

SUPPORTING INFORMATION

Ethynelene-Analogues of Hemicurcuminoids: Synthesis and Ground- and Excited Properties of their Boron Difluoride Complexes

Bogdan Štefane,^{a,*} Franc Požgan,^a Eunsun Kim,^b Eunyoung Choi,^b Jean-Charles Ribierre,^b Jeong Weon Wu,^b Miguel Ponce-Vargas,^c Boris Le Guennic,^{c,*} Denis Jacquemin,^{d,e} Gabriel Canard,^f Elena Zaborova,^f Frédéric Fages,^{f,*} Anthony D’Aléo,^{f,*}

^a Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 114, SI-1000 Ljubljana, Slovenia; ^b Department of Physics, Quantum MetaMaterials Research Center, Ewha Womans University, Seoul, Korea; ^c Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1, 263 Avenue du Général Leclerc, 35042 Rennes Cedex, France; ^d Laboratoire CEISAM, UMR CNRS 6230, Université de Nantes, 2 Rue de la Houssinière, BP 92208, 44322 Nantes Cedex 3, France; ^e Institut Universitaire de France, rue Descartes, 75231 Paris Cedex 05, France; ^f Aix Marseille Univ, CNRS, CINaM UMR 7325, Campus de Luminy, Case 913, 13288 Marseille, France.

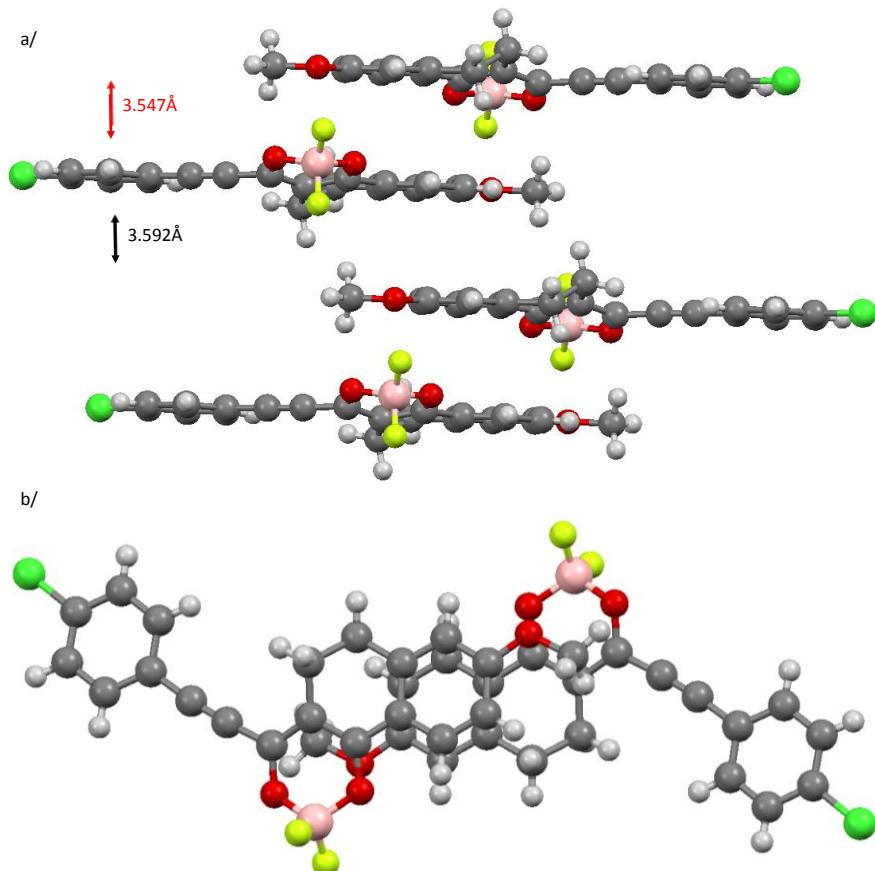


Figure S1. Molecular packing of **3** determined by single-crystal X-ray diffraction.

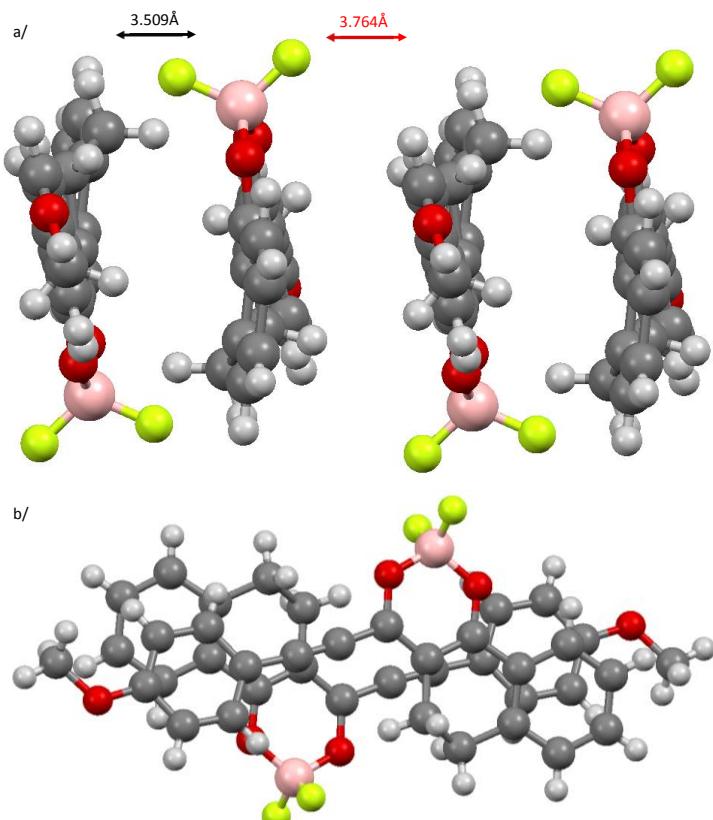


Figure S2. Molecular packing of **4** determined by single-crystal X-ray diffraction.

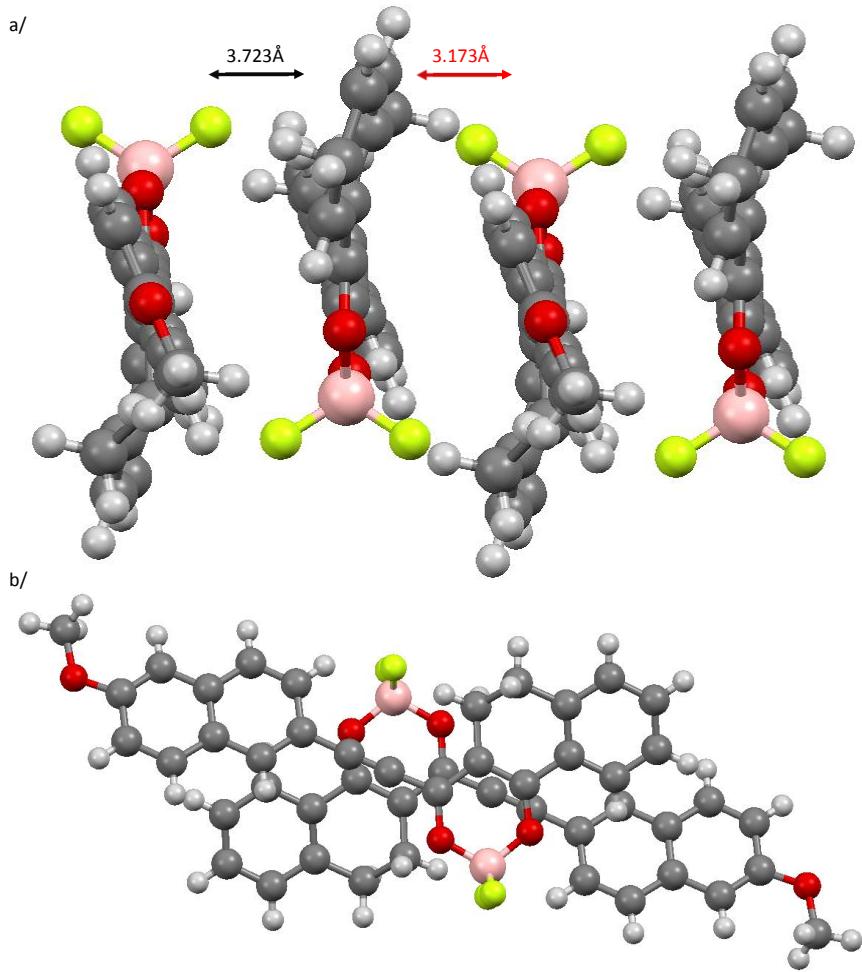


Figure S3. Molecular packing of **6** determined by single-crystal X-ray diffraction.

