SUPPORTING INFORMATION

Effect of the iodine atom position on the phosphorescence of BODIPY derivatives: a combined computational and experimental study

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General methods

^{1}H-NMR, ^{13}C-NMR and ^{13}C-NMR spectra were recorded on a Varian Mercury 400 spectrometer in $CDCl_3$. Trifluoroacetic acid signal (-76.55 ppm) was used as references for ^{19}FNMR spectra. Chemical shifts are reported in parts per million (ppm) of the δ scale relative to TMS for ^{1}H and ^{13}C spectra and $CFCl_3$ for ^{19}FNMR spectra. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = duplet, t = triplet, q = quartet, dd = double duplet, dt = double triplet, bs = broad signal, m = multiplet), coupling constants (Hz). Chromatographic purification was performed with 240-400 mesh silica gel and reagents were purchased from Aldrich and used without further purification, unless specified.

All photophysical analyses were carried out in MeCN at 298 K, unless otherwise specified. Luminescence measurements at 77 K were performed in EtOH/MeOH (1:1 v/v) mixture. UV-Vis absorption spectra were recorded with a PerkinElmer λ40 spectrophotometer and luminescence spectra were performed with a PerkinElmer LS-50, using quartz cells with a path length of 1 cm. Fluorescence lifetimes were measured with an Edinburgh FLS920 spectrofluorometer by time-correlated single-photon counting (TCSPC) technique, whereas phosphorescence lifetimes were measured with an Edinburgh FS5 or PerkinElmer λ40 spectrofluorometer. Emission quantum yields were measured using fluoresceine in NaOH 0.1M as the standard. Singlet oxygen quantum yields were measured with an Edinburgh FLS920 spectrofluorometer equipped with a Ge detector using $[Ru(bpy)_3](PF_6)_2$ as the standard.

Cyclic voltammetries were performed at r.t. by using an EcoChemie Autolab 30 potentiostat in a three-electrode setup (working electrode: glassy carbon; quasi-reference electrode: silver wire; counter electrode: Pt wire) in anhydrous MeCN (supporting electrolyte: TEA PF_6 0.1M) and using Fc^+/Fc as the internal standard. Potentials were converted to V vs. SCE considering Fc^+/Fc= +0.39 V vs. SCE.

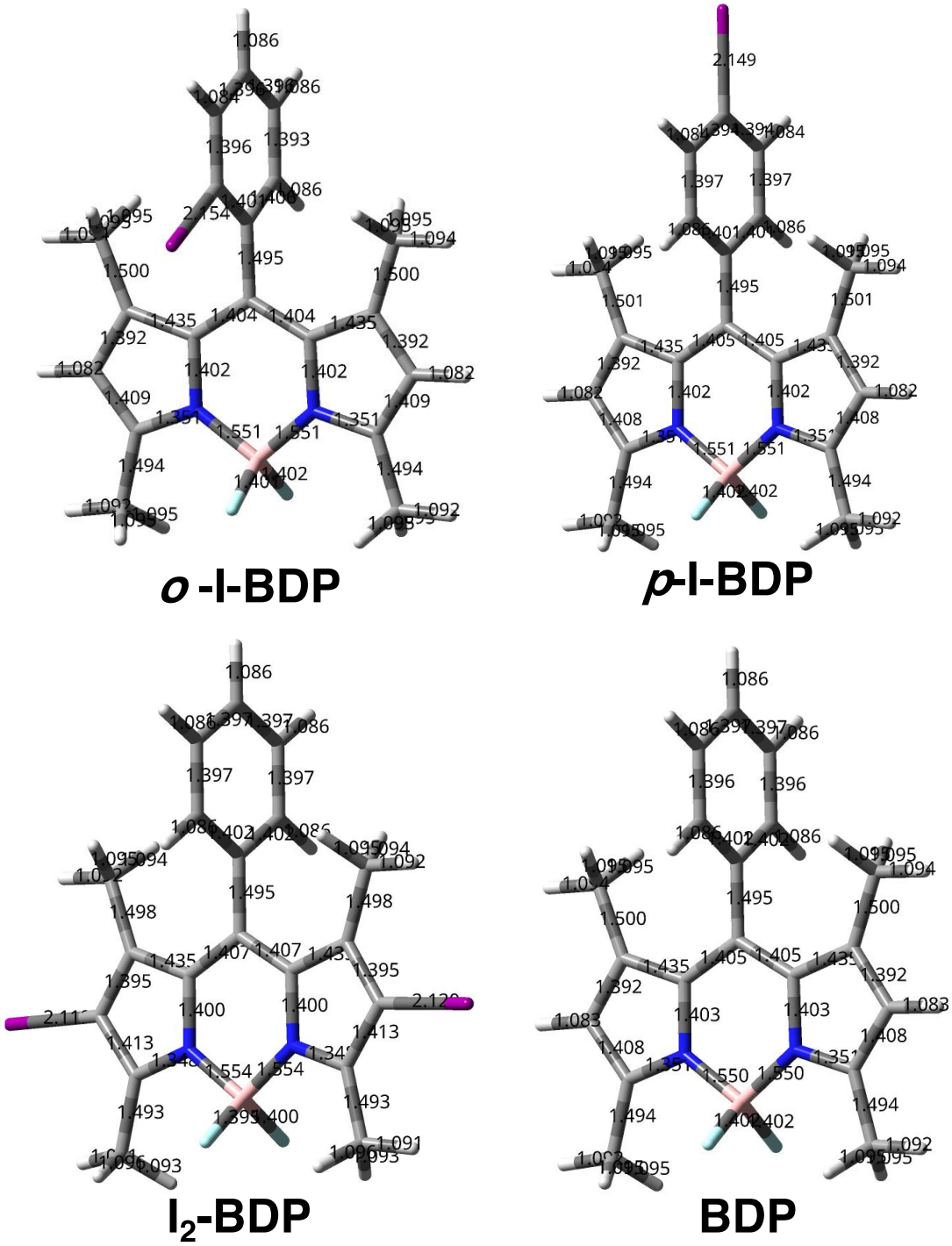


Figure S1. Geometries of **BDP** and its iodinated derivatives optimized at PCM-B3LYP/6-31G* and PCM-B3LYP/6-31G*/LANL2DZ levels of theory.

