Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

SUPPORTING INFORMATION

Chiral diketopyrrolopyrrolo dyes with light emission from solid and aggregate states

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Summary

NMR spectra

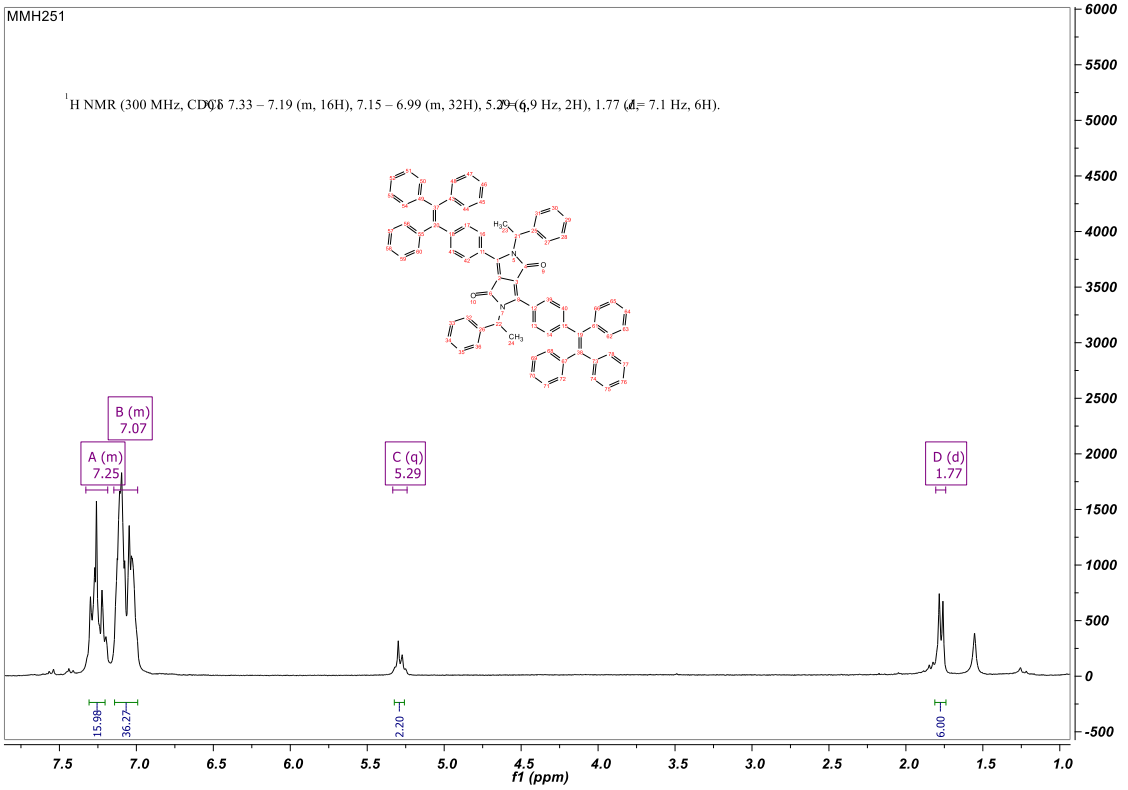

Fig. S1 ^{1}H-NMR spectrum of compound **3*RR*** in CDCl3.

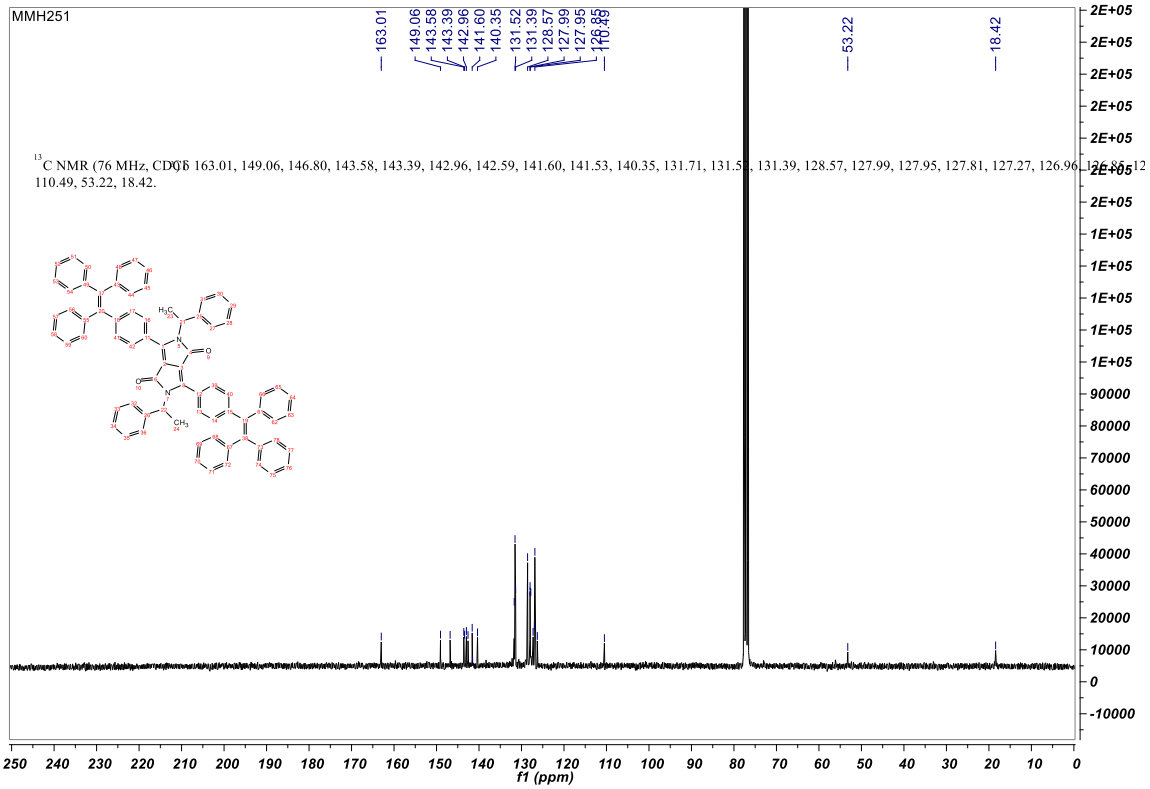

Fig. S2 ^{13}C-NMR spectrum of compound **3*RR*** in CDCl3.

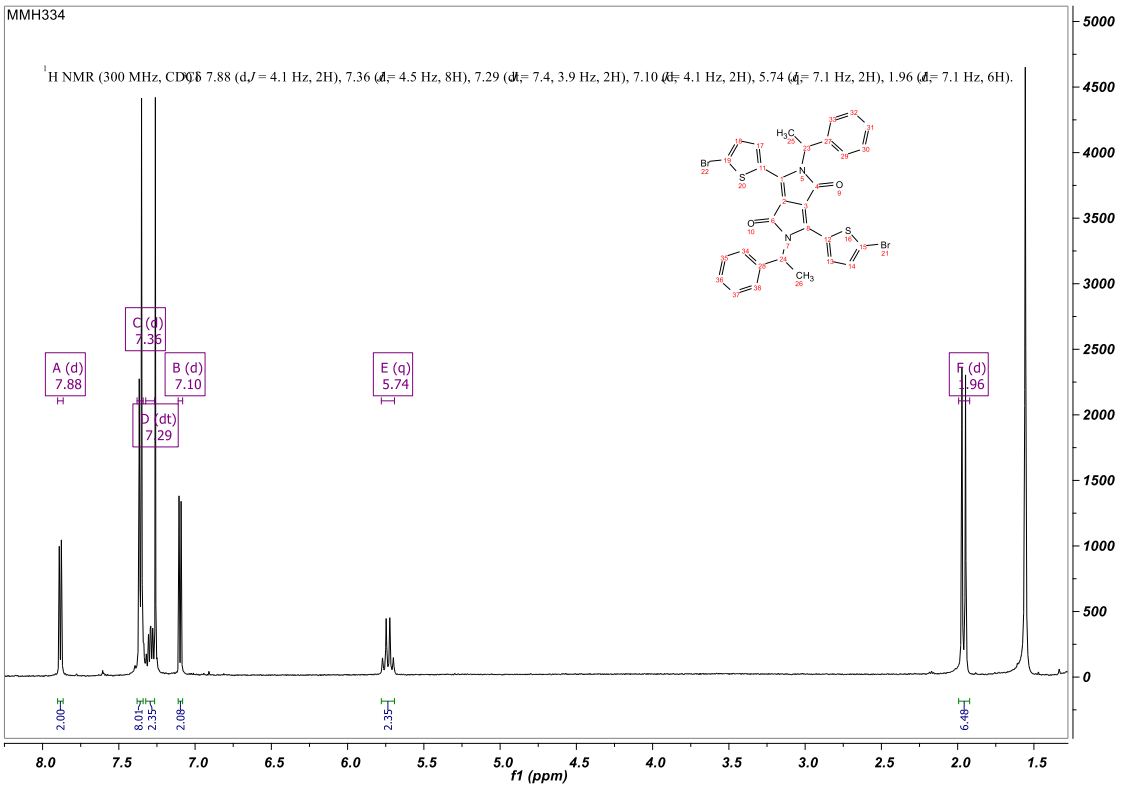

Fig. S3 ^{1}H-NMR spectrum of compound **5*RR*** in CDCl3.

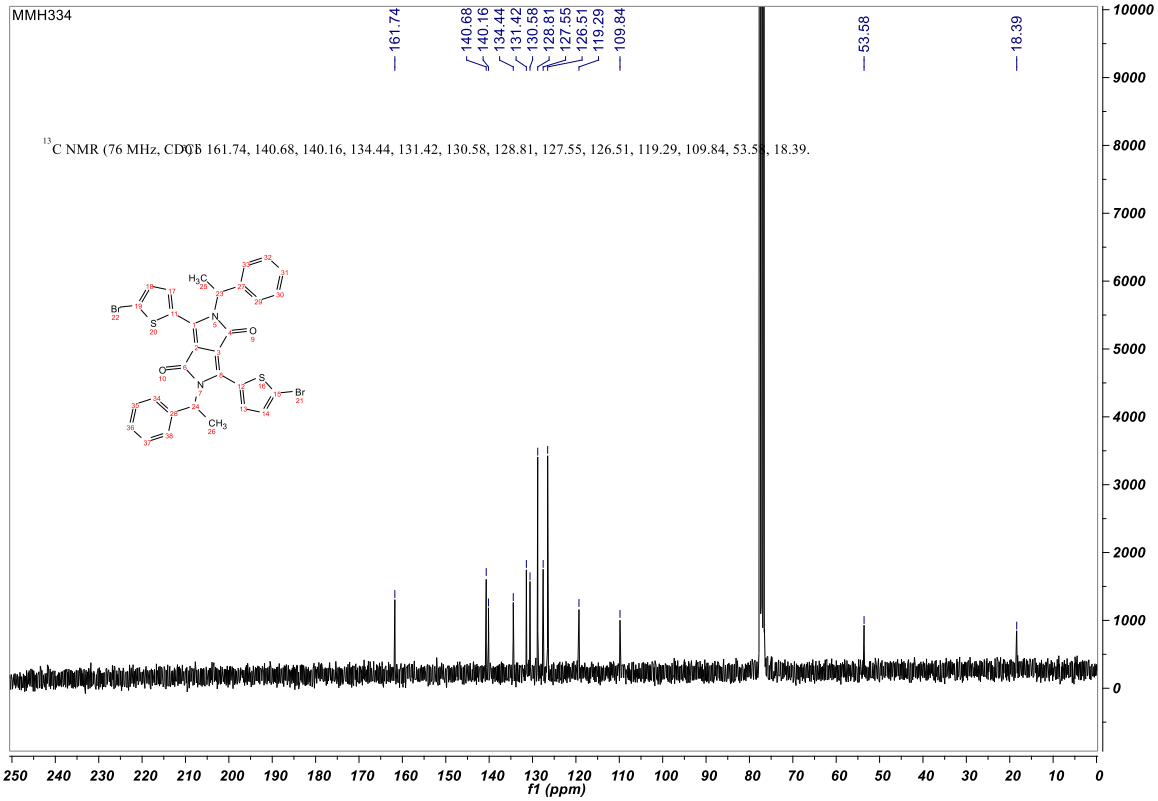

Fig. S4 ^{13}C-NMR spectrum of compound **5*RR*** in CDCl3.

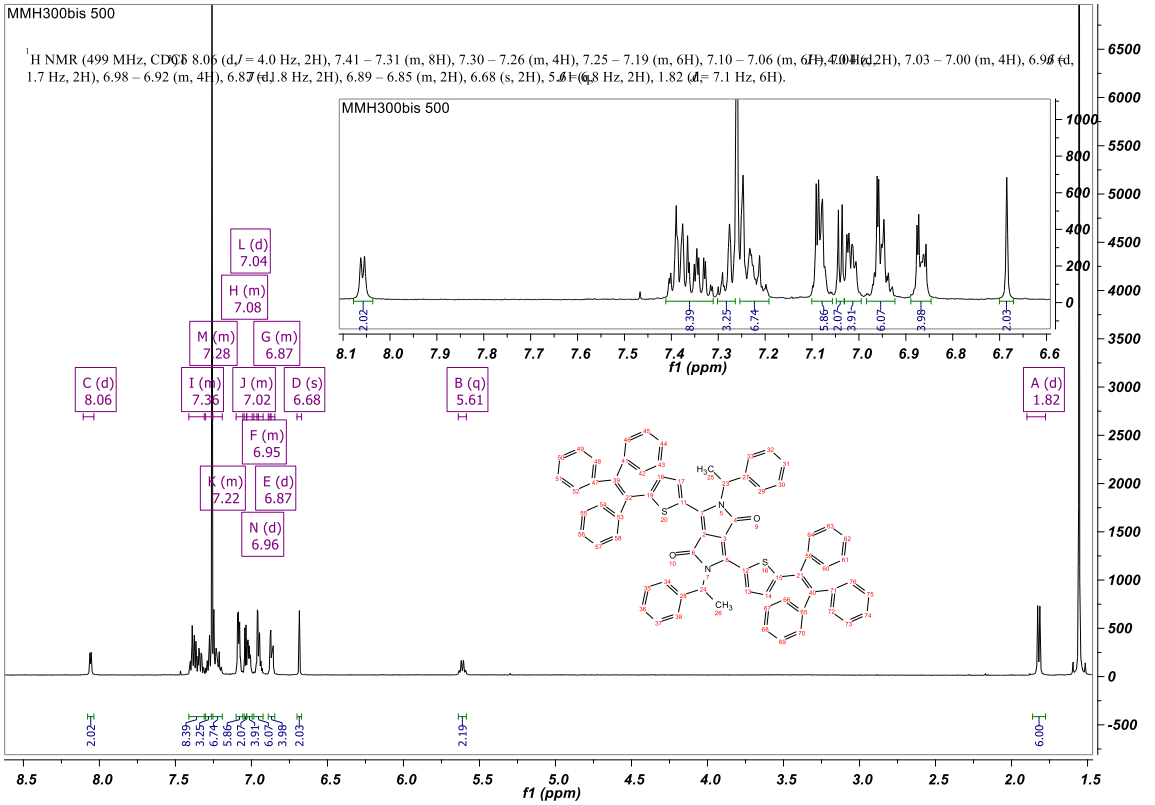

Fig. S5 ^{1}H-NMR spectrum of compound **6*RR*** in CDCl3, with a zoom on the aromatic area in the inset.

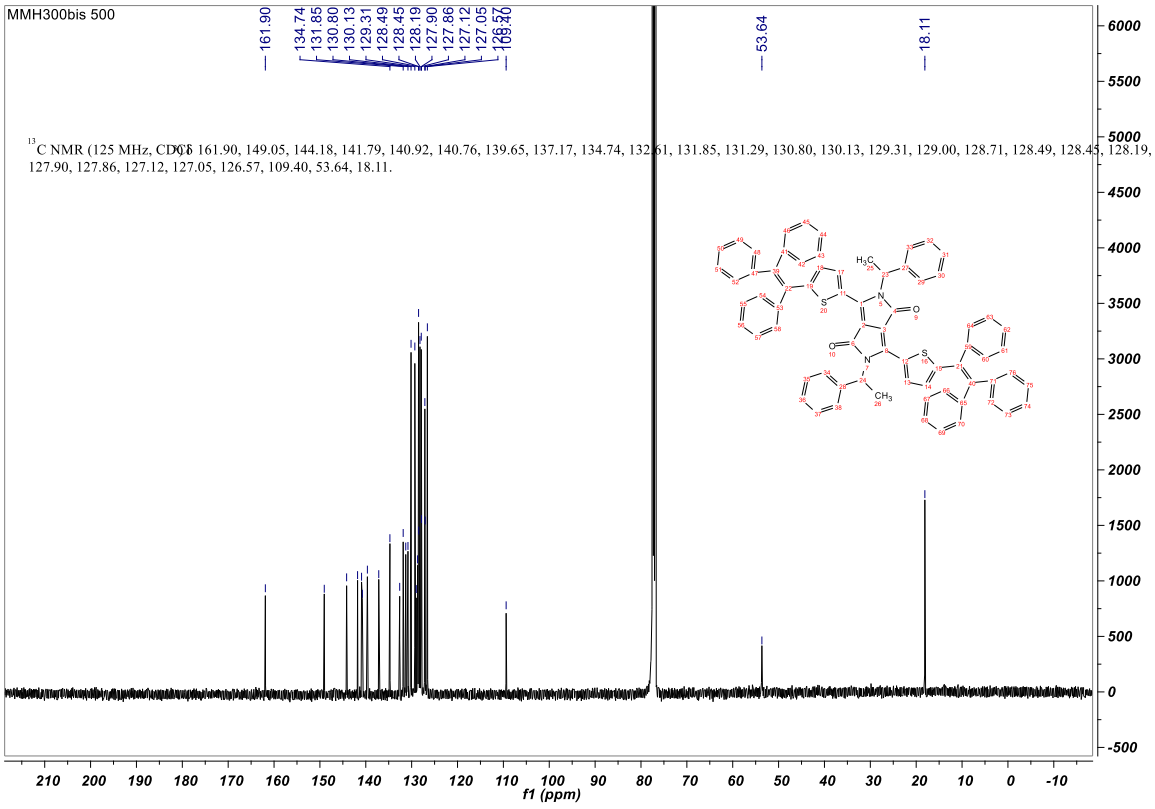

Fig. S6 ^{13}C-NMR spectrum of compound **6*RR*** in CDCl3.

