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

Electronic Supporting Information:

Single crystal spectroscopic measurement details

Spectroscopic measurements on single crystals were performed on a self-built instrument, composed of a halogen light source, a rotating sample stage and a conventional microscope coupled to a spectrometer. A linear polarizer could be inserted between the light source and the condenser lens focusing light on the sample. Using the optical microscope equipped with a 60x objective, individual crystals were selected and illuminated with a focused light beam. The transmitted signal was collected through a slit at the entrance of the spectrometer, in the form of a spatially resolved transmission map: the slit is decomposed in 255 lines along its largest dimension, a spectrum being measured for each of these lines

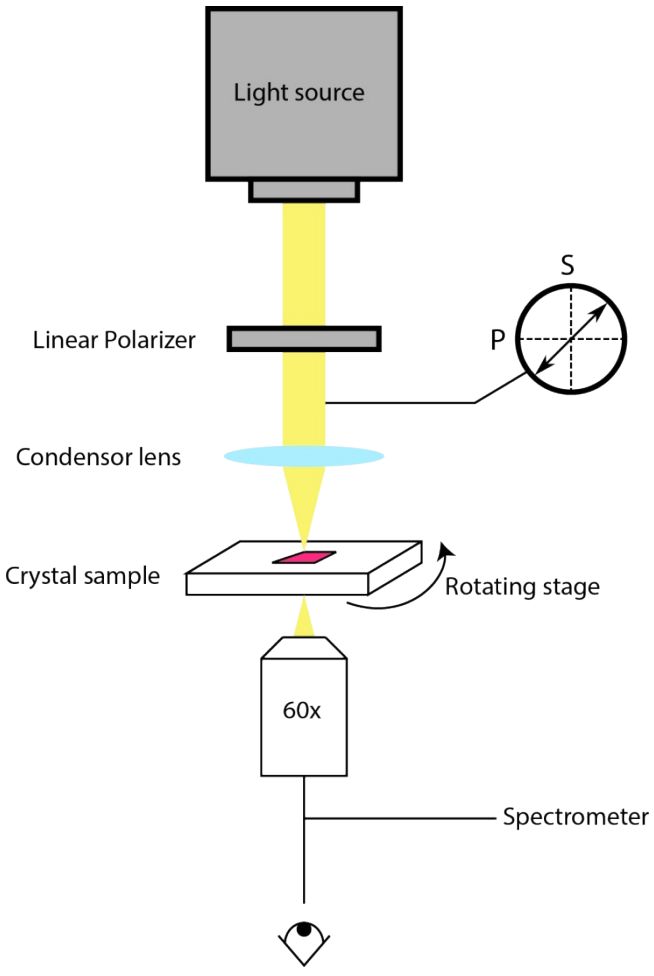

Figure S1: Sketch of the micro-spectrometer

The directly transmitted signal was converted to absorption using the following relation:

$$Abs = -\log\left(\frac{I_{sample}}{I_0}\right) + \log\left(\frac{I_{substrate}}{I_0}\right)$$

where I_{sample} and $I_{substrate}$ are the transmitted intensity of the sample and the substrate, respectively. I_0 is the intensity of the illumination beam (with or without polarizing filter depending on the experiment) measured in the same conditions as the sample.

An example of the raw data is presented in Figure S2. The spatially resolved absorbance spectra of the same crystal are given for c- and b-polarization. The images correspond to the position of the crystal between the slit, as seen by the spectrometer. To achieve good spectral resolution, the slit opening was set to 3 nm.