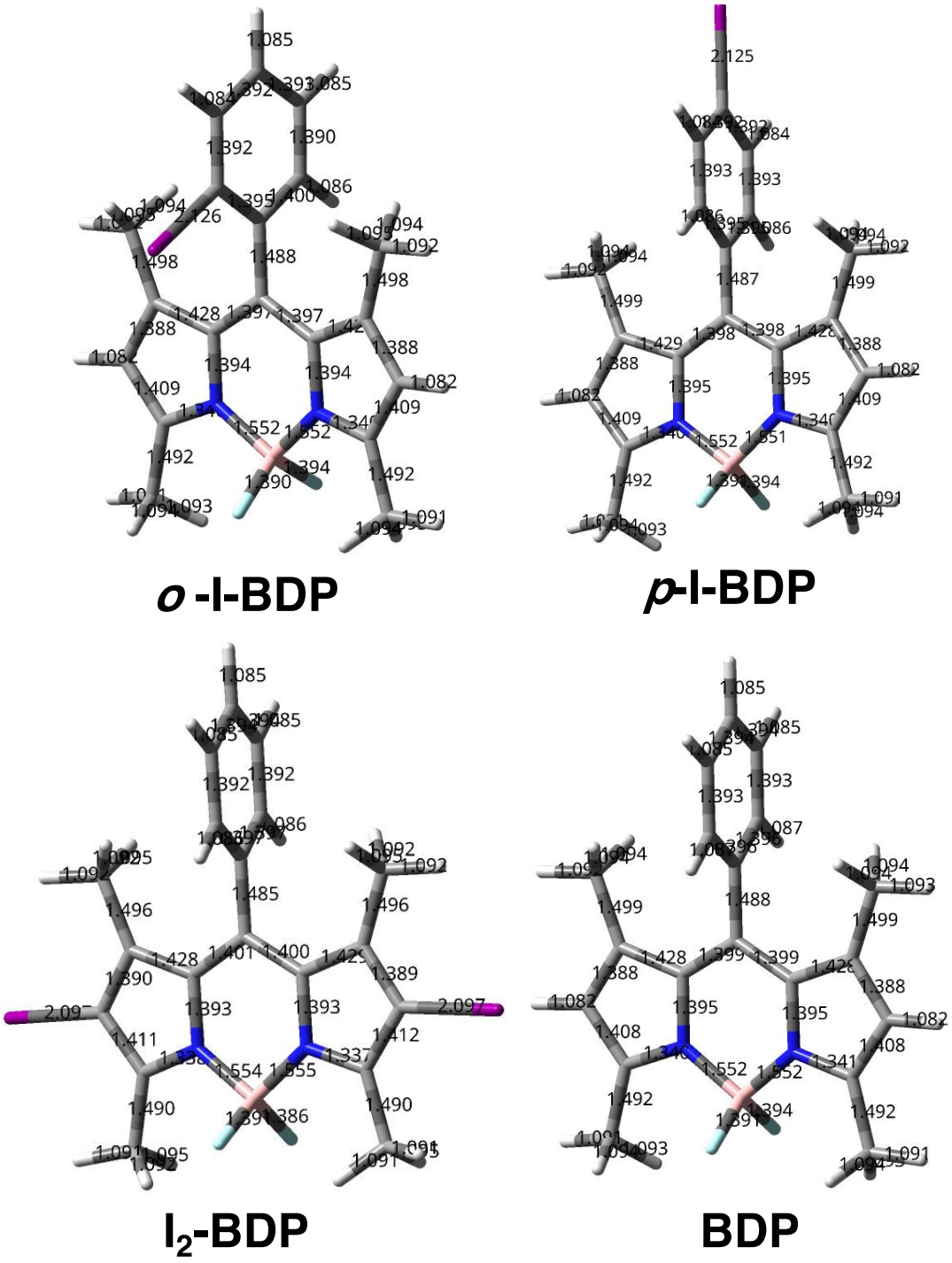


Figure S2. Geometries of **BDP** and its iodinated derivatives optimized at PCM-M06-2X/6-31G* and PCM-M06-2X/6-31G*/LANL2DZ levels of theory.

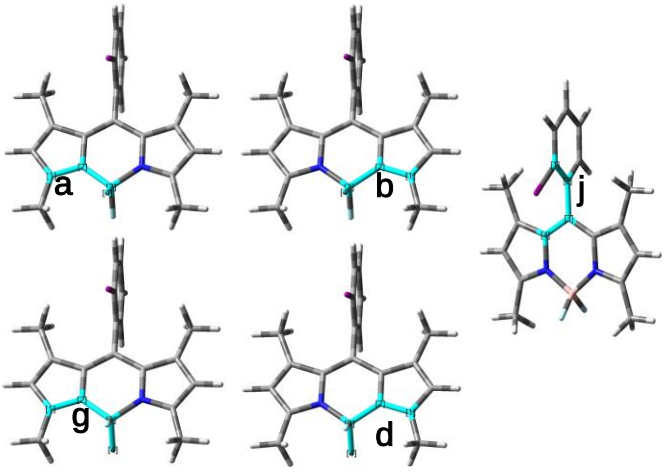


Figure S3: Definition of relevant dihedral angles

Table S1. Dihedral angles of **BDP** and iodinated derivatives. The structure of **BDP** is optimized at PCM-B3LYP/6-31G* level of theory, while the three iodinated derivatives are optimized at PCM-B3LYP/6-31G*/LANL2DZ level. Definition of the five angles can be found in Figure S3.

Molecule	φ (°)	α (°)	β (°)	γ (°)	δ (°)
BDP	90.00	-60.42	60.41	60.39	-60.39
***o*-I-BDP**	91.19	-60.74	60.74	60.09	-60.09
***p*-I-BDP**	90.00	-60.41	60.41	60.41	-60.41
I_2-BDP	89.99	-59.14	59.22	62.25	-62.17

Table S2. Dihedral angles of **BDP** and iodinated derivatives. The structure of **BDP** is optimized at PCM-M06-2X/6-31G* level of theory, while the three iodinated derivatives are optimized at PCM-M06-2X/6-31G*/LANL2DZ level. Definition of the five angles can be found in Figure S3

Molecule	φ (°)	α (°)	β (°)	γ (°)	δ (°)
BDP	99.08	-61.12	64.13	60.22	-57.19
***o*-I-BDP**	90.55	-56.47	56.47	64.93	-64.93
***p*-I-BDP**	99.44	-57.34	60.78	63.99	-60.55
I_2-BDP	103.57	-56.08	60.15	65.71	-61.66

Table S3. Frontier molecular orbital (MOs) energies of BODIPY derivatives calculated at PCM-B3LYP/6-31G* (PCM-B3LYP/6-31G*/LANL2DZ) and PCM-M06-2X/6-31G* (PCM-M06-2X/6-31G*/LANL2DZ) levels.

	PCM-B3LYP		**PCM-M06-2X**	
MOs /eV	L	H	L	H
BDP	-2.52	-5.55	-1.88	-6.70
***o*-I-BDP**	-2.61	-5.58	-1.96	-6.72
***p*-I-BDP**	-2.57	-5.58	-1.93	-6.72
I_2-BDP	-2.81	-5.75	-2.17	-6.86

