

# MCD and Induced CD of a Tetraphenoxyperylene-based Dye in Chiral Solvents: An Experimental and Computational Study

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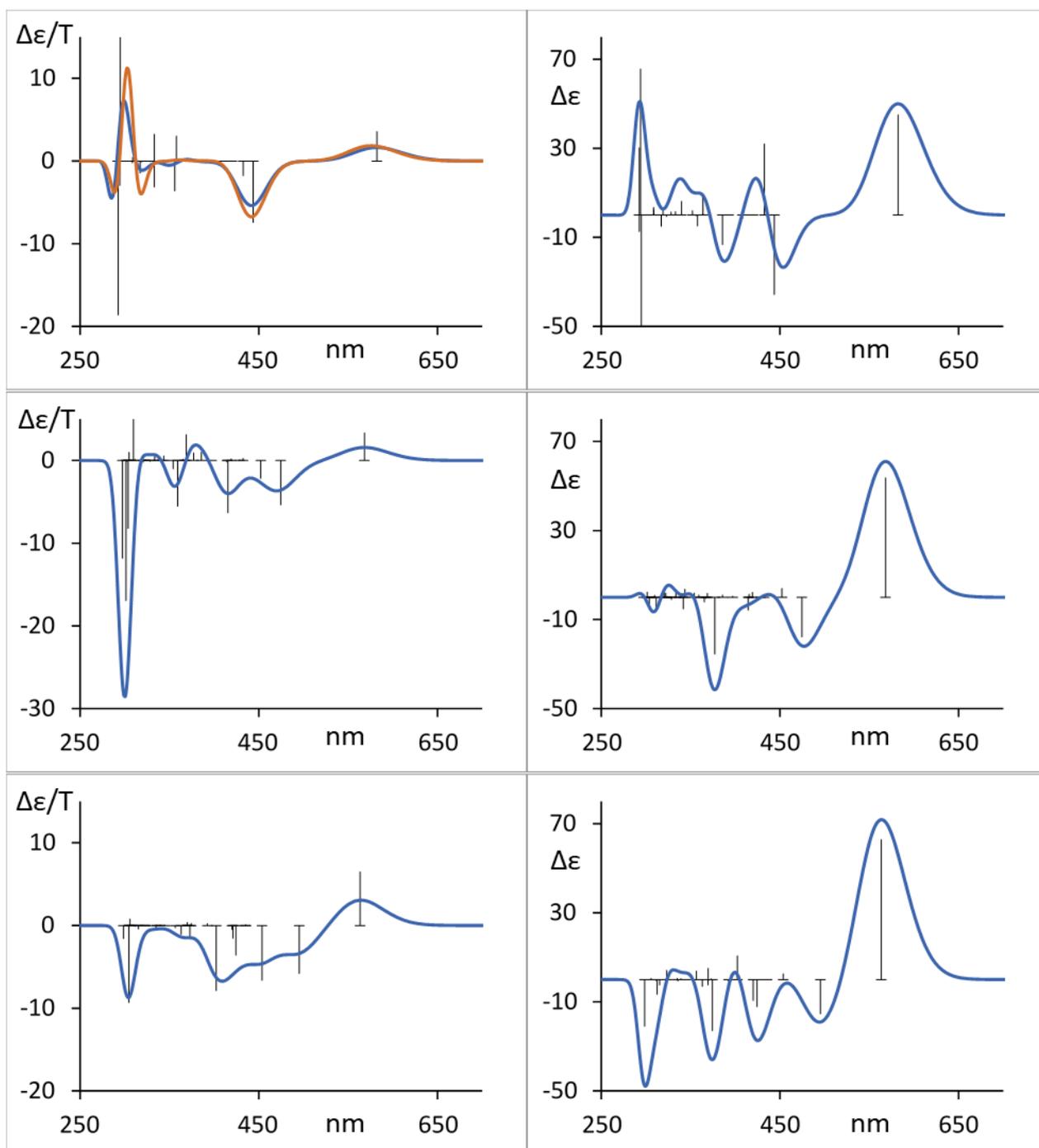
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## Supplementary Information

