Supporting Information

Regioisomeric BODIPY Derivatives: Second-order Nonlinear Optical Properties under the External Electric Field

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Table S1. The μ_g (Debye, D) and E_{gap} (eV) values of **m-AD** and **p-AD** by using the B3LYP functional.

	m-AD	**p-AD**
μ_g (D)	5.33	6.17
E_{gap} (eV)	2.48	2.51

The dipole moments of ground state (μ_g) are calculated in Table S1, the μ_g values of **m-AD** and **p-AD** are 5.33 D and 6.17 D, respectively. The energy gap (E_{gap}) of the highest occupied (HOMO) to lowest unoccupied molecular orbital (LUMO) of **p-AD** (2.51 eV) is higher than that of **m-AD** (2.48 eV).

Table S2. The first hyperpolarizabilities (β_{tot}, a.u.) of **m-AD** and **p-AD** by using the M06-2X, the CAM-BLYP and the BHandHLYP functionals.

		β_x	β_y	β_z	β_{tot}
M06-2X	**m-AD**	9.07×10^2	-3.38×10^2	-3.61×10^2	1.03×10^3
	p-AD	7.484×10^3	3.39×10^2	1.27×10^2	7.49×10^3
BHandHLYP	**m-AD**	5.99×10^2	-3.54×10^2	-4.06×10^2	8.05×10^2
	p-AD	6.96×10^3	3.00×10^2	1.25×10^2	6.97×10^3
CAM-BLYP	**m-AD**	7.17×10^2	-3.38×10^2	-3.83×10^2	8.81×10^2
	p-AD	6.42×10^3	3.02×10^2	1.20×10^2	6.43×10^3

Table S2 results show that the β_{tot} values of **m-AD** and **p-AD** by using the BHandHLYP and the CAM-B3LYP functionals are close to that obtained by the M06-2X functional.

Table S3. The first hyperpolarizabilities (β_{tot}, au) of **m-AD** and **p-AD** by using the M06-2X method with different basis sets (6-31G*, 6-31+G* and 6-31G**).

		6-31G*	6-31+G*	6-s31G**
m-AD	β_x	9.07×10^2	8.31×10^2	9.08×10^2
	β_y	-3.38×10^2	-3.48×10^2	-3.50×10^2
	β_z	-3.61×10^2	-4.19×10^2	-3.66×10^2
	β_{tot}	1.03×10^3	9.93×10^2	1.04×10^3
p-AD	β_x	7.48×10^3	7.97×10^3	7.50×10^3
	β_y	3.39×10^2	3.29×10^2	3.44×10^2
	β_z	1.27×10^2	1.40×10^2	1.28×10^2
	β_{tot}	7.49×10^3	7.98×10^3	7.50×10^3

From Table S3, effect of basis sets (6-31G*, 6-31+G* and 6-31G**) on the first hyperpolarizabilities of **m-AD** and **p-AD** are evaluated. The results from three basis sets present the same trend of the β_{tot} value, and the β_{tot} values are very close.

Cartesian coordinates of the optimized structures of m-AD and **p-AD.**

(1) **m-AD**

m-AD	The total energy = 2323.2452 a.u.		
Atom	X	Y	Z
C	6.76872400	-1.12366700	1.75720400
C	6.17359200	-2.38300600	1.97507200
N	6.00238000	-0.37841900	0.94826000
C	4.98122600	-2.38784000	1.26399500
C	4.87816400	-1.13040400	0.60872900
C	3.88529800	-0.60599900	-0.23674000
C	4.01782300	0.69475000	-0.75474100
C	3.23465400	1.40266100	-1.70662600
N	5.10636700	1.49638100	-0.41644100
C	3.85699600	2.62538100	-1.92115900
C	5.00917300	2.64016800	-1.10913000
B	6.24445700	1.13161800	0.59797500
F	7.47919300	1.29485400	0.00064700
F	6.12563500	1.89942300	1.74208300
H	6.57867600	-3.17750400	2.58645600
C	-1.06844500	-1.13675500	-0.46222500
C	-1.42931400	0.17640800	-0.34325100
S	-2.46309000	-2.21563000	-0.27804100
C	-3.53917600	-0.84875800	-0.04876000
C	-2.82710000	0.37797800	-0.10559500
H	-0.73543200	1.00267800	-0.44536400
C	-3.51195100	1.60841500	0.05740800
C	-4.89677800	1.53256100	0.27625100
C	-5.60824000	0.30484900	0.33647900
C	-4.92273000	-0.92495000	0.17093200
S	-5.97399800	2.90059600	0.51089400
C	-7.34246400	1.82107300	0.68338800
C	-7.01203700	0.50911700	0.57181800
H	-7.72185200	-0.30596600	0.65006100
C	-2.82931400	2.85462700	0.00477000
C	-5.60224400	-2.17346000	0.22450900
C	-2.25589800	3.92353000	-0.03606000
C	-6.17210000	-3.24399200	0.26871600
C	-1.57128700	5.21079700	-0.08217200
H	-1.36841400	5.51768300	-1.11585400
H	-0.61176700	5.16939600	0.44743900
H	-2.17755500	5.99565700	0.38523600
C	-6.85390400	-4.53254200	0.32183800
H	-7.42468900	-4.64256500	1.25213300