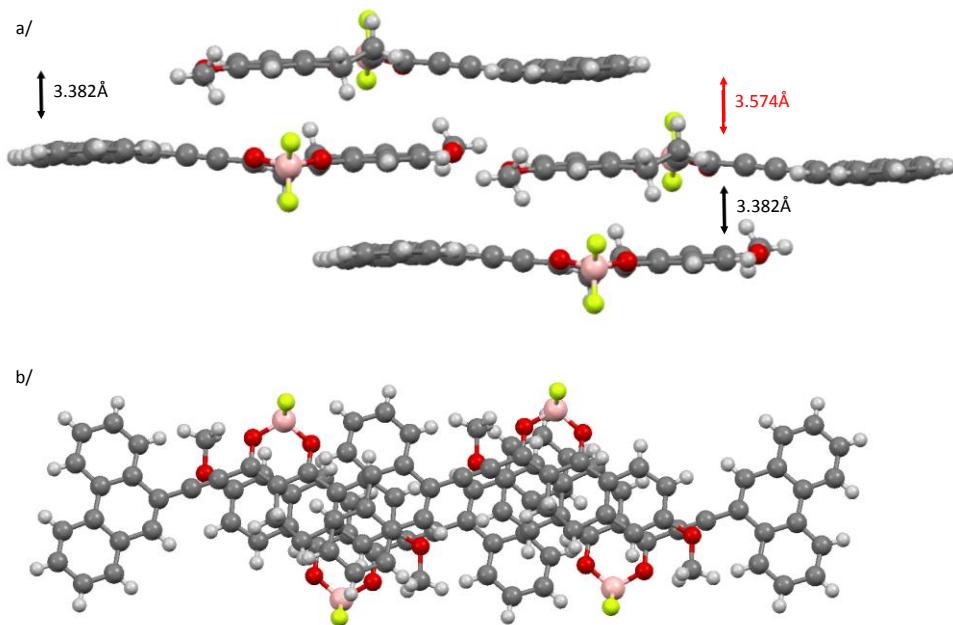


Figure S4. Molecular packing of **7** determined by single-crystal X-ray diffraction.

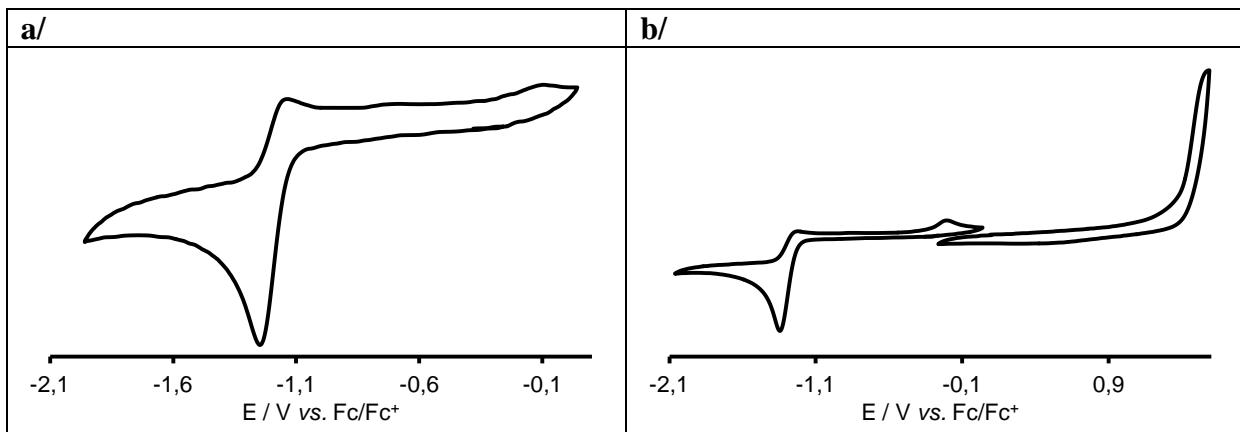


Figure S5. Cyclic voltammogram of the borondifluoride complex a/ **1** and b/ **2** in DCM solution containing 0.1M [$(^n\text{Bu}_4\text{N})\text{PF}_6$] (Scan rate of 100 mV/s).

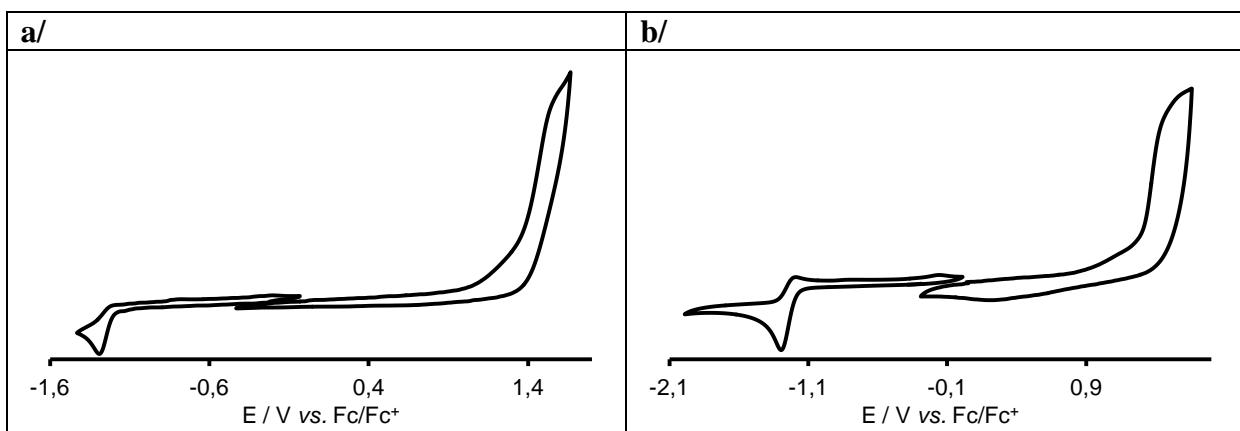


Figure S6. Cyclic voltammogram of the borondifluoride complex a/ **3** and b/ **4** in DCM solution containing 0.1M [$(^n\text{Bu}_4\text{N})\text{PF}_6$] (Scan rate of 100 mV/s).