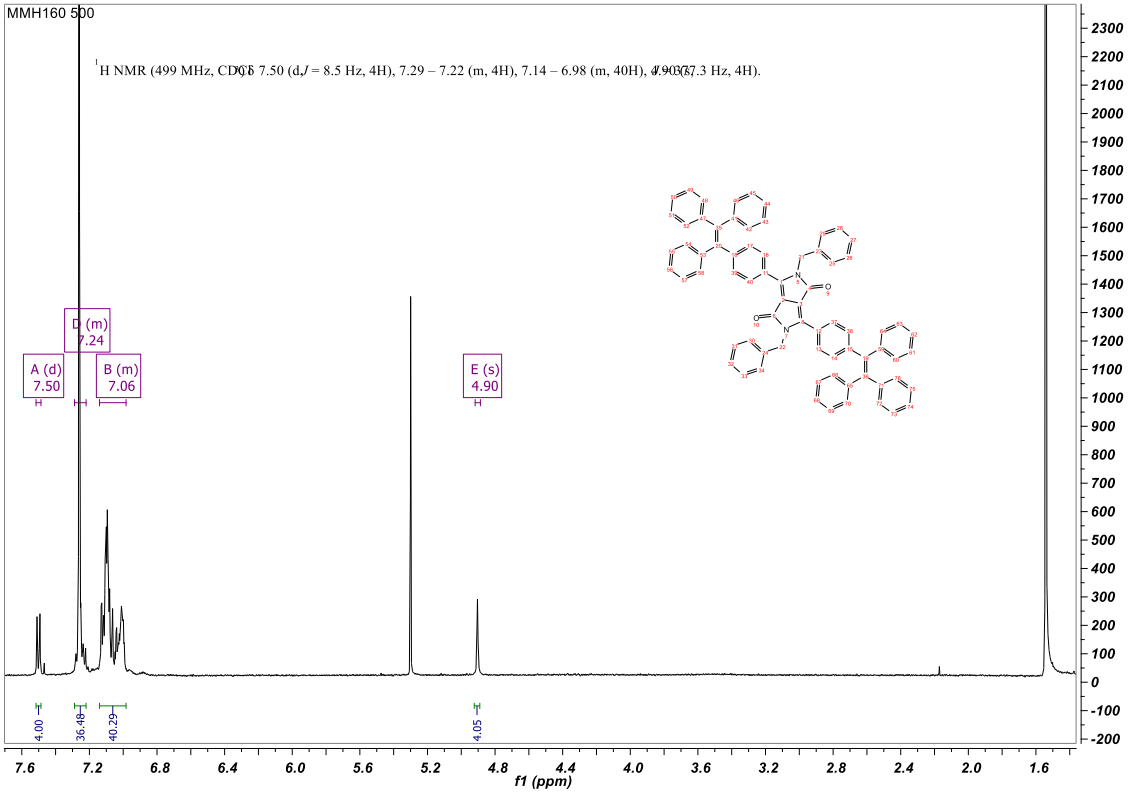

Fig. S7 [1]H-NMR spectrum of compound **8** in CDCl3.

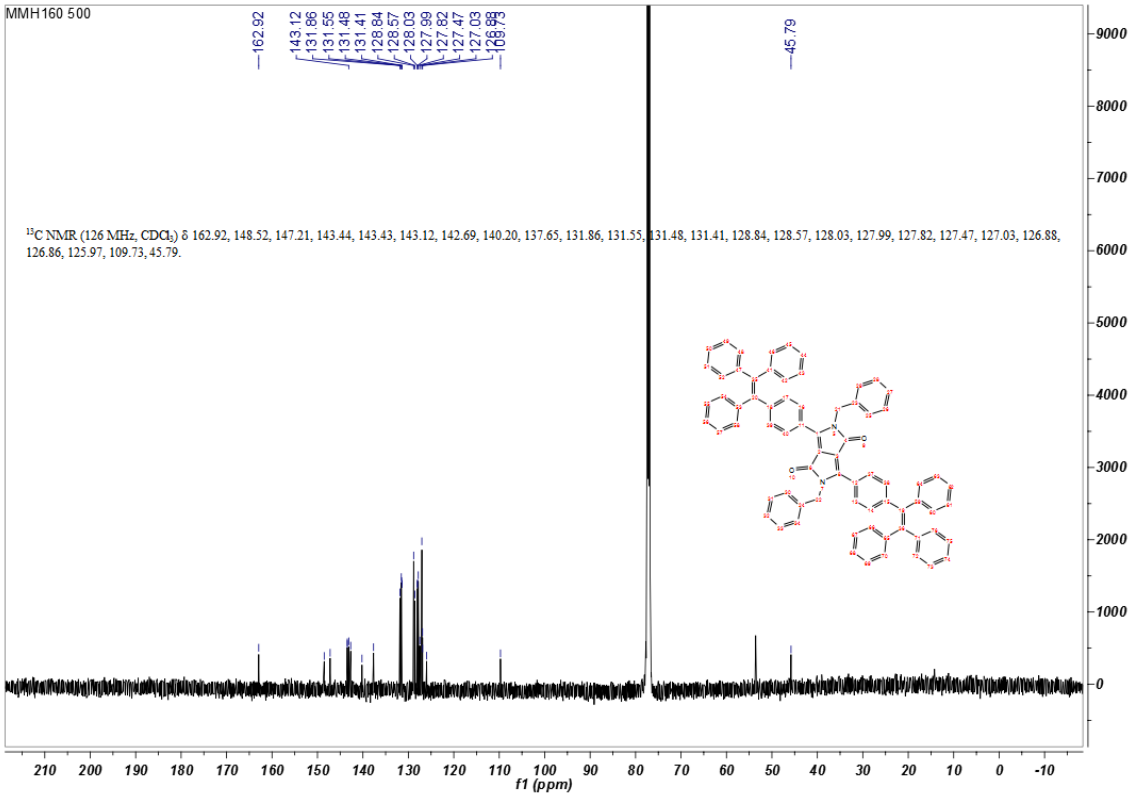

Fig. S8 [13]C-NMR spectrum of compound **8** in CDCl3.

X-ray structure determinations

Compound **3*RR***

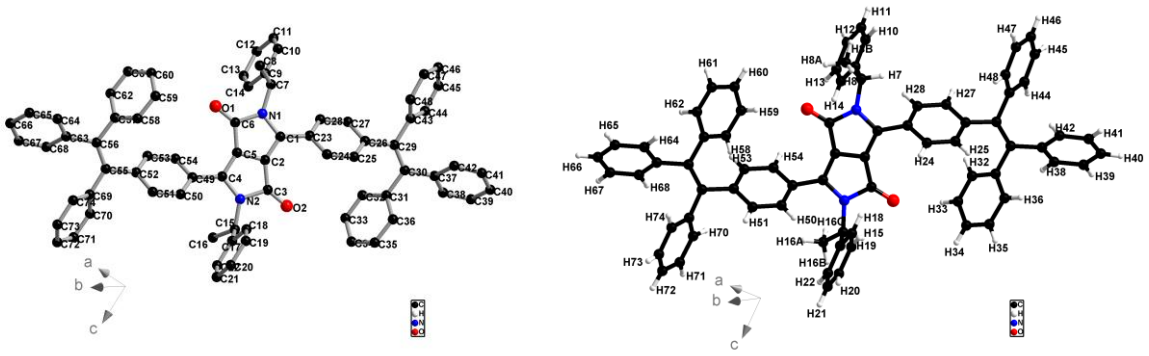

Fig. S9 Molecular structure of compound **3*RR*** in the crystal phase, as result of single crystal X-ray diffraction experiment, with atom numbering (hydrogen omitted for clarity in the left picture, and shown separately in the right one).

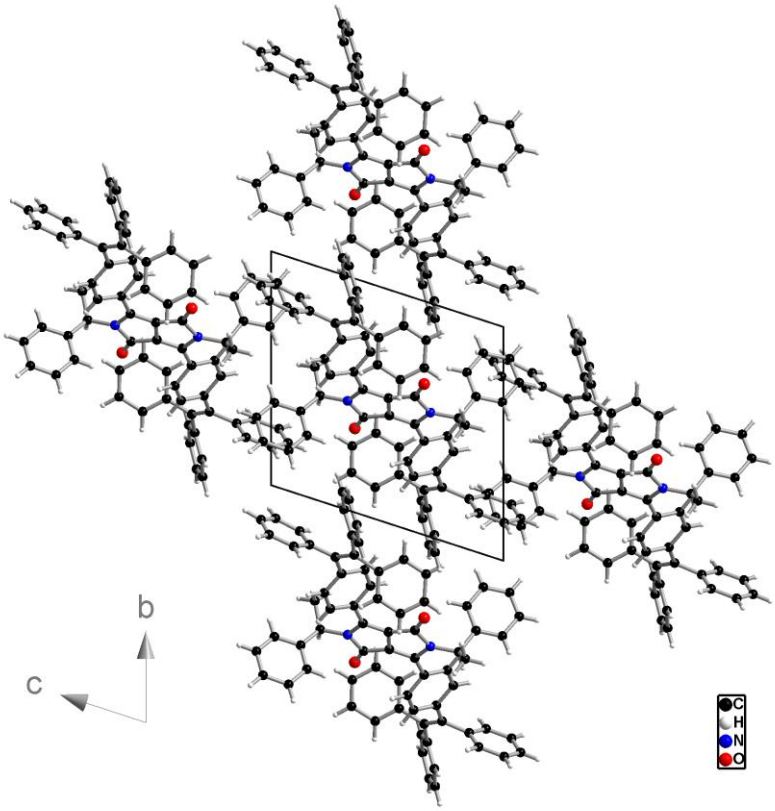

Fig. S10 Crystal packing of compound **3*RR*** in the crystal phase, as result of single crystal X-ray diffraction experiment.

Table S1 Detailed crystallographic data.

	3*RR*	**8**
Chemical formula	$C_{74}H_{56}N_2O_2$	$C_{72}H_{52}N_2O_2$
M_r	1005.20	977.23
Crystal system, space group	Triclinic, *P*1	Triclinic, *P*–1

Temperature (K)	295.0(1)	150.00(10)
a, *b*, *c* (Å)	9.6227(6), 11.8766(7), 12.5108(7)	9.5751(8), 11.3199(9), 12.5471(10)
α, β, γ (°)	71.825(5), 82.689(5), 87.595(5)	72.459(7), 83.128(6), 84.843(6)
V (Å^3)	1347.41(14)	1285.34(18)
Z	1	1
ρ_{calc} (g.cm^{-3})	1.239	1.2624
μ (Cu *K*α) (mm^{-1})	0.567	0.581
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19767 / 9494	9638 / 4845
Flack parameter	0.0(7)	-
R_{int}	0.0448	0.0438
$R[I > 2\sigma(I)]$	R1 = 0.0432, wR2 = 0.0962,	R_1 = 0.0471, wR_2 = 0.1039
$wR(F^2)$, all data	wR2 = 0.1099	wR_2 = 0.1190
$S(F^2)$,[c] all data	0.884	1.045
CCDC number	2237602	2237603

Table S2 Bond Lengths for compound **3*RR*** in the crystal phase.

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
C1—C2	1.369(8)	C35—H35	0.9300
C1—N1	1.404(7)	C36—H36	0.9300
C1—C23	1.462(7)	C37—C38	1.374(9)
C2—C5	1.411(4)	C37—C42	1.408(9)
C2—C3	1.440(8)	C38—C39	1.396(8)
C3—O2	1.212(7)	C38—H38	0.9300
C3—N2	1.444(6)	C39—C40	1.381(11)
C4—C5	1.371(7)	C39—H39	0.9300
C4—N2	1.391(7)	C40—C41	1.374(11)
C4—C49	1.477(7)	C40—H40	0.9300
C5—C6	1.456(8)	C41—C42	1.383(9)
C6—O1	1.229(7)	C41—H41	0.9300
C6—N1	1.419(6)	C42—H42	0.9300
C7—N1	1.473(7)	C43—C44	1.39(1)
C7—C9	1.497(9)	C43—C48	1.393(10)
C7—C8	1.540(8)	C44—C45	1.378(10)
C7—H7	0.9800	C44—H44	0.9300
C8—H8A	0.9600	C45—C46	1.377(14)
C8—H8B	0.9600	C45—H45	0.9300
C8—H8C	0.9600	C46—C47	1.375(15)
C9—C10	1.374(8)	C46—H46	0.9300
C9—C14	1.377(9)	C47—C48	1.384(10)
C10—C11	1.427(10)	C47—H47	0.9300
C10—H10	0.9300	C48—H48	0.9300
C11—C12	1.358(11)	C49—C54	1.380(8)
C11—H11	0.9300	C49—C50	1.392(8)
C12—C13	1.379(9)	C50—C51	1.388(7)
C12—H12	0.9300	C50—H50	0.9300
C13—C14	1.38(1)	C51—C52	1.382(8)
C13—H13	0.9300	C51—H51	0.9300
C14—H14	0.9300	C52—C53	1.391(8)
C15—N2	1.478(7)	C52—C55	1.535(7)
C15—C16	1.493(8)	C53—C54	1.396(7)
C15—C17	1.526(9)	C53—H53	0.9300
C15—H15	0.9800	C54—H54	0.9300
C16—H16A	0.9600	C55—C56	1.366(9)

C16—H16B	0.9600	C55—C69	1.450(8)
C16—H16C	0.9600	C56—C57	1.502(8)
C17—C18	1.362(9)	C56—C63	1.504(8)
C17—C22	1.407(8)	C57—C58	1.385(9)
C18—C19	1.378(9)	C57—C62	1.404(10)
C18—H18	0.9300	C58—C59	1.380(9)
C19—C20	1.384(10)	C58—H58	0.9300
C19—H19	0.9300	C59—C60	1.358(12)
C20—C21	1.372(11)	C59—H59	0.9300
C20—H20	0.9300	C60—C61	1.412(12)
C21—C22	1.328(10)	C60—H60	0.9300
C21—H21	0.9300	C61—C62	1.35(1)
C22—H22	0.9300	C61—H61	0.9300
C23—C24	1.393(8)	C62—H62	0.9300
C23—C28	1.400(8)	C63—C68	1.372(9)
C24—C25	1.370(7)	C63—C64	1.39(1)
C24—H24	0.9300	C64—C65	1.393(8)
C25—C26	1.393(8)	C64—H64	0.9300
C25—H25	0.9300	C65—C66	1.338(11)
C26—C27	1.399(8)	C65—H65	0.9300
C26—C29	1.489(7)	C66—C67	1.413(12)
C27—C28	1.383(7)	C66—H66	0.9300
C27—H27	0.9300	C67—C68	1.368(9)
C28—H28	0.9300	C67—H67	0.9300
C29—C30	1.350(8)	C68—H68	0.9300
C29—C43	1.494(8)	C69—C70	1.372(10)
C30—C37	1.488(7)	C69—C74	1.395(9)
C30—C31	1.494(8)	C70—C71	1.378(9)
C31—C36	1.383(9)	C70—H70	0.9300
C31—C32	1.403(9)	C71—C72	1.344(12)
C32—C33	1.372(9)	C71—H71	0.9300
C32—H32	0.9300	C72—C73	1.386(13)
C33—C34	1.373(11)	C72—H72	0.9300
C33—H33	0.9300	C73—C74	1.383(9)
C34—C35	1.358(11)	C73—H73	0.9300
C34—H34	0.9300	C74—H74	0.9300
C35—C36	1.415(10)		

Table S3 Bond Angles for compound **3*RR*** in the crystal phase.