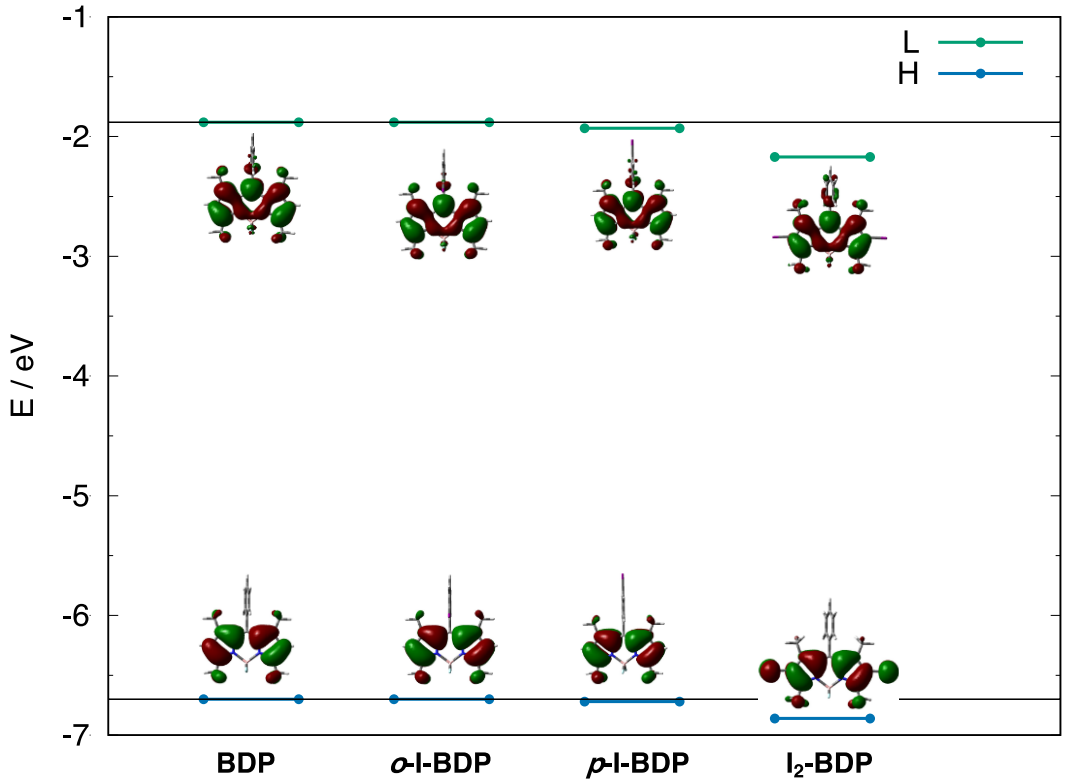


Figure S4. Shapes and energies of HOMO (H) and LUMO (L) calculated at PCM-M06-2X/6-31G* (for **BDP**) and PCM-M06-2X/6-31G*/LANL2DZ levels of theory.

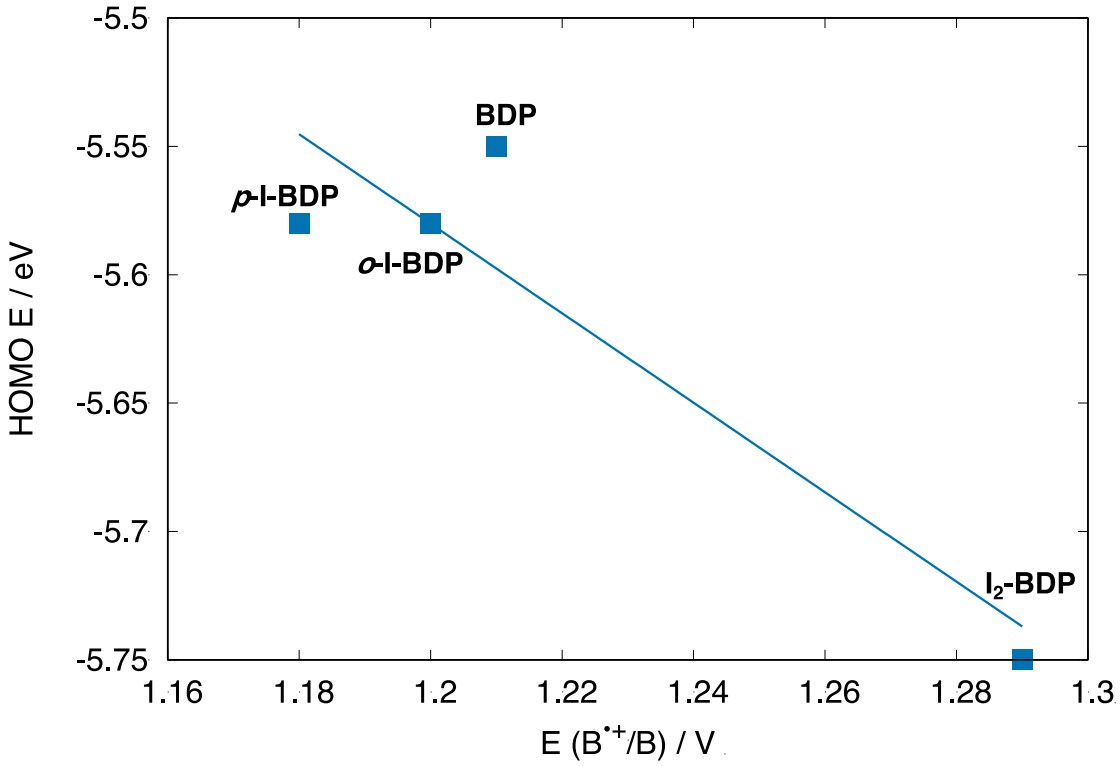


Figure S5. Relationship between the $B^{\bullet+}/B$ redox potentials (see Table 2) and H energies of BODIPY derivatives. H energies are calculated at PCM-B3LYP/6-31G*/LANL2DZ level (see Table S3).

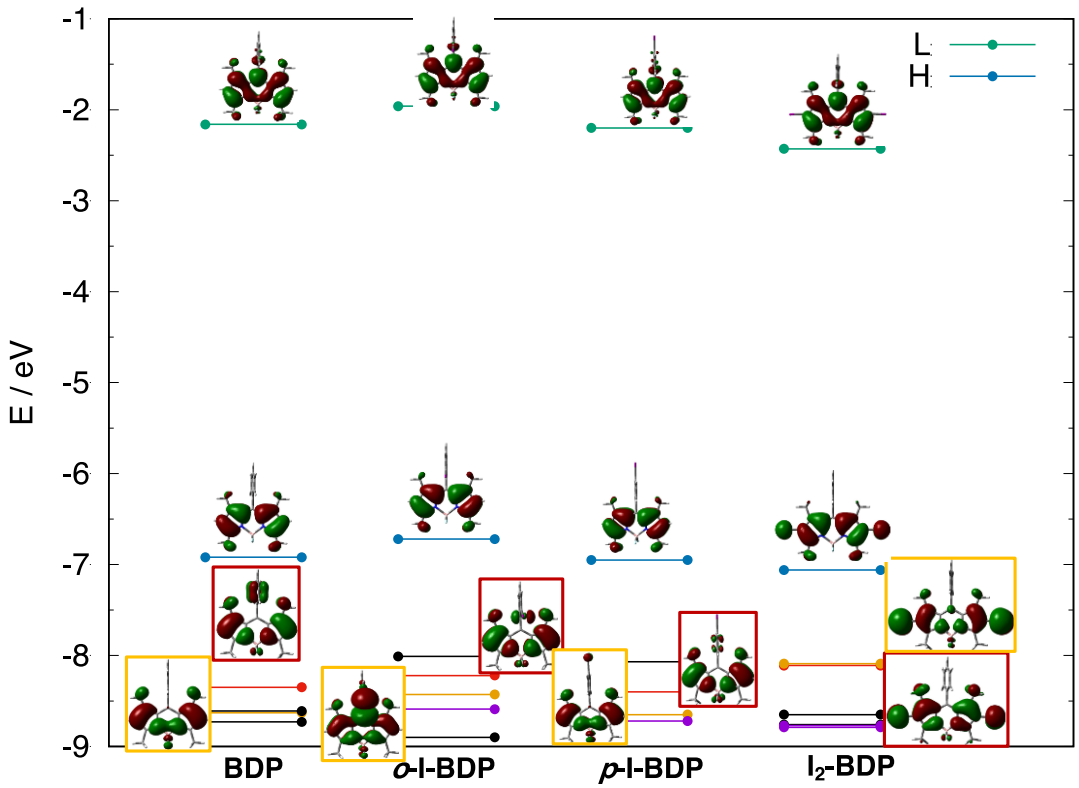


Figure S6. Molecular orbitals involved in low-lying excited states of **BDP** and iodinated derivatives. PCM-TD-M06-2X/6-311G* (PCM-TD-M06-2X/6-311G*/LANL2DZ) at PCM-B3LYP/6-31G* (PCM-B3LYP/6-31G*/LANL2DZ) optimized geometries. Black lines indicate phenyl-localized MOs, while purple lines indicate iodine-centered MOs.