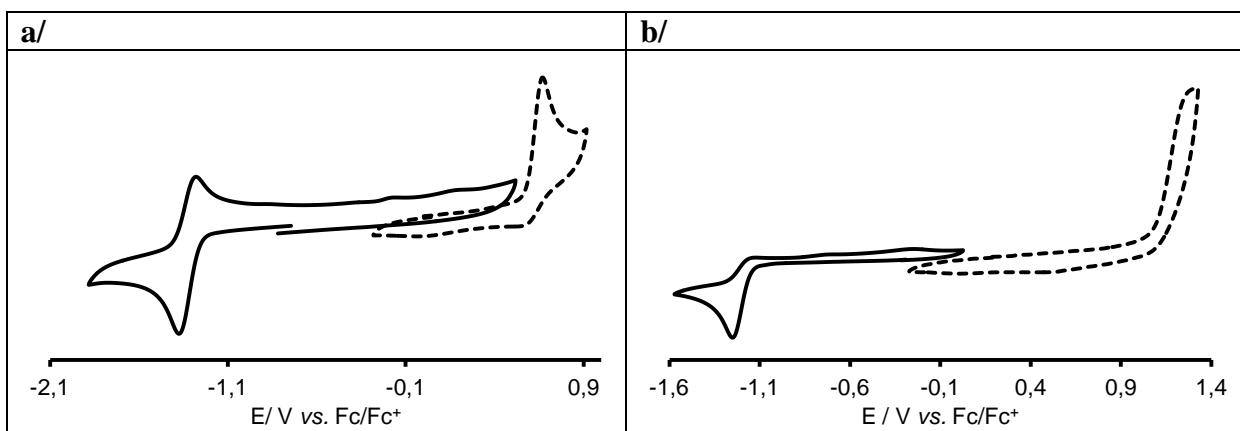


Figure S7. Cyclic voltammogram of the borondifluoride complex a/ **5** and b/ **6** in DCM solution containing 0.1M [$(^n\text{Bu}_4\text{N})\text{PF}_6$] (Scan rate of 100 mV/s).

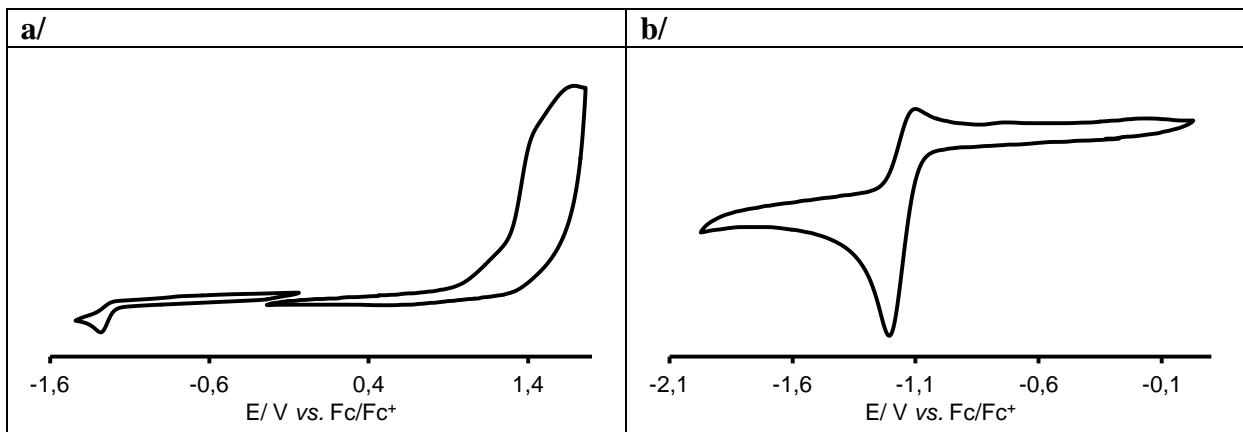


Figure S8. Cyclic voltammogram of the borondifluoride complex a/ **7** and b/ **M1** in DCM solution containing 0.1M [ⁿBu₄N]PF₆] (Scan rate of 100 mV/s).

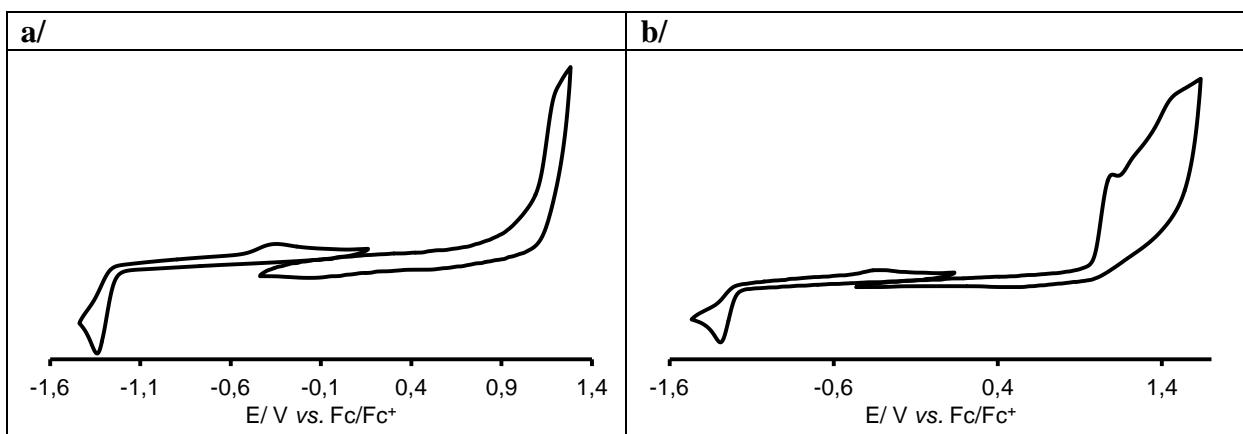


Figure S9. Cyclic voltammogram of the borondifluoride complex a/ **MC4** and b/ **MC6** in DCM solution containing 0.1M [ⁿBu₄N]PF₆] (Scan rate of 100 mV/s).

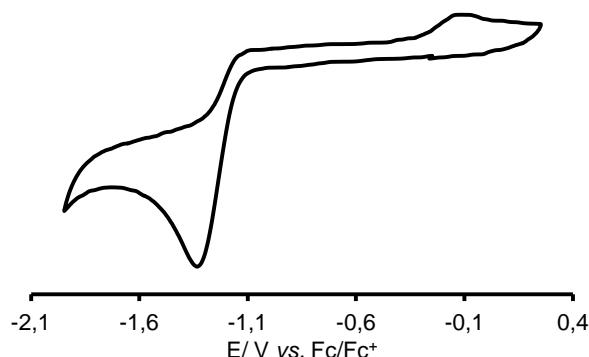


Figure S10. Cyclic voltammogram of the borondifluoride complex **M'1** in DCM solution containing 0.1M [ⁿBu₄N]PF₆] (Scan rate of 100 mV/s).

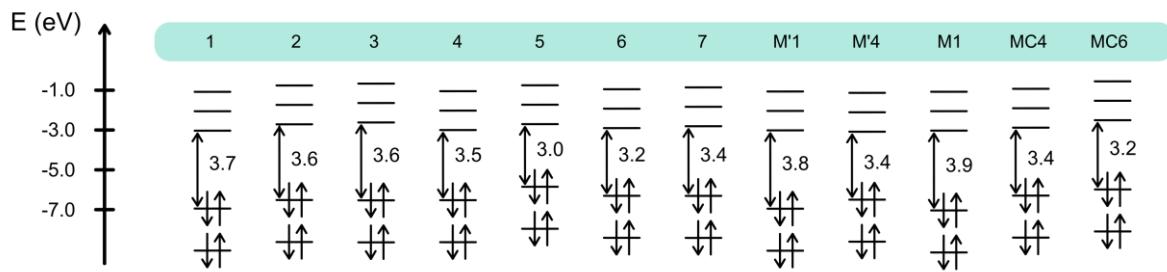


Figure S11. Calculated band gap energies for the studied systems (eV)