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
C2—C1—N1	107.4(4)	C38—C37—C42	119.1(5)
C2—C1—C23	126.8(5)	C38—C37—C30	121.0(5)
N1—C1—C23	125.8(5)	C42—C37—C30	119.7(6)
C1—C2—C5	110.3(4)	C37—C38—C39	120.2(6)
C1—C2—C3	140.7(5)	C37—C38—H38	119.900
C5—C2—C3	108.9(3)	C39—C38—H38	119.900
O2—C3—C2	133.8(5)	C40—C39—C38	120.8(7)
O2—C3—N2	122.8(5)	C40—C39—H39	119.600
C2—C3—N2	103.4(4)	C38—C39—H39	119.600
C5—C4—N2	108.0(4)	C41—C40—C39	118.9(6)
C5—C4—C49	125.4(5)	C41—C40—H40	120.600
N2—C4—C49	126.5(5)	C39—C40—H40	120.600
C4—C5—C2	109.1(4)	C40—C41—C42	121.3(7)
C4—C5—C6	143.7(5)	C40—C41—H41	119.300
C2—C5—C6	107.2(3)	C42—C41—H41	119.300
O1—C6—N1	122.8(5)	C41—C42—C37	119.7(7)
O1—C6—C5	132.3(5)	C41—C42—H42	120.200
N1—C6—C5	104.8(4)	C37—C42—H42	120.200
N1—C7—C9	112.9(5)	C44—C43—C48	117.8(6)
N1—C7—C8	111.8(4)	C44—C43—C29	122.5(6)
C9—C7—C8	113.2(5)	C48—C43—C29	119.7(6)
N1—C7—H7	106.100	C45—C44—C43	121.6(8)
C9—C7—H7	106.100	C45—C44—H44	119.200
C8—C7—H7	106.100	C43—C44—H44	119.200
C7—C8—H8A	109.500	C46—C45—C44	119.9(8)

C7—C8—H8B	109.500	C46—C45—H45	120.000
H8A—C8—H8B	109.500	C44—C45—H45	120.000
C7—C8—H8C	109.500	C47—C46—C45	119.5(7)
H8A—C8—H8C	109.500	C47—C46—H46	120.300
H8B—C8—H8C	109.500	C45—C46—H46	120.300
C10—C9—C14	118.1(7)	C46—C47—C48	120.8(9)
C10—C9—C7	118.2(6)	C46—C47—H47	119.600
C14—C9—C7	123.7(5)	C48—C47—H47	119.600
C9—C10—C11	119.8(7)	C47—C48—C43	120.4(8)
C9—C10—H10	120.100	C47—C48—H48	119.800
C11—C10—H10	120.100	C43—C48—H48	119.800
C12—C11—C10	120.7(6)	C54—C49—C50	117.5(5)
C12—C11—H11	119.700	C54—C49—C4	117.6(5)
C10—C11—H11	119.700	C50—C49—C4	124.7(5)
C11—C12—C13	119.1(7)	C51—C50—C49	121.1(5)
C11—C12—H12	120.400	C51—C50—H50	119.500
C13—C12—H12	120.400	C49—C50—H50	119.500
C12—C13—C14	120.2(7)	C52—C51—C50	121.1(5)
C12—C13—H13	119.900	C52—C51—H51	119.400
C14—C13—H13	119.900	C50—C51—H51	119.400
C9—C14—C13	122.0(6)	C51—C52—C53	118.4(5)
C9—C14—H14	119.000	C51—C52—C55	120.7(5)
C13—C14—H14	119.000	C53—C52—C55	120.8(5)
N2—C15—C16	112.2(5)	C52—C53—C54	119.9(5)
N2—C15—C17	111.4(6)	C52—C53—H53	120.100
C16—C15—C17	117.1(4)	C54—C53—H53	120.100
N2—C15—H15	105.000	C49—C54—C53	122.0(5)
C16—C15—H15	105.000	C49—C54—H54	119.000
C17—C15—H15	105.000	C53—C54—H54	119.000
C15—C16—H16A	109.500	C56—C55—C69	126.7(5)
C15—C16—H16B	109.500	C56—C55—C52	118.2(5)
H16A—C16—H16B	109.500	C69—C55—C52	115.0(5)
C15—C16—H16C	109.500	C55—C56—C57	123.3(5)
H16A—C16—H16C	109.500	C55—C56—C63	121.7(5)
H16B—C16—H16C	109.500	C57—C56—C63	115.1(5)
C18—C17—C22	117.0(6)	C58—C57—C62	118.2(6)
C18—C17—C15	121.3(5)	C58—C57—C56	121.4(6)
C22—C17—C15	121.3(6)	C62—C57—C56	120.5(6)
C17—C18—C19	121.5(6)	C59—C58—C57	120.6(7)
C17—C18—H18	119.200	C59—C58—H58	119.700
C19—C18—H18	119.200	C57—C58—H58	119.700
C18—C19—C20	119.6(7)	C60—C59—C58	120.5(8)
C18—C19—H19	120.200	C60—C59—H59	119.800
C20—C19—H19	120.200	C58—C59—H59	119.800
C21—C20—C19	119.3(7)	C59—C60—C61	120.0(7)
C21—C20—H20	120.400	C59—C60—H60	120.000
C19—C20—H20	120.400	C61—C60—H60	120.000
C22—C21—C20	120.5(7)	C62—C61—C60	119.3(8)
C22—C21—H21	119.800	C62—C61—H61	120.300
C20—C21—H21	119.800	C60—C61—H61	120.300
C21—C22—C17	122.1(8)	C61—C62—C57	121.4(7)
C21—C22—H22	118.900	C61—C62—H62	119.300
C17—C22—H22	118.900	C57—C62—H62	119.300
C24—C23—C28	119.3(5)	C68—C63—C64	117.2(5)
C24—C23—C1	117.0(5)	C68—C63—C56	123.2(6)
C28—C23—C1	123.3(5)	C64—C63—C56	119.6(6)
C25—C24—C23	120.2(5)	C63—C64—C65	120.4(6)
C25—C24—H24	119.900	C63—C64—H64	119.800
C23—C24—H24	119.900	C65—C64—H64	119.800
C24—C25—C26	121.6(5)	C66—C65—C64	121.8(7)
C24—C25—H25	119.200	C66—C65—H65	119.100
C26—C25—H25	119.200	C64—C65—H65	119.100
C25—C26—C27	118.0(5)	C65—C66—C67	118.6(6)
C25—C26—C29	120.3(5)	C65—C66—H66	120.700
C27—C26—C29	121.7(5)	C67—C66—H66	120.700
C28—C27—C26	121.2(5)	C68—C67—C66	119.2(7)
C28—C27—H27	119.400	C68—C67—H67	120.400

C26—C27—H27	119.400	C66—C67—H67	120.400
C27—C28—C23	119.6(5)	C67—C68—C63	122.8(7)
C27—C28—H28	120.200	C67—C68—H68	118.600
C23—C28—H28	120.200	C63—C68—H68	118.600
C30—C29—C26	121.8(5)	C70—C69—C74	116.8(6)
C30—C29—C43	123.6(5)	C70—C69—C55	123.1(6)
C26—C29—C43	114.6(5)	C74—C69—C55	120.1(7)
C29—C30—C37	124.1(5)	C69—C70—C71	122.5(7)
C29—C30—C31	121.1(5)	C69—C70—H70	118.800
C37—C30—C31	114.8(5)	C71—C70—H70	118.800
C36—C31—C32	118.3(6)	C72—C71—C70	119.6(8)
C36—C31—C30	120.4(6)	C72—C71—H71	120.200
C32—C31—C30	121.2(6)	C70—C71—H71	120.200
C33—C32—C31	121.0(6)	C71—C72—C73	120.6(7)
C33—C32—H32	119.500	C71—C72—H72	119.700
C31—C32—H32	119.500	C73—C72—H72	119.700
C32—C33—C34	120.5(7)	C74—C73—C72	118.9(7)
C32—C33—H33	119.800	C74—C73—H73	120.600
C34—C33—H33	119.800	C72—C73—H73	120.600
C35—C34—C33	119.9(7)	C73—C74—C69	121.3(8)
C35—C34—H34	120.000	C73—C74—H74	119.300
C33—C34—H34	120.000	C69—C74—H74	119.300
C34—C35—C36	120.7(8)	C1—N1—C6	110.4(4)
C34—C35—H35	119.700	C1—N1—C7	124.5(4)
C36—C35—H35	119.700	C6—N1—C7	125.1(5)
C31—C36—C35	119.6(7)	C4—N2—C3	110.5(4)
C31—C36—H36	120.200	C4—N2—C15	131.4(4)
C35—C36—H36	120.200	C3—N2—C15	117.2(4)

Compound **8**

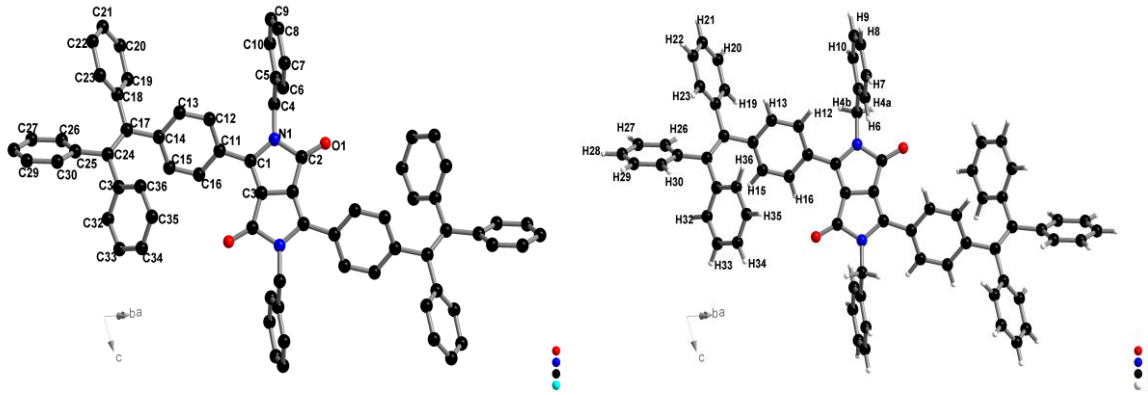

Fig. S11 Molecular structure of compound **8** in the crystal phase, as result of single crystal X-ray diffraction experiment, with atom numbering (hydrogen omitted for clarity in the left picture, and separately numbered in the right one).

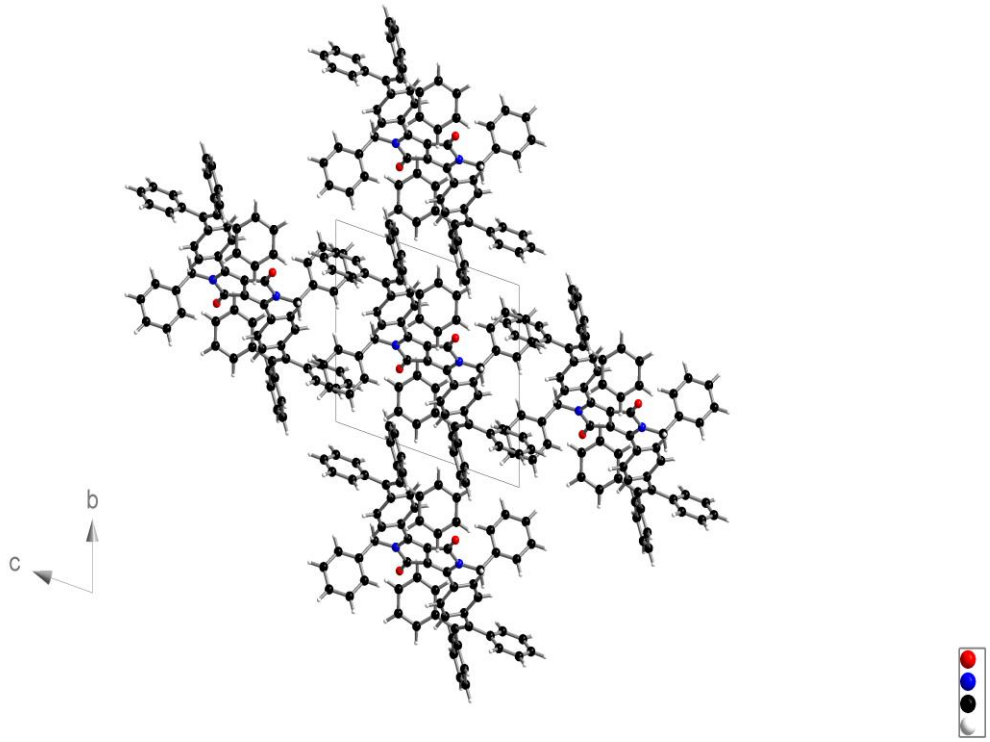

Fig. S12 Crystal packing of compound **8** in the crystal phase, as result of single crystal X-ray diffraction experiment.

Table S4 Bond Lengths for compound **8** in the crystal phase.

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
O1—C2	1.221(2)	C27—C28	1.398(3)
N1—C1	1.390(2)	C30—H30	0.9500
N1—C2	1.427(2)	C30—C29	1.390(3)
N1—C4	1.452(2)	C32—H32	0.9500
C11—C12	1.404(3)	C32—C33	1.383(3)
C11—C1	1.461(3)	C4—H4a	0.9900
C11—C16	1.395(3)	C4—H4b	0.9900
C25—C26	1.395(3)	C28—H28	0.9500
C25—C24	1.488(3)	C28—C29	1.378(3)
C25—C30	1.402(3)	C29—H29	0.9500
C15—H15	0.9500	C6—H6	0.9500
C15—C16	1.377(3)	C6—C7	1.389(3)
C15—C14	1.399(3)	C19—H19	0.9500
C3—C3^{i}	1.420(4)	C19—C20	1.385(3)
C3—C1	1.377(3)	C10—H10	0.9500
C3—C2^{i}	1.450(3)	C10—C9	1.377(3)
C12—H12	0.9500	C36—H36	0.9500
C12—C13	1.386(3)	C36—C35	1.387(3)
C16—H16	0.9500	C35—H35	0.9500
C5—C4	1.513(3)	C35—C34	1.380(3)
C5—C6	1.384(3)	C9—H9	0.9500
C5—C10	1.396(3)	C9—C8	1.383(4)
C17—C18	1.496(3)	C23—H23	0.9500
C17—C24	1.359(3)	C23—C22	1.392(3)
C17—C14	1.488(3)	C33—H33	0.9500
C31—C24	1.496(3)	C33—C34	1.384(4)
C31—C32	1.395(3)	C7—H7	0.9500
C31—C36	1.392(3)	C7—C8	1.396(3)
C13—H13	0.9500	C34—H34	0.9500
C13—C14	1.397(3)	C8—H8	0.9500
C18—C19	1.394(3)	C20—H20	0.9500

C18—C23	1.392(3)	C20—C21	1.384(4)
C26—H26	0.9500	C22—H22	0.9500
C26—C27	1.379(3)	C22—C21	1.381(4)
C27—H27	0.9500	C21—H21	0.9500

Table S5 Bond Angles for compound **8** in the crystal phase.

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
C2—N1—C1	111.63(15)	C33—C32—C31	120.7(2)
C4—N1—C1	128.06(16)	C33—C32—H32	119.65(14)
C4—N1—C2	120.07(15)	C5—C4—N1	114.07(17)
C1—C11—C12	123.32(18)	H4a—C4—N1	108.74(10)
C16—C11—C12	118.40(17)	H4a—C4—C5	108.74(10)
C16—C11—C1	118.03(16)	H4b—C4—N1	108.74(10)
C24—C25—C26	121.55(18)	H4b—C4—C5	108.74(10)
C30—C25—C26	118.16(18)	H4b—C4—H4a	107.600
C30—C25—C24	120.16(18)	H28—C28—C27	120.23(12)
C16—C15—H15	119.33(12)	C29—C28—C27	119.54(19)
C14—C15—H15	119.33(11)	C29—C28—H28	120.23(12)
C14—C15—C16	121.35(18)	C28—C29—C30	120.5(2)
C2^{i}—C3—C1	142.40(18)	H29—C29—C30	119.77(13)
H12—C12—C11	119.93(11)	H29—C29—C28	119.77(12)
C13—C12—C11	120.14(18)	H6—C6—C5	119.49(12)
C13—C12—H12	119.93(11)	C7—C6—C5	121.0(2)
C11—C1—N1	125.61(16)	C7—C6—H6	119.49(14)
C3—C1—N1	107.30(16)	H19—C19—C18	119.45(12)
C3—C1—C11	127.06(18)	C20—C19—C18	121.1(2)
C15—C16—C11	120.93(17)	C20—C19—H19	119.45(15)
H16—C16—C11	119.53(10)	H10—C10—C5	119.73(14)
H16—C16—C15	119.53(11)	C9—C10—C5	120.5(2)
C6—C5—C4	122.04(17)	C9—C10—H10	119.73(13)
C10—C5—C4	119.12(19)	H36—C36—C31	119.50(11)
C10—C5—C6	118.8(2)	C35—C36—C31	121.0(2)
C24—C17—C18	123.21(16)	C35—C36—H36	119.50(14)
C14—C17—C18	114.90(16)	H35—C35—C36	120.11(14)
C14—C17—C24	121.86(17)	C34—C35—C36	119.8(2)
C32—C31—C24	121.11(19)	C34—C35—H35	120.11(13)
C36—C31—C24	120.57(18)	H9—C9—C10	119.75(13)
C36—C31—C32	118.31(18)	C8—C9—C10	120.5(2)
H13—C13—C12	119.22(11)	C8—C9—H9	119.75(13)
C14—C13—C12	121.55(17)	H23—C23—C18	119.78(12)
C14—C13—H13	119.22(10)	C22—C23—C18	120.4(2)
C19—C18—C17	120.58(18)	C22—C23—H23	119.78(15)
C23—C18—C17	120.83(18)	H33—C33—C32	119.95(14)
C23—C18—C19	118.49(18)	C34—C33—C32	120.1(2)
H26—C26—C25	119.40(11)	C34—C33—H33	119.95(13)
C27—C26—C25	121.21(19)	H7—C7—C6	120.30(14)
C27—C26—H26	119.40(13)	C8—C7—C6	119.4(2)
C17—C24—C25	123.38(17)	C8—C7—H7	120.30(15)
C31—C24—C25	115.49(16)	C33—C34—C35	120.0(2)
C31—C24—C17	121.11(17)	H34—C34—C35	119.98(13)
N1—C2—O1	122.35(17)	H34—C34—C33	119.98(13)
C3^{i}—C2—O1	134.15(17)	C7—C8—C9	119.7(2)
C3^{i}—C2—N1	103.50(15)	H8—C8—C9	120.15(13)
C17—C14—C15	121.28(18)	H8—C8—C7	120.15(15)
C13—C14—C15	117.55(17)	H20—C20—C19	120.14(15)
C13—C14—C17	121.17(17)	C21—C20—C19	119.7(2)
H27—C27—C26	119.97(13)	C21—C20—H20	120.14(14)
C28—C27—C26	120.1(2)	H22—C22—C23	119.92(15)
C28—C27—H27	119.97(12)	C21—C22—C23	120.2(2)
H30—C30—C25	119.72(12)	C21—C22—H22	119.92(14)
C29—C30—C25	120.6(2)	C22—C21—C20	120.1(2)
C29—C30—H30	119.72(13)	H21—C21—C20	119.97(14)
H32—C32—C31	119.65(12)	H21—C21—C22	119.97(14)

(i) 2-x, 1-y, 1-z.