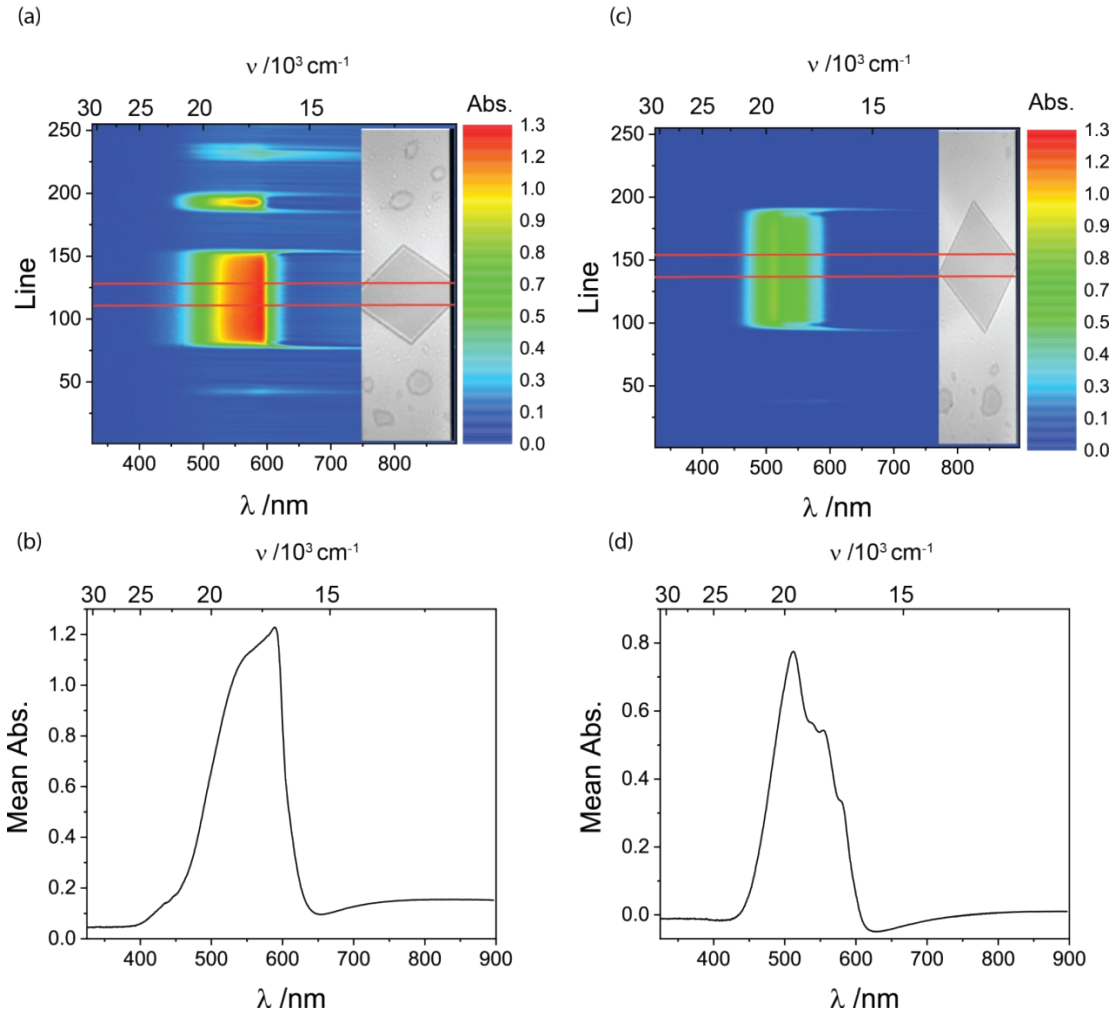

Figure S2: Spatially resolved absorption spectra of a (a) b-polarized and (c) c-polarized CyC crystal. The area between the red lines was used to average the absorption spectra of each polarization. The resulting mean absorbance spectra visible in (b) and (d) for b-polarization and c-polarization, respectively.

As visible from Figure S2, the spatially resolved spectra present some artefacts, mostly at the edges of the crystals where diffraction occurs, resulting in absorbance extending to the infrared. In order to get representative spectra of the crystal absorbance, spectra were averaged over 15-20 lines in the center of the crystal where absorbance is homogenous.

BFDH morphology prediction

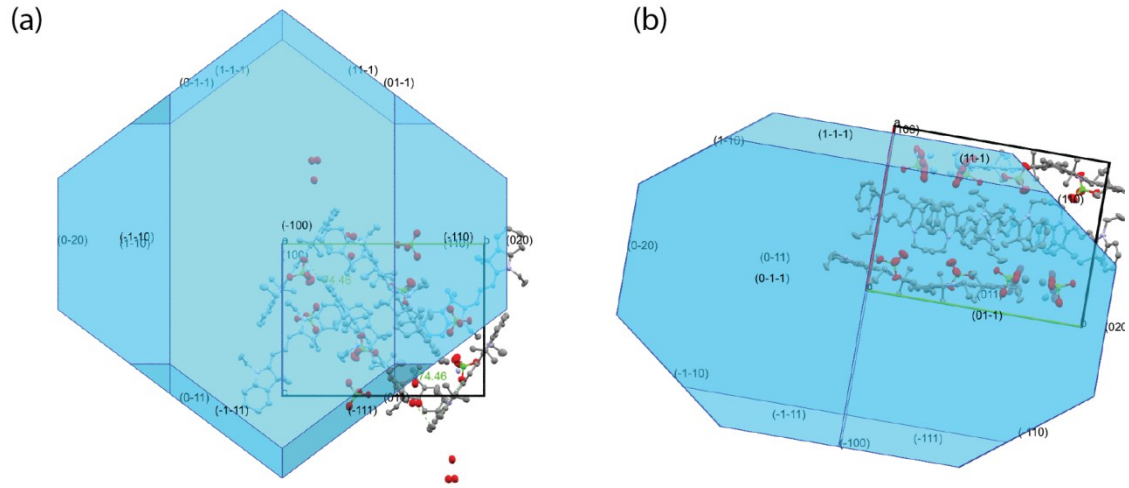

Figure S3: Crystal equilibrium morphology using the BFDH model implemented in the Mercury 3.8 software.(a) View along the [100] direction (b) view along the [001] direction. While the BFDH morphology gives the equilibrium form of the crystal, the final growth form depends on growth conditions. In the present case, growth conditions give rise to crystals composed mainly of {100},{011} and {0-11} faces.

