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

XPS and quantum chemical analysis of 4Me-BODIPY derivatives

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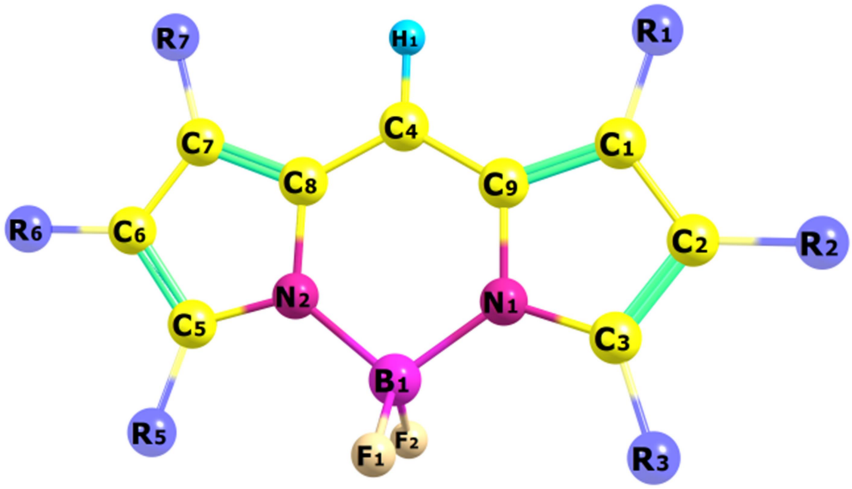
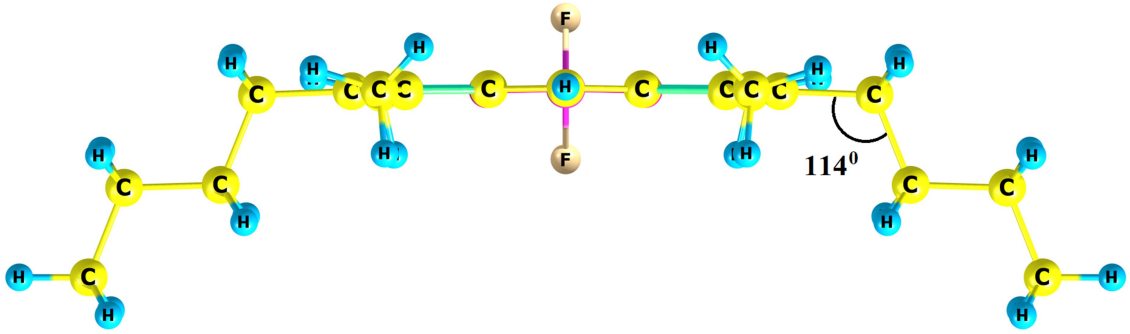