DFT and TD-DFT calculations

Compound ***2RR***

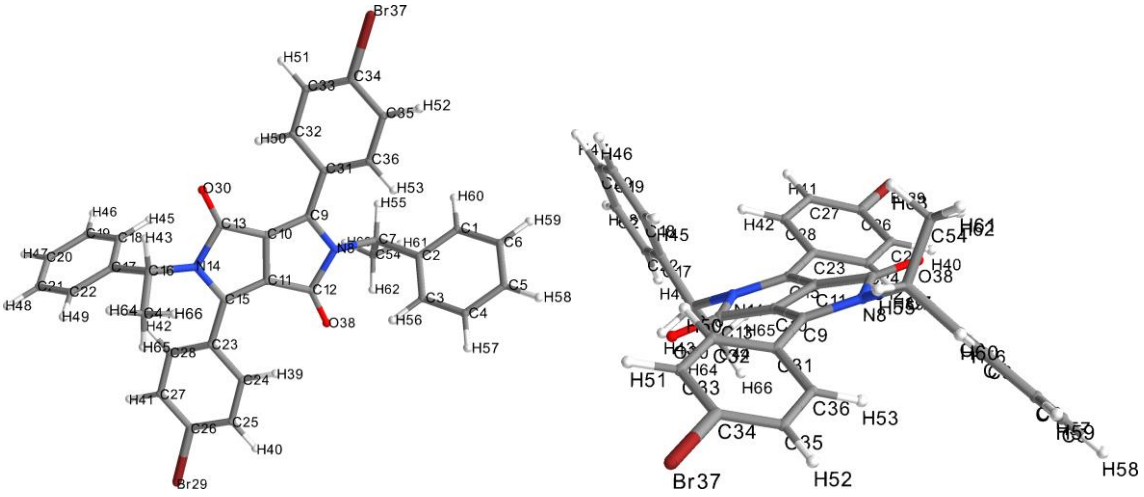

Fig. S13 Two views of the optimized geometry of compound **2*RR*** with atom numbering scheme.

Total molecular energy	-6717.61405 hartrees
HOMO number	165
LUMO+1 energies	-1.22 eV
LUMO energies	-2.76 eV
HOMO energies	-5.86 eV
HOMO-1 energies	-7.22 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	5377.77649 Hartrees
Frequency and Thermochemistry specific results	
Number of negative frequencies	0
Sum of electronic and zero-point energy	-6717.09833 Hartrees
Sum of electronic and thermal energies at 298.15 K	-6717.06360 Hartrees
Enthalpy at 298.15 K	-6717.06266 Hartrees
Gibbs free energy at 298.15 K	-6717.17088 Hartrees
Entropy at 298.15 K	0.00036 Hartrees

Table. Most intense (> 20 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
1794	50	A
1773	1027	A
1662	665	A
1651	71	A
1616	56	A
1532	283	A
1455	78	A
1448	148	A
1434	103	A
1422	67	A
1395	165	A
1373	117	A
1179	86	A
1133	50	A
1104	201	A
1078	51	A
1031	53	A
1030	64	A
760	79	A

Table. Results concerning the calculated mono-electronic excitations

E.S.	Symmetry	nm	cm-1	f	R	Lambda	dCT	qCT	Excitation description in %
1	Singlet-A	462	21643	0.559	1.863	0.85	16.13	0.40	165->166 (100)
2	Singlet-A	360	27718	0.000	-2.221	0.33	125.75	0.77	158->166 (10) 159->166 (14) 160->166 (7) 161->166 (2) 162->166 (8) 163->166 (6) 164->166 (45)
3	Singlet-A	344	29002	0.010	4.386	0.42	124.94	0.65	155->166 (2) 157->166 (53) 159->166 (6) 160->166 (7) 161->166 (11) 162->166 (2) 163->166 (6)
4	Singlet-A	326	30602	0.037	19.854	0.36	88.27	0.68	154->166 (4) 160->166 (2) 161->166 (3) 163->166 (42) 164->166 (32) 165->167 (6)
5	Singlet-A	317	31470	0.015	3.470	0.58	144.80	0.44	160->166 (2) 161->166 (7) 162->166 (18) 163->166 (14) 165->167 (52)
6	Singlet-A	314	31803	0.000	-0.561	0.42	136.41	0.65	157->166 (9) 158->166 (5) 159->166 (8) 160->166 (8) 162->166 (15) 163->166 (22) 164->166 (12) 165->167 (13)
7	Singlet-A	310	32195	0.261	-80.655	0.43	148.61	0.62	154->166 (8) 156->166 (2) 157->166 (16) 159->166 (5) 160->166 (3) 161->166 (32) 162->166 (19) 163->166 (2)
8	Singlet-A	302	33038	0.001	-1.588	0.36	208.77	0.73	159->166 (21) 160->166 (58) 161->166 (12) 165->167 (3)
9	Singlet-A	300	33289	0.001	10.165	0.46	78.85	0.55	157->166 (3) 158->166 (5) 159->166 (15) 161->166 (14) 162->166 (31) 163->166 (2) 165->167 (18)
10	Singlet-A	298	33452	0.020	21.954	0.37	193.35	0.47	154->166 (8) 156->166 (35) 158->166 (15) 159->166 (3) 160->166 (5) 161->166 (7) 165->168 (7) 165->169 (9)
11	Singlet-A	297	33634	0.012	14.023	0.33	311.64	0.67	154->166 (9) 155->166 (3) 156->166 (7) 158->166 (51) 159->166 (16) 165->168 (4)
12	Singlet-A	293	34071	0.004	2.023	0.32	191.67	0.51	154->166 (3) 155->166 (15) 159->166 (2) 165->168 (51) 165->169 (17)
13	Singlet-A	290	34437	0.003	8.219	0.33	207.34	0.51	154->166 (23) 155->166 (2) 158->166 (3) 161->166 (2) 165->168 (14) 165->169 (42)
14	Singlet-A	277	35977	0.017	4.771	0.41	225.20	0.44	154->166 (10) 155->166 (26) 156->166 (27) 157->166 (4) 165->169 (27)
15	Singlet-A	275	36247	0.008	-7.104	0.41	39.64	0.46	154->166 (19) 155->166 (41) 156->166 (16) 165->168 (18)

Table. Atomic charges population analysis. Selection of the most charged atoms based on Hirshfeld analysis

Atom and N°	Hirshfeld charge	CM5 charge	Mulliken charge
O 30	-0.334	-0.285	-0.310
O 38	-0.324	-0.271	-0.299
N 14	-0.301	-0.059	+0.028
N 8	-0.297	-0.058	+0.082
C 44	-0.252	-0.108	-0.405
C 54	-0.252	-0.110	-0.374
C 9	+0.143	+0.079	+0.230
C 15	+0.146	+0.082	+0.096
C 13	+0.266	+0.174	-0.000
C 12	+0.273	+0.180	-0.041

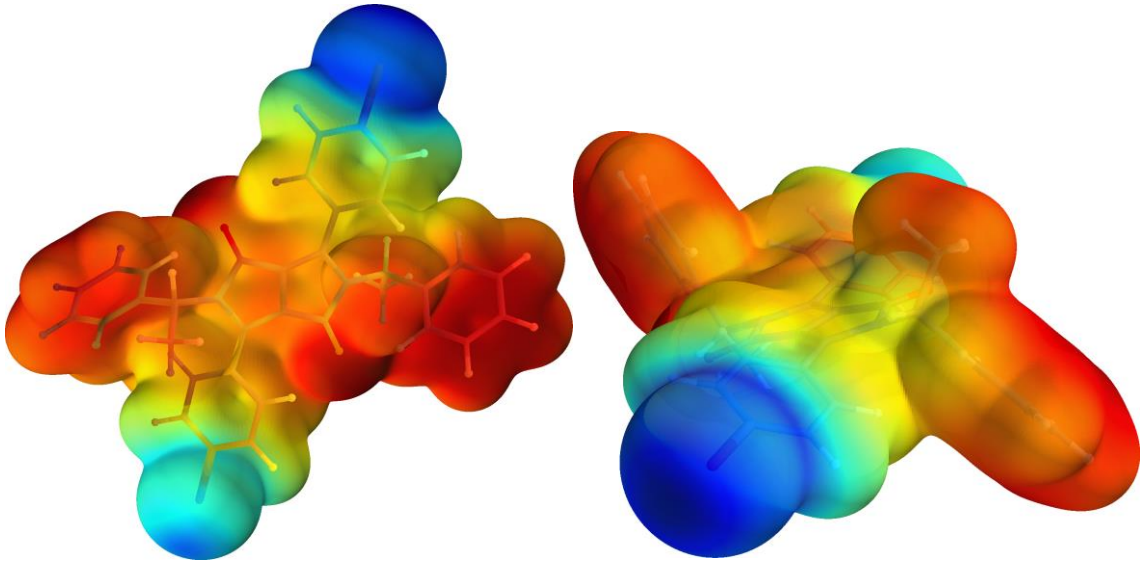

Fig. S14 Representation of the Molecular Electrostatic Potential of **2*RR*** mapped on the electron density (cutoff value of 0.002 e-/bohr3). Red, blue and green regions correspond to the most negative (< -0.1 a.u.), the most positive potentials (> 0.1 a.u.) and intermediate values respectively.

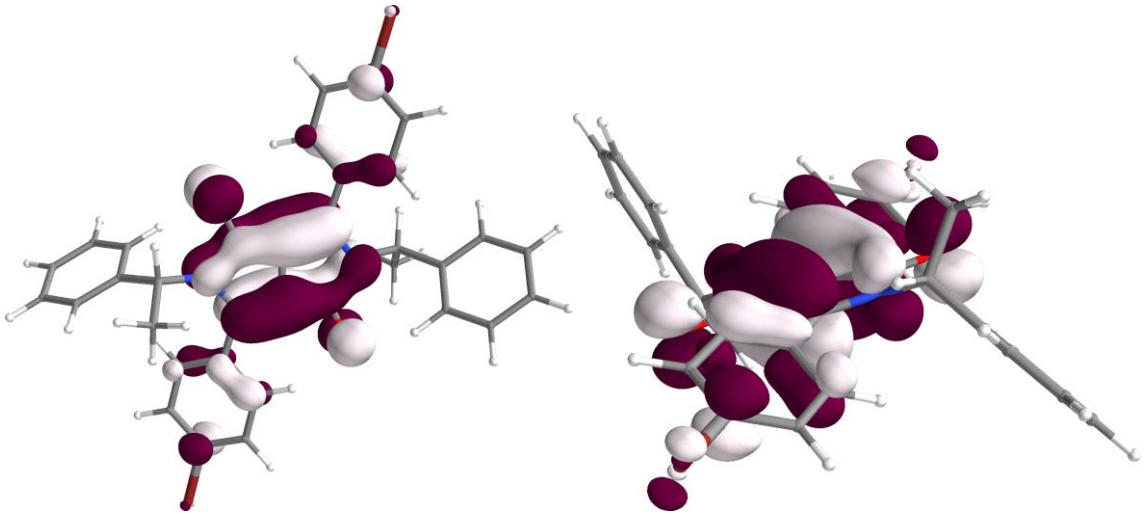

Fig. S15 Representation of the HOMO of **2*RR*** from two points of view.

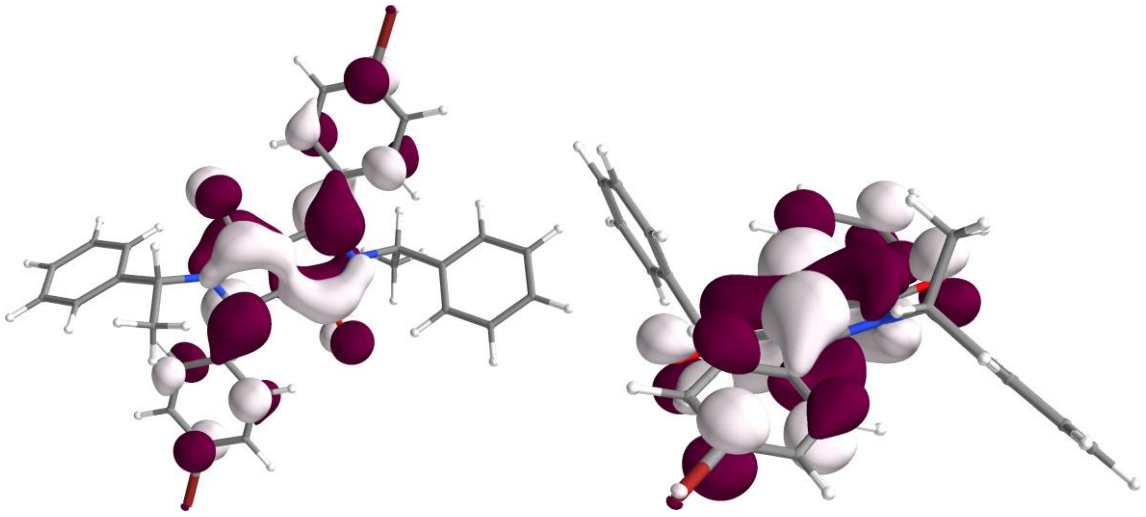

Fig. S16 Representation of the LUMO of **2*RR*** from two points of view.

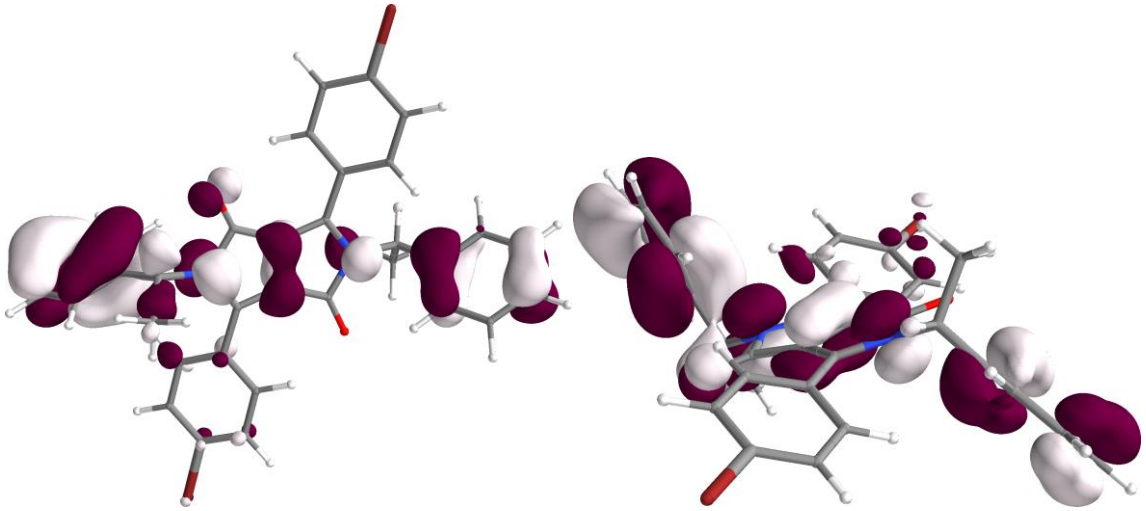

Fig. S17 Representation of the HOMO–1 of **2*RR*** from two points of view.

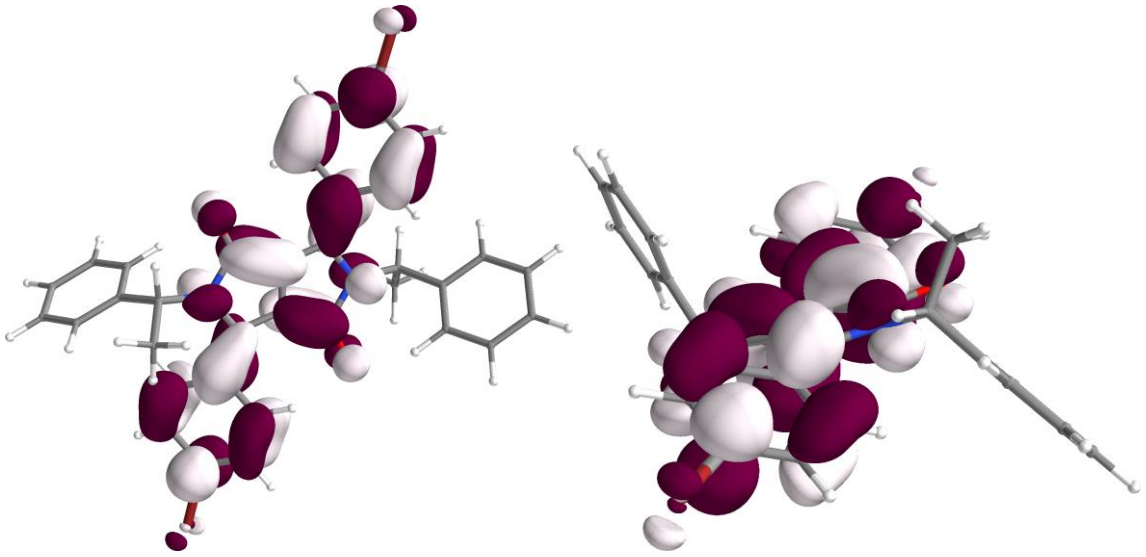

Fig. S18 Representation of the LUMO+1 of **2*RR*** from two points of view.

