Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Crystal structures, intermolecular interactions and fluorescence properties of a series of symmetrical bi-1,3,4-oxadiazole derivatives

Fangyi Chen,[a] Taiji Tian,[a] Binglian Bai,[b] Jian Wang,[c] Haitao Wang*[a] and Min Li*[a]

[a] Key Laboratory of Automobile Materials (MOE) & College of Materials Science and Engineering, Jilin University, Changchun 130012, China

[b] College of Physics, Jilin University, Changchun 130012, China

[c] Institute of Theoretical Chemistry, Jilin University, Changchun 130023, China

Contents

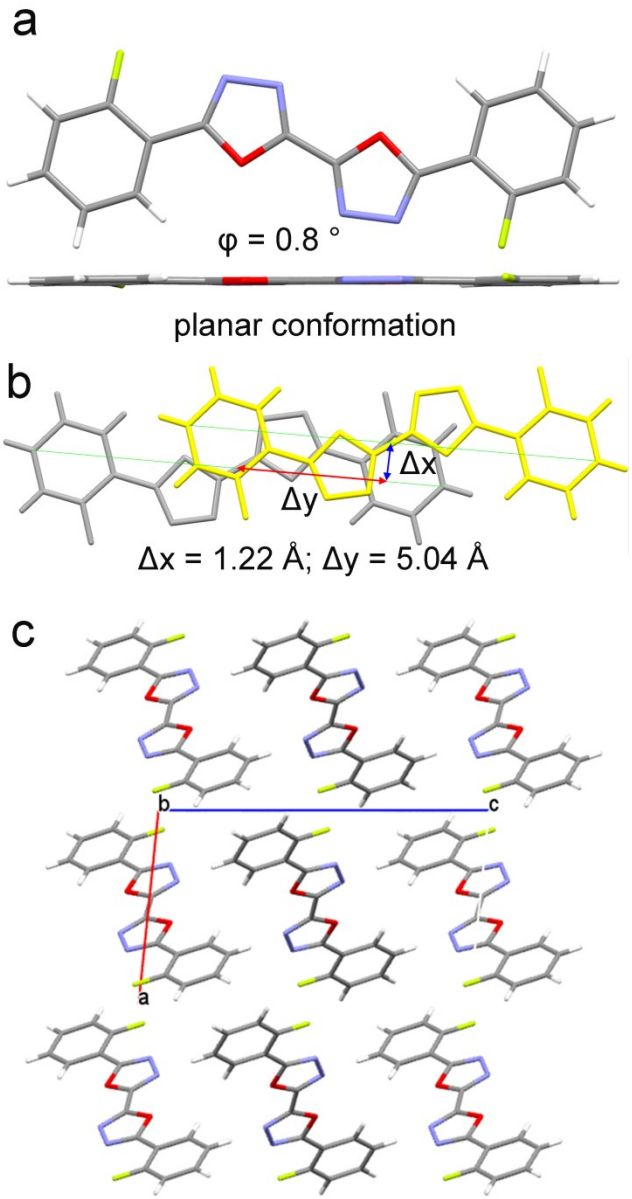

Figure S1 (a) Single crystal structure of BOXD-*o*-F; (b) top view of the nearest dimer along the π-stacking direction of BOXD-*o*-F; (c) the crystal packing of BOXD-*o*-F viewed on the b axis.

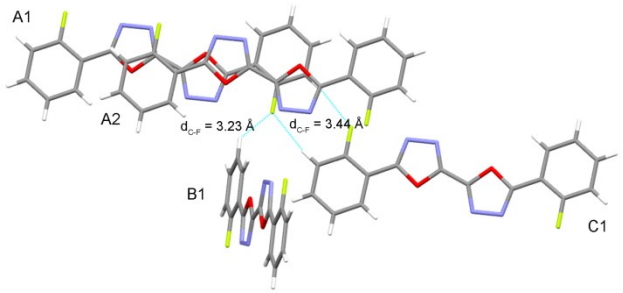

Figure S2 Other short contacts than π-π stacking interactions found in BOXD-*o*-F crystals.

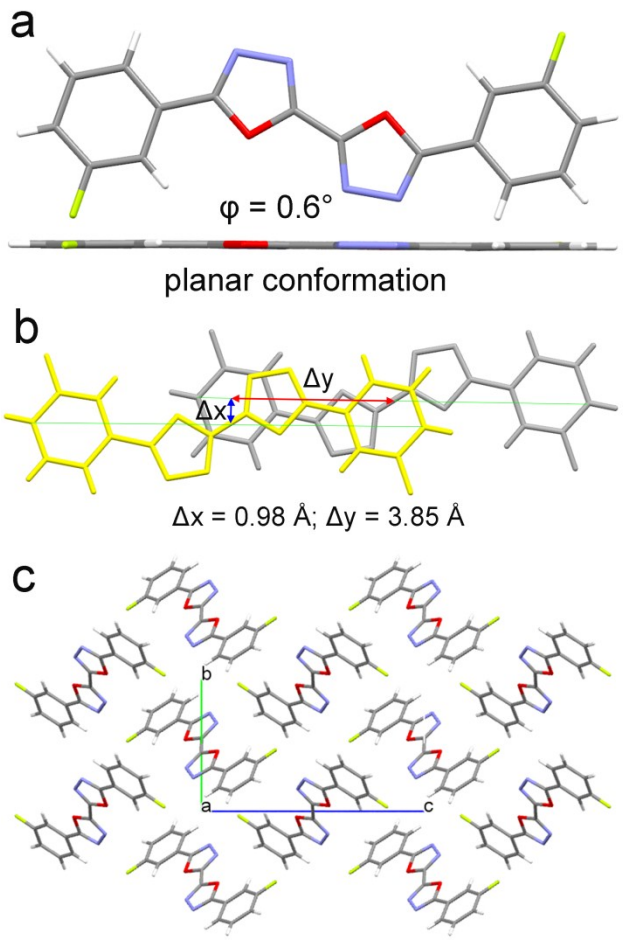

Figure S3 (a) Single crystal structure of BOXD-*m*-F; (b) top view of the nearest dimer along the π-stacking direction of BOXD-*m*-F; (c) the crystal packing of BOXD-*m*-F viewed on the a axis.