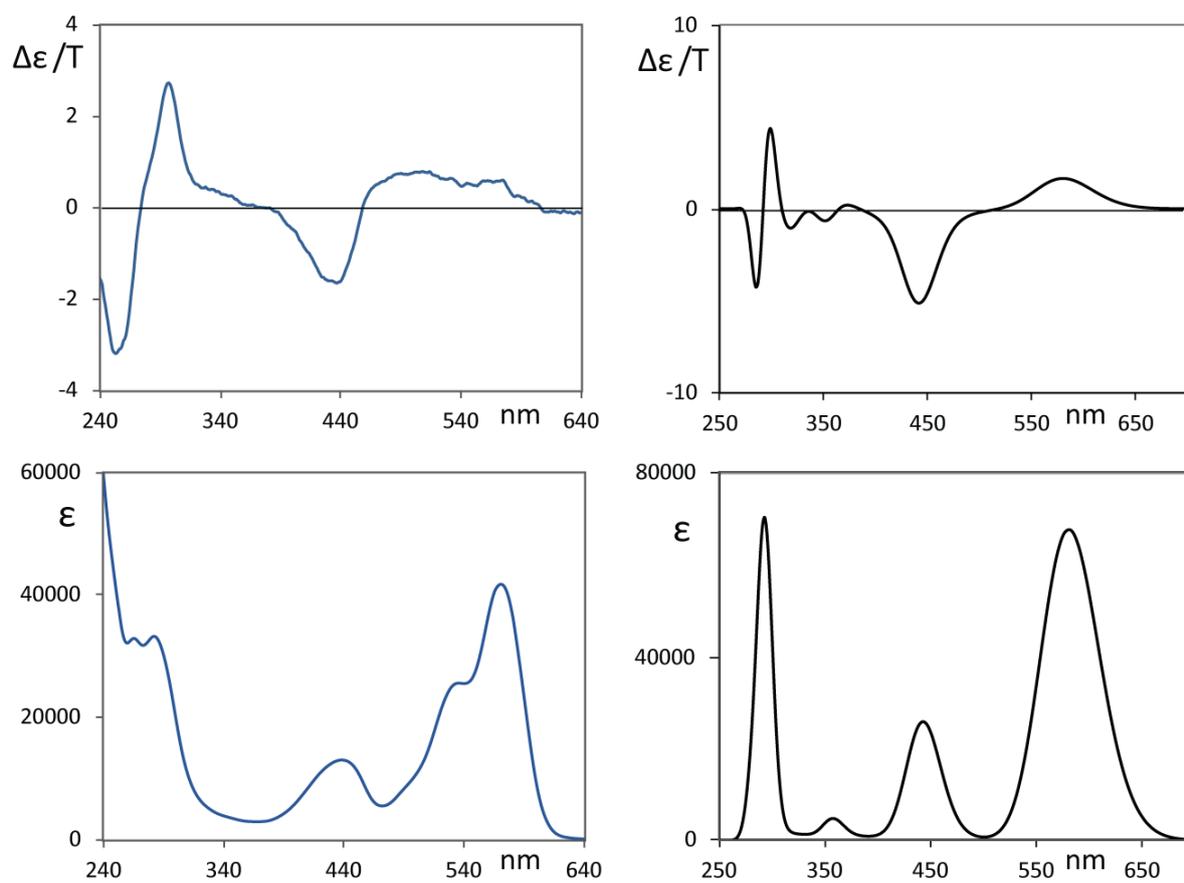
**Table S1.** Calculated wavelength (nm), dipole strength  $D$  ( $10^{-40}$  esu<sup>2</sup>cm<sup>2</sup>), rotational strength  $R$  ( $10^{-40}$  esu<sup>2</sup>cm<sup>2</sup>),  $\mathcal{B}$ -term (a.u.) of the transitions for the three main conformers A, B, C and for the meso form of ROT300 (see text).