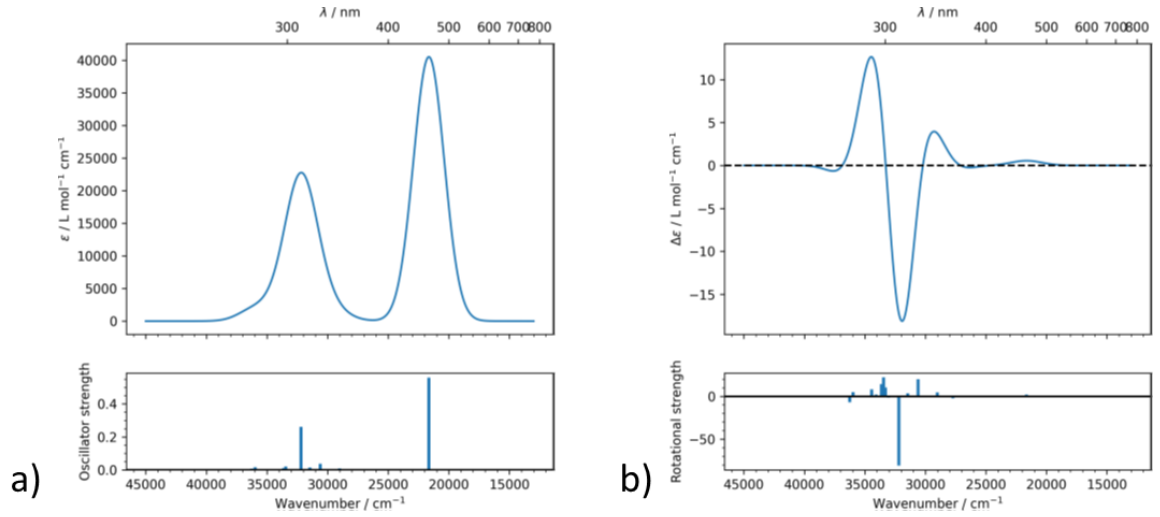

Fig. S19 Simulated spectra for compound **2*RR***, obtained with gaussian broadening (FWHM = 3000 cm^{-1}): *a*) UV-visible absorption and *b*) Circular Dichroism spectrum.

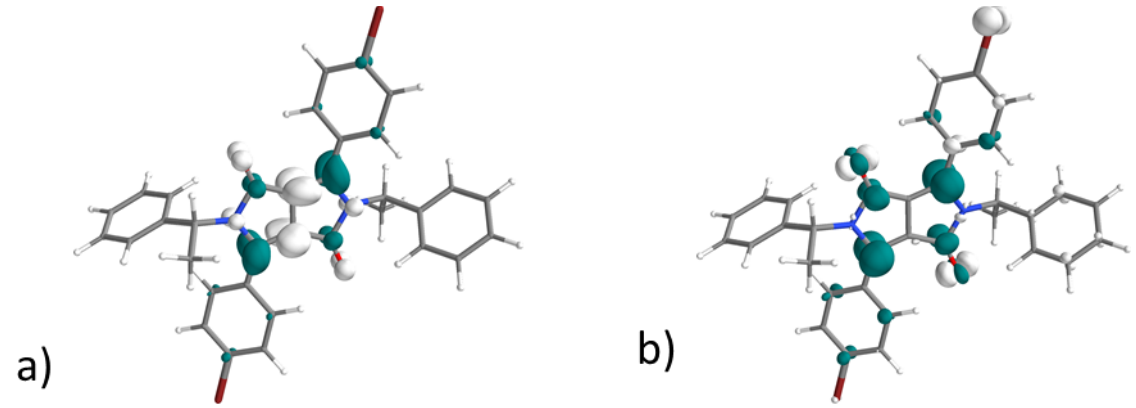

Fig. S20 Representation of the Electron Density Difference (EDD) associated to the strongest transitions calculated for the compound **2*RR***: *a*) S0-S1; *b*) S0-S7; excited electrons and holes indicated by green and white surfaces, respectively.

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
C	-4.2617	-3.8055	0.6102
C	-2.9327	-3.4252	0.4325
C	-2.1547	-4.1230	-0.4870
C	-2.7002	-5.1724	-1.2139
C	-4.0247	-5.5441	-1.0306
C	-4.8060	-4.8580	-0.1115
C	-2.3857	-2.2982	1.2858
N	-1.4729	-1.3906	0.5772
C	-1.7819	-0.0812	0.2303
C	-0.6097	0.5639	-0.0780
C	0.4693	-0.3472	0.0450
C	-0.0660	-1.6247	0.4659
C	-0.0809	1.8312	-0.5194
N	1.3321	1.6072	-0.6033
C	1.6460	0.2945	-0.2691
C	2.1361	2.6317	-1.2732
C	2.9904	3.4470	-0.3171
C	2.4986	3.7707	0.9469
C	3.2384	4.5550	1.8180
C	4.4840	5.0388	1.4388
C	4.9778	4.7323	0.1804
C	4.2359	3.9445	-0.6910
C	2.9867	-0.2799	-0.2183
C	3.1514	-1.6266	-0.5599
C	4.3944	-2.2300	-0.4962
C	5.4870	-1.4896	-0.0712
C	5.3479	-0.1604	0.2972
C	4.1017	0.4378	0.2226
Br	7.1921	-2.3093	0.0203
O	-0.5969	2.8995	-0.7790
C	-3.1334	0.4597	0.1576
C	-3.3454	1.8044	0.4778
C	-4.6048	2.3676	0.3786
C	-5.6648	1.5876	-0.0588
C	-5.4778	0.2588	-0.4085
C	-4.2160	-0.2998	-0.2986
Br	-7.3916	2.3528	-0.1968
O	0.4573	-2.7022	0.6704
H	2.2946	-2.2124	-0.8663
H	4.5107	-3.2711	-0.7691
H	6.2030	0.4038	0.6477
H	3.9997	1.4700	0.5294
H	1.3609	3.3217	-1.6268
C	2.8520	2.0908	-2.5032
H	1.5257	3.4012	1.2505
H	2.8384	4.7925	2.7977
H	5.0634	5.6516	2.1201
H	5.9479	5.1055	-0.1293
H	4.6456	3.7108	-1.6661
H	-2.5120	2.4194	0.7928
H	-4.7595	3.4083	0.6335
H	-6.3078	-0.3337	-0.7725
H	-4.0728	-1.3306	-0.6001
C	-1.7810	-2.8172	2.5907
H	-3.2353	-1.6706	1.5623
H	-1.1130	-3.8572	-0.6173
H	-2.0815	-5.7065	-1.9268
H	-4.4462	-6.3644	-1.6008
H	-5.8428	-5.1377	0.0403
H	-4.8819	-3.2670	1.3218
H	-2.5541	-3.3561	3.1416
H	-0.9474	-3.4909	2.4052
H	-1.4336	-1.9852	3.2081
H	3.1973	2.9170	-3.1267
H	3.7100	1.4655	-2.2544
H	2.1548	1.4997	-3.0994

Compound **2*SS***

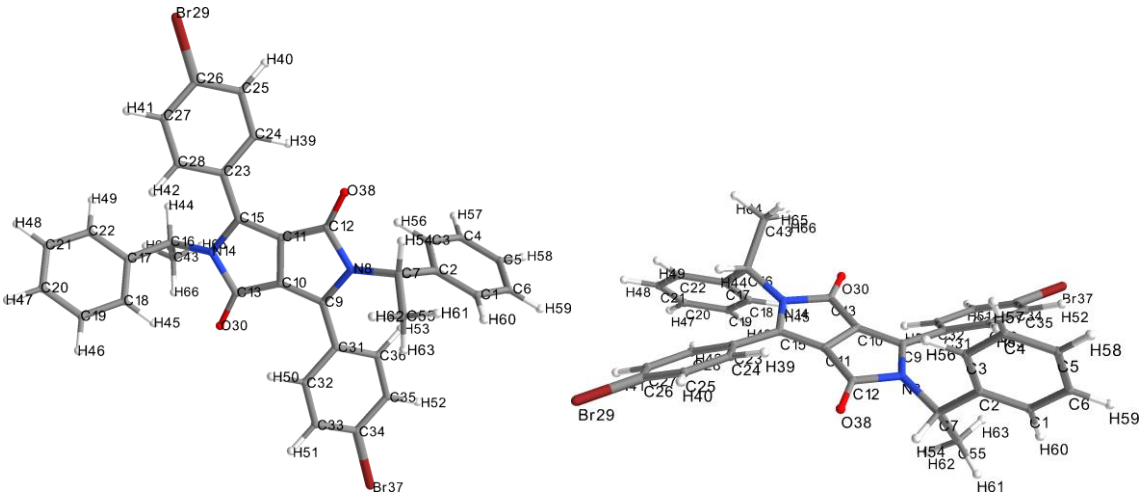

Fig. S21 Two views of the optimized geometry of compound **2*SS*** with atom numbering scheme.

Total molecular energy	-6717.61405 hartrees
HOMO number	165
LUMO+1 energies	-1.22 eV
LUMO energies	-2.76 eV
HOMO energies	-5.86 eV
HOMO-1 energies	-7.22 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	5377.77692 Hartrees
Frequency and Thermochemistry specific results	
Number of negative frequencies	0
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Sum of electronic and thermal energies at 298.15 K	-6717.06360 Hartrees
Enthalpy at 298.15 K	-6717.06266 Hartrees
Gibbs free energy at 298.15 K	-6717.17088 Hartrees
Entropy at 298.15 K	0.00036 Hartrees

Table. Most intense (> 20 km/mol) molecular vibrations in wavenumbers

Frequencies	Intensity	Symmetry
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1773	1027	A
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1651	71	A
1616	56	A
1532	283	A
1455	78	A
1448	148	A
1434	103	A
1422	67	A
1395	165	A
1373	117	A
1179	86	A
1133	50	A
1104	202	A
1078	51	A
1031	53	A
1030	64	A
760	80	A

Table. Results concerning the calculated mono-electronic excitations

E.S.	Symmetry	nm	cm-1	f	R	Lambda	dCT	qCT	Excitation description in %
1	Singlet-A	462	21643	0.559	-1.863	0.85	16.13	0.40	165->166 (100)
2	Singlet-A	360	27718	0.000	2.221	0.33	125.75	0.77	158->166 (10) 159->166 (14) 160->166 (7) 161->166 (2) 162->166 (8) 163->166 (6) 164->166 (45)
3	Singlet-A	344	29002	0.010	-4.386	0.42	124.94	0.65	155->166 (2) 157->166 (53) 159->166 (6) 160->166 (7) 161->166 (11) 162->166 (2) 163->166 (6)
4	Singlet-A	326	30602	0.037	-19.854	0.36	88.27	0.68	154->166 (4) 160->166 (2) 161->166 (3) 163->166 (42) 164->166 (32) 165->167 (6)
5	Singlet-A	317	31470	0.015	-3.470	0.58	144.80	0.44	160->166 (2) 161->166 (7) 162->166 (18) 163->166 (14) 165->167 (52)
6	Singlet-A	314	31803	0.000	0.561	0.42	136.41	0.65	157->166 (9) 158->166 (5) 159->166 (8) 160->166 (8) 162->166 (15) 163->166 (22) 164->166 (12) 165->167 (13)
7	Singlet-A	310	32195	0.261	80.655	0.43	148.61	0.62	154->166 (8) 156->166 (2) 157->166 (16) 159->166 (5) 160->166 (3) 161->166 (32) 162->166 (19) 163->166 (2)
8	Singlet-A	302	33038	0.001	1.588	0.36	208.77	0.73	159->166 (21) 160->166 (58) 161->166 (12) 165->167 (3)
9	Singlet-A	300	33289	0.001	-10.165	0.46	78.85	0.55	157->166 (3) 158->166 (5) 159->166 (15) 161->166 (14) 162->166 (31) 163->166 (2) 165->167 (18)
10	Singlet-A	298	33452	0.020	-21.954	0.37	193.35	0.47	154->166 (8) 156->166 (35) 158->166 (15) 159->166 (3) 160->166 (5) 161->166 (7) 165->168 (7) 165->169 (9)
11	Singlet-A	297	33634	0.012	-14.023	0.33	311.64	0.67	154->166 (9) 155->166 (3) 156->166 (7) 158->166 (51) 159->166 (16) 165->168 (4)
12	Singlet-A	293	34071	0.004	-2.023	0.32	191.66	0.51	154->166 (3) 155->166 (15) 159->166 (2) 165->168 (51) 165->169 (17)
13	Singlet-A	290	34437	0.003	-8.219	0.33	207.33	0.51	154->166 (23) 155->166 (2) 158->166 (3) 161->166 (2) 165->168 (14) 165->169 (42)
14	Singlet-A	277	35977	0.017	-4.771	0.41	225.21	0.44	154->166 (10) 155->166 (26) 156->166 (27) 157->166 (4) 165->169 (27)
15	Singlet-A	275	36247	0.008	7.104	0.41	39.64	0.46	154->166 (19) 155->166 (41) 156->166 (16) 165->168 (18)

Table. Atomic charges population analysis. Selection of the most charged atoms based on Hirshfeld analysis

Atom and N°	Hirshfeld charge	CM5 charge	Mulliken charge
O 38	-0.334	-0.285	-0.310
O 30	-0.324	-0.271	-0.299
N 8	-0.301	-0.059	+0.028
N 14	-0.297	-0.058	+0.082
C 55	-0.252	-0.108	-0.405
C 43	-0.252	-0.110	-0.374
C 15	+0.143	+0.079	+0.230
C 9	+0.146	+0.082	+0.096
C 12	+0.266	+0.174	-0.000
C 13	+0.273	+0.180	-0.041

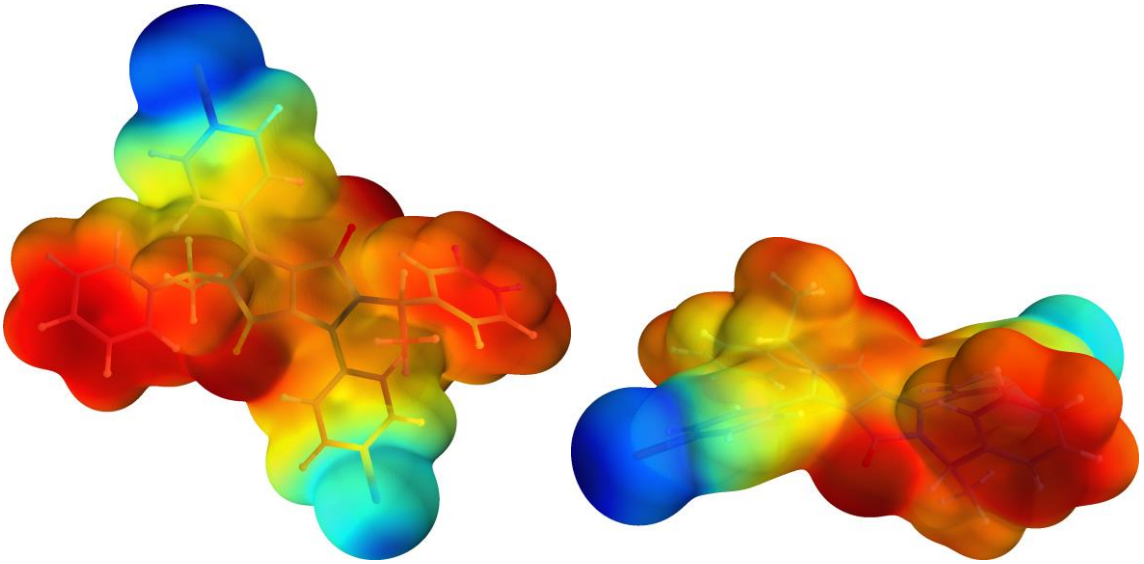


Fig. S22 Representation of the Molecular Electrostatic Potential of **2*SS*** mapped on the electron density (cutoff value of 0.002 e-/bohr3). Red, blue and green regions correspond to the most negative (< -0.1 a.u.), the most positive potentials (> 0.1 a.u.) and intermediate values respectively.

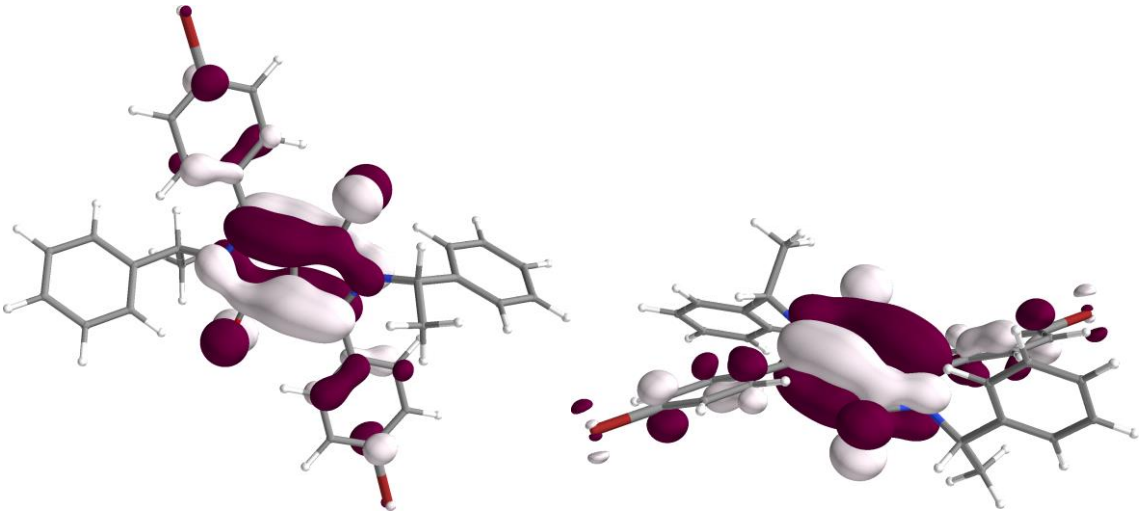


Fig. S23 Representation of the HOMO of **2*SS*** from two points of view.

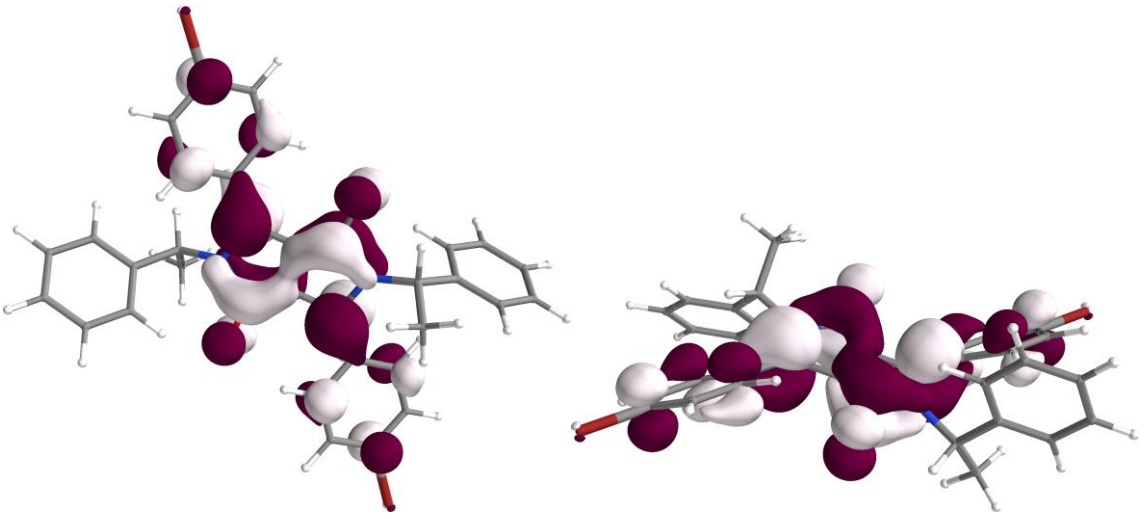


Fig. S24 Representation of the LUMO of **2*SS*** from two points of view.

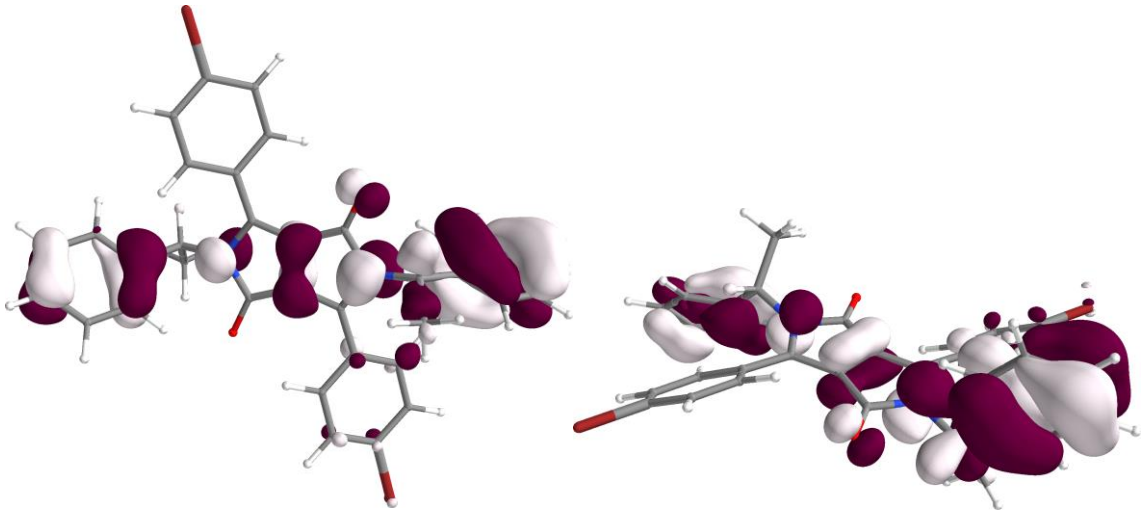


Fig. S25 Representation of the HOMO–1 of **2*SS*** from two points of view.

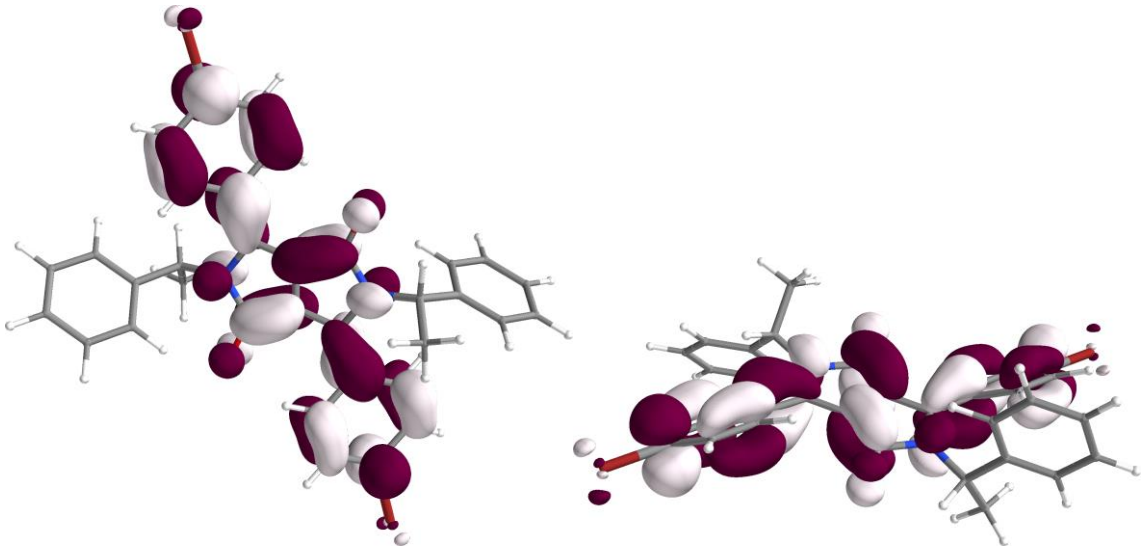
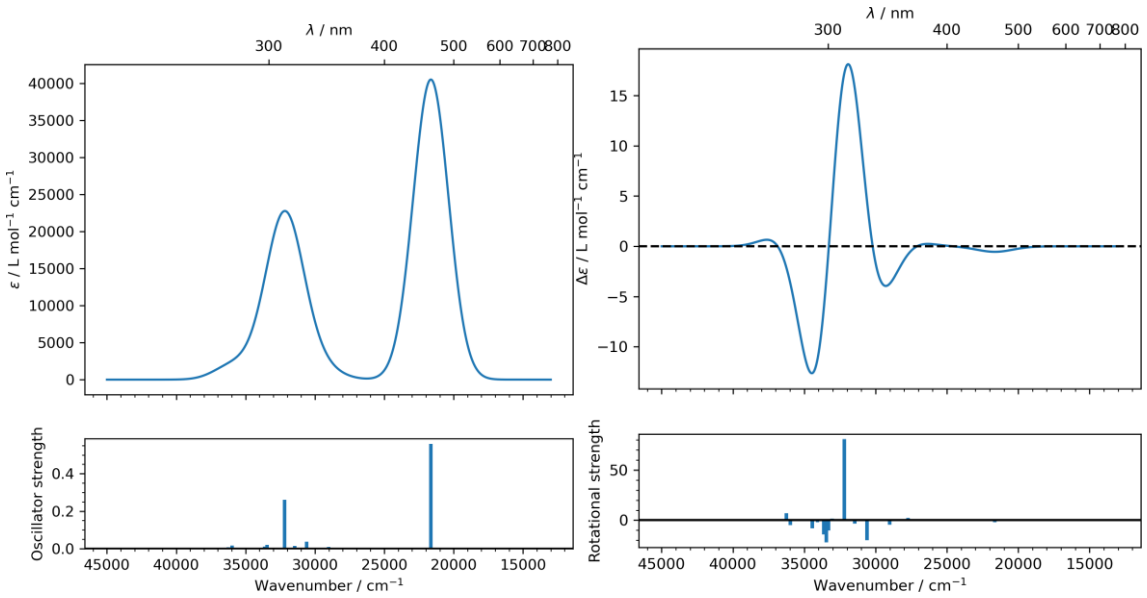


Fig. S26 Representation of the LUMO+1 of **2*SS*** from two points of view.



a) b)

Fig. S27 Simulated spectra for compound **2*SS***, obtained with gaussian broadening (FWHM = 3000 cm^{-1}): *a*) UV-visible absorption and *b*) Circular Dichroism spectrum.

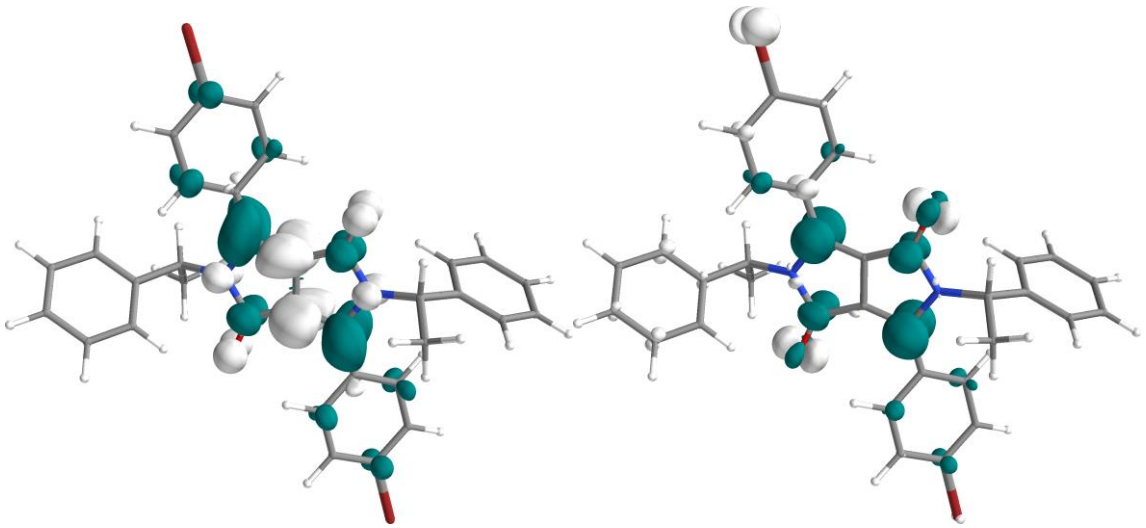


Fig. S28 Representation of the Electron Density Difference (EDD) associated to the strongest transitions calculated for the compound **2*SS***: *a*) S0-S1; *b*) S0-S7; excited electrons and holes indicated by green and white surfaces, respectively.

Compound **3*RR***

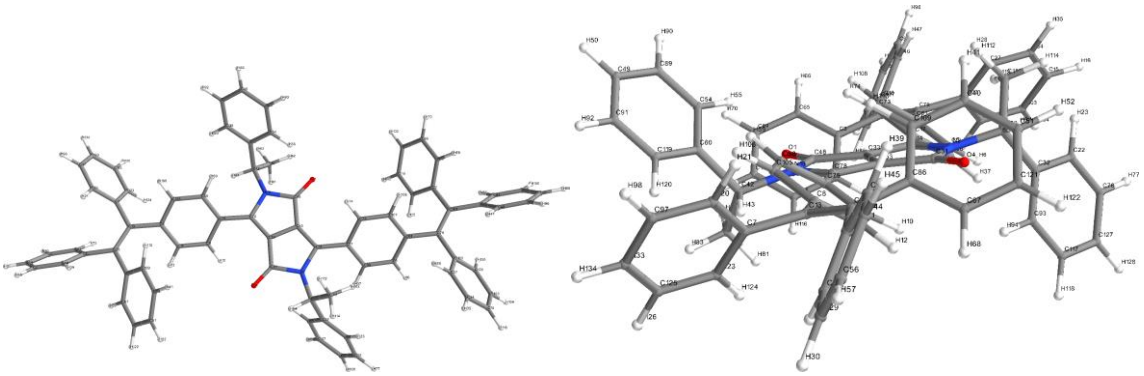


Fig. S29 Two views of the optimized geometry of compound **3*RR*** with atom numbering scheme.

Total molecular energy	-3110.83781 hartrees
HOMO number	265
LUMO+1 energies	-1.54 eV
LUMO energies	-2.48 eV
HOMO energies	-5.43 eV
HOMO-1 energies	-5.92 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	11489.65179 Hartrees

Table. First five calculated mono-electronic excitations and those with f > 0.1 or R > 10.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	501	19921	0.859	-16.3	0.81	59.78	0.42	265-266(98);
2	Singlet-A	419	23811	0.001	16.5	0.44	192.27	0.79	264-266(97);
3	Singlet-A	402	24849	0.142	-11.6	0.61	219.90	0.63	263-266(96);
4	Singlet-A	370	27013	0.001	14.4	0.61	154.13	0.59	265-267(89);
5	Singlet-A	358	27897	0.000	-2.0	0.38	187.47	0.71	255-266(11); 261-266(10); 262-266(53); 265-267(6);
6	Singlet-A	345	28923	0.163	-4.3	0.48	172.76	0.40	251-266(8); 252-266(6); 256-266(17); 265-268(43);
7	Singlet-A	343	29135	0.207	-8.4	0.49	137.60	0.41	251-266(7); 252-266(6); 256-266(14); 265-268(44);
8	Singlet-A	321	31138	0.215	6.6	0.73	342.43	0.35	263-268(13); 264-267(70); 265-268(7);
9	Singlet-A	319	31321	0.014	-42.1	0.34	316.73	0.64	242-266(8); 255-266(10); 259-266(11); 261-266(18); 262-266(19);
10	Singlet-A	317	31484	0.002	49.0	0.73	67.17	0.36	263-267(56); 264-268(32);
15	Singlet-A	301	33159	0.061	-18.6	0.33	155.72	0.48	245-266(8); 256-266(17); 257-266(8); 258-266(8); 260-266(10); 265-270(6); 265-271(10);
21	Singlet-A	294	33915	0.022	-42.8	0.42	297.80	0.34	251-266(9); 256-266(8); 263-267(7); 264-268(14); 265-271(22);
22	Singlet-A	293	34031	0.016	29.0	0.57	207.35	0.29	256-266(6); 263-267(15); 264-268(36); 265-271(14);
23	Singlet-A	291	34355	0.008	12.9	0.30	107.51	0.53	242-266(9); 251-266(8); 252-266(10); 253-266(29); 254-266(8); 265-270(10);
24	Singlet-A	289	34564	0.063	-13.7	0.61	210.96	0.33	251-266(6); 263-268(46); 264-267(6); 264-269(7); 265-272(9);
27	Singlet-A	281	35573	0.174	-4.2	0.32	169.50	0.46	245-266(6); 249-266(10); 250-266(9); 252-266(27); 265-272(9);
28	Singlet-A	279	35727	0.033	17.1	0.29	89.50	0.63	249-266(15); 250-266(46);
30	Singlet-A	276	36151	0.020	32.1	0.36	218.21	0.31	247-266(13); 248-266(17); 264-272(7); 265-273(22);
31	Singlet-A	275	36331	0.272	21.3	0.36	77.88	0.47	244-266(8); 245-266(10); 247-266(22); 248-266(25); 265-272(9);
32	Singlet-A	274	36392	0.049	-18.6	0.37	623.86	0.41	245-266(15); 263-270(22); 264-270(16);
33	Singlet-A	273	36518	0.005	10.2	0.34	207.00	0.39	246-266(8); 247-266(14); 248-266(6); 249-266(15); 250-266(6); 265-273(19);
34	Singlet-A	273	36617	0.005	-16.1	0.35	71.95	0.36	245-266(13); 248-266(10); 249-266(18); 265-273(17);
49	Singlet-A	258	38741	0.007	-45.1	0.30	531.36	0.43	259-267(9); 261-267(19); 261-268(13); 262-267(7);
50	Singlet-A	257	38861	0.024	55.2	0.35	815.56	0.44	260-267(39); 260-268(15); 261-267(8);

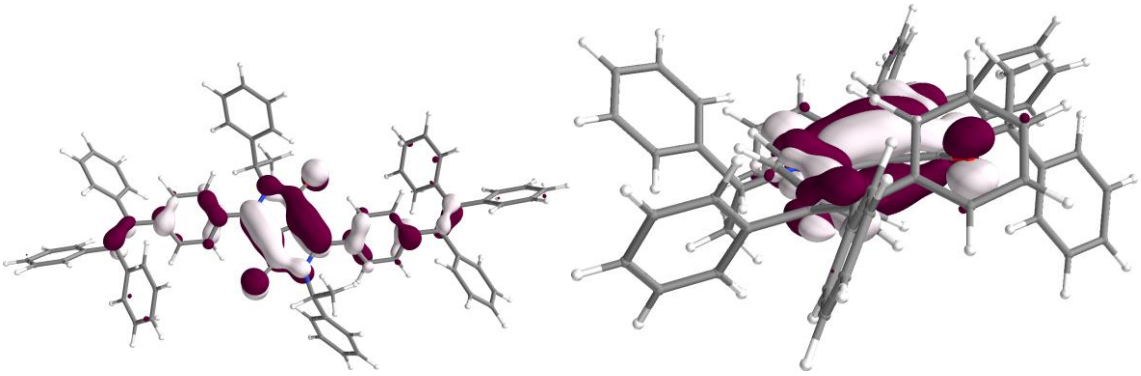


Fig. S30 Representation of the HOMO of **3*RR*** from two points of view.