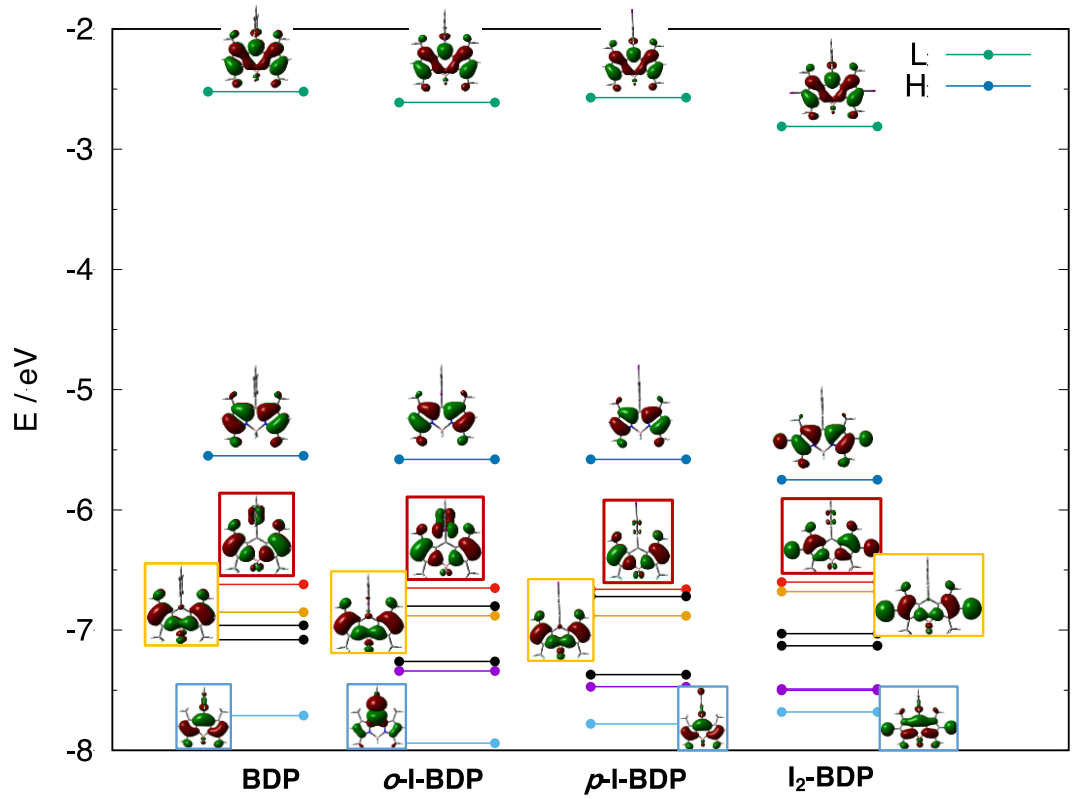


Figure S7. Molecular orbitals of **BDP** and iodinated derivatives calculated with PCM-B3LYP/6-31G* (PCM-B3LYP/6-31G*/LANL2DZ) level of theory based on PCM-B3LYP/6-31G* (PCM-B3LYP/6-31G*/LANL2DZ) optimized geometries. Black lines indicate phenyl-localized MOs, while purple lines indicate iodine-centered MOs

Table S4. Excitation energies, λ_{abs}, oscillator strengths and wavefunctions of the low-lying excited states of **BDP** and iodinated derivatives. Excited states of **BDP** and iodinated derivatives are calculated at PCM-TD-M06-2X level of theory using 6-311G*, 6-311+G* and def2-TZVP basis sets. LANL2DZ is used for Iodine. The TD calculations were carried out at PCM-B3LYP/6-31G* (PCM-B3LYP/6-31G*/LANL2DZ) optimized geometries.

BDP

	6-311G*					6-311+G*	def2-TZVP
State	**E (eV)**	**λ_{abs} (nm)**	**osc.str**	**S**2**	**wavefunction**	**E (eV)**	**E (eV)**
T_1	1.50	824	0	2	0.72 H→ L	1.50	1.50
S_1	2.87	432	0.6261	0	0.7 H→ L	2.84	2.83
T_2	3.12	397	0	2	0.67 H-1 → L	3.12	3.14

***o*-I-BDP**

	6-311G*/ LANL2DZ					6-311+G*/LANL2DZ	def2-TZVP/LANL2DZ
State	**E (eV)**	**λ_{abs} (nm)**	**osc.str**	**S**2**	**wavefunction**	**E (eV)**	**E (eV)**
T_1	1.45	856	0	2	0.72 H→ L	1.45	1.45
S_1	2.84	437	0.6156	0	0.70 H→ L	2.80	2.80
T_2	3.09	402	0	2	0.66 H-2[a] → L	3.09	3.11

***p*-I-BDP**

	6-311G*/ LANL2DZ					6-311+G*/LANL2DZ	def2-TZVP/LANL2DZ
State	**E (eV)**	**λ_{abs} (nm)**	**osc.str**	**S**2**	**wavefunction**	**E (eV)**	**E (eV)**
T_1	1.48	837	0	2	0.72H → L	1.48	1.48
S_1	2.86	434	0.6265	0	0.70H → L	2.83	2.82
T_2	3.11	399	0	2	0.68 H-2 [a] → L	3.11	3.13

I_2-BDP

	6-311G*/ LANL2DZ					6-311+G*/LANL2DZ	def2-TZVP/LANL2DZ
State	**E (eV)**	**λ_{abs}(nm)**	**osc.str**	**S**2**	**wavefunction**	**E (eV)**	**E (eV)**
T_1	1.50	828	0	2	0.69 H → L	1.49	1.48
S_1	2.73	454	0.7603	0	0.70 H → L	2.71	2.69
T_2	2.92	425	0	2	0.64 H-2 [a] → L	2.91	2.92

[a] shapes of ***o*-I-BDP**, ***p*-I-BDP** and **I_2-BDP**'s H-2 correspond to that of **BDP**'s H-1, see Figure S.

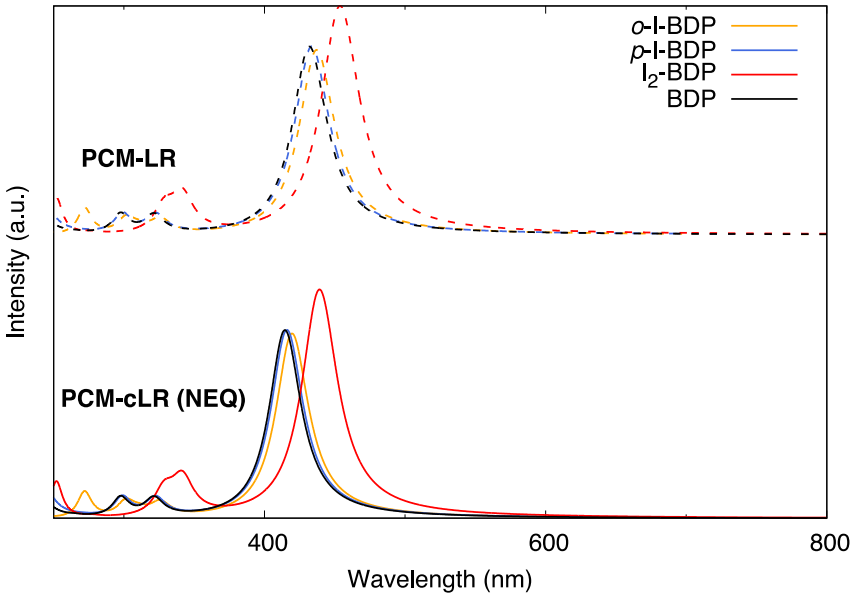


Figure S8. Absorption spectra of **BDP** and iodinated derivatives calculated at PCM-TD-M06-2X/6-311G* (PCM-TD-M06-2X/6-311G*/LANL2DZ) level of theory with (bottom, solid lines) and without (top, dashed lines) cLR (NEQ) solvent correction.