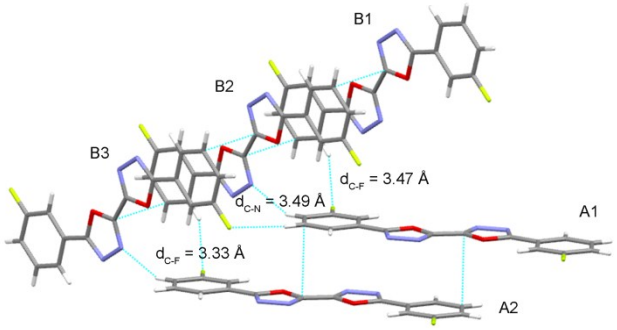

Figure S4 Other short contacts than π-π stacking interactions found in BOXD-*m*-F crystals.

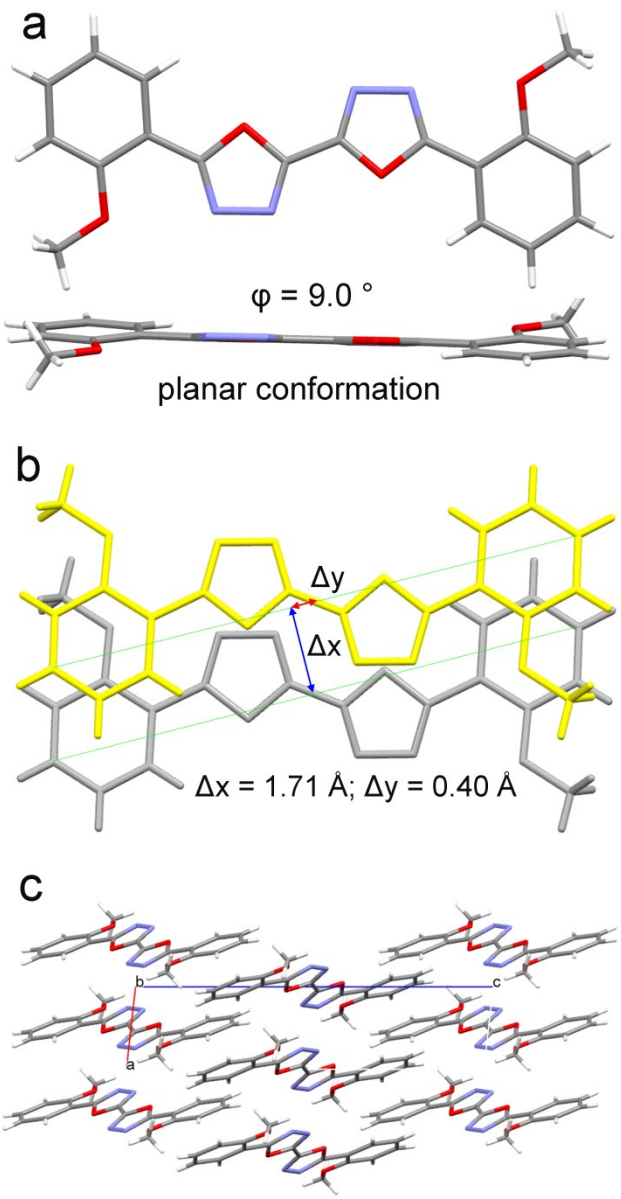

Figure S5 (a) Single crystal structure of BOXD-*o*-OCH_3; (b) top view of the nearest dimer along the π-stacking direction of BOXD-*o*-OCH_3; (c) the crystal packing of BOXD-*o*-OCH_3 viewed on the b axis.

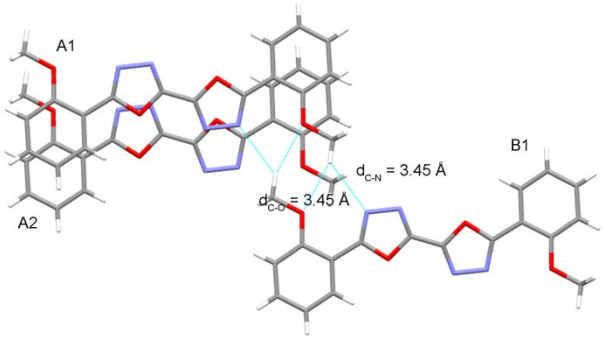

Figure S6 Other short contacts than π-π stacking interactions found in BOXD-*o*-OCH_3 crystals.

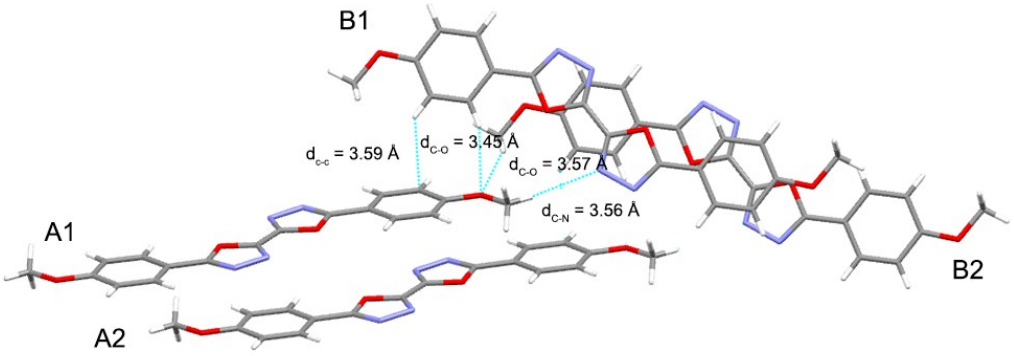

Figure S7 Other short contacts than π-π stacking interactions found in BOXD-1 crystals.

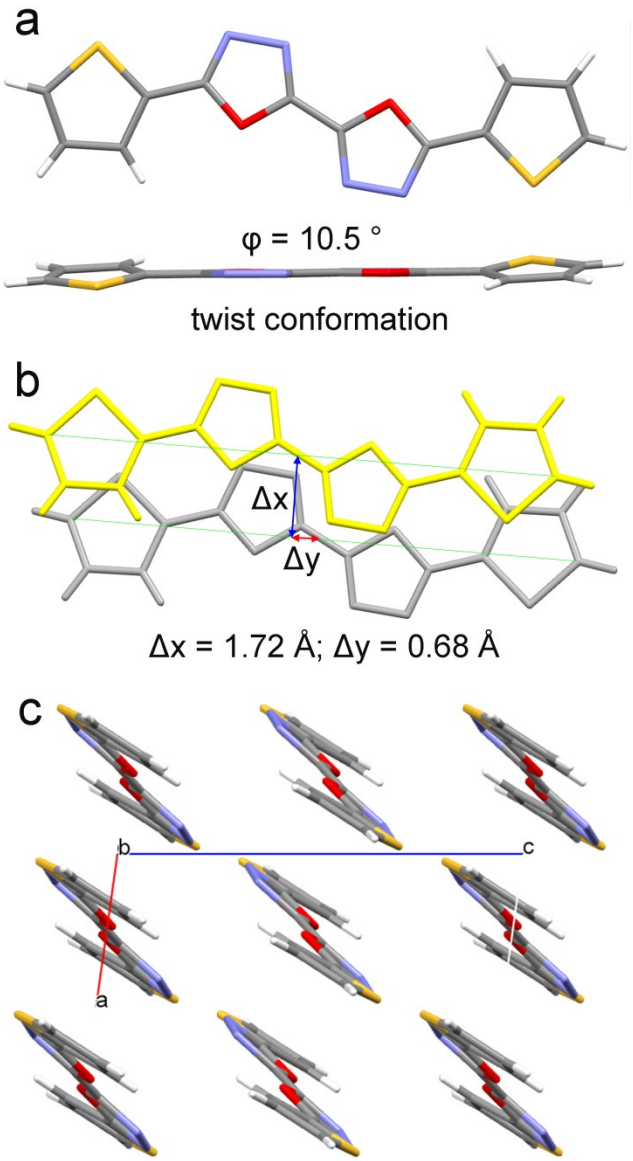

Figure S8 (a) Single crystal structure of TBOX; (b) top view of the nearest dimer along the π-stacking direction of TBOXD; (c) the crystal packing of TBOXD viewed on the b axis.

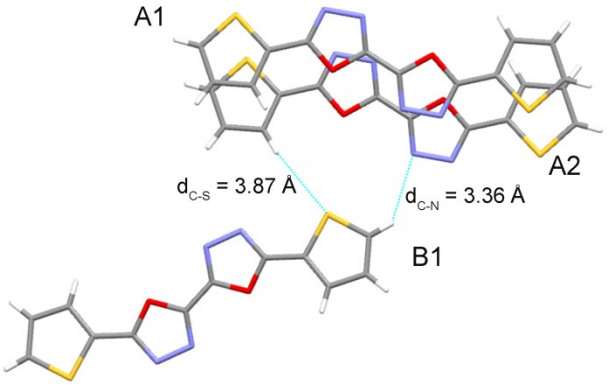

Figure S9 Other short contacts than π-π interactions found in TBOXD crystals.

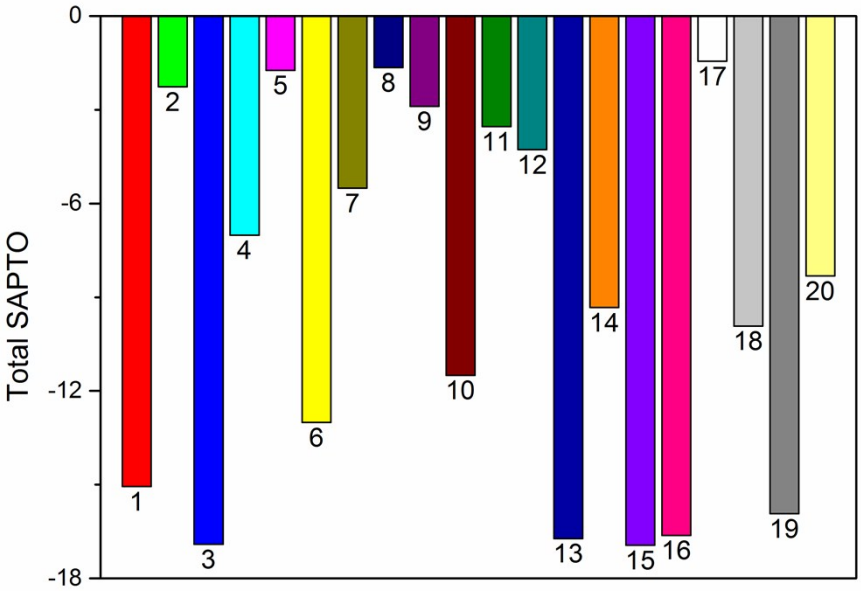

Figure S10 Calculated total SPAT0 energy of all the structures. The number stands for the structure corresponding with the number in table S3.

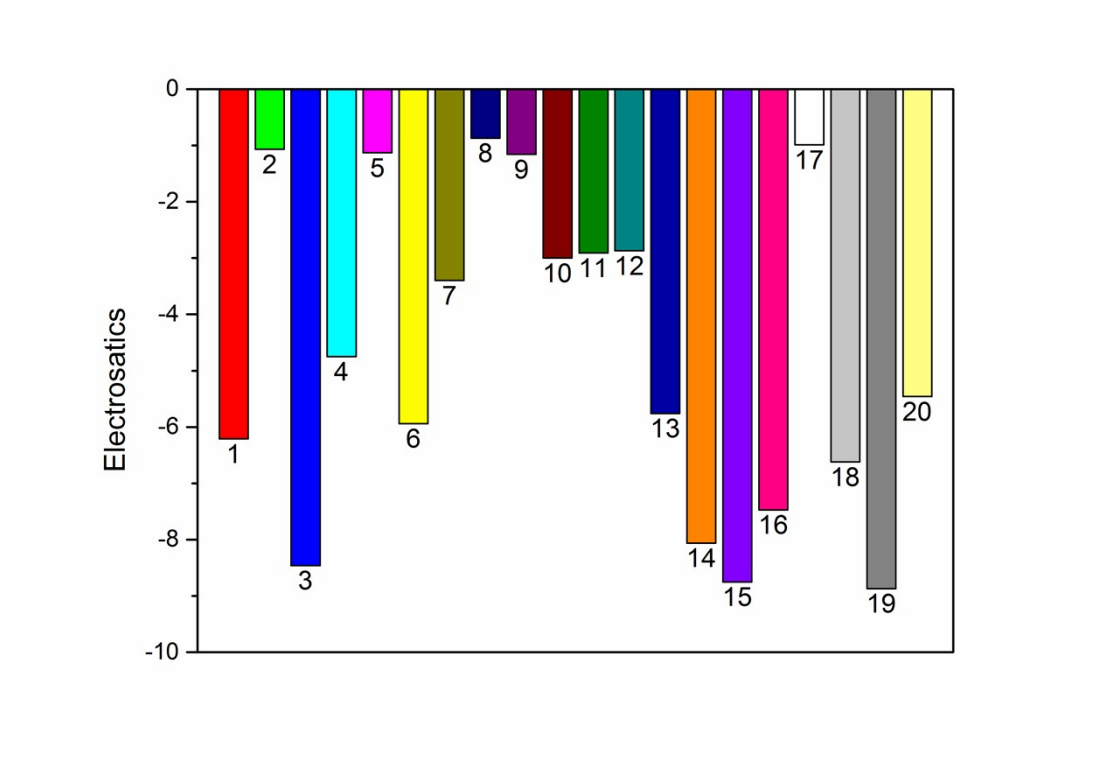

Figure S11 Calculated electrostatics of all the structures. The number stands for the structure corresponding with the number in table S3.

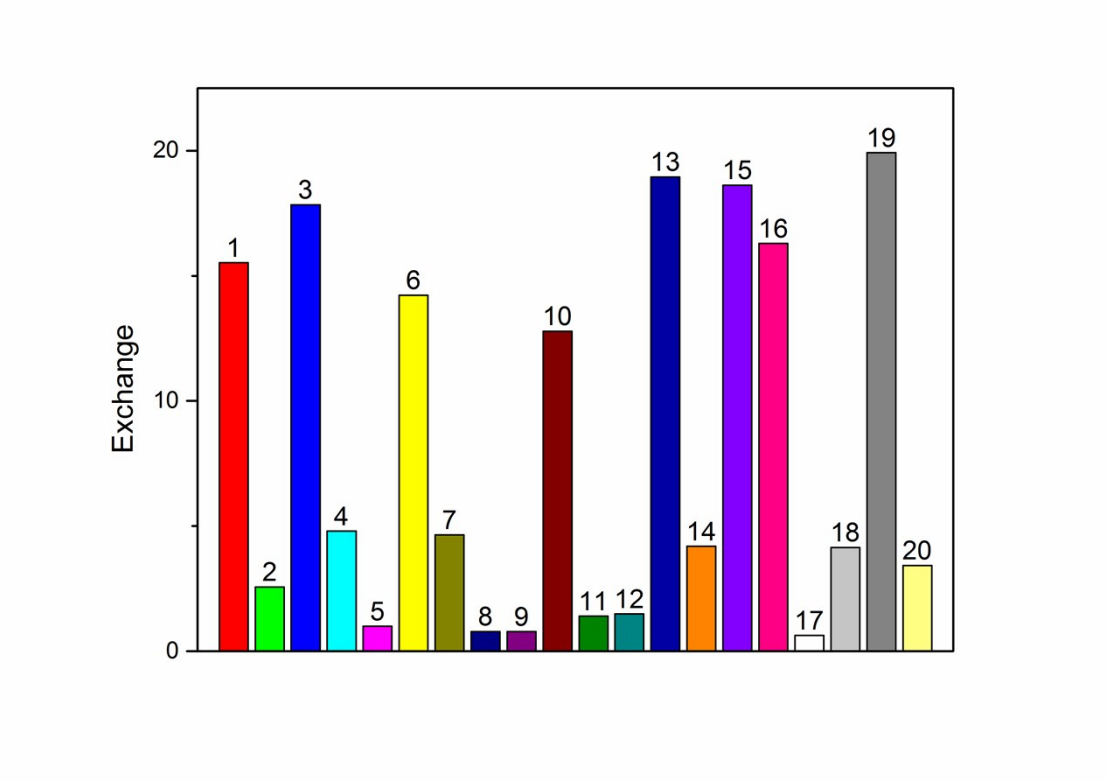

Figure S12 Calculated exchange of all the structures. The number stands for the structure corresponding with the number in table S3.

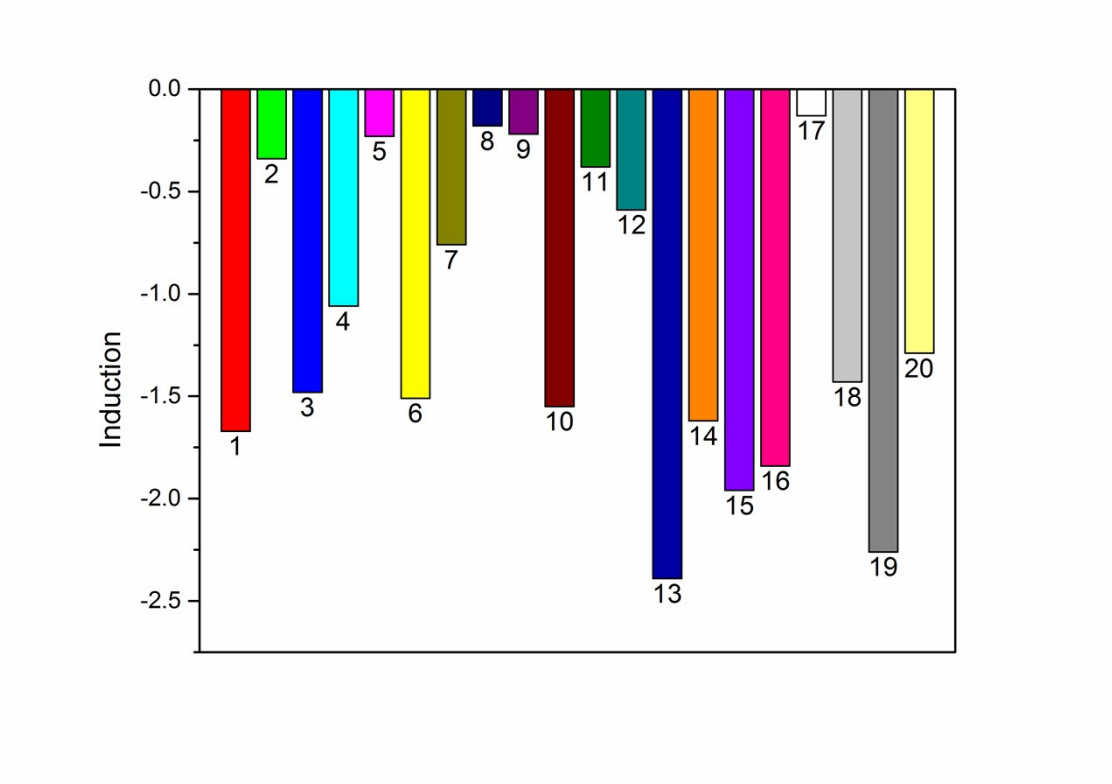

Figure S13 Calculated induction of all the structures. The number stands for the structure corresponding with the number in table S3.

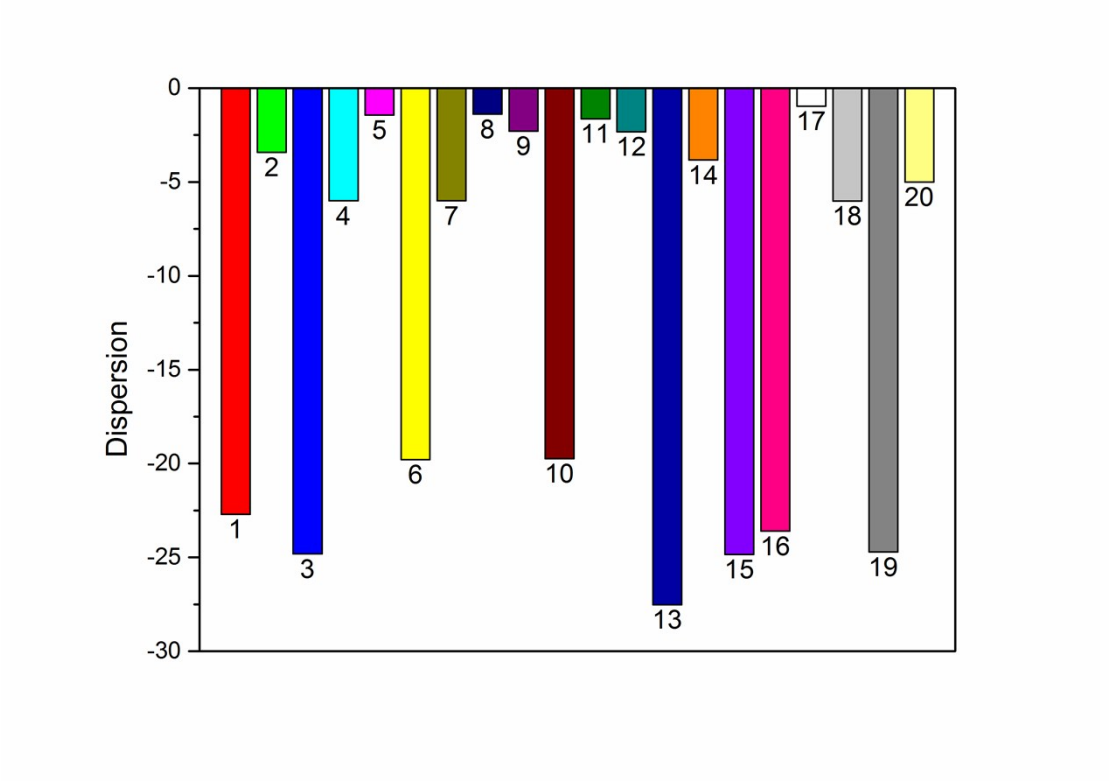

Figure S14 Calculated dispersion of all the structures. The number stands for the structure corresponding with the number in table S3.

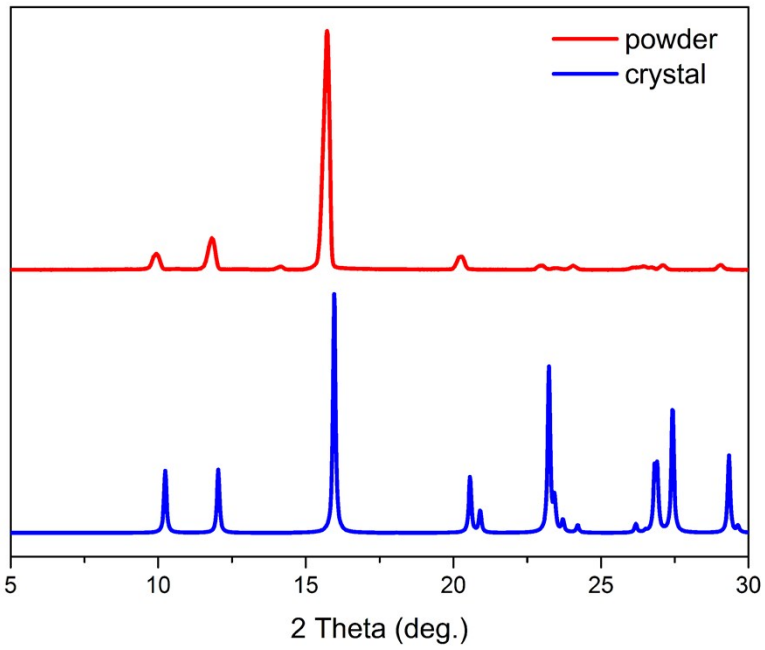

Figure S15 X-ray diffraction pattern of BOXD

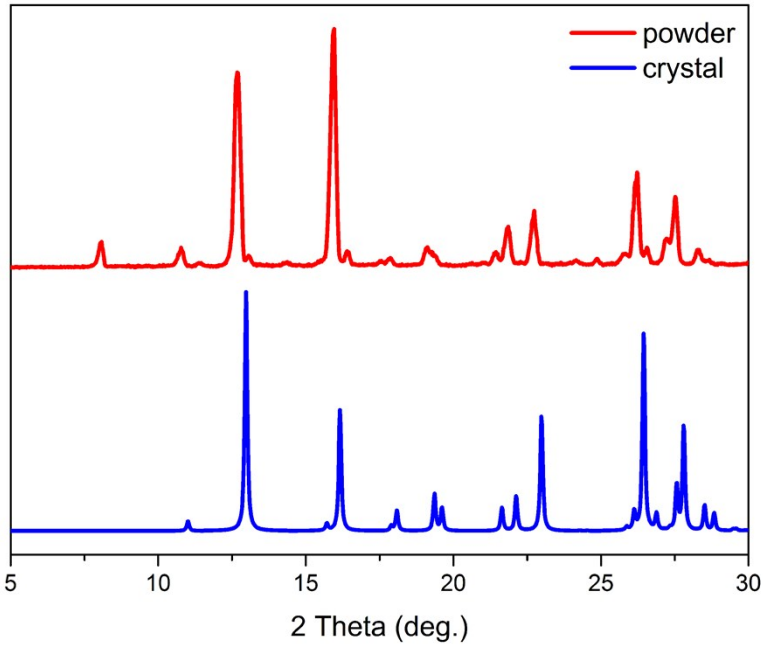

Figure S16 X-ray diffraction pattern of BOXD-*o*-F

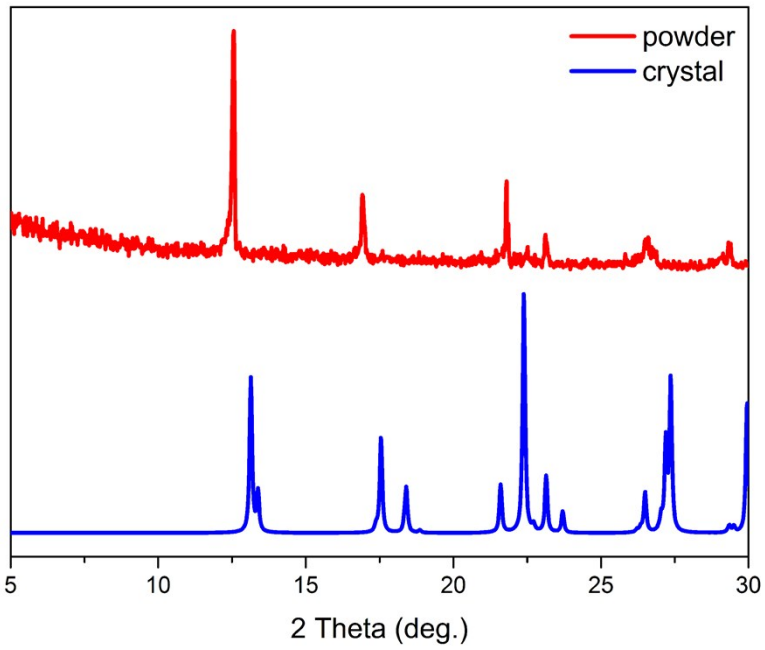

Figure S17 X-ray diffraction pattern of BOXD-*m*-F

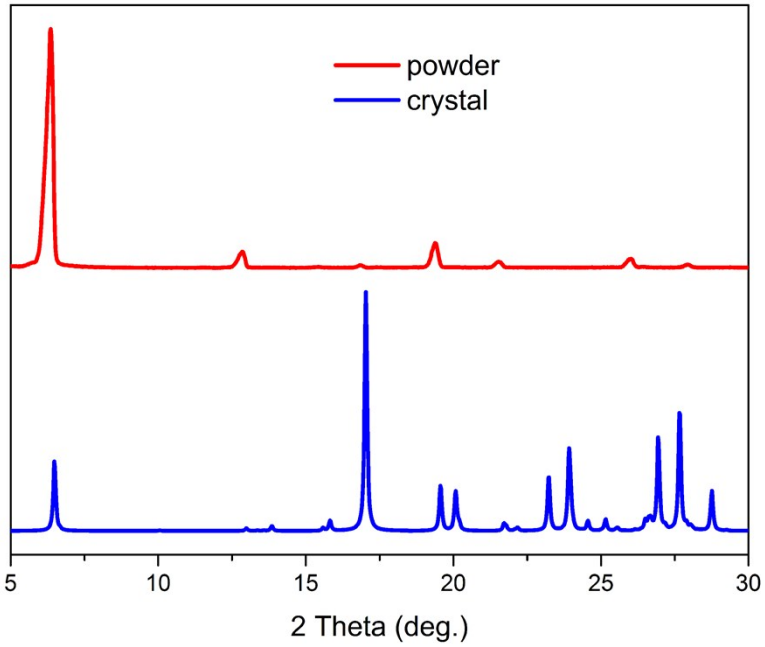

Figure S18 X-ray diffraction pattern of BOXD-*p*-F

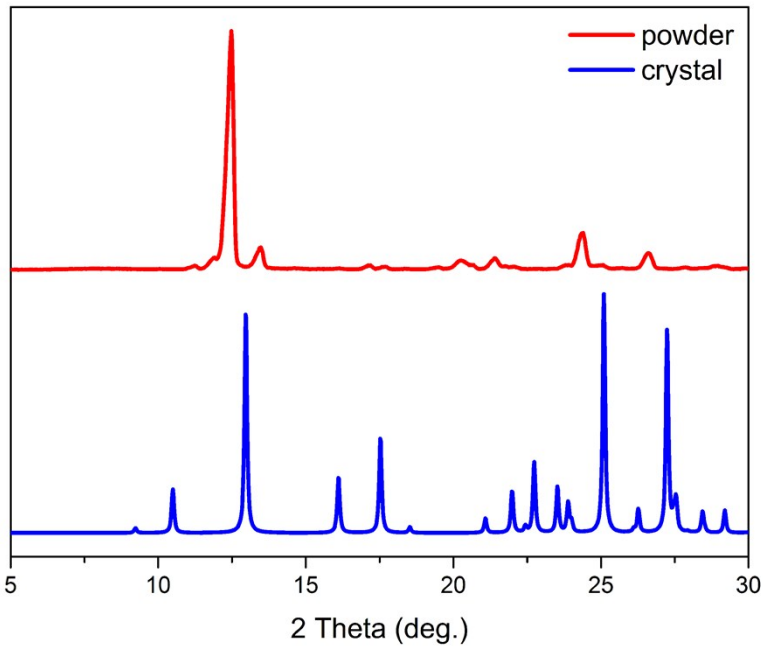

Figure S19 X-ray diffraction pattern of BOXD-*o*-OCH_3

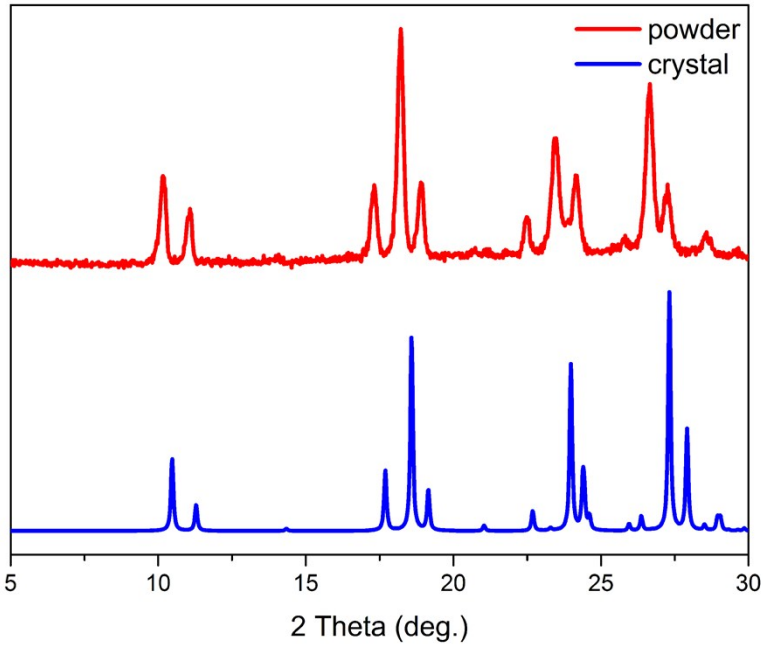

Figure S20 X-ray diffraction pattern of TBOXD

Table S1 Bond length of these bi-1,3,4-oxadiazole derivatives.

Length (Å)	BOXD	BOXD-*m*-F	BOXD-*o*-F	BOXD-*o*-OCH3	BOXD-*p*-F		TBOXD
O1-C8	1.359	1.35	1.34	1.35	1.35	1.36	1.36
O1-C7	1.37	1.36	1.37	1.37	1.36	1.37	1.37
N1-C7	1.30	1.28	1.29	1.29	1.29	1.29	1.29
N1-N2	1.40	1.40	1.40	1.40	1.41	1.40	1.40
N2-C8	1.28	1.27	1.27	1.28	1.28	1.28	1.29
C1-C2	1.37	1.36	1.38	1.38	1.36	1.36	1.36
C2-C3	1.38	1.37	1.38	1.38	1.38	1.38	1.42
C1-C6	1.38	1.38	1.38	1.38	1.36	1.36	-
C5-C6	1.38	1.38	1.37	1.39	1.38	1.37	-
C4-C5	1.39	1.39	1.39	1.40	1.39	1.40	-
C3-C4	1.39	1.38	1.39	1.40	1.38	1.38	1.38
C4-C7	1.45	1.46	1.46	1.45	1.45	1.44	1.38
C8-C8	1.44	1.45	1.46	1.45	1.44	1.43	1.43

Table S2 Bond angle of these bi-1,3,4-oxadiazole derivatives.

Angle (°)	BOXD	BOXD-*m*-F	BOXD-*o*-F	BOXD-*o*-OCH3	BOXD-*p*-F		TBOXD
C8-O1-C7	102.0	101.6	101.6	102.0	102.0	102.2	101.6
C7-N1-N2	106.5	106.1	106.6	106.6	106.3	106.6	106.1
C8-N2-N1	105.4	105.6	105.2	105.5	105.4	105.9	105.9
N1-C7-O1	112.1	112.6	111.9	111.7	112.3	111.7	112.9
NI-C7-C4	128.5	127.8	130.8	131.7	129.2	129.4	128.9
O1-C7-C4	119.2	119.4	117.2	116.4	118.3	118.8	118.1
N2-C8-O1	113.8	113.8	114.4	114.0	113.7	113.4	113.3
C1-C2-C3	120.6	123.4	119.8	119.1	118.2	118.6	112.8
C2-C1-C6	119.9	118.1	120.3	120.8	123.5	123.1	-
C1-C6-C5	120.2	120.6	119.2	120.6	118.1	118.2	-
C4-C5-C6	119.8	119.5	122.0	119.0	120.0	120.6	-
C3-C4-C5	119.6	120.7	117.8	118.8	119.7	119.3	-
C3-C4-C7	121.3	120.7	120.9	119.1	120.7	121.2	127.4
C5-C4-C7	119.0	118.5	121.4	121.9	119.4	119.4	-
C2-C3-C4	119.6	117.5	120.9	121.4	120.2	120.2	111.0
N2-C8-C8#1	128.1	128.0	128.0	128.0	128.2	128.5	128.4
01-C8-C8#1	117.9	118.1	117.5	117.9	118.1	118.1	118.3

TableS3 The calculated result of these bi-1,3,4-oxadiazole derivatives. .

Compound	No.	molecules	Total SAPT	Electrostatics	Exchange	Induction	Dispersion	Interaction	Distance (Å)
BOXD	1	A1A2	-15.06	-6.21	15.52	-1.67	-22.70	π-π	3.35
	2	A1B1	-2.27	-1.07	2.57	-0.34	-3.42	C-H-π	3.72
BOXD-1	3	A1A2	-16.91	-8.46	17.84	-1.48	-24.81	π-π	3.33
	4	A1B1	-7.01	-4.75	4.80	-1.06	-6.00	C-H-N,C-H-O,C-H-π	3.56,3.45,3.59
	5	A1B2	-1.74	-1.13	1.0	-0.23	-1.43	C-H-O	3.57
BOXD-*m*-F	6	A1A2	-13.01	-5.94	14.23	-1.51	-19.79	π-π	3.36
	7	A1B2	-5.51	-3.40	4.65	-0.76	-6.00	C-H-N	3.49
	8	A1B3	-1.65	-0.87	0.79	-0.18	-1.39	C-H-F	3.33
	9	A1B1	-2.89	-1.16	0.78	-0.22	-2.29	C-H-F	3.47
BOXD-*o*-F	10	A1A2	-11.50	-3.00	12.79	-1.55	-19.74	π-π	3.36
	11	A1C1	-3.54	-2.91	1.40	-0.38	-1.63	C-H-F	3.44
	12	A1B1	-4.28	-2.87	1.49	-0.59	-2.32	C-H-F	3.23
BOXD-*o*-OCH_3	13	A1A2	-16.72	-5.76	18.95	-2.39	-27.52	π-π	3.52
	14	A1B1	-9.33	-8.06	4.19	-1.62	-3.83	C-H-N, C-H-O	3.45, 3.45
BOXD-*p*-F	15	A1A2	-16.94	-8.75	18.62	-1.96	-24.84	π-π	3.36
	16	B1B2	-16.62	-7.47	16.29	-1.84	-23.60	π-π	3.44
	17	A1C1	-1.45	-0.99	0.63	-0.13	-0.96	C-H-F	3.38
	18	A2B1	-9.92	-6.62	4.15	-1.43	-6.01	C-H-N	3.32, 3.41
TBOXD	19	A1A2	-15.93	-8.87	19.92	-2.26	-24.71	π-π	3.37
	20	A1B1	-8.32	-5.46	3.43	-1.29	-5.00	C-H-S, C-H-N	3.87, 3.36