Conoscopy analysis

Optical microscopy was performed on a polarizing microscope equipped with a universal stage (Leitz-Orthoplan-Pol with Leitz universal stage). Due to the high absorbance of all crystals, thick specimens appear dark red, and all colour effects related to birefringence disappear. We therefore selected a sample with thin crystal, yet having lateral sizes of several micrometers. Spacers were placed in the corners of the sample (to protect the fragile crystals from being crunched) and immersion oil was placed on it before it was clamped between the two glass hemispheres of the universal stage.

The crystals extinguish symmetrically, with the diagonals parallel to polarizer and analyzer. They expose a complete isogyre cross in conoscopic view, two adjacent quadrants are tainted blue, the other two are red, see Figure S4. The isogyre perpendicular to the long rhomb diagonal serves as a mirror plane (m) in the field of view. From these observations one can conclude that a) the crystals are monoclinic, b) the crystallographic b-axis is in the substrate plane and parallel to the long rhomb diagonal, c) the crystals have a (h0l) out-of-plane orientation, d) the crystals show horizontal dispersion (i.e. b-axis || X- or Z-axis of indicatrix). It proved impossible to bring an optic axis into the field of view by tilting the sample. Therefore, the acute bisectrix (AB) must be in the substrate plane and the angle between the two optical axes (2V) must be less than 60°.[1]

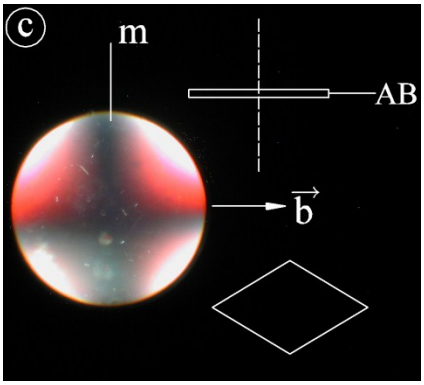

Figure S4. Conoscopic view of the crystal, schematic top view of the crystal (lower) and schematic side view of the crystal (upper) corresponding to the microscope image. The dotted line indicates the microscope axis. The rhomb shaped crystal shows horizontal dispersion.

Atomic displacements in CyC platelet crystals

In total 6 parameters per atom were refined using the SHELXL program[2] to obtain the anisotropic displacements *U* which include thermal motion as well as disorder (see ellipsoid representation in Figure S5). The six eigenvalues of *U* are represented in the isotropic displacement parameter *Ueq* as the mean-square displacement $\langle u^2 \rangle$ averaged over all directions ($Ueq = \langle u^2 \rangle$). All *U* values are small (see figure below). Additionally, it was possible to solve the positional disorder which is related to one of the two perchlorate anions in the asymmetric unit. As seen in Figure S5, there is rotational disorder around the Cl2-O5 bond resulting in an atom position splitting for O6, O7 and O8.