Table S5: Excitation energies of the first three excited states of **BDP** and derivatives. Calculations done at PCM-TD-M06-2X/6-311G* (for **BDP**) and PCM-TD-M06-2X/6-311G*/LANL2DZ levels of theory. LR, cLR(NEQ) and cLR(EQ) solvent corrections are considered.

			S_1		
Molecule	**gas phase** (eV)	**LR** (eV)	**cLR (NEQ)** (eV)	**cLR (EQ)** (eV)	**S1 exp. (eV)**
***o*-I-BDP**	2.94	2.84	2.96	2.95	2.46
***p*-I-BDP**	2.97	2.86	2.98	2.98	2.49
I_2-BDP	2.81	2.73	2.84	2.83	2.34
BDP	2.97	2.87	2.99	2.99	2.45
			T_1		
Molecule	**gas phase** (eV)	**LR** (eV)	**cLR (NEQ)** (eV)	**cLR (EQ)** (eV)	
***o*-I-BDP**	1.41	1.45	1.44	1.44	
***p*-I-BDP**	1.44	1.48	1.48	1.47	
I_2-BDP	1.45	1.50	1.49	1.48	
BDP	1.46	1.50	1.50	1.49	
			T_2		
Molecule	**gas phase** (eV)	**LR**(eV)	**cLR (NEQ)** (eV)	**cLR (EQ)** (eV)	
***o*-I-BDP**	3.04	3.09	3.08	3.07	
***p*-I-BDP**	3.06	3.11	3.10	3.08	
I_2-BDP	2.86	2.92	2.90	2.88	
BDP	3.07	3.12	3.11	2.99	

Table S6. Dipole moments μ of the ground state (GS) and the first three excited states of **BDP** and iodinated derivatives. Ground states are calculated at PCM-B3LYP/6-31G* (for **BDP**) and PCM-B3LYP/6-31G*/LANL2DZ levels of theory; excited states are evaluated at PCM-TD-M06-2X/6-311G* (PCM-TD-M06-2X/6-311G*/LANL2DZ for iodinated derivatives) level, cLR is included for solvent correction.

Molecule	μ @ GS (Debye)	μ @ S_1 (Debye)	μ @ T_1 (Debye)	μ @ T_2 (Debye)
***o*-I-BDP**	6.507	6.098	5.346	6.453
***p*-I-BDP**	3.405	3.068	2.228	3.381
I_2-BDP	6.283	5.192	4.649	5.880
BDP	6.045	5.333	4.571	5.704

Table S7. SOC matrix elements components (in cm^{-1}) on Cartesian basis. The corresponding magnitudes are collected in Table 3[a]. SOC values are calculated at SOMF(1X) level of theory with excited states calculated at TDA-M06-2X/ZORA-def2-TZVP/SARC-ZORA-TZVP[1] level. The relativistic correction is considered using ZORA scheme of ORCA 5.0.1. The real and imaginary parts are in parenthesis. Calculations were carried out at PCM-B3LYP equilibrium geometries.

Molecule	ZORA-def2-TZVP/SARC-ZORA-TZVP @ geo PCM-B3LYP			
		X(Re, Im)	Y (Re, Im)	Z (Re, Im)
***o*-I-BDP**	S_1/T_1	(0.00 , 0.00)	(-0.00 , 1.09)	(0.00 , -0.00)
	S_1/T_2	(0.00 , 0.00)	(-0.00 , -0.14)	(0.00 , -0.00)
***p*-I-BDP**	S_1/T_1	(0.00 , -0.00)	(-0.00 , 0.00)	(0.00 , -0.00)
	S_1/T_2	(0.00 , 0.00)	(-0.00 , -0.00)	(0.00 , 0.00)
I_2-BDP	S_1/T_1	(0.00 , -2.64)	(-0.00 , -0.03)	(0.00 , -0.00)
	S_1/T_2	(0.00 , -11.70)	(-0.00 , -0.05)	(0.00 , 0.00)
BDP	S_1/T_1	(0.00 , 0.00)	(-0.00 , 0.00)	(0.00 , 0.00)
	S_1/T_2	(0.00 , 0.00)	(-0.00 , 0.00)	(0.00 , 0.00)

[a] SOC values in Table 3 are calculated as the square-root of the sum of the squared matrix elements of the three components.

Table S8. SOC matrix elements components (in cm-1) on Cartesian basis. SOC values are calculated at SOMF(1X) level of theory with excited states calculated at TDA-M06-2X/ZORA-def2-TZVP/SARC-ZORA-TZVP level. The relativistic correction is considered using ZORA scheme of ORCA 5.0.1. The real and imaginary parts are in parenthesis. Calculations were carried out at PCM-M06-2X equilibrium geometries.

Molecule	**ZORA-def2-TZVP/SARC-ZORA-TZVP@ geo PCM-M06-2X**			
		X(Re, Im)	**Y (Re, Im)**	**Z (Re, Im)**
***o*-I-BDP**	S_1/T_1	(0.00 , 0.00)	(-0.00 , 1.00)	(0.00 , -0.00)
	S_1/T_2	(0.00 , -0.00)	(-0.00 , 0.20)	(0.00 , -0.00)
***p*-I-BDP**	S_1/T_1	(0.00 , -0.20)	(-0.00 , 0.01)	(0.00 , 0.01)
	S_1/T_2	(0.00 , -0.01)	(-0.00 , -0.01)	(0.00 , -0.02)
I_2-BDP	S_1/T_1	(0.00 , -4.20)	(-0.00 , -1.52)	(0.00 , -0.24)
	S_1/T_2	(0.00 , 19.70)	(-0.00 , 3.96)	(0.00 , 0.53)
BDP	S_1/T_1	(0.00 , 0.03)	(-0.00 , 0.01)	(0.00 , -0.00)
	S_1/T_2	(0.00 , -0.02)	(-0.00 , 0.02)	(0.00 , -0.00)

References

1 J. D. Rolfes, F. Neese and D. A. Pantazis, All-electron scalar relativistic basis sets for the elements Rb–Xe, *J. Comput. Chem.*, 2020, **41**, 1842–1849.