Fig. S1. Chemical structure of compounds II-V**.**

IV



V

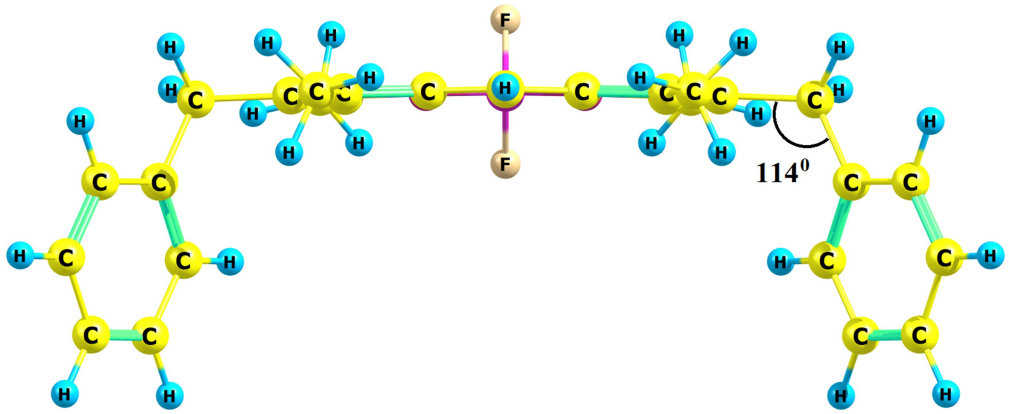


Fig. S2. Chemical structure of compounds IV and V**.**

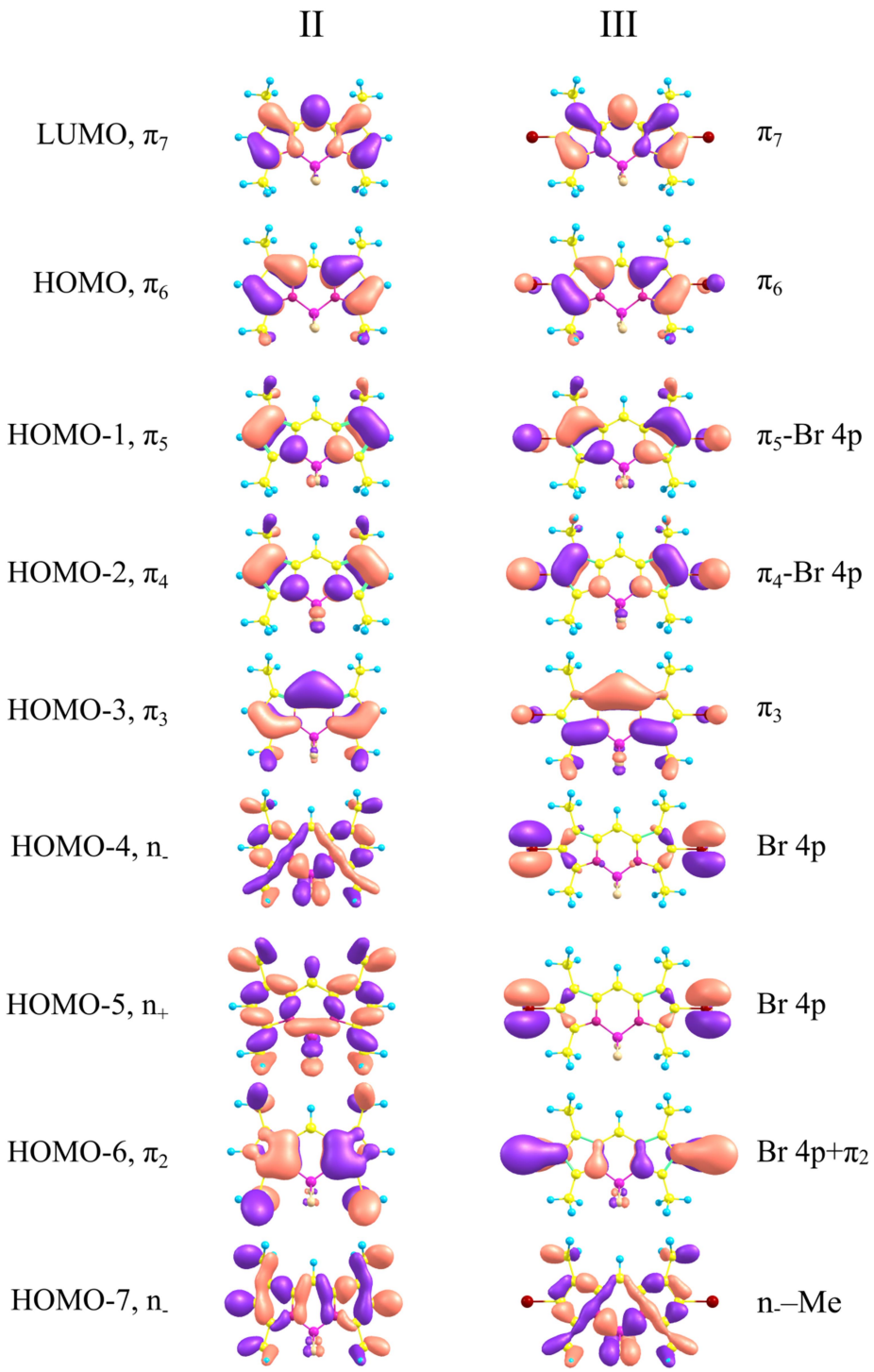


Fig. S3. Molecular orbitals of compounds II and III.