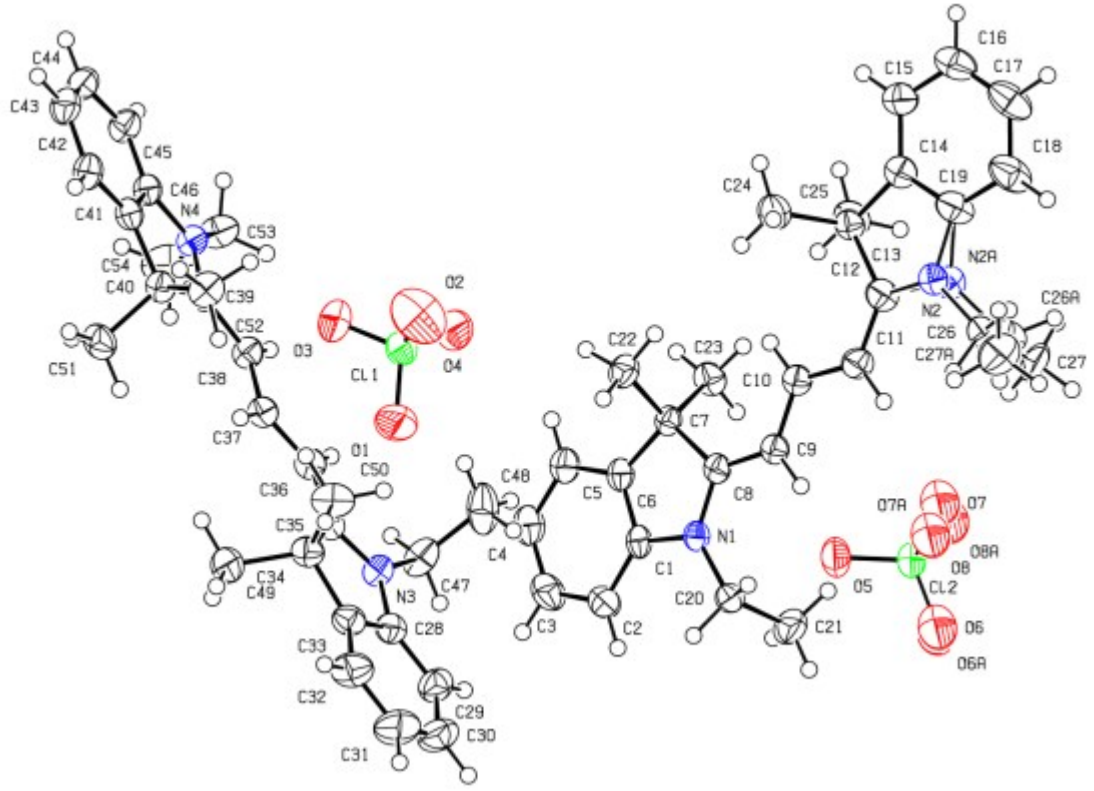

Figure S5. Ellipsoid representation (50% probability) of the anisotropic displacement parameters of the atoms in the molecules composing the asymmetric unit of the crystal structure. The atoms are labeled in the Figure, which was prepared using PLATON.[3]

Franck-Condon analysis

The observed spectrum of CyC in chloroform solution (Fig. 4a) is fitted to a three-mode Franck-Condon model and the results shown in Figure S6. The 0-1 primary shoulder at 15500 cm^{-1} is not represented in the fit as sharply as it is observed, but all other spectral features, including the long tail extending up to 23000 cm^{-1}, are well reproduced. While the addition of a fourth mode could allow the shoulder to sharpen, it is questionable as to whether or not the data supports unique optimization of the two additional parameters required. Here, only the simplest realistic fit to the data is presented.

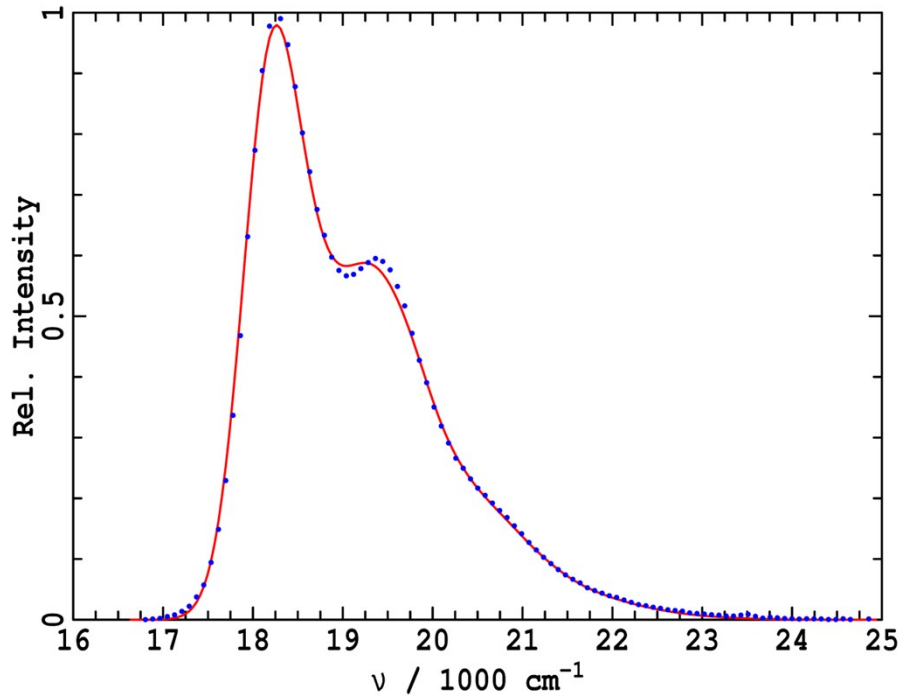

Figure S6. Fit of the observed spectrum of CyC in chloroform to a 3-model Franck-Condon model (see Table 1) blue points- observed spectrum, red line- fit.