Cartesian coordinates

1. PCM-B3LYP geometries

o-I-BDP

C	-2.479754	2.530615	0.087381
C	-1.389391	3.373672	0.378485
C	-0.280768	2.582497	0.663660
C	-0.723575	1.223126	0.539444
N	-2.079608	1.243968	0.184305
H	-1.421363	4.455652	0.377288
B	-2.975223	0.000170	-0.052081
N	-2.079846	-1.243908	0.183735
C	-2.480241	-2.530434	0.086223
C	-0.723809	-1.223490	0.538880
C	-1.390048	-3.373834	0.376973
C	-0.281279	-2.583002	0.662532
H	-1.422235	-4.455806	0.375308
C	-0.053786	-0.000283	0.703432
C	1.384342	-0.000511	1.112202
C	1.688814	-0.001042	2.484728
C	2.452783	-0.000219	0.205562
C	3.007942	-0.001286	2.933663
H	0.870289	-0.001272	3.198571
C	3.778946	-0.000447	0.641769
C	4.054491	-0.000987	2.010187
H	3.215598	-0.001704	3.999287
H	4.591730	-0.000205	-0.075690
H	5.086969	-0.001166	2.346710
I	2.108881	0.000652	-1.920884
F	-4.048371	0.000067	0.849713
F	-3.468884	0.000517	-1.363435
C	1.074796	-3.117391	1.018345
H	1.842585	-2.799351	0.304690
H	1.403069	-2.783539	2.008419
H	1.050049	-4.211178	1.020771
C	-3.875521	-2.922281	-0.277781
H	-4.594295	-2.508233	0.437570
H	-4.144555	-2.527218	-1.263504
H	-3.974014	-4.010135	-0.292173
C	1.075433	3.116461	1.019630
H	1.403679	2.782145	2.009555
H	1.843126	2.798547	0.305814
H	1.050914	4.210252	1.022496
C	-3.874962	2.922896	-0.276434
H	-4.144089	2.528311	-1.262323
H	-4.593806	2.508682	0.438749

H	-3.973240	4.010775	-0.290354

***p*-I-BDP**

C	-2.530317	-3.555728	0.000000
C	-3.373654	-2.427658	0.000000
C	-2.582828	-1.282433	0.000000
C	-1.223034	-1.741357	0.000000
N	-1.243887	-3.143679	0.000000
H	-4.455667	-2.459272	0.000000
B	0.000001	-4.069373	0.000000
F	-0.000023	-4.879194	1.144054
F	-0.000023	-4.879194	-1.144054
N	1.243954	-3.143755	0.000000
C	2.530347	-3.555906	0.000000
C	2.583051	-1.282617	0.000000
C	3.373778	-2.427907	0.000000
H	4.455788	-2.459616	0.000000
C	0.000098	-1.050232	0.000000
C	1.223203	-1.741424	0.000000
C	3.119946	0.118695	0.000000
H	2.794192	0.684634	0.879262
H	4.213769	0.093432	0.000000
H	2.794192	0.684634	-0.879262
C	2.922806	-4.997814	0.000000
H	2.518876	-5.510292	0.879837
H	2.518876	-5.510292	-0.879837
H	4.010831	-5.095942	0.000000
C	-3.119564	0.118939	0.000000
H	-2.793739	0.684841	0.879262
H	-2.793739	0.684841	-0.879262
H	-4.213390	0.093808	0.000000
C	-2.922891	-4.997605	0.000000
H	-2.519001	-5.510115	-0.879837
H	-2.519001	-5.510115	0.879837
H	-4.010923	-5.095647	0.000000
C	0.000084	0.445007	0.000000
C	0.000027	1.154722	1.207457
C	0.000027	1.154722	-1.207457
C	-0.000023	2.551702	1.214921
H	0.000031	0.617545	2.151425
C	-0.000023	2.551702	-1.214921
H	0.000031	0.617545	-2.151425
C	-0.000039	3.235635	0.000000

H	-0.000054	3.085914	2.158356
H	-0.000054	3.085914	-2.158356
I	-0.000133	5.384527	0.000000

I_2-BDP

C	-2.524478	-1.588472	0.013997
C	-3.360332	-0.449038	0.001467
C	-2.579630	0.706509	0.008979
C	-1.223949	0.236393	0.024116
N	-1.245107	-1.163249	0.027706
B	0.000042	-2.093073	0.056767
F	-0.000825	-2.857934	1.228973
F	0.000958	-2.931072	-1.058931
N	1.245208	-1.163167	0.029245
C	1.223920	0.236486	0.024446
C	2.524595	-1.588260	0.015590
C	2.579588	0.706710	0.008200
C	3.360355	-0.448757	0.001661
C	-0.000033	0.930877	0.025799
C	-0.000095	2.425623	0.021187
C	-0.003371	3.128480	-1.191670
C	0.003095	3.135359	1.230123
C	-0.003336	4.525024	-1.193740
H	-0.005835	2.581793	-2.130489
C	0.002929	4.531916	1.224158
H	0.005605	2.594078	2.172061
C	-0.000232	5.228951	0.013186
H	-0.005779	5.060934	-2.138596
H	0.005317	5.073251	2.165913
H	-0.000283	6.315170	0.010090
I	-5.477865	-0.533506	-0.033884
I	5.477848	-0.533397	-0.034314
C	3.081166	2.118114	-0.001111
H	2.737035	2.663288	-0.885605
H	2.732581	2.676663	0.872924
H	4.173400	2.129138	0.001082
C	2.890020	-3.035458	0.001970
H	2.648381	-3.482811	-0.969146
H	3.956491	-3.168089	0.189977

H	2.319775	-3.578873	0.760193
C	-3.081317	2.117890	0.001645
H	-2.725617	2.677841	0.871841
H	-2.744473	2.661658	-0.886578
H	-4.173500	2.128896	0.012540
C	-2.889399	-3.035795	-0.000032
H	-3.957960	-3.168392	0.175466
H	-2.635151	-3.485787	-0.966610

BDP

C	-1.902799	2.530811	-0.000006
C	-0.774825	3.373079	0.000140
C	0.370128	2.581807	0.000111
C	-0.088755	1.222637	-0.000014
N	-1.491362	1.244181	-0.000090
H	-0.806033	4.455200	0.000246
B	-2.416594	0.000076	-0.000251
N	-1.491462	-1.244103	-0.000046
C	-1.903018	-2.530697	0.000127
C	-0.088851	-1.222683	0.000023
C	-0.775126	-3.373067	0.000103
C	0.369905	-2.581901	-0.000042
H	-0.806432	-4.455184	0.000141
F	-3.226621	0.000128	1.143578
F	-3.226156	0.000093	-1.144437
C	1.771001	-3.118514	-0.000192
H	2.336666	-2.790917	-0.878774
H	2.336699	-2.791290	0.878507
H	1.746093	-4.212356	-0.000417
C	-3.344355	-2.924786	0.000330
H	-3.857328	-2.522544	0.880577
H	-3.857934	-2.521235	-0.878948
H	-3.440856	-4.012930	-0.000409
C	1.771288	3.118256	0.000267
H	2.336883	2.790630	0.878886
H	2.336975	2.790918	-0.878396
H	1.746513	4.212101	0.000444
C	-3.344099	2.925037	0.000064

H	-3.857650	2.521474	-0.879225
H	-3.857176	2.522903	0.880299
H	-3.440496	4.013190	-0.000756
C	0.603600	-0.000045	0.000024
C	2.099055	-0.000072	0.000038
C	2.806796	0.000076	1.209830
C	2.806820	-0.000186	-1.209741
C	4.203170	0.000088	1.208500
H	2.262841	0.000196	2.150338
C	4.203195	-0.000207	-1.208382
H	2.262885	-0.000284	-2.150259
C	4.903916	-0.000069	0.000066
H	4.741755	0.000208	2.152003
H	4.741800	-0.000319	-2.151874
H	5.990252	-0.000070	0.000077