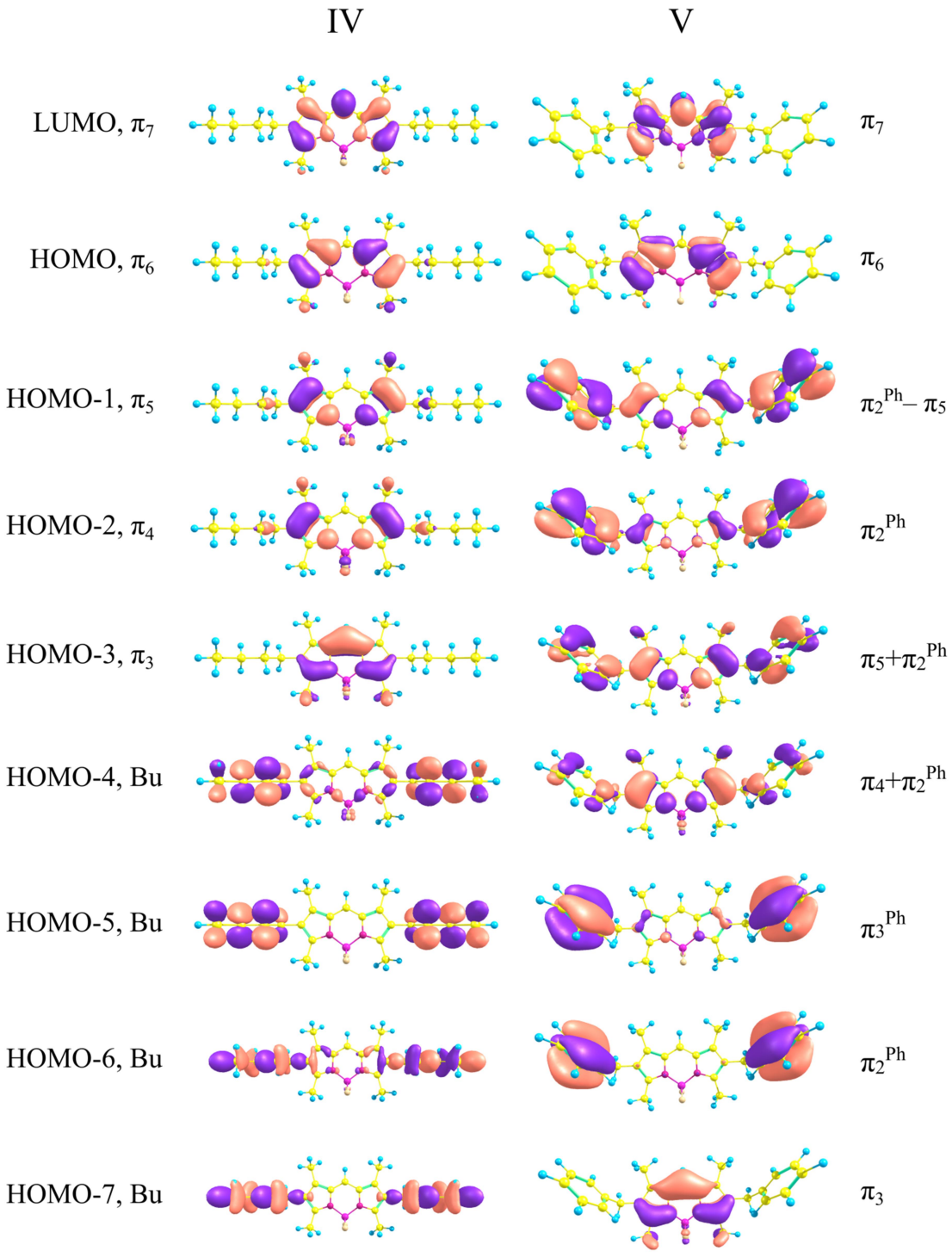


Fig. S4. Molecular orbitals of compounds IV and V.

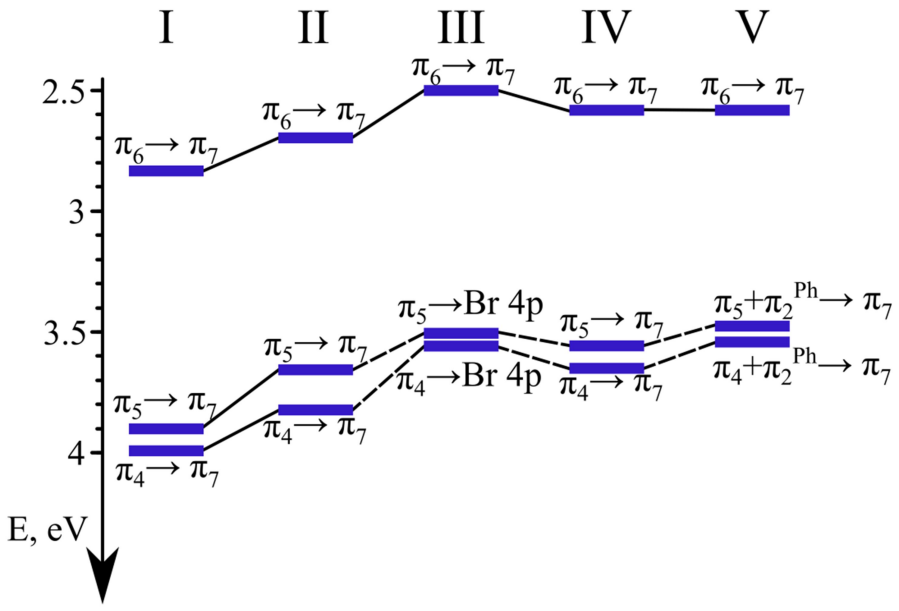


Fig. S5. Correlation diagram of excited states of compounds I–V**.**

Table S1

Vertical ionization energies I_n (eV) and pole strengths f (a.u.) of the BODIPY core outer valence MOs computed at OVGF level of theory using different basis sets. The vertical electron attachment energy and the corresponding pole strength for the lowest unoccupied MO, $7b_1$ (π_7*), is also included.

Molecular orbital	cc-pVDZ		aug-cc-pVDZ		cc-pVTZ	
	I_n	f	I_n	f	I_n	f
L, π_7 ($7b_1$)	0.92	0.89	1.27	0.89	1.20	0.89
H, π_6 ($4a_2$)	7.62	0.88	7.83	0.88	7.84	0.88
H–1, π_5 ($3a_2$)	9.20	0.86	9.40	0.85	9.42	0.85
H–2, π_4 ($6b_1$)	9.40	0.85	9.61	0.84	9.62	0.84
H–3, π_3 ($5b_1$)	10.32	0.81	10.51	0.80	10.51	0.80
H–4, n_- ($11b_2$)	12.15	0.89	12.45	0.88	12.42	0.88
H–5, n_+ ($14a_1$)	12.96	0.88	13.22	0.87	13.20	0.87
H–7, π_2 ($2a_2$)	13.22	0.80	13.48	0.77	13.49	0.78
H–6, n_- ($10b_2$)	13.31	0.87	13.49	0.87	13.45	0.87

Table S2
Energies E (eV) and oscillator strength *f* (a.u.) of vertical singlet excitations of the BODIPY I, calculated using ADC(2) and different basis sets.

Excitation	cc-pVDZ		aug-cc-pVDZ		cc-pVTZ	
	E	*f*	E	*f*	E	*f*
1^1B_2	2.83	0.50	2.76	0.50	2.77	0.49
2^1B_2	3.85	0.23	3.77	0.21	3.78	0.21
2^1A_1	3.95	0.04	3.88	0.04	3.89	0.04
3^1A_1	5.41	0.07	5.31	0.06	5.30	0.07

Table S3
Energies (eV) of vertical singlet excitations of the BODIPY I obtained at the ADC(2)/cc-pVDZ level in the gas phase and considering solvation within different solvents using SS(V)PE continuum solvation model compared with experiment [81].