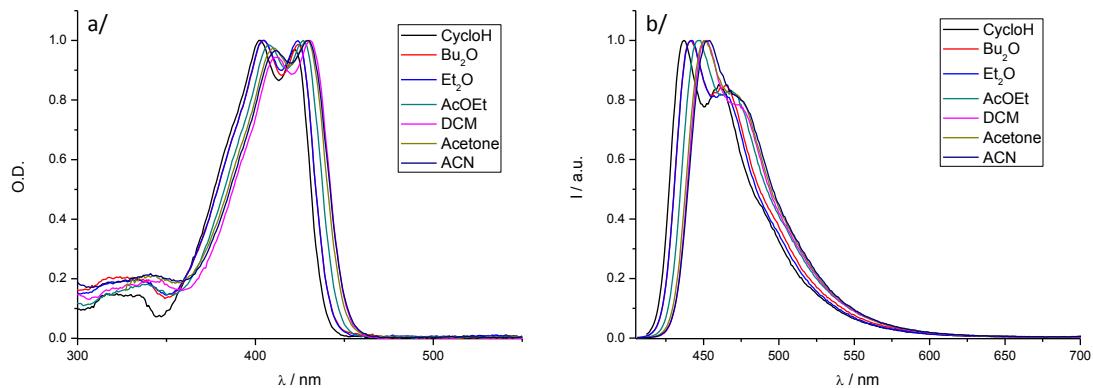


Figure S12. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **1** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

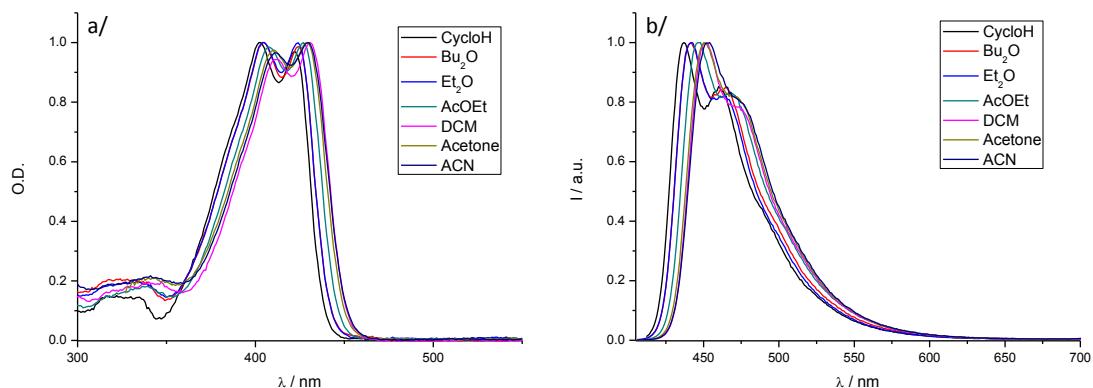


Figure S13. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **2** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

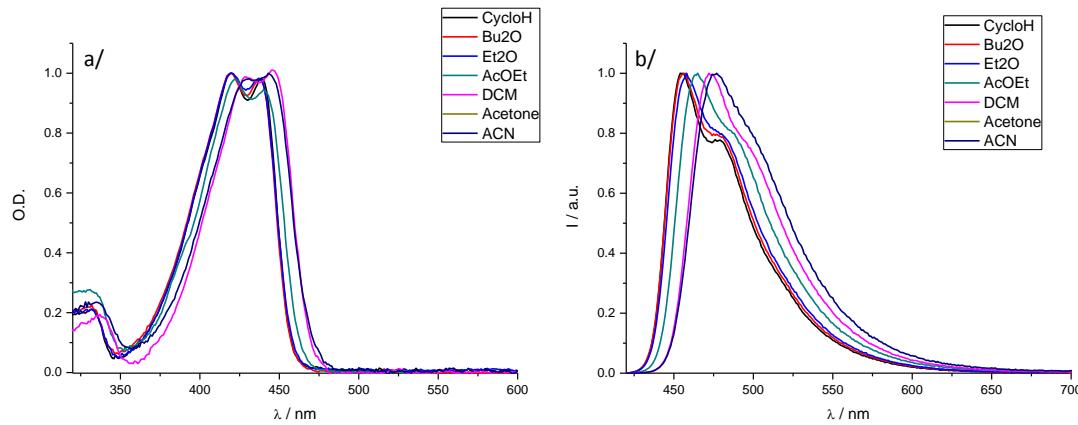


Figure S14. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **3** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

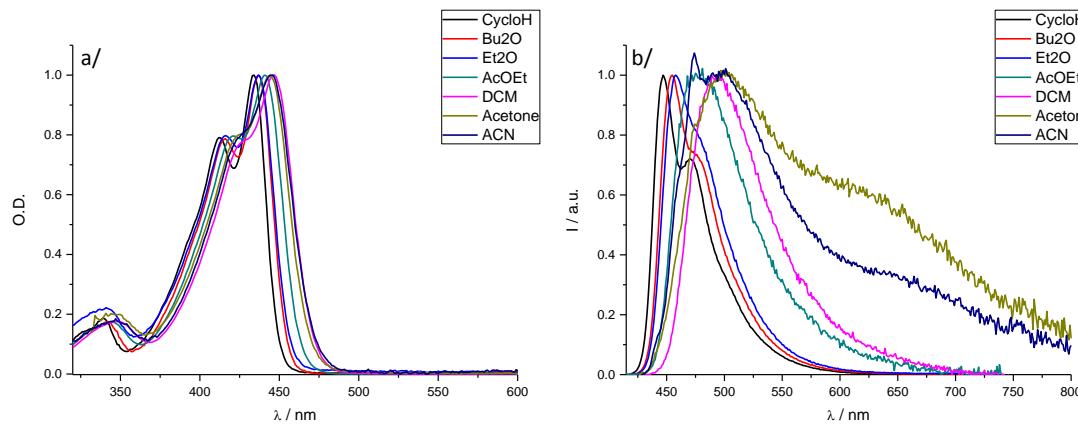


Figure S15. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **4** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

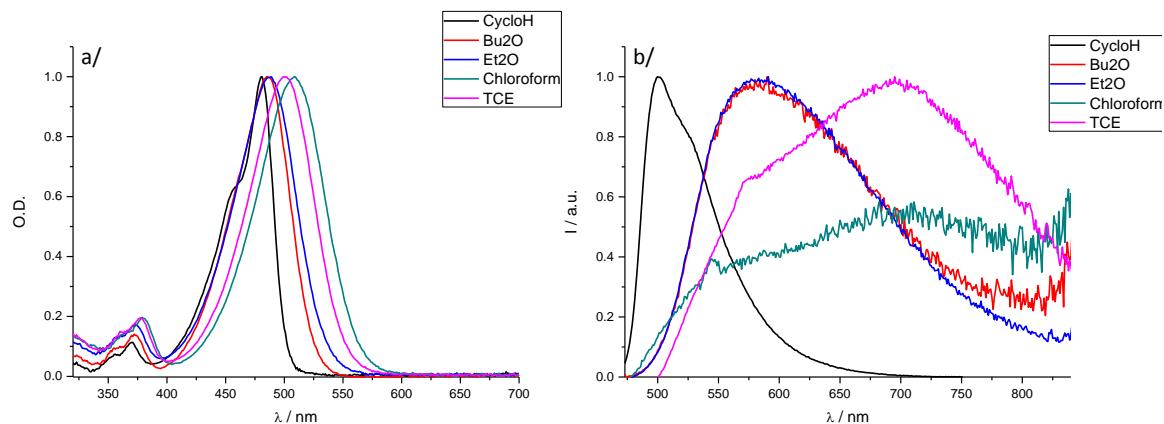


Figure S16. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **5** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; TCE: 1,1,1-Trichloroethane).