A				B				C				meso		
nm	$D$	$R$	$\mathcal{B}$	nm	$D$	$R$	$\mathcal{B}$	nm	$D$	$R$	$\mathcal{B}$	nm	$D$	$\mathcal{B}$
582	734191	135.2	42.7	568	650215	161.0	40.1	563	609912	188.5	77.9	576	783041	47.8
444	206319	-107.1	-89.2	475	53237	-53.5	-64.4	495	44336	-46.1	-69.7	442	212667	-133.3
433	16893	96.0	-21.3	452	124925	12.0	-26.0	454	23998	7.8	-79.6	427	0	0.0
420	548	-0.2	-0.1	432	281	-0.1	3.3	435	34	0.0	0.0	414	0	0.0
410	0	0.0	0.0	428	291	-0.1	0.9	435	502	-0.2	1.3	411	0	0.0
408	95	0.2	0.2	419	5540	6.7	2.3	424	75158	-36.5	-43.1	411	524	1.3
408	725	-4.8	-0.5	415	11657	4.3	-76.0	421	662	-0.5	-18.7	403	0	0.0
392	0	0.0	0.0	414	24700	-17.3	-2.3	420	15465	-28.2	-6.0	399	0	0.0
386	2085	-39.9	-2.0	397	771	1.7	-0.3	402	33765	31.9	-94.6	399	424	0.2
364	1489	28.3	3.1	386	30072	3.1	12.0	392	595	-1.7	2.8	391	0	0.0
364	130	1.5	0.6	377	3455	-76.5	11.0	374	6149	-69.0	3.2	357	152	0.3

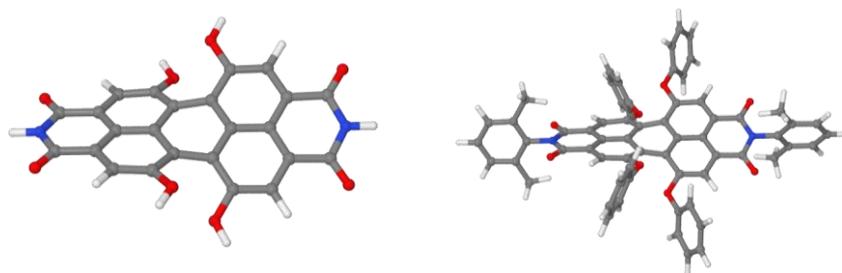




**Figure S1.** Calculated MCD (*left*) and CD (*right*) spectra for the three principal conformer A (*top*), B (*middle*), C (*bottom*). The red trace in the *top-left* square is the calculated MCD spectrum for the meso form and is superimposed to the MCD spectrum for the A conformer (see text).



**Figure S2.** Experimental (*left*) and calculated (*right*) spectra of MCD (*top*) and UV (*bottom*) for ROT300 in acetonitrile.



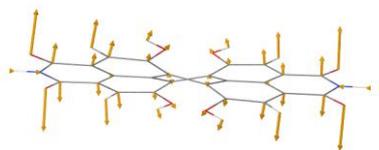
**Figure SI-3.** Representations of the model system (*left*) and of conformer A of full ROT300 molecule (*right*).

**Table S2.** Calculated wavelength (nm), dipole strength  $D$  ( $10^{-40}$  esu<sup>2</sup>cm<sup>2</sup>), rotational strength  $R$  ( $10^{-40}$  esu<sup>2</sup>cm<sup>2</sup>),  $\mathcal{B}$ -term (a.u.) for the main conformer A of ROT300 and of the model system.