Excitation	Gas phase	Chloroform	Cyclohexane	THF	Ethanol	H_2O	H_2O[a]	DMSO	DMSO[a]
$1\,^1B_{2\,expl}$		2.46[81]	2.46[81]	2.48[81]	2.49[81]				
$1\,^1B_2$	2,83	2.83	2,84	2,86	2,87	2,87	2,84	2,87	2,84
$2\,^1B_2$	3,85	3.89	3,89	3,92	3,94	3,94	3,88	3,94	3,89
$2\,^1A_1$	3,95	3.99	4,00	4,04	4,06	4,06	4,01	4,06	4,01
$3\,^1A_1$	5,41	5.42	5,42	5,44	5,44	5,44	5,40	5,44	5,41

[a] calculations with geometrical parameters pre-optimized accounting for solvation effects at the SS(V)PE level.

Table S4
Geometric parameters of compounds I-V in the S_0 ground state [a] and S_1 excited state [b].

Compound	Chemical bond, Å													
	F_1-B_1		B_1-N_1		N_1-C_9		C_9-C_4		C_1-R_1		C_3-R_3		C_2-R_2	
	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1
I	1.38	1.38	1.58	1.54	1.39	1.41	1.40	1.38	1.09	1.09	1.09	1.09	1.09	1.09
II	1.39	1.40	1.57	1.56	1.40	1.41	1.39	1.41	1.50	1.50	1.49	1.50	1.09	1.09
III	1.39	1.40	1.57	1.56	1.39	1.41	1.39	1.41	1.50	1.49	1.49	1.49	1.89	1.87
IV	1.39	1.39	1.57	1.57	1.39	1.39	1.39	1.39	1.50	1.50	1.50	1.50	1.50	1.50
V	1.39	1.40	1.57	1.55	1.39	1.42	1.39	1.41	1.50	1.50	1.50	1.49	1.51	1.50

[a] The equilibrium S_0 geometry was computed using DFT/CAM-B3LYP/Def2-SVP approach.
[b] The equilibrium S_1 geometry was computed using TD-DFT/CAM-B3LYP/Def2-SVP approach.

Table S5
Relative photoionization cross sections σ [86] for the radiation source MgKα (hν = 1253.6 eV).

Atom	2p	2s
C	1.0	66.0
N	7.2	110.0
F	68.0	280.0
B	0.2	28.0
	4p	-
Br	450.0	-
	-	1s
H	-	0.2

Table S6
Localization (Mulliken populations according to the CAM-B3LYP method) and calculated energies of some lower valence MOs of the compound II which correspond to maxima 2-5 in the X-ray photoelectron spectra.

Peak.	MO	$-\varepsilon_i$ eV	Localization (%)			
			C 2s/2p	N 2s/2p	F 2s/2p	Br 4s/4p
2	67, $11a_1$	15.88	5/48	1/2	2/26	0/2
	66, $8b_1$	16.08	11/38	1/16	0/5	6/11
	65, $7b_1$	16.99	12/49	1/24	0/1	1/1
2’	64, $6b_1$	17.69	23/52	2/5	0/2	0/1
	63, $10a_1$	17.78	13/40	1/19	2/8	0/0
	62, $9a_1$	18.17	20/29	0/20	1/5	9/5
	61, $8a_1$	19.21	40/23	0/13	0/0	0/0
3	60, $5b_1$	20.67	45/28	0/7	0/0	3/0
	59, $4b_1$	21.63	34/28	6/2	0/0	10/0
	58, $7a_1$	21.84	37/26	4/5	0/1	5/0
	57, $6a_1$	22.55	52/20	4/1	0/0	2/0
	56, $3b_1$	22.76	43/14	4/4	0/0	20/0
	55, $5a_1$	23.44	27/17	1/3	0/0	45/0
	54, $3b_1$	24.09	56/12	0/4	0/0	19/0
	53, $4a_1$	25.01	71/7	6/6	0/0	1/0
	52, $2b_1$	25.12	41/7	10/0	0/0	35/2
	51, $3a_1$	25.36	50/7	5/3	0/0	29/2
4	50, $1b_1$	29.29	42/5	45/4	0/0	0/0
	49, $2a_1$	29.71	39/7	47/3	1/0	0/0
5	48, $1b_2$	33.06	0/0	0/0	88/1	0/0
	47, $1a_1$	33.99	0/1	1/1	85/2	0/0

Table S7

Localization (Mulliken populations according to the CAM-B3LYP method) and calculated energies of some lower valence MOs of the compound III which correspond to maxima 2-5 in the X-ray photoelectron spectra.

Peak.	MO	$-\varepsilon_i$ eV	Localization (%)		
			C 2s/2p	N 2s/2p	F 2s/2p
2’	36 $8b_1$	16.21	7/51	0/15	0/4
	35 $7b_1$	16.91	18/39	3/21	0/0
	34 $6b_1$	17.06	25/50	2/6	0/3
	33 $9a_1$	17.35	13/34	1/20	2/11
2	32 $8a_1$	18.50	18/33	1/23	1/3
	31 $7a_1$	18.81	43/25	0/8	0/0
3	30 $5b_1$	20.38	46/28	2/6	0/0
	29 $4b_1$	21.51	44/27	3/2	0/0
	28 $6a_1$	21.60	44/24	3/4	0/0
	27 $5a_1$	22.23	54/21	4/0	0/0
	26 $3b_1$	22.93	61/12	6/6	0/0
	25 $2b_1$	24.07	65/14	9/1	0/0
	24 $4a_1$	24.16	62/16	9/3	0/0
	23 $3a_1$	24.60	74/7	3/8	0/0
4	22 $1b_1$	28.76	41/6	46/4	0/0
	21 $2a_1$	29.21	38/7	48/2	0/0
5	20 $1b_2$	32.69	0/0	0/0	88/1
	19 $1a_1$	33.63	0/0	1/1	85/2

Table S8
Localization (Mulliken populations according to the CAM-B3LYP method) and calculated energies of some lower valence MOs of the compound IV which correspond to maxima 2-5 in the X-ray photoelectron spectra.