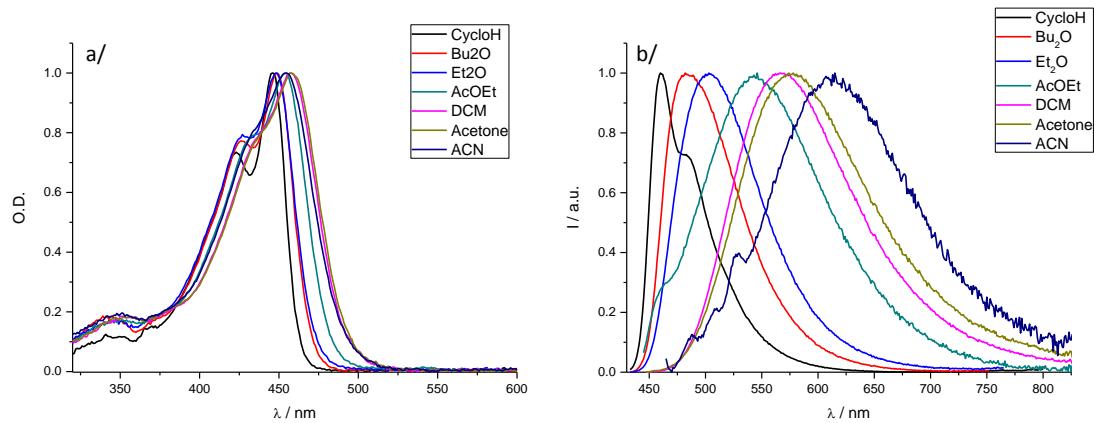


Figure S17. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **6** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

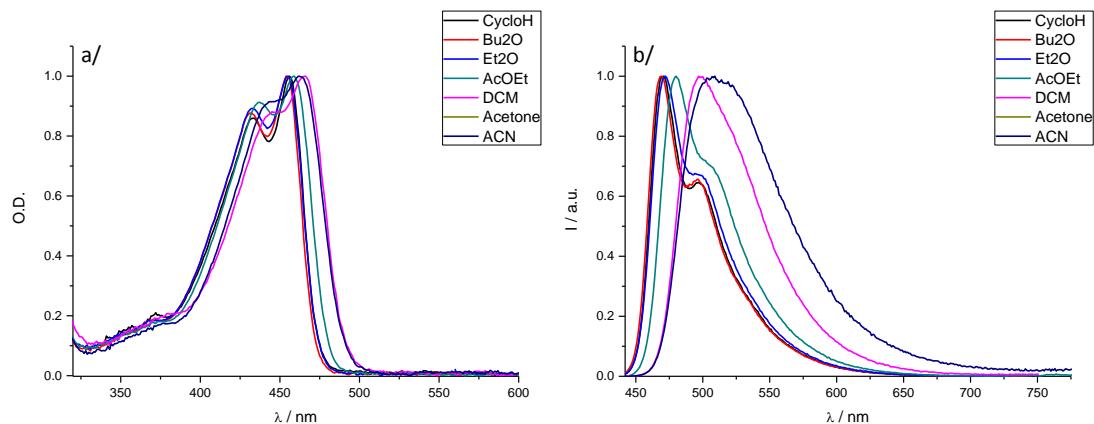


Figure S18. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **7** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

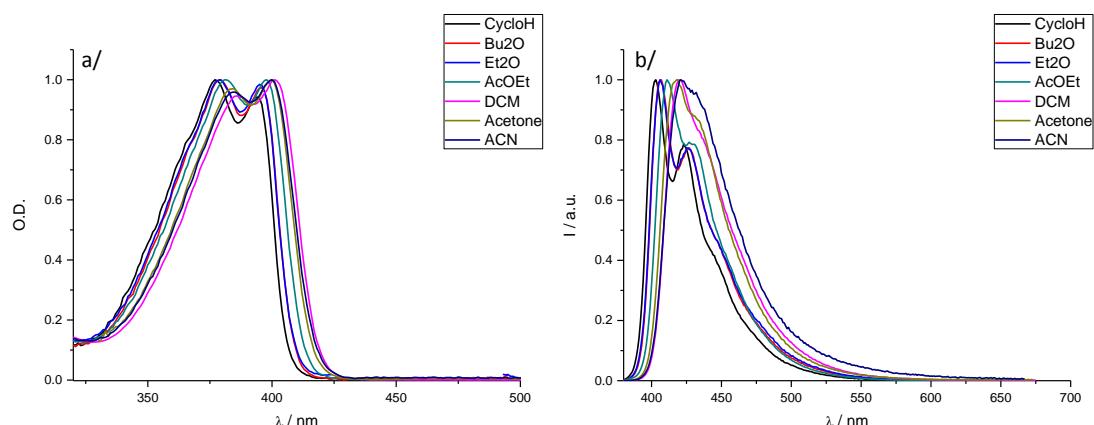


Figure S19. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **M1** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

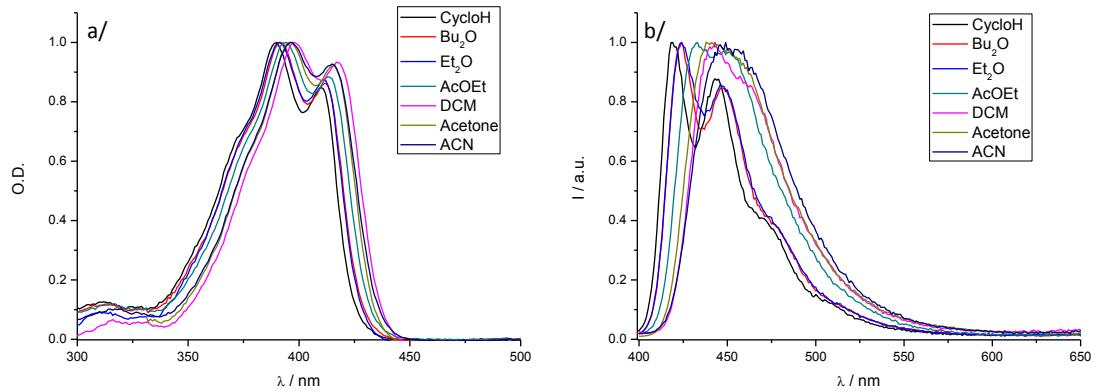


Figure S20. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **M'1** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

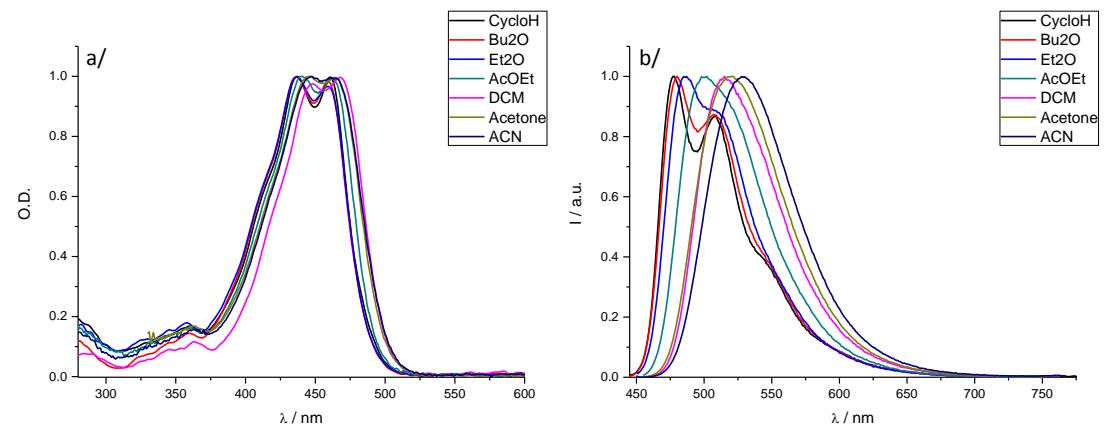


Figure S21. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **MC4** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