PL Measurements

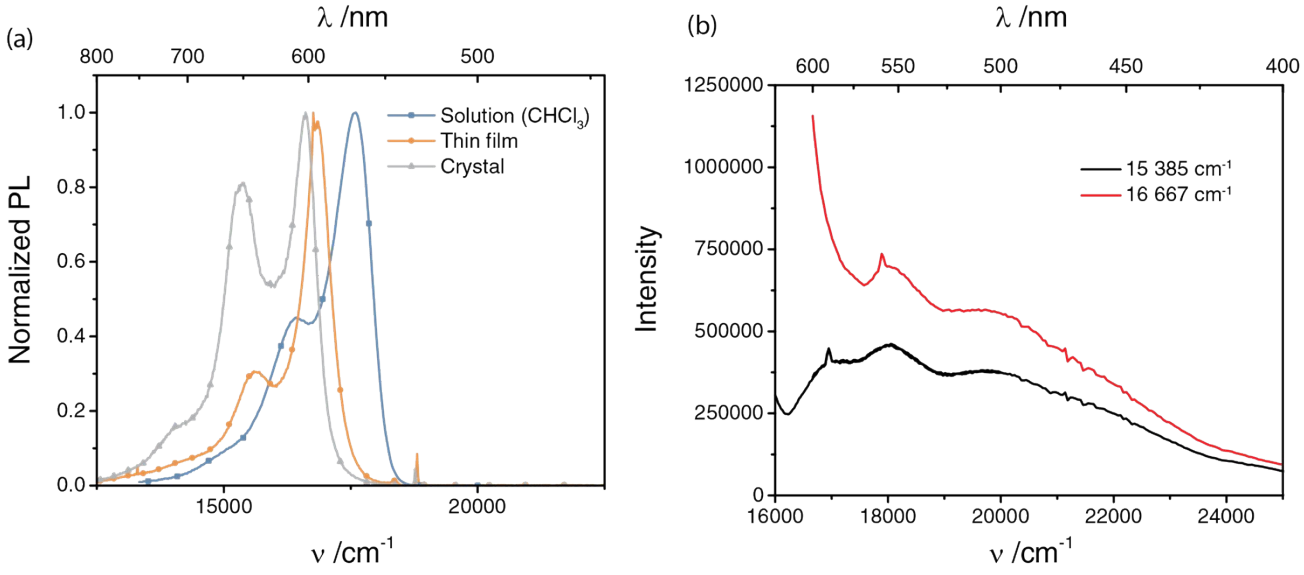

Figure S7:(a) Compared emission of CyC solution, thin film and single crystal. (b) Excitation scan of a collection of single crystals grown on a substrate for emission at 16 667 cm^{-1} and 15 385 cm^{-1}

Reflection

The reflection resulting from a CyC amorphous thin film of about 50 nm was evaluated by comparing the absorbance of the film as measured in a UV-vis spectrometer to that measured in an integrating sphere. While the UV-vis measurement gives the transmission of the film (T=1-A-R), the integrating sphere measurement give the "true" absorption of the film.[4] The two spectra are compared in Figure S8 below. At the main resonances, a difference of 28-38% is found and attributed to reflection from the film surface.

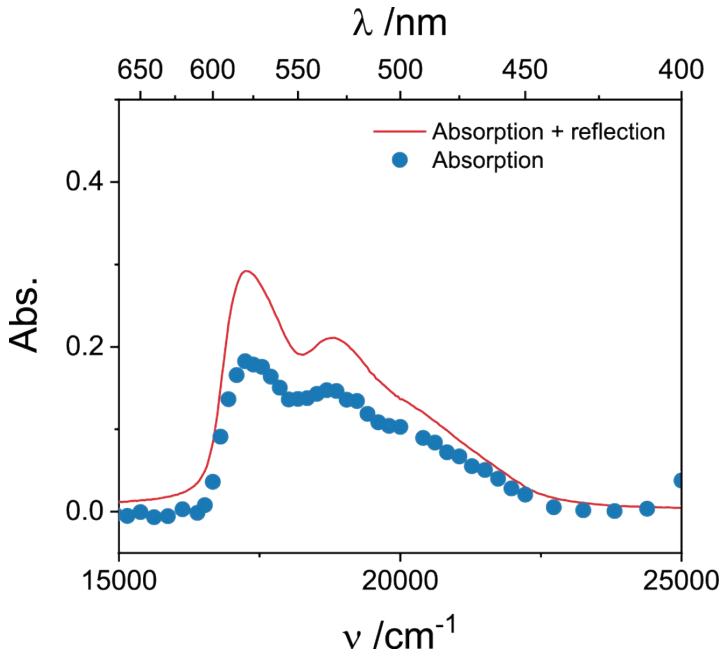

Figure S8: Compared spectra of a 50 nm CyC film measured with a UV-vis spectrometer (red line) and in an integrating sphere (blue dots)

Polarized transmission spectra of CyC platelet crystals

Transmission microscopy of rhombic CyC crystal platelets did not show identical spectral shapes. As mentioned in the main text, reflectance and interference severely affect the transmission signal and depend strongly on crystal thickness. Figure S9 shows the angular dependence of polarized transmission spectra of a 50-60 nm thick crystal. In this thinner crystal, the peak observed at about 19 000 cm^{-1} is not as prominent as in Figure 4 of the main text. However, the angular dependence can be rationalized as a combination of two components. Defining spectrum S_0 as the one obtained with

polarization parallel to c ($\theta = 0°$) and S_{90} as the spectrum obtained with θ=90° polarization (parallel to b) the spectra S_θ at varying angle θ reasonably follow the relationship $S_\theta = S_0 \cos^2 \theta + S_{90} \sin^2 \theta$. For larger crystals this cannot clearly be observed, which could be due to thickness inhomogeneity.