Peak.	MO	$-\varepsilon_i$ eV	Localization (%)		
			C 2s/2p	N 2s/2p	F 2s/2p
2’	52, 14a_1	15.58	4/54	0/2	1/17
	51, 10b_1	16.46	11/52	1/22	0/1
	50, 9b_1	17.11	22/53	2/5	0/2
	49, 13a_1	17.18	16/55	0/10	0/1
	48, 12a_1	17.35	16/21	1/22	2/13
	47, 8b_1	17.83	28/29	0/0	0/0
	46, 11a_1	17.89	30/27	0/2	0/0
2	45, 10a_1	18.67	39/22	0/15	0/0
	44, 7b_1	19.26	42/24	1/4	0/0
	43, 9a_1	19.71	42/25	1/4	0/1
	42, 6b_1	20.29	46/26	1/6	0/0
3	41, 5b_1	21.18	43/26	5/1	0/0
	40, 8a_1	21.37	40/24	4/4	0/1
	39, 4b_1	22.04	52/20	1/2	0/0
	38, 7a_1	22.05	53/20	2/1	0/0
	37, 6a_1	22.29	59/20	1/0	0/0
	36, 3b_1	23.07	67/11	3/4	0/0
	35, 5a_1	23.72	66/14	2/2	0/0
	34, 2b_1	23.80	67/12	3/1	0/0
	33, 4a_1	24.45	71/6	7/6	0/0
	32, 1b_1	24.46	71/8	7/0	00
	31, 3a_1	24.65	75/8	3/4	0/0
4	30, 1b_1	28.65	41/6	46/4	0/0
	29, 2a_1	29.10	38/7	48/2	0/0
5	28, 1b_2	32.62	0/0	0/0	88/1
	27, 1a_1	33.56	0/0	1/1	85/2

Table S9
Localization (Mulliken populations according to the CAM-B3LYP method) and calculated energies of some lower valence MOs of the compound V which correspond to maxima 2-5 in the X-ray photoelectron spectra.

Peak.	MO	$-\varepsilon_i$ eV	Localization (%)		
			C 2s/2p	N 2s/2p	F 2s/2p
2	61, $13b_1$	16.56	11/52	1/22	0/1
	60, $12b_1$	17.18	23/52	2/4	0/2
	59, $15a_1$	17.23	17/55	0/9	0/1
	58, $14a_1$	17.42	17/26	1/20	2/12
	57, $11b_1$	18.01	33/47	0/1	0/0
	56, $13a_1$	18.28	31/46	0/7	0/1
	55, $10b_1$	18.53	35/44	0/0	0/0
	54, $12a_1$	18.55	34/43	0/2	0/0
	53, $11a_1$	18.78	42/24	0/12	0/0
3	52, $9b_1$	20.13	46/31	0/7	0/0
	51, $8b_1$	20.72	42/29	6/2	0/0
	50, $10a_1$	20.93	42/30	3/5	0/1
	49, $9a_1$	21.69	47/28	1/2	0/0
	48, $7b_1$	21.70	48/29	0/1	0/0
	47, $8a_1$	22.25	54/21	4/0	0/0
	46, $6b_1$	22.48	67/20	0/0	0/0
	45, $7a_1$	22.49	67/20	0/0	0/0
	44, $5b_1$	22.73	64/16	4/3	0/0
	43, $6a_1$	23.16	65/21	1/2	0/0
	42, $4b_1$	23.56	70/15	0/3	0/0
	41, $3b_1$	24.35	69/12	9/0	0/0
	40, $5a_1$	24.49	68/10	11/2	0/0
	39, $4a_1$	24.62	76/9	0/8	00
	38, $2b_1$	25.71	86/8	0/0	0/0
	37, $3a_1$	25.72	86/8	0/0	0/0
4	36, $1b_1$	28.72	42/6	45/4	0/0
	35, $2a_1$	29.17	39/7	48//2	1/0
5	34, $1b_2$	32.68	0/0	0/0	88/1
	33, $1a_1$	33.61	0/1	1/1	85/2

Table S10
Experimental energies and half-widths of bands in X-ray photoelectron spectra of 1s-Electrons of compounds II-IV.

Compound, electron levels	II		III		IV		V	
	E_b	Half-width	E_b	Half-width	E_b	Half-width	E_b	Half-width
F 1s	686.0	1.8	686.0	1.7	686.0	1.8	686.0	1.6
N 1s	399.8	1.7	399.8	1.7	399.8	2.2	399.9	1.4
C 1s	285.4	1.9	285.3	1.9	285.5	1.6	285.5	1.4
B 1s	193.3	1.9	193.5	1.5	193.4	1.7	193.4	1.3
Br 3p 3/2	-	-	191.1	2.6	-	-	-	-
Br 3p 1/2	-	-	184.6	2.6	-		-	-
Br 3d	-	-	71.4	2.0	-	-	-	-

Table S11
Differences in the calculated energy intervals (eV) between I_1-I_n, in comparison with the OVGF method data (ΔOVGF).