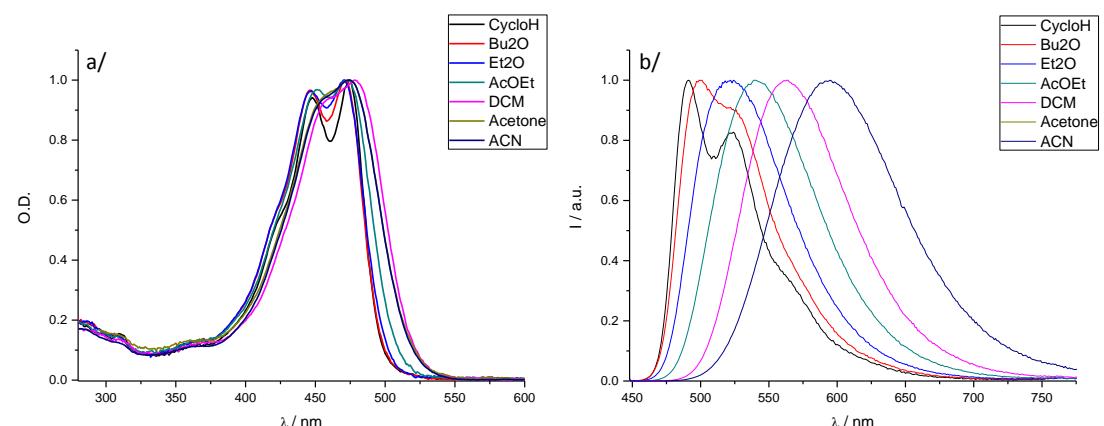


Figure S22. Solvatochromic shifts of the UV/visible absorption spectra (a) and emission spectra (b) of **MC6** in different solvent having different polarities. (CycloH: cyclohexane; Bu₂O: dibutylether; Et₂O: diethylether; AcOEt: ethylacetate; DCM: dichloromethane; ACN: acetonitrile).

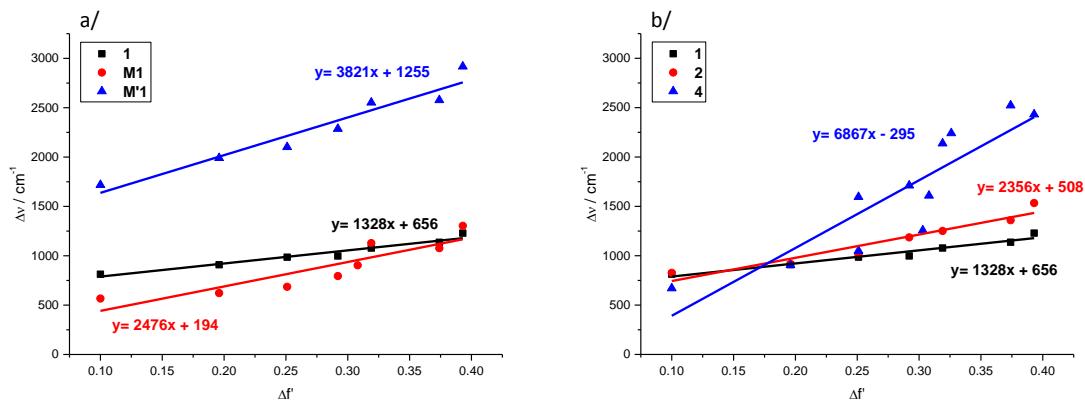


Figure S23. Stokes shifts of a/ **1** (■), **M1** (●) and **M'1** (▲) and b/ **1** (■), **2** (●) and **4** (▲) as a function of the Stokes shift of the solvent polarity $\Delta f'$ and their linear fit.

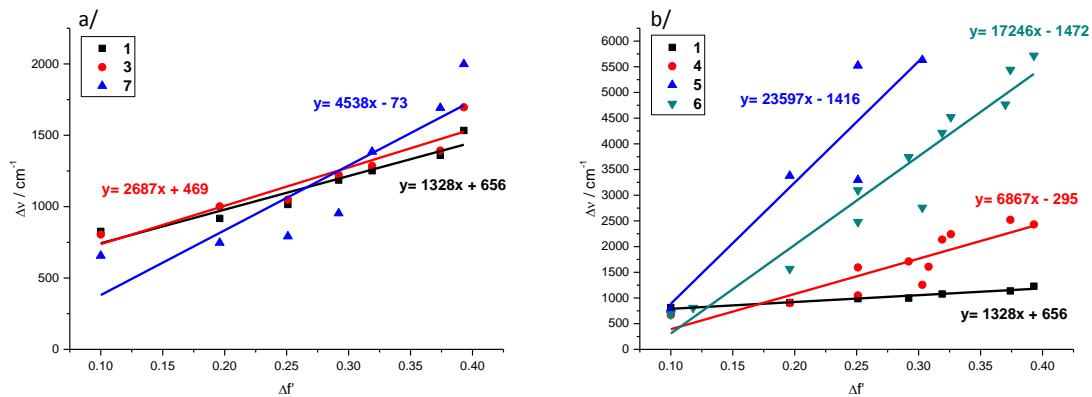


Figure S24. Stokes shifts of a/ **1** (■), **3** (●) and **7** (▲) and b/ **1** (■), **4** (●), **5** (▲) and **6** (▼) as a function of the Stokes shift of the solvent polarity $\Delta f'$ and their linear fit.

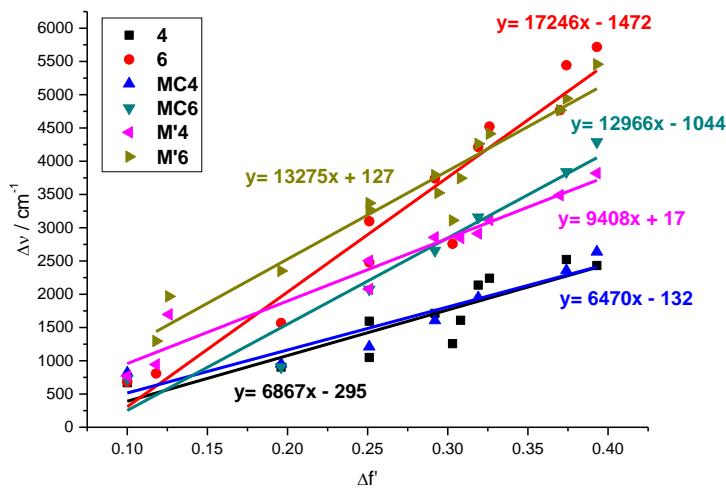


Figure S25. Stokes shifts of **4** (■), **6** (●), **MC4** (▲), **MC6** (▼), **M'4** (◀) and **M'6** (▶) as a function of the Stokes shift of the solvent polarity $\Delta f'$ and their linear fit.

Table S1. Selected crystal data for compounds **3**, **4**, **6** and **7**.