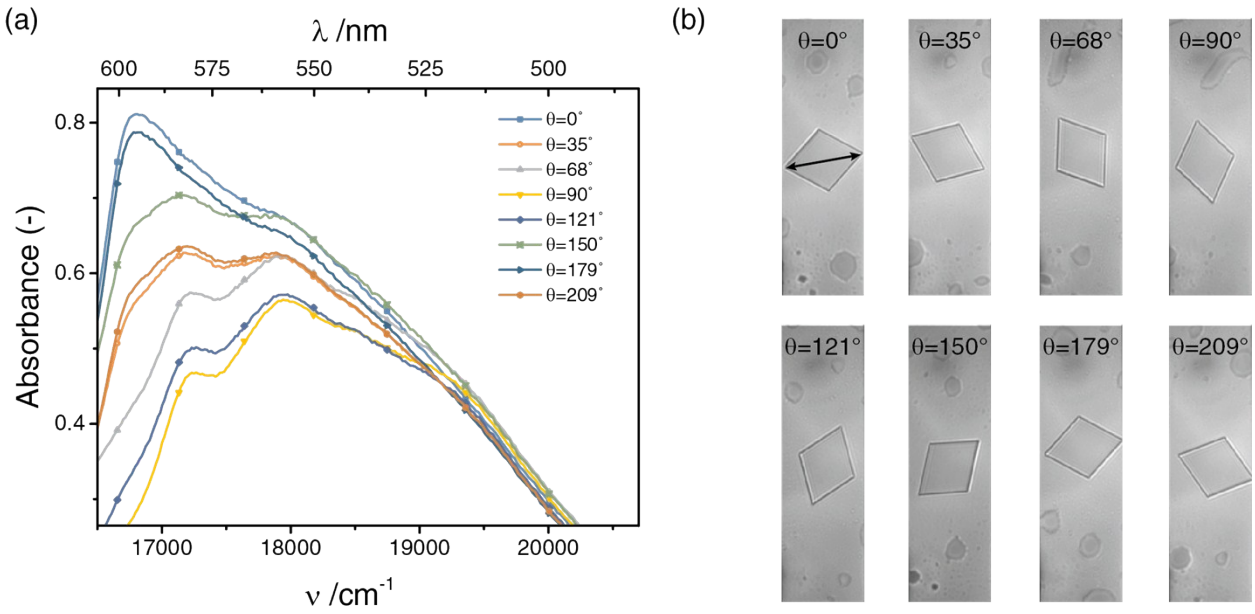

Figure S9: (a) Transmission spectra of CyC single crystals under linearly polarized light, the absorbance of the crystal varies as a function of the crystal orientation (b) Relative position of the crystal and light polarization direction (double arrows) at all angles presented in (a).

Exciton coupling energy

To get an estimation of the exciton coupling strength in the layered crystal structure, the exciton coupling energy J_D of selected chromophore pairs was calculated according to the extended dipole model. [5]

$$J_D = \frac{1}{4\pi\varepsilon\varepsilon_0}\left(\frac{\mu}{L}\right)^2\left(R_1^{-1} + R_2^{-1} - R_3^{-1} - R_4^{-1}\right)$$

where μ is the transition dipole moment, R_i (i=1…4) are the distances between the charges of the dipoles in a pair of molecules, and $\varepsilon_0 = 8.85 \cdot 10^{-12}$ Fm^{-1} is the vacuum permittivity and $\varepsilon = 4$ was taken for the relative permittivity of the dye according to similar trimethine dyes.[6,7] L is the dipole length taken to be 9.5 Å in agreement with previous works [8-10] on different trimethine cyanine dyes.

The transition dipole moment was obtained from the absorption spectrum in chloroform solution according to

$$|\mu|^2 = \frac{f}{4.702 \cdot 10^{-7} \bar{\nu}_{max}}$$

where μ is the transition dipole moment in Debye, $\bar{\nu}_{max}$ is the maximum absorption wavenumber, f is the oscillator strength measured in chloroform solution, $4.702 \cdot 10^{-7}$ D^{-2} cm is a collection of physical constants. This yielded a transition dipole moment of $\mu = 10.9$ D.

The strongest exciton coupling energies of neighboring molecules within layers 1, as well as the interlayer couplings between layers 1 - 2 and 1a – 1b are given in Table S1 below:

Table S1: Intralayer and interlayer exciton coupling energies J_D in the layered crystal structure of cyanine dye CyC. Layers 1a, 1b and 2 follow the notation given in Figure 2a. The various exciton coupling terms J_1-J_{11} are identified in Figure S7. Our sign convention uses that all transition dipole moments are oriented in the direction of the crystallographic c-axis.