2. PCM-M06-2X geometries

o-I-BDP

C	-2.440068	2.515941	0.059318
C	-1.337994	3.360394	0.302212
C	-0.241043	2.566349	0.604665
C	-0.704507	1.217170	0.540486
N	-2.055936	1.239747	0.199825
H	-1.357730	4.441100	0.254516
B	-2.978853	0.000003	0.056517
N	-2.055940	-1.239731	0.199730
C	-2.440055	-2.515925	0.059151
C	-0.704519	-1.217161	0.540437
C	-1.338002	-3.360377	0.302084
C	-0.241085	-2.566341	0.604690
H	-1.357730	-4.441081	0.254336
C	-0.041886	0.000001	0.714219
C	1.390944	-0.000012	1.116113
C	1.701569	0.000000	2.480761
C	2.437120	-0.000041	0.193583
C	3.023908	-0.000031	2.909664
H	0.888421	0.000031	3.200672
C	3.765109	-0.000073	0.611121

C	4.055107	-0.000073	1.973068
H	3.247918	-0.000024	3.970875
H	4.567882	-0.000094	-0.117549
H	5.090427	-0.000100	2.297138
I	2.032110	0.000027	-1.893895
F	-3.945003	-0.000098	1.061090
F	-3.594878	0.000056	-1.189747
C	1.137384	-3.070740	0.904638
H	1.858794	-2.736450	0.151099
H	1.499975	-2.720250	1.875405
H	1.133910	-4.163035	0.910511
C	-3.835829	-2.889996	-0.312091
H	-4.552926	-2.374774	0.332835
H	-4.049569	-2.590420	-1.342536
H	-3.975952	-3.967806	-0.219813
C	1.137451	3.070736	0.904514
H	1.500009	2.720403	1.875352
H	1.858855	2.736262	0.151055
H	1.134032	4.163031	0.910188
C	-3.835837	2.890009	-0.311960
H	-4.049123	2.591450	-1.342796
H	-4.553004	2.373915	0.332176
H	-3.976307	3.967685	-0.218633

***p*-I-BDP**

C	-3.530863	-2.516610	-0.030890
C	-2.403982	-3.361570	-0.062470
C	-1.265412	-2.568451	-0.046084
C	-1.728425	-1.217607	0.000190
N	-3.122948	-1.240544	0.005569
H	-2.435396	-4.442458	-0.098534
B	-4.055626	-0.000921	0.031914
F	-4.899804	-0.011812	-1.073956
F	-4.812170	0.009540	1.202238
N	-3.124324	1.239071	-0.010928
C	-3.533941	2.515295	-0.001441
C	-1.268654	2.569904	0.023629
C	-2.408417	3.361941	0.019004
H	-2.441215	4.443294	0.033585
C	-1.042195	0.000558	0.003665

C	-1.729887	1.218129	0.000432
C	0.137554	3.087527	0.052623
H	0.652743	2.907531	-0.896055
H	0.125226	4.164946	0.232777
H	0.732776	2.610664	0.836636
C	-4.978839	2.887044	-0.010673
H	-5.462778	2.512166	-0.917216
H	-5.492792	2.434941	0.842396
H	-5.091741	3.970938	0.034148
C	0.141611	-3.083536	-0.078554
H	0.734969	-2.602440	-0.861483
H	0.657661	-2.905977	0.870062
H	0.131129	-4.160175	-0.263278
C	-4.974922	-2.891294	-0.052600
H	-5.516079	-2.371243	0.742243
H	-5.430397	-2.598286	-1.003439
H	-5.088197	-3.968445	0.076900
C	0.445116	0.001014	0.003507
C	1.145360	0.202633	-1.186508
C	1.146157	-0.200970	1.192917
C	2.537977	0.199556	-1.193928
H	0.601457	0.361365	-2.113167
C	2.538855	-0.198338	1.199157
H	0.603023	-0.359911	2.119956
C	3.220440	0.000492	0.002365
H	3.075486	0.353089	-2.122839
H	3.077065	-0.352185	2.127607
I	5.345258	0.000061	0.001454

I_2-BDP

C	-2.507068	-1.580740	-0.006708
C	-3.346682	-0.446712	0.010780
C	-2.568297	0.703683	0.057841
C	-1.219582	0.234978	0.047717
N	-1.238233	-1.157469	0.019773
B	0.001250	-2.091362	0.106754
F	-0.035023	-2.820099	1.291262
F	0.037037	-2.948305	-0.981798
N	1.242149	-1.154251	0.093080

C	1.218733	0.238193	0.054273
C	2.511291	-1.573980	0.065755
C	2.565636	0.709956	-0.016462
C	3.347149	-0.438184	-0.000922
C	-0.000876	0.926627	0.053259
C	-0.001734	2.411884	0.041295
C	-0.290428	3.099355	-1.139751
C	0.287520	3.118801	1.210455
C	-0.282880	4.491600	-1.150678
H	-0.515589	2.541555	-2.044360
C	0.280190	4.511194	1.198027
H	0.513147	2.576374	2.124198
C	-0.001301	5.197822	0.017913
H	-0.500705	5.024148	-2.070632
H	0.498202	5.059020	2.108918
H	-0.001221	6.282908	0.008891
I	-5.441125	-0.530425	-0.050419
I	5.440391	-0.529863	-0.081332
C	3.063838	2.117882	-0.106664
H	2.464850	2.715428	-0.797121
H	3.029794	2.613567	0.868831
H	4.100289	2.121060	-0.450881
C	2.880813	-3.017364	0.070561
H	2.894458	-3.407755	-0.952684
H	3.874428	-3.153857	0.501109
H	2.154748	-3.593920	0.645460
C	-3.075880	2.109754	0.123220
H	-2.480155	2.724226	0.801004
H	-3.050080	2.587549	-0.861657
H	-4.111695	2.110628	0.469983
C	-2.865139	-3.025917	-0.065822
H	-3.896696	-3.178121	0.254465
H	-2.760842	-3.399452	-1.089792
H	-2.197644	-3.606571	0.573648

