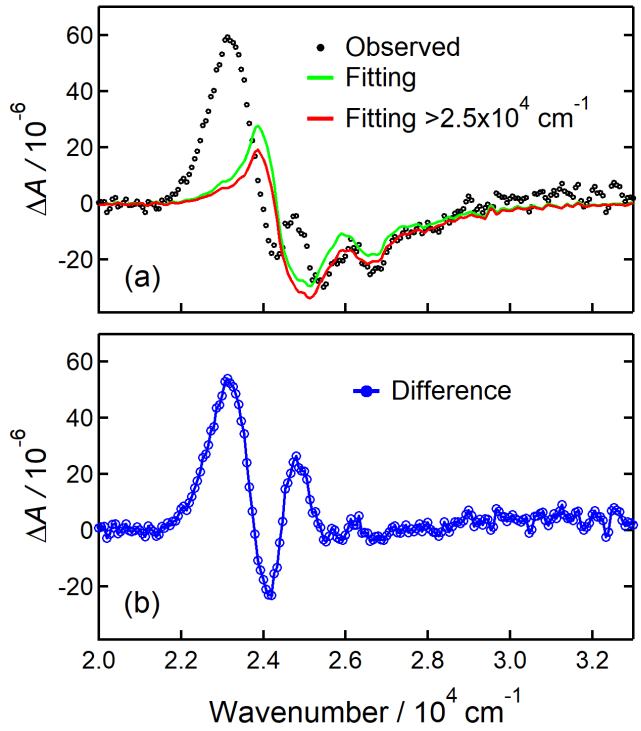

Fig. S1. (a) The electroabsorption (EA) spectrum (black circle), the fitting result using a single set of coefficients and the entire absorption spectrum without band separation at the entire wavenumbers (green line), and the fitting result at higher wavenumbers than 2.5×10^4 cm^{-1} (red line). (b) Difference between the observed EA spectrum and the fitting spectrum at wavenumbers higher than 2.5×10^4 cm^{-1}.

Gaussian band fitting of absorption and electroabsorption (EA) spectra

In our analysis, the sum of eight Gaussian band shapes was used to reproduce the absorption spectrum.

$$A(\bar{\nu}) = \sum_{i=1}^{8} a_i \exp\left\{-\frac{(\bar{\nu}-c_i)^2}{b_i^2}\right\}, \qquad \text{(S1)}$$

where $\bar{\nu}$ is the wavenumber of light, and a_i, b_i, c_i are parameters representing the maximum amplitude, line width (cm^{-1}), and wavenumber (cm^{-1}) at the maximum, respectively. The parameter values are shown in Table S1.

Table S1. Parameters of the Eight Gaussian Bands

Gaussian band	parameters	values
G-1	a_1	0.0816
	b_1	892.69
	c_1	24014
G-2	a_2	0.2182
	b_2	592.93
	c_2	24564
G-3	a_3	0.0480
	b_3	424.91
	c_3	25092
G-4	a_4	0.1849
	b_4	701.84
	c_4	25411
G-5	a_5	0.1033
	b_5	702.65
	c_5	26381
G-6	a_6	0.0625
	b_6	1191.98
	c_6	27113
G-7	a_7	0.0657
	b_7	2483
	c_7	27279
G-8	a_8	0.0296
	b_8	9250.54
	c_8	40012