R_1 (Å)	R_2 (Å)	R_3 (Å)	R_4 (Å)	J_D (cm^{-1})	identifier
5.784	5.784	12.799	9.209	263.2	J_1
11.361	11.361	3.849	20.617	-218.9	J_2
8.046	14.902	7.312	17.265	-5.4	J_3
5.923	16.107	11.417	15.13	127.8	J_4
10.59	10.59	7.91	18.47	13.7	J_5
7.242	7.242	14.849	7.99	138.4	J_6
6.024	17.334	14	12.571	120.3	J_7
8.419	17.666	17.576	9.556	22.9	J_8
15.652	15.652	23.501	10.82	-11.9	J_9
7.056	6.822	8.866	14.021	172.4	J_{10}
6.252	15.23	13.249	11.69	106.9	J_{11}

The various exciton coupling energies J_1 to J_{11} are identified with the help of the crystal structure projections below (Figure S10):

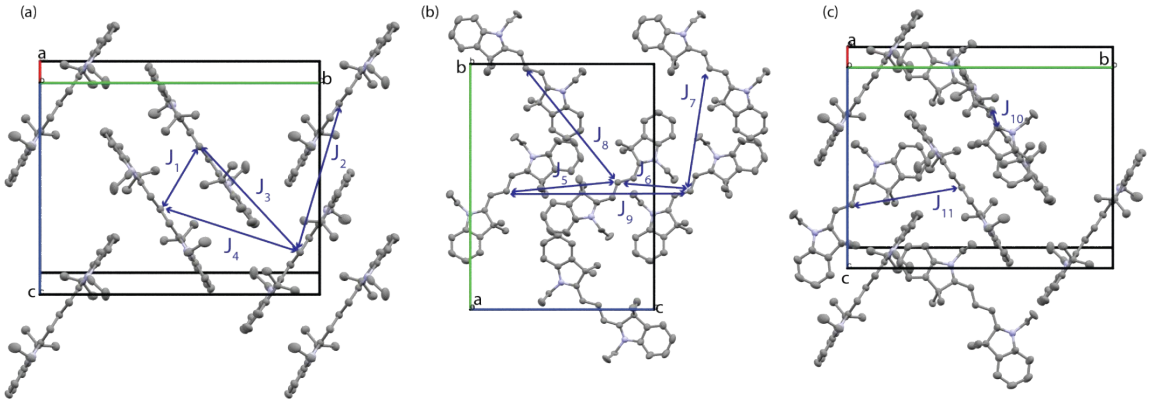

Figure S10: Identification of exciton coupling terms J_1 to J_{11} viewed at different projections. (a) Intralayer couplings in layer 2 (b) Interlayer (J_5 to J_8) and intralayer (J_9) couplings between layers 1a and 1b (c) interlayer couplings between layers 1 and 2.

TDDFT prediction of the spectrum of isolated CyC

Table S2: Cam-B3LYP/6-31G* TDDFT predictions of the absorption spectrum of an isolated CyC cation in chloroform.

Layer 1		Layer 2	
Energy / cm^{-1}	Oscillator strength	Energy / cm^{-1}	Oscillator strength
22400	1.59	22080	1.62
34700	0.02	34340	0.01
38370	0.01	38170	0.01
38630	0.00	38380	0.00
41090	0.11	40800	0.09
42400	0.09	42160	0.10

DFT optimized coordinates for the translationally optimized unit cell, no symmetry

```
box: 15.825751   0.00 -1.606683   0.00 20.7468   0.00   0.00   0.00 15.6519
Kpoints:   2   2   2
basis: NGX= 108 NGY= 140 NGZ= 108 NGXF= 216 NGYF= 280 NGZF= 216

  6    1.584647    6.736895    7.290021
  6   14.241104   14.009904    6.755196
  6   14.241103   17.110295   -1.070753
  6    1.584647    3.636505   15.115971
  6    1.503718    6.062622    6.075231
  6   14.322035   14.684177    7.969986
```

```
6   14.322034   16.436022    0.144036
6    1.503717    4.310777   13.901181
6    1.124381    4.715954    6.129960
6   14.701370   16.030845    7.915256
6   14.701370   15.089355    0.089306
6    1.124381    5.657446   13.955911
6    0.851093    4.082127    7.343507
6   14.974657   16.664672    6.701711
6   14.974657   14.455527   -1.124240
6    0.851094    6.291273   15.169457
6    0.951456    4.781347    8.553052
6   14.874295   15.965452    5.492164
6   14.874295   15.154747   13.318115
6    0.951455    5.592053    0.727102
6    1.317072    6.117038    8.514736
6   14.508678   14.629762    5.530481
6   14.508678   16.490437   13.356432
6    1.317073    4.256362    0.688786
6    1.528703    7.113729    9.634985
6   14.297048   13.633071    4.410232
6   14.297048   17.487128   12.236183
6    1.528703    3.259671    1.809035
6    1.913228    8.371568    8.851851
6   13.912523   12.375231    5.193365
6   13.912523   18.744968   13.019315
6    1.913228    2.001832    1.025902
6    2.183347    9.649867    9.341084
6   13.642404   11.096932    4.704133
6   13.642404   20.023267   12.530083
6    2.183346    0.723533    1.515133
6    2.208328    9.998214   10.689400
6   13.617423   10.748585    3.355817
6   13.617422   20.371614   11.181767
6    2.208329    0.375185    2.863449
6    2.438520   11.295977   11.145864
6   13.387231    9.450822    2.899352
6   13.387231    0.922578   10.725303
6    2.438520   19.824222    3.319914
6    2.452717   11.678019   12.484060
6   13.373034    9.068781    1.561158
6   13.373035    1.304619    9.387108
6    2.452717   19.442180    4.658109
6    2.226352   10.818069   13.732898
6   13.599399    9.928730    0.312318
6   13.599399    0.444669    8.138268
6    2.226352   20.302130    5.906948
6    2.369931   11.843030   14.838324
6   13.455820    8.903770   -0.793108
6   13.455819    1.469630    7.032843
6    2.369932   19.277169    7.012374
6    2.305367   11.706038    0.565637
6   13.520384    9.040762   13.479580
6   13.520383    1.332638    5.653630
6    2.305368   19.414161    8.391587
6    2.432752   12.857699    1.356316
6   13.392999    7.889100   12.688900
6   13.392999    2.484300    4.862951
6    2.432751   18.262500    9.182267
6    2.633624   14.109116    0.767430
6   13.192127    6.637684   13.277787
6   13.192127    3.735716    5.451837
6    2.633623   17.011084    8.593381
6    2.724454   14.254622   15.031794
6   13.101297    6.492177   -0.986578
6   13.101297    3.881222    6.839372
6    2.724454   16.865577    7.205844
6    2.594394   13.100034   14.269394
6   13.231357    7.646766   -0.224176
```