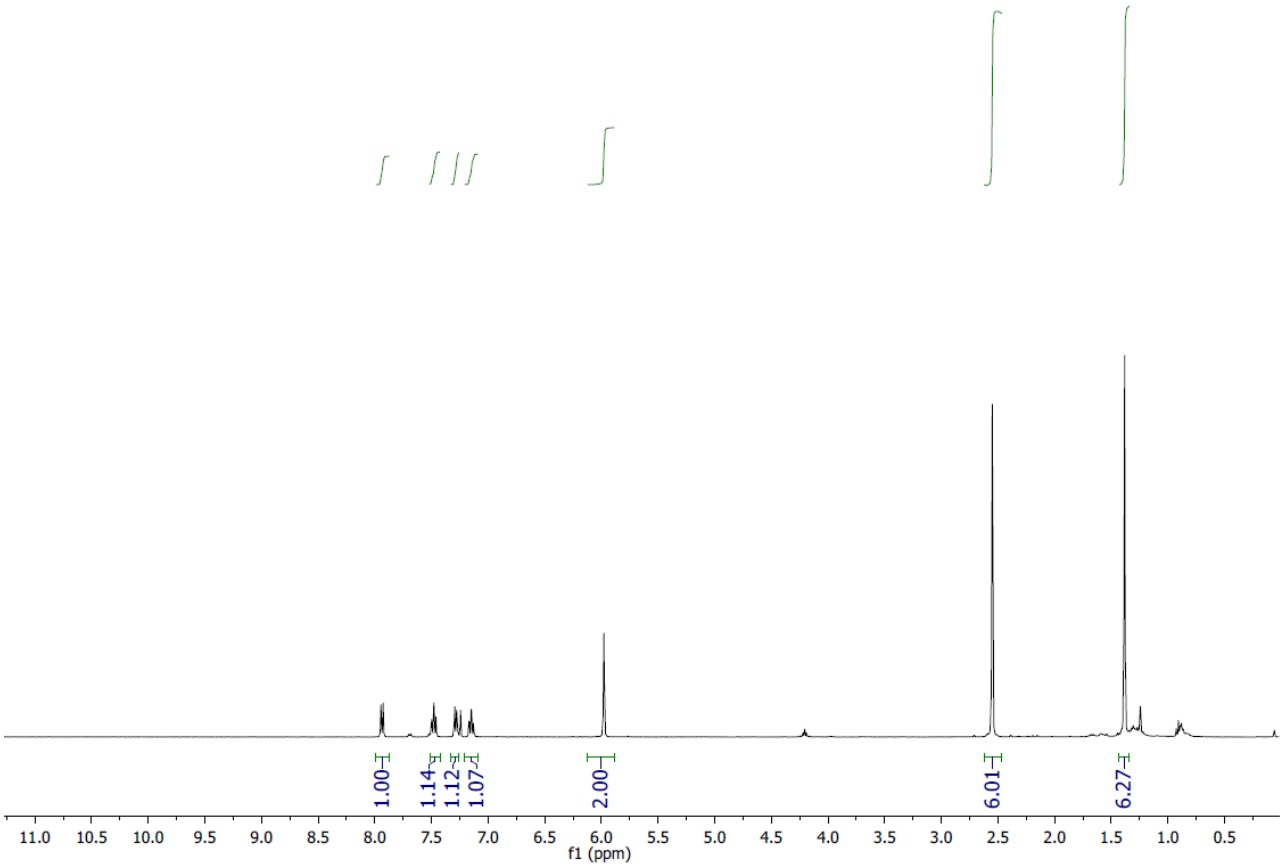
BDP

C	1.893789	2.515839	0.004791
C	0.768110	3.361682	-0.012965

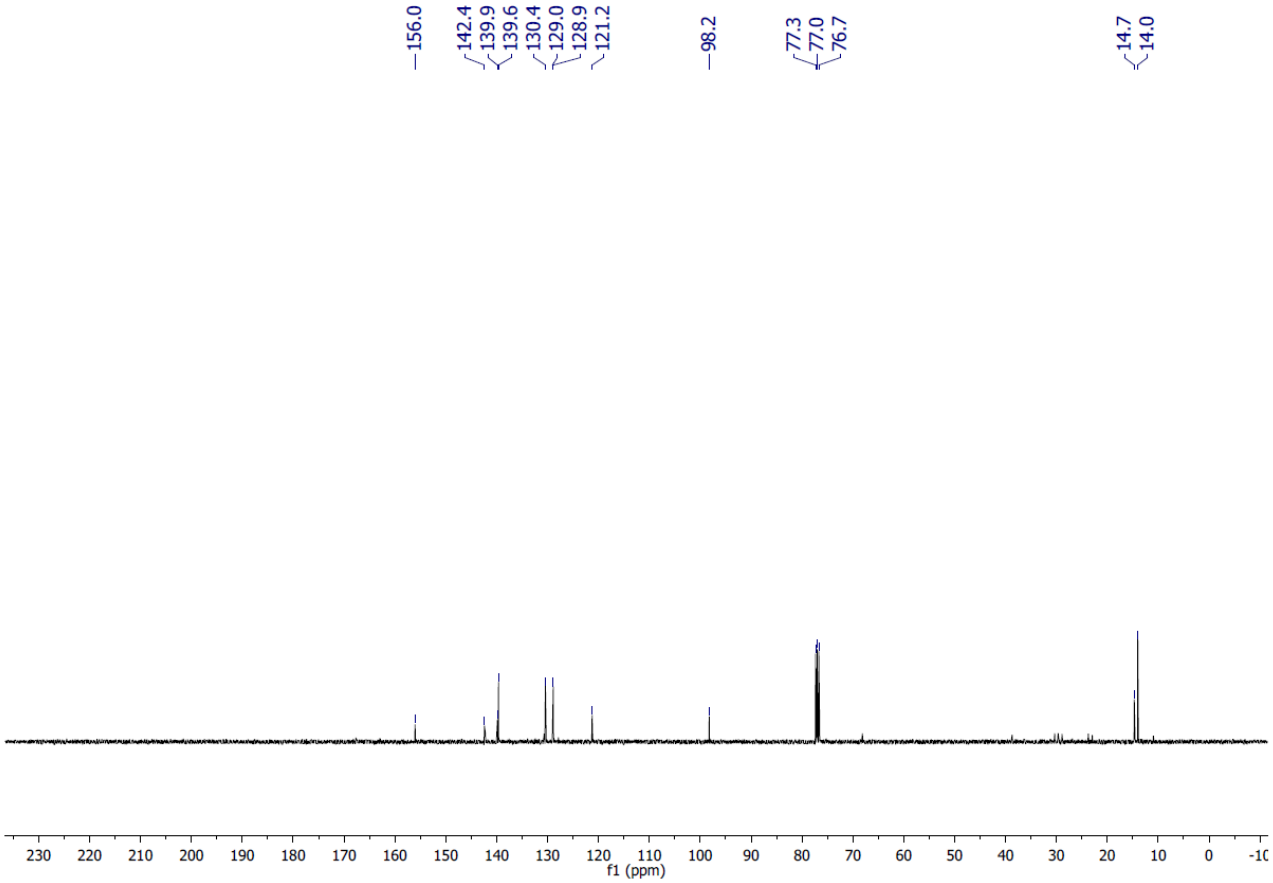
C	-0.371500	2.569063	-0.019721
C	0.089912	1.217690	-0.001115
N	1.484809	1.239159	0.009809
H	0.800566	4.443280	-0.024159
B	2.415345	-0.001521	-0.038423
N	1.482878	-1.241138	-0.003089
C	1.890085	-2.517598	0.035079
C	0.088000	-1.217477	-0.000483
C	0.762986	-3.361591	0.065118
C	-0.375397	-2.567744	0.045560
H	0.793894	-4.442658	0.102010
F	3.162082	0.005285	-1.215172
F	3.268227	-0.009423	1.059982
C	-1.782955	-3.081522	0.074350
H	-2.375069	-2.604125	0.860427
H	-2.298960	-2.893905	-0.872239
H	-1.773976	-4.159646	0.250609
C	3.334022	-2.893421	0.059037
H	3.876356	-2.375414	-0.736373
H	3.789309	-2.599448	1.009613
H	3.446278	-3.970896	-0.068845
C	-1.778086	3.085777	-0.045775
H	-2.371745	2.613202	-0.833483
H	-2.293863	2.895556	0.900479
H	-1.766728	4.164741	-0.216864
C	3.338160	2.890258	0.023195
H	3.800687	2.582273	0.965684
H	3.873765	2.382700	-0.783619
H	3.450522	3.969146	-0.091602
C	-0.599320	0.000526	-0.005378
C	-2.087170	0.001200	-0.005986
C	-2.785790	-0.185239	-1.200529
C	-2.786144	0.187425	1.188459
C	-4.178456	-0.180734	-1.199490
H	-2.235775	-0.331756	-2.126051
C	-4.178725	0.182925	1.187215
H	-2.236224	0.333557	2.114144
C	-4.875556	0.001099	-0.006237
H	-4.718397	-0.321585	-2.130388
H	-4.718846	0.323648	2.118033
H	-5.960888	0.001075	-0.006353

NMR spectra of *o*-I-BDP

^{1}H-NMR:



^{13}C-NMR:



^{19}F-NMR: