Electronic structure and second-order nonlinear optical properties of linear [3]spirobifluorenylene compounds

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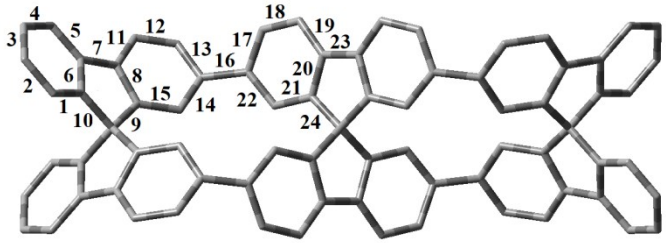
Table S1. The selected bond lengths for compound **1** between experiment and calculation.



Optimized geometry of compound **1** (not show hydrogens)

Bond	B3LYP-D3	Experiment（	Difference
1	1.385	1.384	0.001
2	1.399	1.394	0.005
3	1.399	1.387	0.012
4	1.397	1.384	0.013
5	1.395	1.402	-0.007
6	1.409	1.404	0.005
7	1.467	1.457	0.010
8	1.411	1.415	-0.004
9	1.526	1.531	-0.005
10	1.543	1.543	0.000
11	1.396	1.392	0.004
12	1.393	1.378	0.015
13	1.410	1.419	-0.009
14	1.411	1.406	0.005
15	1.387	1.379	0.008
16	1.490	1.486	0.004
17	1.413	1.411	0.002
18	1.387	1.371	0.016

19	1.394	1.394	0.000
20	1.406	1.396	0.010
21	1.391	1.376	0.015
22	1.412	1.412	0.000
23	1.456	1.451	0.005
24	1.540	1.555	-0.015

Note: the difference is equal to calculation value minus experimental value

Table S2. The computed absorption wavelengths (λ, nm) using the B3LYP functional at the different basis sets level for compound **1** along with the experimental values.

Basis set	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	Exp
λ_1	389.62	397.32	398.13	380
λ_2	410.66	419.56	420.12	405

Table S3. The computed absorption wavelengths (λ, nm) in gas and solution (in parentheses) phases, using the different functionals at 6-31G(d, p) basis set level for compound **1** along with the experimental values.

Functional	B3LYP	CAM-B3LYP	M06-2X	BH&HLYP	Exp
λ_1	389.62（397.39）	341.00	340.65	345.74	380
λ_2	410.66（412.39）				405