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6	2.594394	18.020166	6.443443
6	2.273270	9.014491	6.452863
6	13.552481	11.732308	7.592354
6	13.552481	19.387891	-0.233597
6	2.273270	1.358908	14.278813
6	1.046785	9.769150	5.959357
6	14.778966	10.977649	8.085860
6	14.778966	20.142550	0.259910
6	1.046785	0.604249	13.785307
6	2.685149	6.645005	10.548308
6	13.140602	14.101795	3.496909
6	13.140602	17.018404	11.322860
6	2.685149	3.728395	2.722358
6	0.214920	7.309934	10.416124
6	15.610831	13.436866	3.629093
6	15.610831	17.683334	11.455043
6	0.214920	3.063466	2.590174
6	3.280564	9.710935	13.895060
6	12.545188	11.035865	0.150157
6	12.545187	20.084334	7.976108
6	3.280564	0.662465	6.069110
6	0.796462	10.236752	13.753723
6	15.029289	10.510048	0.291493
6	15.029289	20.610151	8.117444
6	0.796462	0.136647	5.927774
6	2.846689	14.103460	11.969806
6	12.979062	6.643340	2.075411
6	12.979062	3.730060	9.901361
6	2.846690	17.016740	4.143856
6	1.517881	14.627877	11.437747
6	14.307870	6.118923	2.607469
6	14.307870	4.254477	10.433419
6	1.517881	16.492323	3.611797
6	7.013656	6.120229	13.308556
6	8.812095	14.626570	0.736660
6	8.812095	16.493629	8.562611
6	7.013656	4.253170	5.482607
6	6.512410	5.315961	12.286259
6	9.313340	15.430838	1.758958
6	9.313340	15.689361	9.584908
6	6.512410	5.057438	4.460309
6	7.442452	4.775879	11.390145
6	8.383299	15.970921	2.655072
6	8.383300	15.149279	10.481023
6	7.442452	5.597521	3.564195
6	8.810892	5.027050	11.528540
6	7.014859	15.719750	2.516677
6	7.014858	15.400449	10.342627
6	8.810893	5.346350	3.702590
6	9.292957	5.831091	12.570688
6	6.532794	14.915709	1.474529
6	6.532794	16.204490	9.300479
6	9.292957	4.542309	4.744738
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6	8.592531	7.249715	14.683244
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6	7.233221	17.623114	7.187924
6	8.592530	3.123685	6.857293
6	7.149393	7.479454	-0.502694
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6	8.676358	17.852853	6.721961
6	7.149393	2.893946	7.323256
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6	9.155073	12.534745	13.464364

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6	6.670679	2.161345	8.406803
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6	7.429786	1.444727	9.338493
6	6.850218	9.619281	2.574670
6	8.975532	11.127519	11.470546
6	8.975532	19.992680	3.644596
6	6.850219	0.754119	10.400621
6	7.525977	10.315123	3.580811
6	8.299775	10.431677	10.464406
6	8.299775	20.688522	2.638455
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6	9.031591	10.524726	3.768353
6	6.794160	10.222073	10.276864
6	6.794160	0.151327	2.450915
6	9.031591	20.595473	11.594303
6	9.067537	11.286067	5.080388
6	6.758214	9.460733	8.964829
6	6.758214	0.912667	1.138879
6	9.067537	19.834132	12.906338
6	10.133461	11.730120	5.849048
6	5.692290	9.016679	8.196169
6	5.692290	1.356721	0.370219
6	10.133460	19.390079	13.674998
6	9.861749	12.440848	7.027233
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6	8.544069	12.717999	7.406541
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6	7.460089	12.273373	6.643392
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6	7.757783	11.545833	5.492611
6	8.067967	9.200966	8.552606
6	8.067968	1.172434	0.726656
6	7.757783	19.574366	13.318562
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