	3	4	6	7
Formula	C ₂₀ H ₁₄ BClF ₂ O ₃	C ₂₀ H ₁₅ BF ₂ O ₃	C ₂₄ H ₁₇ BF ₂ O ₃	C ₂₈ H ₁₉ BF ₂ O ₃
M _r / g/mol	386.57	352.13	402.18	452.24
Size / mm ³	0.40 × 0.18 × 0.08	0.22 × 0.12 × 0.04	0.50 × 0.15 × 0.04	0.38 × 0.25 × 0.05
Crystal System	triclinic	monoclinic	monoclinic	monoclinic
Space group	P -1	P 21/c	P 21/c	P 21/c
<i>a</i> / Å	7.3491(5)	7.8064(6)	6.9275(3)	11.6684(3)
<i>b</i> / Å	7.6278(5)	12.5650(10)	21.1323(8)	15.1963(4)
<i>c</i> / Å	17.5011(11)	17.6579(11)	12.7437(5)	12.2324(2)
α / deg	101.372(5)	90	90	90
β / deg	90.133(5)	98.492(7)	92.586(4)	91.415(2)
γ / deg	116.501(6)	90	90	90
<i>V</i> / Å ³	856.175	1713.03	1863.7	2168.35
<i>Z</i>	2	4	4	4
$\lambda(Mo/K\alpha)$ / Å	0.71073	0.71073	0.71073	0.71073
<i>T</i> / K	150	293	150	293
D _c / g.cm ⁻³	1.500	1.365	1.433	1.385
θ range / deg	3.0–27.5	2.8–30.4	2.9–27.5	2.2–27.5
<i>hkl</i> ranges	$h = -6 \rightarrow 9$ $k = -9 \rightarrow 9$ $l = -22 \rightarrow 22$	$h = -11 \rightarrow 8$ $k = -17 \rightarrow 14$ $l = -23 \rightarrow 24$	$h = -6 \rightarrow 8$ $k = -27 \rightarrow 24$ $l = -16 \rightarrow 15$	$h = -15 \rightarrow 15$ $k = -19 \rightarrow 19$ $l = -15 \rightarrow 15$
R _{int}	0.020	0.032	0.033	0.024
Refln measured	7477 (3935 independent reflections)	10579 (4518 independent reflections)	10646 (4257 independent reflections)	9665 (4932 independent reflections)
Refln <i>I</i> > 2σ(<i>I</i>)	2998	2332	3080	3407
R1 <i>I</i> > 2σ(<i>I</i>)	0.0432	0.0534	0.0465	0.0450
R1 all data	0.0609	0.1105	0.0678	0.0725
wR2 <i>I</i> > 2σ(<i>I</i>)	0.1002	0.1241	0.1101	0.1133
wR2 all data	0.1088	0.1559	0.1199	0.1320
Δρ (+/-) / e. Å ⁻³	0.64 / -0.49	0.15 / -0.18	0.22 / -0.24	0.20 / -0.24

Table S2. Selected bond lengths (Å) and angles (°) for compounds **3**, **4**, **6** and **7**.

	C1-C2 (endo)	C2-C12 (exo)	C1-O1	C12-O2	O1-B1	O2-B2	ψ
3	1.406	1.380	1.303	1.315	1.480	1.479	2.0°
4	1.394	1.379	1.301	1.313	1.479	1.475	20.1°
6	1.403	1.380	1.291	1.316	1.486	1.480	37.2°
7	1.408	1.377	1.301	1.316	1.489	1.476	3.8°

Table S3. Calculated electronic absorption data for the studied compounds.

		Calculated			
		λ_{\max}		<i>f</i>	Assignment (%)
		(nm)	(cm ⁻¹)		
1	I	404	24 752	1.051	HOMO→LUMO (98.85)
	II	335	29 851	0.149	HOMO-1→LUMO (89.09)
	III	307	32 573	0.097	HOMO-2→LUMO (88.34)
2	I	416	24 038	1.243	HOMO→LUMO (98.63)
	II	318	31 447	0.182	HOMO-2→LUMO (71.64)
	III	265	37 736	0.053	HOMO-1→LUMO (22.88) HOMO→LUMO+1 (94.72)
3	I	420	23 809	1.364	HOMO→LUMO (98.69)
	II	322	31 055	0.152	HOMO-2→LUMO (80.09)
	III	332	30 120	0.077	HOMO-1→LUMO (84.48)
4	I	426	23 474	1.272	HOMO→LUMO (97.63)
	II	265	37 736	0.157	HOMO→LUMO+1 (92.92)
	III	340	29 412	0.102	HOMO-1→LUMO (81.93) HOMO-2→LUMO (15.18)
5	I	486	20 576	1.351	HOMO→LUMO (97.78)
	II	290	34 483	0.228	HOMO→LUMO+1 (91.66)
	III	354	28 249	0.169	HOMO-1→LUMO (93.65)
6	I	465	21 505	1.239	HOMO→LUMO (97.22)
	II	375	26 667	0.256	HOMO-1→LUMO (95.13)
	III	269	37 175	0.151	HOMO-5→LUMO (82.15)
7	I	450	22 222	1.383	HOMO→LUMO (97.54)
	II	369	27 100	0.122	HOMO-2→LUMO (82.52)
	III	273	36 630	0.113	HOMO-1→LUMO+1 (50.81)
M'1	I	393	25 445	1.463	HOMO→LUMO (98.91)
	II	227	44 053	0.071	HOMO-5→LUMO (56.19)
	III	258	38 760	0.061	HOMO-6→LUMO (12.03) HOMO→LUMO+1 (90.79)
M'4	I	440	22 727	1.422	HOMO→LUMO (98.49)
	II	281	35 587	0.190	HOMO→LUMO+1 (94.84)
	III	338	29 586	0.116	HOMO-1→LUMO (95.96)
M1	I	382	26 178	1.316	HOMO→LUMO (98.61)
	II	303	33 003	0.134	HOMO-1→LUMO (81.69)
	III	249	40 161	0.092	HOMO→LUMO+1 (85.83)
MC4	I	439	22 779	1.459	HOMO→LUMO (98.43)
	II	279	35 842	0.106	HOMO→LUMO+1 (81.12)
	III	247	40 486	0.084	HOMO-4→LUMO (14.06) HOMO-5→LUMO (69.85)
MC6	I	473	21 142	1.492	HOMO→LUMO (98.01)
	II	379	26 385	0.225	HOMO-1→LUMO (93.95)
	III	262	38 168	0.126	HOMO-1→LUMO+1 (86.32)

Table S4. HOMO, LUMO and band gap energies (eV) for the studied systems.

	1	2	3	4	5	6	7	M'1	M'4	M1	MC4	MC6
LUMO	-3.1	-3.0	-3.0	-3.0	-2.9	-3.1	-3.0	-3.1	-3.1	-3.2	-2.9	-2.9
Band gap	3.7	3.6	3.6	3.5	3.0	3.2	3.4	3.8	3.4	3.9	3.4	3.2
HOMO	-6.9	-6.6	-6.6	-6.6	-5.9	-6.3	-6.3	-6.9	-6.4	-7.1	-6.3	-6.1

Table S5. Spectroscopic data and photophysical properties of compounds **1** and **2** in solvents of different polarity at room temperature^a

solvent	1							2						
	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}
CycloH	422	437	813	0.89	2.81	3.2	0.4	432	448	827	0.80	2.51	3.2	0.8
Bu ₂ O	424	441	909	0.83	2.97	2.8	0.6	434	452	918	0.82	2.62	3.1	0.7
Et ₂ O	424	442	960	0.86	3.01	2.9	0.5	434	454	1015	0.89	2.75	3.2	0.4
AcOEt	427	446	998	0.89	3.09	2.9	0.4	438	462	1186	0.975	2.74	3.6	0.1
DCM	431	452	1078	0.83	2.79	3.0	0.6	443	469	1251	0.80	2.61	3.1	0.8
Acetone	429	451	1137	0.79	3.07	2.6	0.7	440	468	1360	0.845	2.82	3.0	0.6
ACN	430	454	1229	0.795	3.19	2.5	0.6	441	473	1534	0.865	2.90	3.0	0.5

^a Absorption maximum wavelengths λ_{abs} (nm), fluorescence maximum wavelengths λ_{em} (nm), Stokes shifts $\Delta\nu_{ST}$ (cm^{-1}), fluorescence quantum yields Φ_f , fluorescence lifetimes τ_f (ns), radiative k_f (10^8 s^{-1}) and nonradiative $k_{\text{nr}} = (1 - \Phi_f)/\tau_f$ (10^8 s^{-1}) rate constants, oscillator strength $f = 4.32 \times 10^{-9} \int \epsilon(\nu)d\nu$; CycloH: cyclohexane, Et₂O: ethylic ether, AcOEt: ethyl acetate, DCM: dichloromethane, ACN: acetonitrile.

Table S6. Spectroscopic data and photophysical properties of compounds **3** and **4** in solvents of different polarity at room temperature^a

solvent	3							4						
	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}
CycloH	438	454	804	0.65	2.45	2.7	1.4	434	447	670	0.785	2.26	3.5	1.0
Bu ₂ O	437	457	1001	0.70	2.44	2.9	1.2	437	455	905	0.795	2.22	3.6	0.9
Et ₂ O	437	458	1049	0.71	2.47	2.9	1.2	437	458	1049	0.58	1.83	3.2	2.3
AcOEt	440	465	1222	0.75	2.61	2.9	1.0	441	477	1711	0.12	1.39	0.86	6.3
DCM	445	472	1285	0.72	2.53	2.8	1.1	446	493	2138	0.145	1.49	0.97	5.7
Acetone	442	471	1393	0.68	2.67	2.5	1.2	445	500	2472	0.01	n.d.	n.d.	n.d.
ACN	443	479	1697	0.665	2.61	2.5	1.3	445	498	2391	0.005	n.d.	n.d.	n.d.

^a Absorption maximum wavelengths λ_{abs} (nm), fluorescence maximum wavelengths λ_{em} (nm), Stokes shifts $\Delta\nu_{ST}$ (cm^{-1}), fluorescence quantum yields Φ_f , fluorescence lifetimes τ_f (ns), radiative k_f (10^8 s^{-1}) and nonradiative $k_{\text{nr}} = (1 - \Phi_f)/\tau_f$ (10^8 s^{-1}) rate constants, oscillator strength $f = 4.32 \times 10^{-9} \int \epsilon(\nu)d\nu$; Et₂O: ethylic ether, AcOEt: ethyl acetate, DCM: dichloromethane, ACN: acetonitrile.

Table S7. Spectroscopic data and photophysical properties of compounds **5** and **6** in solvents of different polarity at room temperature^a

solvent	5							6						
	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}
CycloH	481	501	830	0.285	1.11	2.6	6.4	446	460	682	0.32	0.91	4.3	6.7
Bu ₂ O	485	579	3347	0.01	n.d.	n.d.	n.d.	449	483	1568	0.47	1.32	3.6	4.0
Et ₂ O	489	586	3385	0.005	n.d.	n.d.	n.d.	448	504	2480	0.435	1.88	2.3	3.0
AcOEt	496	-	-	-	n.d.	n.d.	n.d.	452	544	3742	0.165	1.30	1.3	6.4
DCM	514	-	-	-	n.d.	n.d.	n.d.	457	566	4214	0.16	1.69	0.95	5.0
Acetone	508	-	-	-	n.d.	n.d.	n.d.	454	603	5443	0.01	n.d.	n.d.	n.d.
ACN	510	-	-	-	n.d.	n.d.	n.d.	455	615	5718	0.005	n.d.	n.d.	n.d.

^a Absorption maximum wavelengths λ_{abs} (nm), fluorescence maximum wavelengths λ_{em} (nm), Stokes shifts $\Delta\nu_{ST}$ (cm^{-1}), fluorescence quantum yields Φ_f , fluorescence lifetimes τ_f (ns), radiative k_f (10^8 s^{-1}) and nonradiative $k_{\text{nr}} = (1 - \Phi_f)/\tau_f$ (10^8 s^{-1}) rate constants, oscillator strength $f = 4.32 \times 10^9 \int \epsilon(\nu) d\nu$; Et₂O: ethylic ether, AcOEt: ethyl acetate, DCM: dichloromethane, ACN: acetonitrile.

Table S8. Spectroscopic data and photophysical properties of compounds **7** in solvents of different polarity at room temperature^a

solvent	7						
	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}
CycloH	455	469	656	0.37	1.11	3.3	5.7
Bu ₂ O	455	471	747	0.40	1.15	3.5	5.2
Et ₂ O	455	472	792	0.425	1.19	3.6	4.8
AcOEt	459	480	953	0.395	1.14	3.5	5.3
DCM	465	497	1385	0.425	1.33	3.2	4.3
Acetone	461	500	1692	0.40	1.43	2.9	4.3
ACN	462	509	1999	0.39	1.41	2.8	4.3

Table S9. Spectroscopic data and photophysical properties of compounds **M1** and **M'1** in solvents of different polarity at room temperature^a

solvent	M1							M'1						
	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}
CycloH	394	403	567	0.22	0.65	3.4	12.0	390	418	1718	0.025	0.13	1.9	75.0
Et ₂ O	395	406	685	0.145	0.53	2.7	16.1	391	426	2101	0.025	0.11	2.3	88.6
AcOEt	398	411	795	0.33	0.73	4.5	9.2	394	433	2286	0.03	0.12	2.5	80.8
DCM	401	420	1128	0.43	0.94	4.6	6.1	398	443	2552	0.02	0.10	2.0	98.0
Acetone	399	419	1196	0.275	0.85	3.2	8.5	396	441	2577	0.02	0.09	2.2	108.9
ACN	400	422	1303	0.16	0.92	1.7	9.1	397	449	2917	0.02	0.10	2.0	98.0

^a Absorption maximum wavelengths λ_{abs} (nm), fluorescence maximum wavelengths λ_{em} (nm), Stokes shifts $\Delta\nu_{ST}$ (cm^{-1}), fluorescence quantum yields Φ_f , fluorescence lifetimes τ_f (ns), radiative k_f (10^8 s^{-1}) and nonradiative $k_{\text{nr}} = (1 - \Phi_f)/\tau_f$ (10^8 s^{-1}) rate constants, oscillator strength $f = 4.32 \times 10^9 \int \epsilon(\nu) d\nu$; Et₂O: ethylic ether, AcOEt: ethyl acetate, DCM: dichloromethane, ACN: acetonitrile.

Table S10. Spectroscopic data and photophysical properties of compounds **MC4** and **MC6** in solvents of different polarity at room temperature^a

solvent	MC4							MC6						
	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}	λ_{abs}	λ_{em}	$\Delta\nu_{ST}$	Φ_f	τ_f	k_f	k_{nr}
CycloH	460	478	819	0.025	0.14	1.8	69.6	461	477	728	0.05	0.97	0.5	9.8
Bu ₂ O	459	480	953	0.03	0.16	1.0	60.6	460	480	906	0.10	1.00	1.0	9.0
Et ₂ O	459	486	1210	0.035	0.17	2.1	56.8	471	522	2074	0.135	1.03	1.3	8.4
AcOEt	462	499	1605	0.045	0.22	2.0	43.4	473	541	2657	0.25	1.28	2.0	5.9
DCM	468	515	1950	0.04	0.24	1.6	38.4	478	563	3159	0.33	1.60	2.1	4.2
Acetone	464	521	2358	0.065	0.35	1.9	26.7	473	578	3841	0.46	2.21	2.1	2.4
ACN	465	530	2637	0.085	0.40	2.0	23.0	474	595	4290	0.485	2.19	2.2	2.4

^a Absorption maximum wavelengths λ_{abs} (nm), fluorescence maximum wavelengths λ_{em} (nm), Stokes shifts $\Delta\nu_{ST}$ (cm^{-1}), fluorescence quantum yields Φ_f , fluorescence lifetimes τ_f (ns), radiative k_f (10^8 s^{-1}) and nonradiative $k_{\text{nr}} = (1 - \Phi_f)/\tau_f$ (10^8 s^{-1}) rate constants, oscillator strength $f = 4.32 \times 10^{-9} \int \epsilon(\nu) d\nu$; Et₂O: ethylic ether, AcOEt: ethyl acetate, DCM: dichloromethane, ACN: acetonitrile.