Energy	ΔOVGF		
	BHHLYP	CAM-B3LYP	ωB97X
	I		
I_2–I_1	0.01	–0.09	0.09
I_3–I_1	0.01	–0.10	0.08
I_4–I_1	0.08	0.07	0.28
I_5–I_1	–0.12	–0.89	–0.72
I_6–I_1	–0.21	–1.00	–0.83
I_7–I_1	–0.14	–1.14	0.97
I_8–I_1	–0.03	–0.52	–0.35
	II		
I_2–I_1	0.03	–0.09	0.09
I_3–I_1	0.02	–0.11	0.07
I_4–I_1	0.11	0.04	0.23
I_5–I_1	–0.17	–0.78	–0.61
I_6–I_1	–0.10	–0.63	–0.45
I_7–I_1	–0.04	–0.64	–0.08
I_8–I_1	–0.16	–0.67	0.15
	III		
I_2–I_1	–0.06	–0.15	0.01
I_3–I_1	–0.08	–0.19	–0.03
I_4–I_1	–0.02	–0.09	0.09
I_5–I_1	**–0.38**	–0.60	–0.39
I_6–I_1	**–0.40**	–0.61	–0.39
I_7–I_1	**–0.30**	–0.49	–0.27
I_8–I_1	**–0.24**	–0.37	–0.29
I_2–I_1	–0.25	–0.85	–0.54
	IV		
I_2–I_1	0.04	–0.07	0.09
I_3–I_1	0.05	–0.07	0.08
I_4–I_1	0.08	–0.01	0.18
I_5–I_1	**–0.36**	–0.59	–0.50
I_6–I_1	**–0.55**	–1.02	–0.85
I_7–I_1	**–0.43**	–0.83	–0.61
I_8–I_1	**–0.41**	–0.72	–0.62
I_9–I_1	**–0.23**	–0.97	–0.63
	V		
I_2–I_1	–0.24	–0.30	–0.14
I_3–I_1	–0.26	–0.29	0.19
I_4–I_1	–0.19	–0.21	–0.06
I_5–I_1	–0.01	–0.18	–0.37
I_6–I_1	–0.14	–0.18	–0.01
I_7–I_1	–0.27	–0.26	–0.10
I_8–I_1	0.07	–0.01	0.17
I_9–I_1	–0.15	–0.70	–0.53

Table S12
Equilibrium geometrical parameters of BODIPY II in its S_0 ground state obtained at the CAM-B3LYP/cc-pVTZ level of theory without C_{2v} point group symmetry constraints in terms of Cartesian coordinates (Å).

Atom	X	Y	Z
H	0.000000	2.761008	0.000000
C	1.212318	0.996267	0.000000
C	-1.212318	0.996267	0.000000
C	2.549030	1.479014	0.000000
C	-2.549030	1.479014	0.000000
C	-3.361516	0.354340	0.000000
C	3.361516	0.354340	0.000000
C	-2.527403	-0.786823	0.000000
C	2.527403	-0.786823	0.000000
N	-1.246589	-0.396015	0.000000
N	1.246589	-0.396015	0.000000
C	0.000000	1.669731	0.000000
C	2.970912	2.912704	0.000000
C	-2.970912	2.912704	0.000000
H	-4.448857	0.334551	0.000000
H	4.448857	0.334551	0.000000
C	-2.917277	-2.223374	0.000000
C	2.917277	-2.223374	0.000000
H	2.593975	3.445617	0.886900
H	-2.593975	3.445617	0.886900
H	2.593975	3.445617	-0.886900
H	-2.593975	3.445617	-0.886900
H	4.065636	2.997349	0.000000
H	-4.065636	2.997349	0.000000
H	-2.496995	-2.729462	0.881311
H	2.496995	-2.729462	0.881311
H	-2.496995	-2.729462	-0.881311
H	2.496995	-2.729462	-0.881311
H	4.008742	-2.331937	0.000000
H	-4.008742	-2.331937	0.000000
B	0.000000	-1.323170	0.000000
F	0.000000	-2.126079	1.144240
F	0.000000	-2.126079	-1.144240

Table S13
Equilibrium geometrical parameters of BODIPY II in its S_1 excited state obtained at the CAM-B3LYP/cc-pVTZ level of theory without C_{2v} point group symmetry constraints in terms of Cartesian coordinates (Å).

Atom	X	Y	Z
H	0.000000	2.799799	0.000000
C	1.212003	1.003258	0.000000
C	-1.212003	1.003258	0.000000
C	2.564063	1.479752	0.000000
C	-2.564063	1.479752	0.000000
C	-3.363303	0.347051	0.000000
C	3.363303	0.347051	0.000000
C	-2.520761	-0.796154	0.000000
C	2.520761	-0.796154	0.000000
N	-1.234172	-0.393060	0.000000
N	1.234172	-0.393060	0.000000
C	0.000000	1.712000	0.000000
C	2.963328	2.915484	0.000000
C	-2.963328	2.915484	0.000000
H	-4.451053	0.315450	0.000000
H	4.451053	0.315450	0.000000
C	-2.891471	-2.230867	0.000000
C	2.891471	-2.230867	0.000000
H	2.573288	3.445954	0.885540
H	-2.573288	3.445954	0.885540
H	2.573288	3.445954	-0.885540
H	-2.573288	3.445954	-0.885540
H	4.056346	3.021693	0.000000
H	-4.056346	3.021693	0.000000
H	-2.456763	-2.735669	0.878574
H	2.456763	-2.735669	0.878574
H	-2.456763	-2.735669	-0.878574
H	2.456763	-2.735669	-0.878574
H	3.980852	-2.358056	0.000000
H	-3.980852	-2.358056	0.000000
B	0.000000	-1.319251	0.000000
F	0.000000	-2.133017	1.142066
F	0.000000	-2.133017	-1.142066