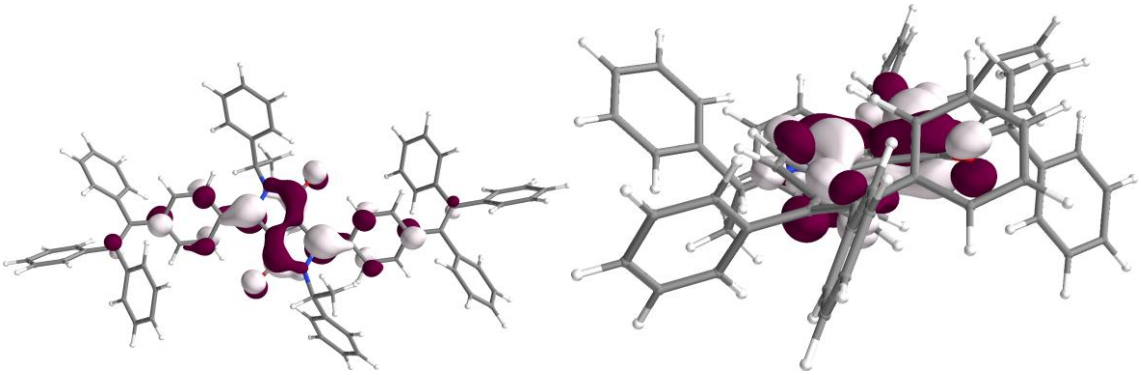
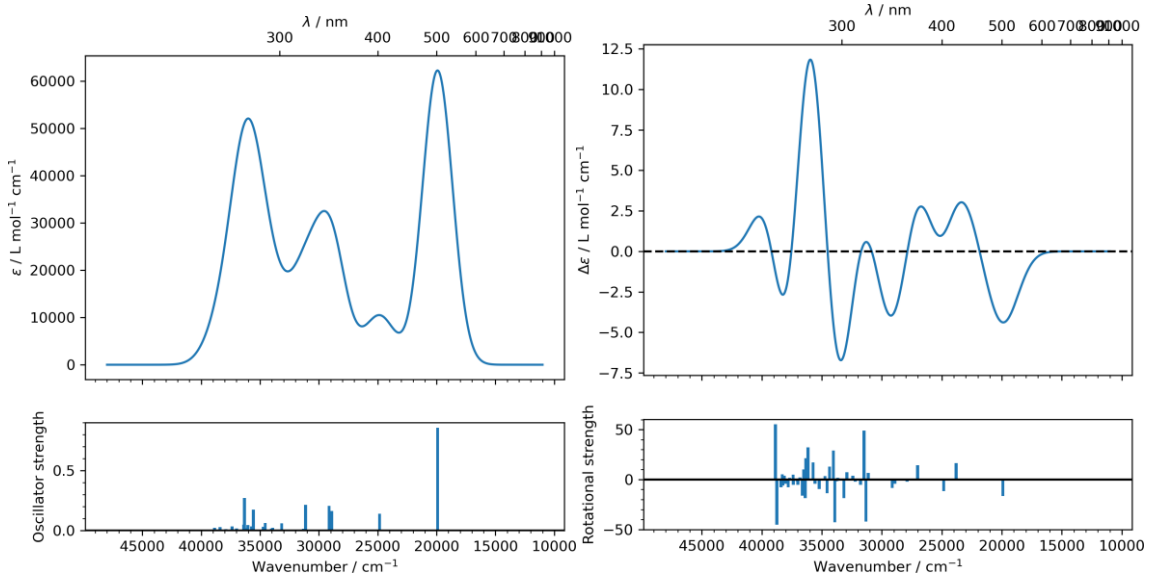


Fig. S31 Representation of the LUMO of **3*RR*** from two points of view.



a) b)

Fig. S32 Simulated spectra for compound **3*RR***, obtained with gaussian broadening (FWHM = 3000 cm^{-1}): *a*) UV-visible absorption and *b*) Circular Dichroism spectrum.

Compound **3*SS***

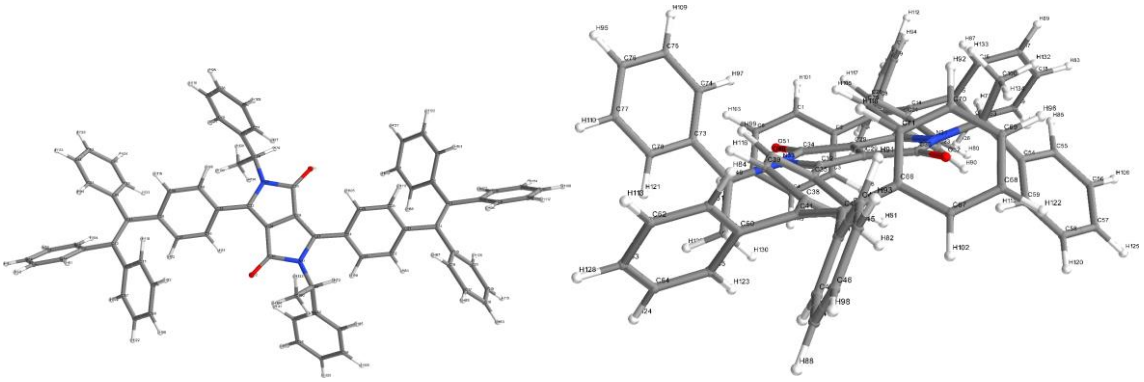


Fig. S33 Two views of the optimized geometry of compound **3*SS*** with atom numbering scheme.

Total molecular energy	-3110.83781 hartrees
HOMO number	265
LUMO+1 energies	-1.54 eV
LUMO energies	-2.48 eV
HOMO energies	-5.43 eV
HOMO-1 energies	-5.92 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	11489.62360 Hartrees
Enthalpy at 298.15 K	-3109.68262 Hartrees
Gibbs free energy at 298.15 K	-3109.85930 Hartrees
Entropy at 298.15 K	0.00059 Hartrees

Table. First five calculated mono-electronic excitations and those with f > 0.1 or R > 10.

E.S.	Symmetry	nm	cm^{-1}	f	R	Λ	d_{CT}	q_{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-A	502	19918	0.859	16.2	0.81	59.75	0.42	265-266(98);
2	Singlet-A	420	23809	0.001	-16.5	0.44	192.36	0.79	264-266(97);
3	Singlet-A	402	24848	0.142	11.6	0.61	219.95	0.63	263-266(96);
4	Singlet-A	370	27013	0.001	-14.3	0.61	153.86	0.59	265-267(89);
5	Singlet-A	358	27896	0.000	2.0	0.38	187.29	0.71	255-266(11); 261-266(10); 262-266(53); 265-267(6);
6	Singlet-A	345	28923	0.162	4.2	0.48	174.44	0.40	251-266(8); 252-266(6); 256-266(17); 265-268(43);
7	Singlet-A	343	29133	0.209	8.5	0.49	136.03	0.40	251-266(7); 252-266(6); 256-266(14); 265-268(45);
8	Singlet-A	321	31138	0.215	-6.8	0.73	342.45	0.35	263-268(13); 264-267(70); 265-268(7);
9	Singlet-A	319	31320	0.014	42.1	0.34	316.59	0.64	242-266(8); 255-266(10); 259-266(11); 261-266(18); 262-266(19);
10	Singlet-A	317	31484	0.002	-48.8	0.73	67.34	0.36	263-267(56); 264-268(32);
15	Singlet-A	301	33158	0.061	18.6	0.33	153.18	0.48	245-266(8); 256-266(17); 257-266(8); 258-266(8); 260-266(10); 265-270(6); 265-271(10);
21	Singlet-A	294	33914	0.022	42.7	0.42	302.26	0.34	251-266(9); 256-266(8); 263-267(7); 264-268(14); 265-271(22);
22	Singlet-A	293	34031	0.016	-29.0	0.57	207.15	0.29	256-266(6); 263-267(15); 264-268(36); 265-271(14);
23	Singlet-A	291	34353	0.008	-13.0	0.30	107.80	0.53	242-266(9); 251-266(8); 252-266(10); 253-266(29); 254-266(8); 265-270(10);
24	Singlet-A	289	34564	0.063	13.8	0.61	210.20	0.33	251-266(6); 263-268(46); 264-267(6); 264-269(7); 265-272(9);
27	Singlet-A	281	35571	0.174	4.2	0.32	169.75	0.46	245-266(6); 249-266(10); 250-266(9); 252-266(27); 265-272(9);
28	Singlet-A	279	35725	0.033	-17.1	0.29	89.67	0.63	249-266(15); 250-266(46);
30	Singlet-A	276	36150	0.020	-31.8	0.36	217.40	0.31	247-266(13); 248-266(17); 264-272(7); 265-273(22);
31	Singlet-A	275	36329	0.272	-21.6	0.36	75.11	0.47	244-266(8); 245-266(10); 247-266(23); 248-266(24); 265-272(9);
32	Singlet-A	274	36392	0.050	18.7	0.37	625.04	0.41	245-266(15); 263-270(22); 264-270(16);
33	Singlet-A	273	36517	0.005	-10.3	0.34	205.96	0.39	246-266(8); 247-266(14); 248-266(6); 249-266(15); 250-266(6); 265-273(19);
34	Singlet-A	273	36615	0.005	16.1	0.35	71.67	0.35	245-266(13); 248-266(10); 249-266(18); 265-273(17);
49	Singlet-A	258	38741	0.007	45.2	0.29	560.73	0.43	259-267(9); 261-267(19); 261-268(13); 262-267(7);
50	Singlet-A	257	38861	0.024	-55.2	0.35	815.83	0.44	260-267(39); 260-268(15); 261-267(8);

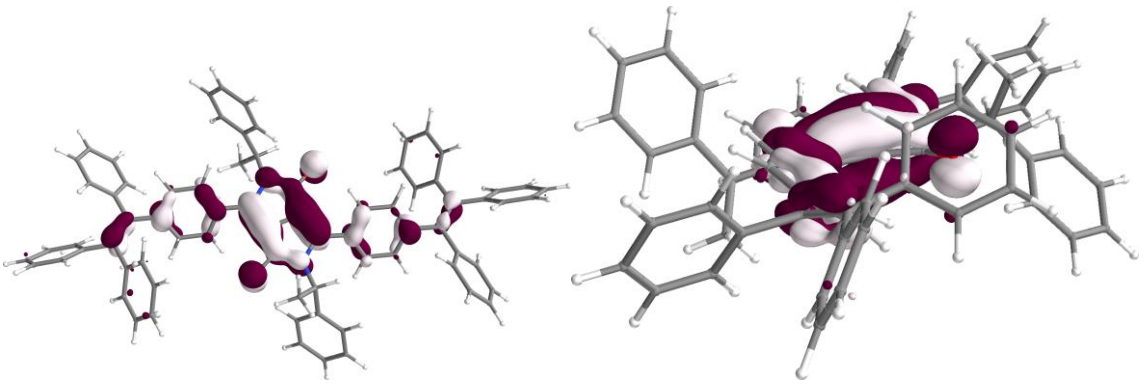


Fig. S34 Representation of the HOMO of **3*SS*** from two points of view.

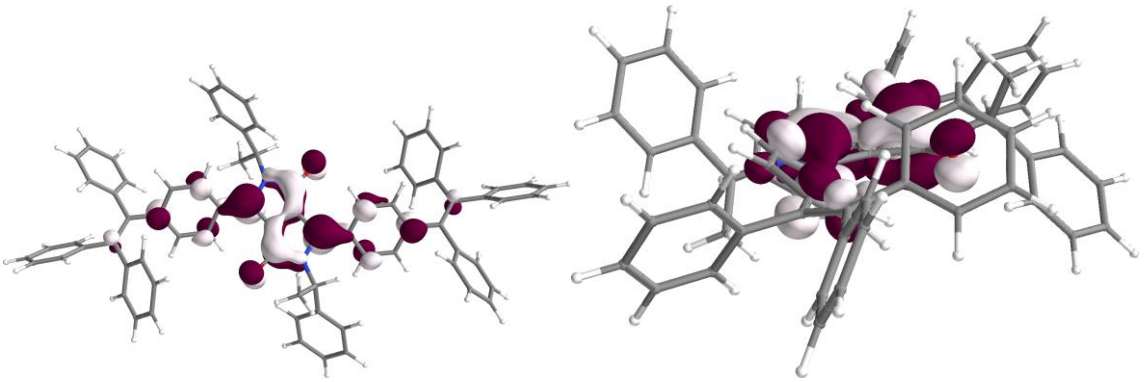
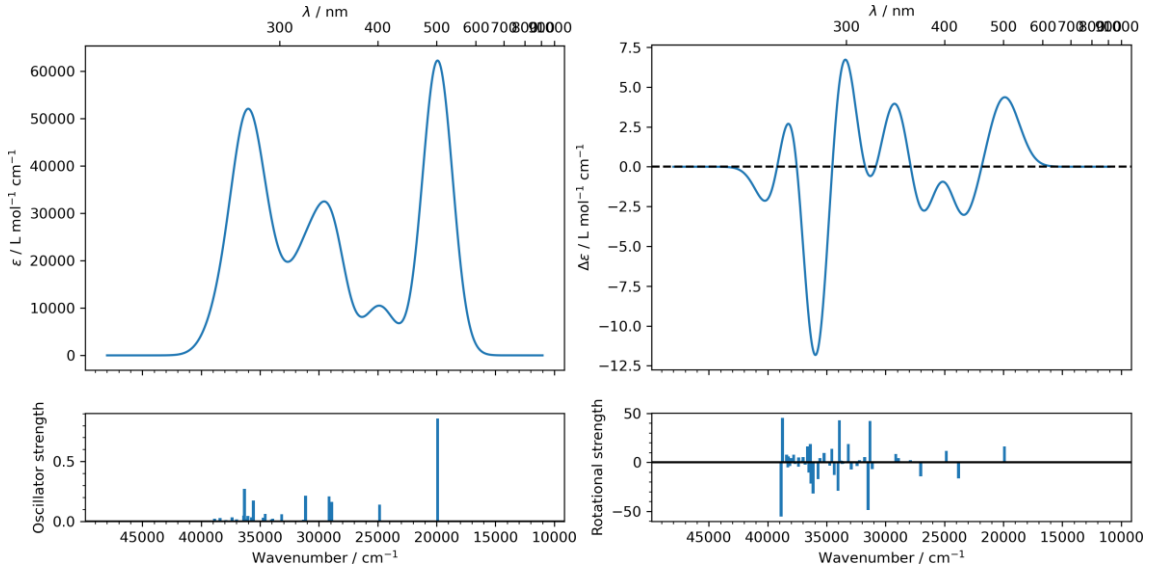


Fig. S35 Representation of the LUMO of **3*SS*** from two points of view.



a) b)

Fig. S36 Simulated spectra for compound **3*SS***, obtained with gaussian broadening (FWHM = 3000 cm^{-1}): *a*) UV-visible absorption and *b*) Circular Dichroism spectrum.

Compound **8**

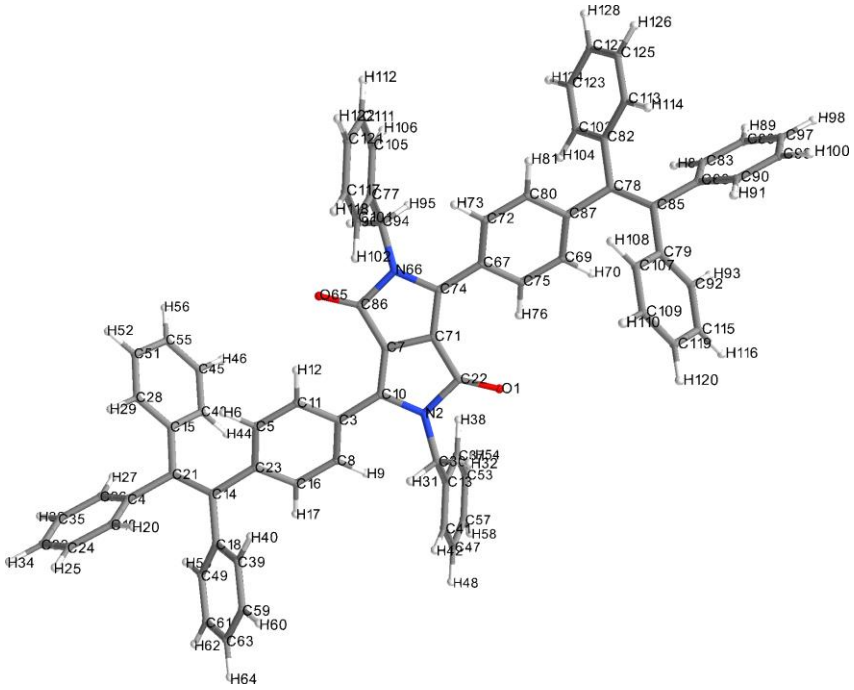


Fig. S37 Optimized geometry of compound **8** with atom numbering scheme.