H	-6.13634100	-5.35990300	0.27107800
H	-7.55504300	-4.64723700	-0.51415900
C	0.45610900	-2.95792900	-1.27445100
C	0.27120400	-1.68452200	-0.70700100
C	1.73704400	-3.45770300	-1.49807300
C	2.86035000	-2.70448900	-1.16354700
C	1.41166000	-0.93263700	-0.37500000
C	2.70289300	-1.42629600	-0.60027800
H	1.29470100	0.03341200	0.10398900
H	1.86024300	-4.43889100	-1.94770700
H	-8.32471300	2.23987600	0.86034700
H	4.25151000	-3.18301100	1.21076600
H	7.69490400	-0.72723000	2.15173000
H	-0.40806000	-3.55127800	-1.55906200
H	3.85717200	-3.08777100	-1.35603300
H	2.33933000	1.02837800	-2.18220700
H	3.54300900	3.41563400	-2.58907600
H	5.76267800	3.40930400	-1.00335500

(2) **p-AD**

p-AD	The total energy = -2323.2460 a.u.		
Atom	X	Y	Z
C	6.99829800	2.26501000	-0.97682500
C	5.90257600	3.07135900	-1.34441900
N	6.57099200	1.10452800	-0.45830200
C	4.75674200	2.34951100	-1.03705500
C	5.17693400	1.11637000	-0.46824000
C	4.43949900	0.01982900	0.01584400
C	5.11113200	-1.11157900	0.51595800
C	4.61866000	-2.27695500	1.16401700
N	6.50268700	-1.18343700	0.50946300
C	5.72007500	-3.04011700	1.52881700
C	6.86146500	-2.32703500	1.11085600
B	7.48315300	-0.11598300	-0.08604100
F	8.41522200	0.25137300	0.86519000
F	8.08838900	-0.60895700	-1.22794300
H	5.96100400	4.05648800	-1.78629100
C	-1.34493200	0.14006600	0.00869700
C	-2.19680600	-0.92182200	-0.12603000
S	-2.22984300	1.66534800	0.19407200
C	-3.76888400	0.82933900	0.09515800
C	-3.58280200	-0.56698800	-0.08305100

H	-1.86616200	-1.94889700	-0.22691300
C	-4.70419400	-1.42844200	-0.18704100
C	-5.96943100	-0.82484800	-0.10991300
C	-6.15487100	0.57256300	0.06437700
C	-5.03306400	1.43265100	0.17190400
S	-7.51186600	-1.65989200	-0.21265700
C	-8.36939600	-0.14447300	-0.02351400
C	-7.54742000	0.92769800	0.10944600
H	-7.89236500	1.94710600	0.23628800
C	-4.55465900	-2.83156800	-0.36222900
C	-5.18023200	2.83616000	0.35024100
C	-4.44333900	-4.03079700	-0.51236600
C	-5.29289500	4.03479500	0.50292800
C	-4.31704600	-5.47281100	-0.69275600
H	-5.30132900	-5.94162500	-0.80798000
H	-3.82343200	-5.94045500	0.16819200
H	-3.72662700	-5.71247800	-1.58573500
C	-5.42426800	5.47599200	0.68646300
H	-6.02374800	5.71107600	1.57457400
H	-5.91145300	5.94472100	-0.17752900
H	-4.44255000	5.94757100	0.81209000
C	0.82499900	-0.94691500	-0.57420800
C	0.12011000	0.12292400	0.01103600
C	2.21301600	-0.98610400	-0.55967300
C	2.95975100	0.05806500	0.01589400
C	0.87095900	1.16099500	0.59297100
C	2.26074200	1.13468300	0.58760900
H	0.36084600	1.98870900	1.07723300
H	2.73223800	-1.81333500	-1.03334700
H	2.81453800	1.93805000	1.06286400
H	5.72092700	-3.98900900	2.04723300
H	-9.45173800	-0.14825100	-0.02326900
H	3.73113800	2.64704200	-1.20147600
H	8.05744400	2.46354100	-1.07339600
H	7.90710600	-2.58048500	1.22408800
H	3.57737300	-2.49608200	1.35197900
H	0.27722800	-1.743483000	-1.06755000