Table S14

Franck-Condon structure of the $S_0 \rightarrow S_1$ photoabsorption spectrum of BODIPY II: transition energies E (eV), intensities I (a.u.) and assignment of the vibronic states in terms of the quanta of the S_1 vibrational modes computed using CAM-B3LYP/cc-pVTZ results for S_0 and S_1 states.

Transition	E	I
0-0	2.841	1.000
14^1	2.868	0.106
4^2	2.869	0.186
5^2	2.869	0.190
4^4	2.897	0.052
$5^2\ 4^2$	2.898	0.035
5^4	2.898	0.054
24^1	2.902	0.076
27^1	2.914	0.038
30^1	2.926	0.038
39^1	2.957	0.057
55^1	2.992	0.044
58^1	3.006	0.056

Table S15

Franck-Condon structure of the $S_1 \rightarrow S_0$ photoemission spectrum of BODIPY II: transition energies E (eV), intensities I (a.u.) and assignment of the vibronic states in terms of the quanta of the S_0 vibrational modes computed using CAM-B3LYP/cc-pVTZ results for S_0 and S_1 states.

Transition	E	I
70^1	2.657	0.029
55^1	2.686	0.050
38^1	2.723	0.049
31^1	2.754	0.031
26^1	2.767	0.035
24^1	2.778	0.064
13^1	2.813	0.098
2^4	2.829	0.068
$2^2\ 1^2$	2.829	0.044
1^4	2.829	0.065
2^2	2.835	0.212
1^2	2.835	0.208
0-0	2.841	1.000

Table S16

Harmonic frequencies ω (cm^{-1}) of the vibrational normal modes of BODIPY II in its S_0 ground state and S_1 excited state obtained at the CAM-B3LYP/cc-pVTZ level of theory.

S_0				S_1			
Mode	Assignment		ω	Mode	Assignment		ω
ν_1	1	a_2	23.5	ν'_1	1	b_1	43.7
ν_2	1	b_1	23.9	ν'_2	1	a_2	62.9
ν_3	2	b_1	43.2	ν'_3	2	b_1	84.9
ν_4	2	a_2	69.9	ν'_4	2	a_2	114.6
ν_5	3	b_1	93.7	ν'_5	3	b_1	115.6
ν_6	3	a_2	107.6	ν'_6	3	a_2	138.3
ν_7	4	b_1	109.7	ν'_7	4	b_1	145.3
ν_8	1	a_1	150.2	ν'_8	1	a_1	149.3
ν_9	4	a_2	150.6	ν'_9	4	a_2	156.0
ν_{10}	5	a_2	203.5	ν'_{10}	5	b_1	197.9
ν_{11}	5	b_1	204.5	ν'_{11}	5	a_2	200.8
ν_{12}	1	b_2	207.5	ν'_{12}	1	b_2	208.2
ν_{13}	2	a_1	223.9	ν'_{13}	6	b_1	216.9
ν_{14}	6	b_1	252.1	ν'_{14}	2	a_1	221.5
ν_{15}	2	b_2	256.8	ν'_{15}	2	b_2	252.7
ν_{16}	3	a_1	302.5	ν'_{16}	3	a_1	299.6
ν_{17}	3	b_2	316.1	ν'_{17}	3	b_2	315.2
ν_{18}	6	a_2	321.5	ν'_{18}	6	a_2	325.3
ν_{19}	7	a_2	385.8	ν'_{19}	7	a_2	357.2
ν_{20}	4	a_1	426.1	ν'_{20}	7	b_1	379.9
ν_{21}	7	b_1	469.1	ν'_{21}	4	a_1	417.0
ν_{22}	4	b_2	485.4	ν'_{22}	8	b_1	466.6
ν_{23}	8	b_1	496.8	ν'_{23}	4	b_2	484.8
ν_{24}	5	a_1	501.3	ν'_{24}	5	a_1	494.0
ν_{25}	5	b_2	593.1	ν'_{25}	6	a_1	576.0
ν_{26}	6	a_1	593.3	ν'_{26}	5	b_2	580.3
ν_{27}	7	a_1	604.8	ν'_{27}	7	a_1	594.8
ν_{28}	9	b_1	668.9	ν'_{28}	9	b_1	633.3
ν_{29}	8	a_2	674.5	ν'_{29}	8	a_2	645.4
ν_{30}	6	b_2	689.8	ν'_{30}	8	a_1	690.7
ν_{31}	8	a_1	701.7	ν'_{31}	6	b_2	694.8
ν_{32}	9	a_2	712.8	ν'_{32}	10	b_1	697.0
ν_{33}	10	b_1	752.5	ν'_{33}	9	a_2	698.6
ν_{34}	10	a_2	834.0	ν'_{34}	11	b_1	769.0
ν_{35}	11	b_1	835.4	ν'_{35}	12	b_1	830.4