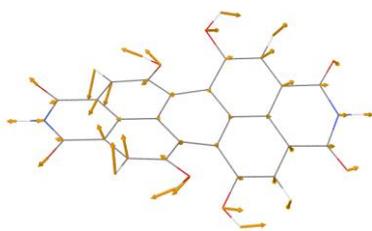
nm	$D$	$R$	$\mathcal{B}$	nm	$D$	$R$	$\mathcal{B}$
582	734191	135.2	42.7	555	592817	118.9	24.9
444	206319	-107.1	-89.2	403	81127	-55.9	-50.1
433	16893	96.0	-21.3	402	0	0.0	0.0
420	548	-0.2	-0.1	400	9477	49.6	-19.2
410	0	0.0	0.0	378	2605	-70.8	-2.6
408	95	0.2	0.2	362	93	1.1	0.1
408	725	-4.8	-0.5	361	16	2.0	0.0
392	0	0.0	0.0	341	76	-15.2	0.3
386	2085	-39.9	-2.0	324	0	0.0	0.0
364	1489	28.3	3.1	310	1283	13.9	-0.5
364	130	1.5	0.6	309	0	0.0	0.0
358	28468	-14.7	36.2	306	0	-0.3	0.2
356	2398	-1.0	-43.4	302	56	1.7	1.0
352	3	5.8	-0.3	290	1167	-6.3	1.1
340	152	18.6	0.6	288	4794	-23.5	-1.5
336	0	0.0	0.0	279	51196	-48.5	242.8
333	1813	4.8	-37.7	278	0	0.0	0.0
333	3523	0.6	38.9	277	82786	43.3	-218.4
328	354	4.3	-0.8				
326	0	0.0	0.0				
323	237	-2.0	-0.3				
319	624	8.4	-1.2				
319	0	0.0	0.0				
317	5230	-15.1	-17.6				
309	1437	7.1	5.5				
309	894	10.4	-2.6				
300	400	-0.2	0.1				
300	0	0.0	0.0				
295	238788	-152.0	316.4				
294	0	0.0	-35.5				
294	25881	196.9	-18.0				
292	477	-22.1	11.7				
292	14672	0.7	37.1				
292	82168	90.7	-223.3				

**Table S3.** Vibronic transitions of the first electronic transition of the model system (see Figure SI-3): relative energy with respect to the  $|0\rangle \rightarrow |0\rangle$  at  $16627.0560 \text{ cm}^{-1}$ , dipole strength  $D$  (a.u.) and rotational strength  $R$  (a.u.).

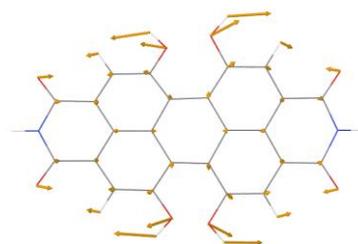
Transition	Energy wrt 0-0 ( $\text{cm}^{-1}$ )	$D$ (au)	$R$ (au)
$ 0\rangle \rightarrow  0\rangle$	0	2.75E+00	4.79E-02
$ 0\rangle \rightarrow  2^1\rangle$	47.589	4.82E-01	8.39E-03
$ 0\rangle \rightarrow  6^1\rangle$	116.6678	1.04E-01	1.81E-03
$ 0\rangle \rightarrow  13^1\rangle$	202.5159	8.76E-01	1.52E-02
$ 0\rangle \rightarrow  13^1;2^1\rangle$	250.105	1.54E-01	2.67E-03
$ 0\rangle \rightarrow  20^1\rangle$	307.9915	1.83E-01	3.18E-03
$ 0\rangle \rightarrow  13^2\rangle$	405.0319	1.39E-01	2.42E-03
$ 0\rangle \rightarrow  34^1\rangle$	459.96	1.24E-01	2.16E-03
$ 0\rangle \rightarrow  35^1\rangle$	483.5743	1.75E-01	3.04E-03
$ 0\rangle \rightarrow  56^1\rangle$	760.9046	1.33E-01	2.31E-03
$ 0\rangle \rightarrow  87^1\rangle$	1301.1039	1.40E-01	2.44E-03
$ 0\rangle \rightarrow  96^1\rangle$	1405.8053	1.88E-01	3.26E-03
$ 0\rangle \rightarrow  99^1\rangle$	1434.2419	1.59E-01	2.76E-03
$ 0\rangle \rightarrow  107^1\rangle$	1590.2188	3.46E-01	6.01E-03
$ 0\rangle \rightarrow  107^1;13^1\rangle$	1792.7347	1.10E-01	1.91E-03