Total molecular energy	-3032.29162 hartrees
HOMO number	257
LUMO+1 energies	-1.56 eV
LUMO energies	-2.57 eV
HOMO energies	-5.39 eV
HOMO-1 energies	-5.94 eV
Geometry optimization specific results	
Converged nuclear repulsion energy	10779.04579 Hartrees

Table. Results concerning the calculated mono-electronic excitations

E.S.	Symmetry	nm	cm-1	f	R	Lambda	dCT	qCT	Excitation description in %
1	Singlet-A	521	19158	0.988	-0.635	0.82	0.14	0.42	257->258 (98)
2	Singlet-A	428	23318	0.000	0.651	0.45	0.68	0.80	256->258 (97)
3	Singlet-A	410	24378	0.136	-0.365	0.62	0.73	0.64	255->258 (96)
4	Singlet-A	374	26716	0.000	1.583	0.65	2.76	0.59	248->258 (2) 256->260 (2) 257->259 (91)
5	Singlet-A	357	27977	0.000	-0.004	0.38	4.81	0.73	244->258 (3) 246->258 (5) 248->258 (39) 250->258 (5) 252->258 (36) 257->259 (4)
6	Singlet-A	346	28873	0.292	-1.551	0.59	2.74	0.60	256->259 (5) 257->260 (86)
7	Singlet-A	340	29397	0.029	-0.118	0.39	0.49	0.66	236->258 (2) 237->258 (9) 241->258 (30) 243->258 (12) 245->258 (15) 247->258 (17) 257->260 (4)
8	Singlet-A	320	31194	0.237	-9.379	0.75	2.43	0.34	255->260 (12) 256->259 (75) 257->260 (5)
9	Singlet-A	320	31194	0.008	8.212	0.40	16.67	0.62	234->258 (4) 240->258 (4) 246->258 (5) 248->258 (22) 252->258 (7) 254->258 (40) 256->259 (2) 257->262 (3)
10	Singlet-A	316	31576	0.005	0.910	0.34	14.48	0.65	237->258 (3) 239->258 (2) 247->258 (6) 249->258 (15) 251->258 (5) 253->258 (50) 257->263 (6)
11	Singlet-A	316	31606	0.000	0.495	0.75	1.39	0.36	255->259 (53) 256->260 (29) 257->261 (11)
12	Singlet-A	313	31901	0.000	0.080	0.37	4.37	0.69	234->258 (2) 246->258 (17) 248->258 (18) 250->258 (9) 252->258 (33) 254->258 (9) 257->262 (3)
13	Singlet-A	312	31971	0.007	-0.043	0.25	2.42	0.84	247->258 (9) 249->258 (78) 253->258 (7)
14	Singlet-A	308	32461	0.000	0.134	0.62	2.66	0.38	246->258 (7) 254->258 (2) 255->259 (13) 257->261 (65)
15	Singlet-A	305	32749	0.051	-0.290	0.35	20.42	0.59	237->258 (6) 241->258 (6) 247->258 (26) 251->258 (27) 253->258 (14) 257->263 (9)

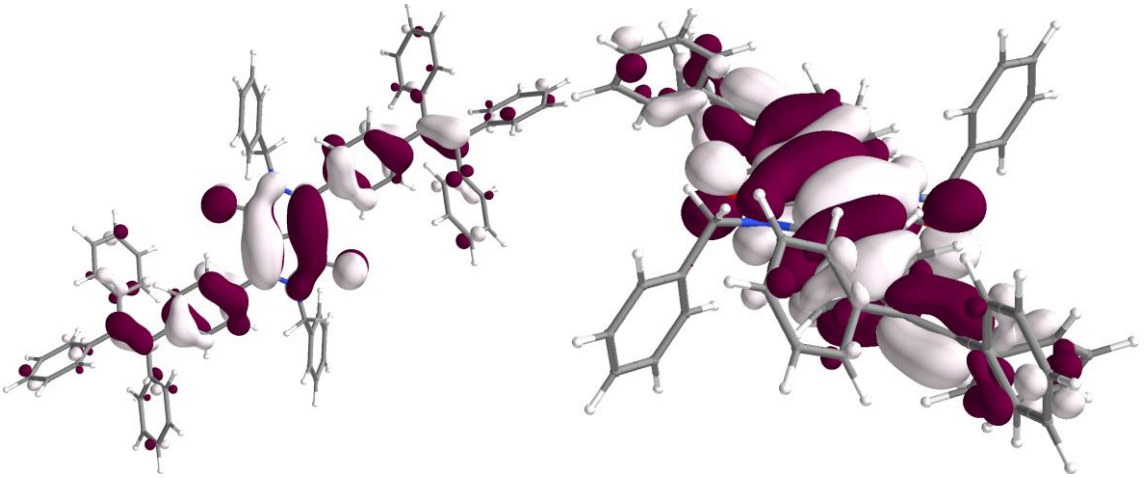


Fig. S38 Representation of the HOMO of **8** from two points of view.

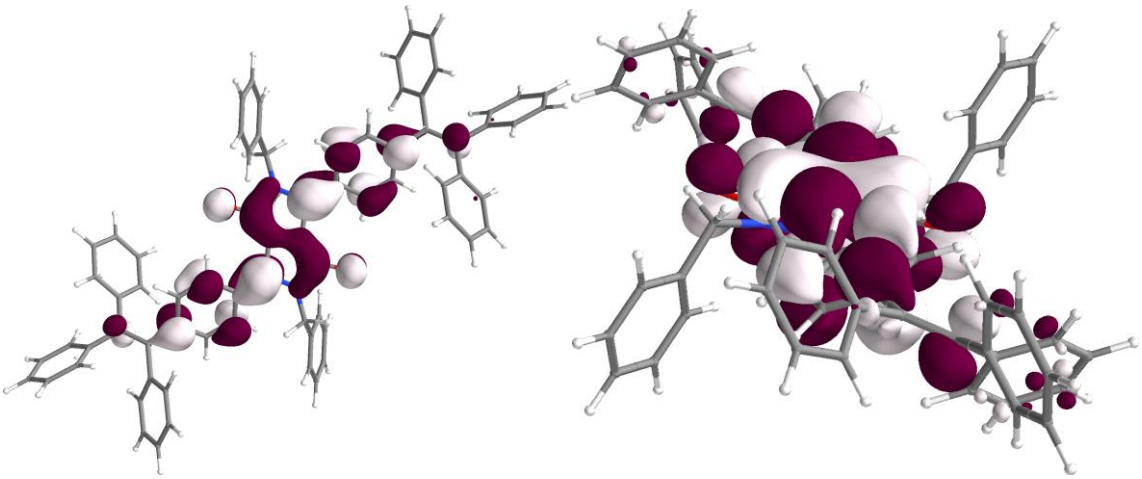


Fig. S39 Representation of the LUMO of **8** from two points of view.

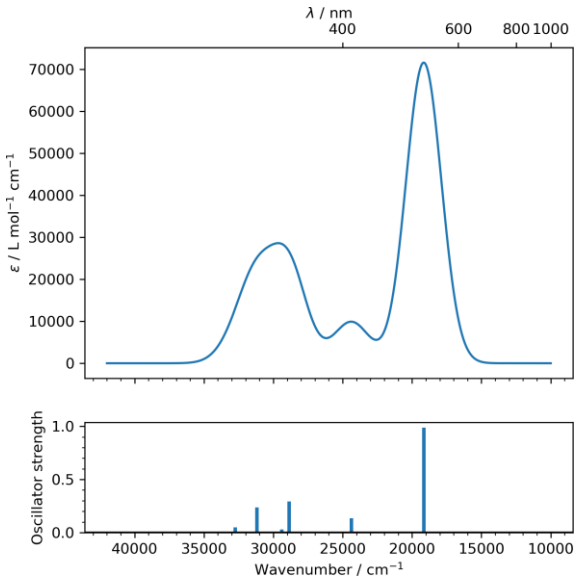


Fig. S40 Simulated UV-visible absorption spectrum for compound **8**, obtained with gaussian broadening (FWHM = 3000 cm^{-1}).

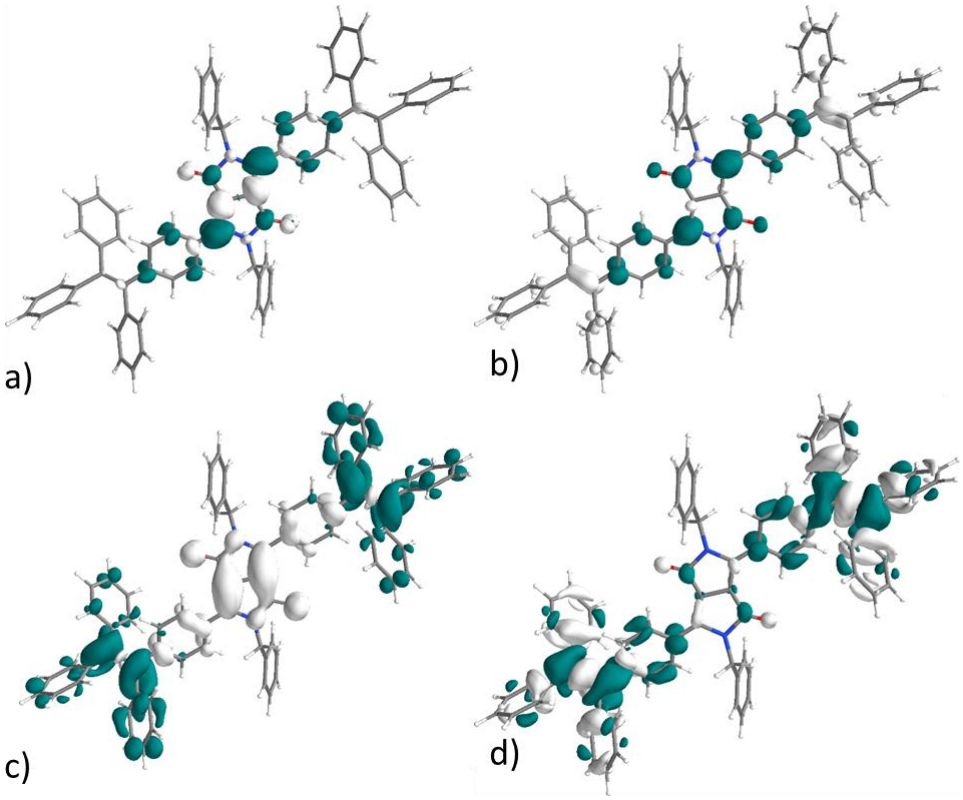
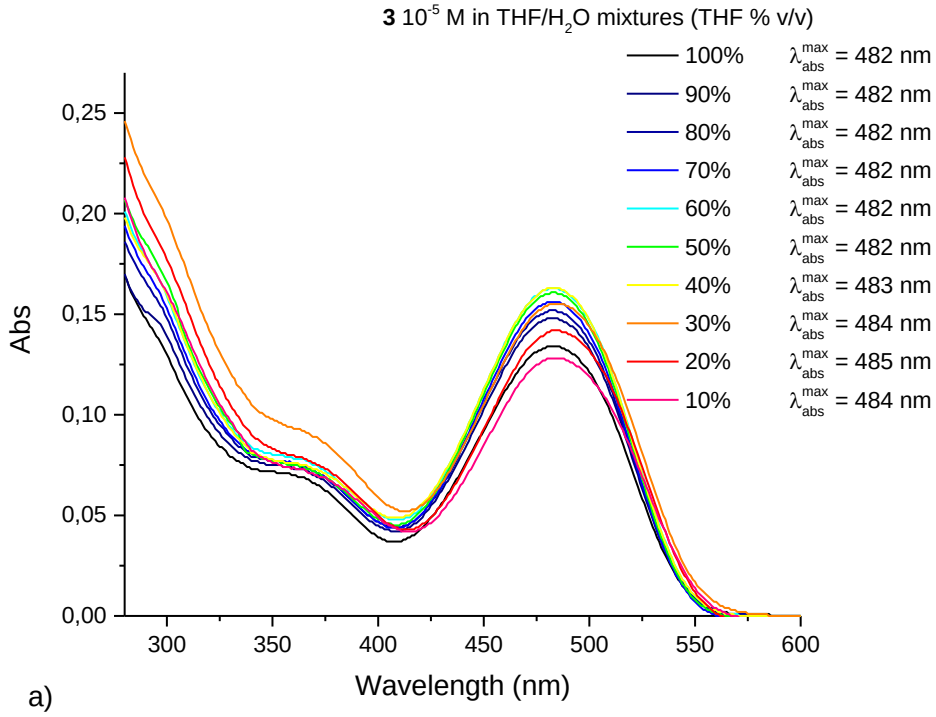


Fig. S41 Representation of the Electron Density Difference (EDD) associated to the strongest transitions calculated for the compound **8**: *a*) S0-S1; *b*) S0-S3; *c*) S0-S6; *d*) S0-S8; excited electrons and holes indicated by green and white surfaces, respectively.

UV-vis spectroscopy and CPL measurements



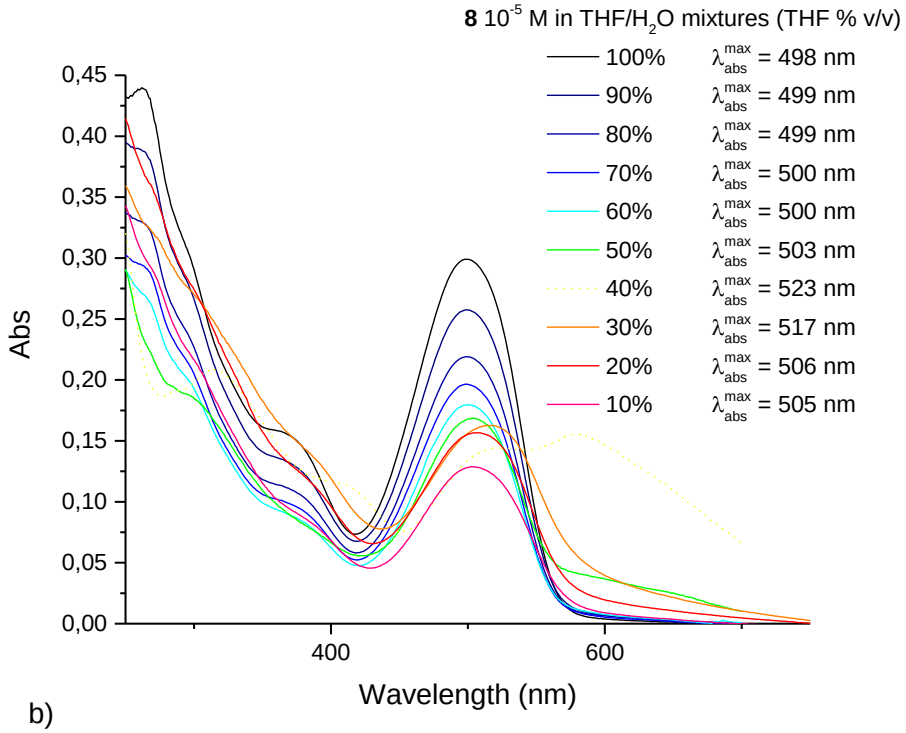


Fig. S42 UV-visible absorption spectra of compounds **3** and **8** in THF/water mixtures: a) absorption spectra of **3** in a series of THF/water mixtures, from 100% THF (black line) to 10% THF (red line), showing little solvatocromism; d) absorption spectra of **8** in a series of THF/water mixtures, from 100% THF (black line) to 10% THF (red line), showing important variations due to precipitation as water fraction increases; at 40% THF the measurements are heavily affected by scattering.

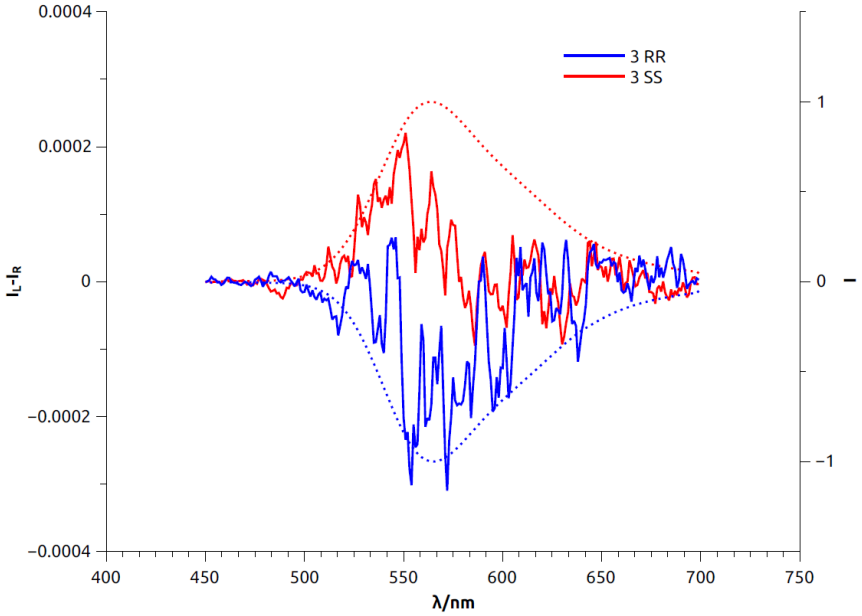


Fig. S43 CPL signal measured for compounds **3*RR*** (blue lines) and **3*SS*** (red lines) in $CHCl_3$ solution (10^{-6} M , λ_{exc} = 365 nm) where the emission traces (original and inverted one) are overlapped with CPL curves.