ν_{36}	7	b_2	850.1	ν'_{36}	10	a_2	834.0
ν_{37}	8	b_2	902.5	ν'_{37}	7	b_2	865.6
ν_{38}	9	a_1	944.1	ν'_{38}	8	b_2	875.4
ν_{39}	12	b_1	957.5	ν'_{39}	9	a_1	939.2
ν_{40}	9	b_2	993.0	ν'_{40}	10	a_1	984.8
ν_{41}	10	a_1	995.6	ν'_{41}	9	b_2	991.7
ν_{42}	11	a_1	1003.9	ν'_{42}	11	a_1	998.9
ν_{43}	10	b_2	1008.6	ν'_{43}	10	b_2	1003.0
ν_{44}	11	a_2	1052.6	ν'_{44}	13	b_1	1042.1
ν_{45}	13	b_1	1054.5	ν'_{45}	11	a_2	1045.1
ν_{46}	14	b_1	1058.5	ν'_{46}	12	a_2	1047.8
ν_{47}	12	a_2	1058.8	ν'_{47}	14	b_1	1047.9
ν_{48}	12	a_1	1090.1	ν'_{48}	12	a_1	1080.5
ν_{49}	11	b_2	1126.7	ν'_{49}	11	b_2	1082.5
ν_{50}	13	a_1	1132.7	ν'_{50}	13	a_1	1095.1
ν_{51}	15	b_1	1147.9	ν'_{51}	15	b_1	1124.7
ν_{52}	12	b_2	1179.5	ν'_{52}	12	b_2	1177.7
ν_{53}	14	a_1	1189.5	ν'_{53}	14	a_1	1183.0
ν_{54}	13	b_2	1210.8	ν'_{54}	13	b_2	1199.5
ν_{55}	15	a_1	1243.8	ν'_{55}	15	a_1	1218.1
ν_{56}	14	b_2	1262.2	ν'_{56}	14	b_2	1265.2
ν_{57}	15	b_2	1396.0	ν'_{57}	15	b_2	1329.6
ν_{58}	16	a_1	1398.6	ν'_{58}	16	a_1	1334.9
ν_{59}	16	b_2	1400.9	ν'_{59}	16	b_2	1389.9
ν_{60}	17	a_1	1404.7	ν'_{60}	17	a_1	1392.5
ν_{61}	17	b_2	1417.4	ν'_{61}	17	b_2	1403.9
ν_{62}	18	a_1	1430.5	ν'_{62}	18	a_1	1404.7
ν_{63}	18	b_2	1433.6	ν'_{63}	18	b_2	1418.2
ν_{64}	13	a_2	1445.5	ν'_{64}	13	a_2	1431.8
ν_{65}	16	b_1	1447.8	ν'_{65}	16	b_1	1433.9
ν_{66}	19	a_1	1456.4	ν'_{66}	19	b_2	1437.4
ν_{67}	14	a_2	1462.3	ν'_{67}	19	a_1	1444.7
ν_{68}	17	b_1	1462.6	ν'_{68}	14	a_2	1453.1
ν_{69}	19	b_2	1473.6	ν'_{69}	17	b_1	1453.5
ν_{70}	20	a_1	1476.2	ν'_{70}	20	a_1	1456.3
ν_{71}	20	b_2	1480.5	ν'_{71}	20	b_2	1459.7
ν_{72}	21	a_1	1516.2	ν'_{72}	21	b_2	1485.9
ν_{73}	21	b_2	1527.8	ν'_{73}	21	a_1	1507.2
ν_{74}	22	a_1	1531.6	ν'_{74}	22	a_1	1518.0

ν_{75}	22	b_2	1604.7	ν'_{75}	22	b_2	1523.8
ν_{76}	23	a_1	1608.5	ν'_{76}	23	a_1	1525.1
ν_{77}	24	a_1	1621.3	ν'_{77}	23	b_2	1600.1
ν_{78}	23	b_2	1681.2	ν'_{78}	24	a_1	1605.9
ν_{79}	24	b_2	3057.6	ν'_{79}	24	b_2	3033.1
ν_{80}	25	a_1	3057.9	ν'_{80}	25	a_1	3033.8
ν_{81}	25	b_2	3072.9	ν'_{81}	26	a_1	3047.1
ν_{82}	26	a_1	3073.2	ν'_{82}	25	b_2	3047.5
ν_{83}	15	a_2	3120.2	ν'_{83}	18	b_1	3085.5
ν_{84}	18	b_1	3120.4	ν'_{84}	15	a_2	3086.0
ν_{85}	16	a_2	3145.5	ν'_{85}	19	b_1	3104.4
ν_{86}	19	b_1	3146.1	ν'_{86}	16	a_2	3106.2
ν_{87}	26	b_2	3152.7	ν'_{87}	26	b_2	3147.3
ν_{88}	27	a_1	3152.8	ν'_{88}	27	a_1	3147.4
ν_{89}	27	b_2	3173.0	ν'_{89}	27	b_2	3167.7
ν_{90}	28	a_1	3173.2	ν'_{90}	28	a_1	3167.8
ν_{91}	29	a_1	3222.6	ν'_{91}	29	a_1	3252.6
ν_{92}	28	b_2	3258.7	ν'_{92}	28	b_2	3253.2
ν_{93}	30	a_1	3258.8	ν'_{93}	30	a_1	3253.3

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