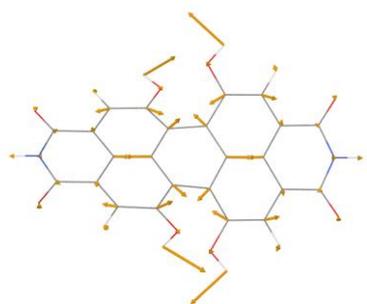
**2:** 47.6  $\text{cm}^{-1}$



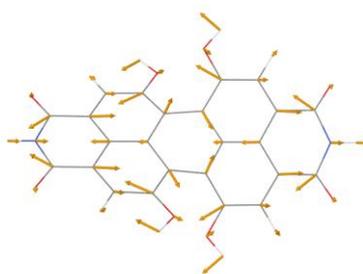
**13:** 202.5  $\text{cm}^{-1}$



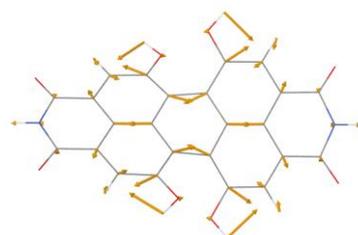
**20:** 308.0  $\text{cm}^{-1}$



**96:** 1405.8  $\text{cm}^{-1}$

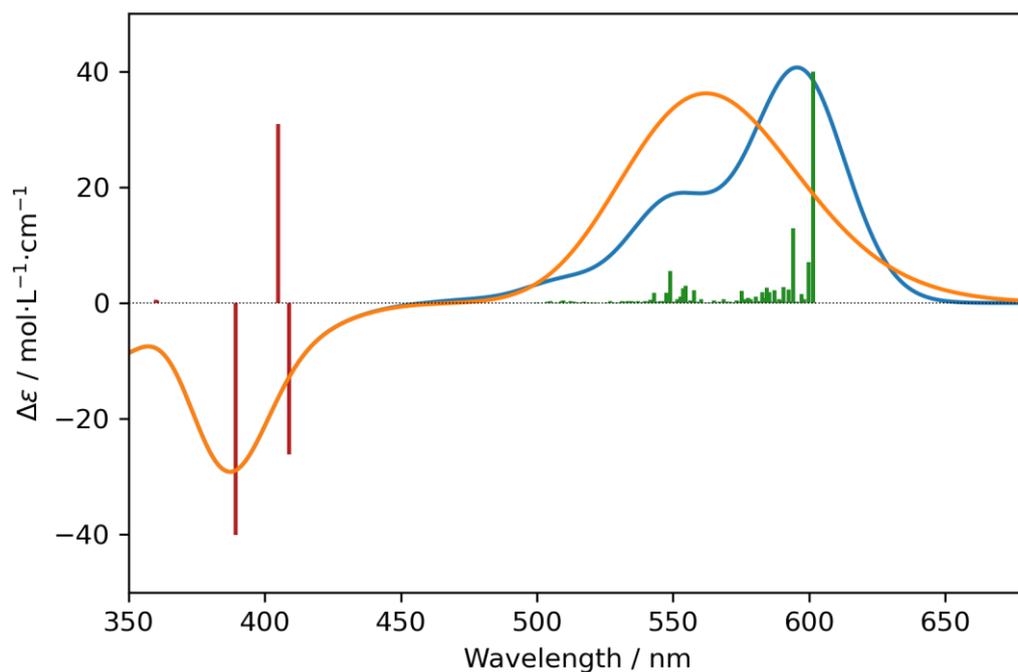


**99:** 1434.2  $\text{cm}^{-1}$



**107:** 1590.2  $\text{cm}^{-1}$

**Figure S4.** Representation of the most relevant normal modes related to the vibronic contributions.



**Figure S5.** Computed CD spectra of the model molecule (see Figure SI-3). The purely electronic spectra (orange) and hybrid spectra in which the first electronic transition was simulated employing the VG|FC vibronic model (blue) are reported. Purely electronic transitions (red vertical lines) were broadened by means of Gaussian distribution functions with HWHMs =  $800\text{ cm}^{-1}$ , while HWHMs of  $500\text{ cm}^{-1}$  was used for the vibronic model (green vertical lines). The most relevant vibronic transitions are annotated.