Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Experimental and Theoretical study on molecular aggregation and its effect on photo-physical properties of mesogenic bi-1,3,4-thiadiazole derivative

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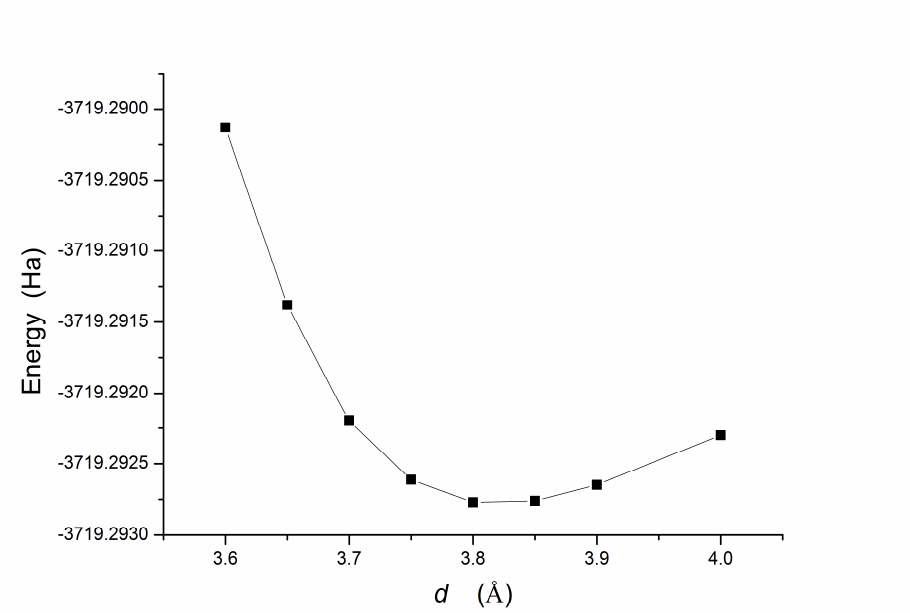

Figure S1 M062x/6-31G** Potential Energy Curve of BTD-1 dimer for the face-to-face molecular packing geometry.

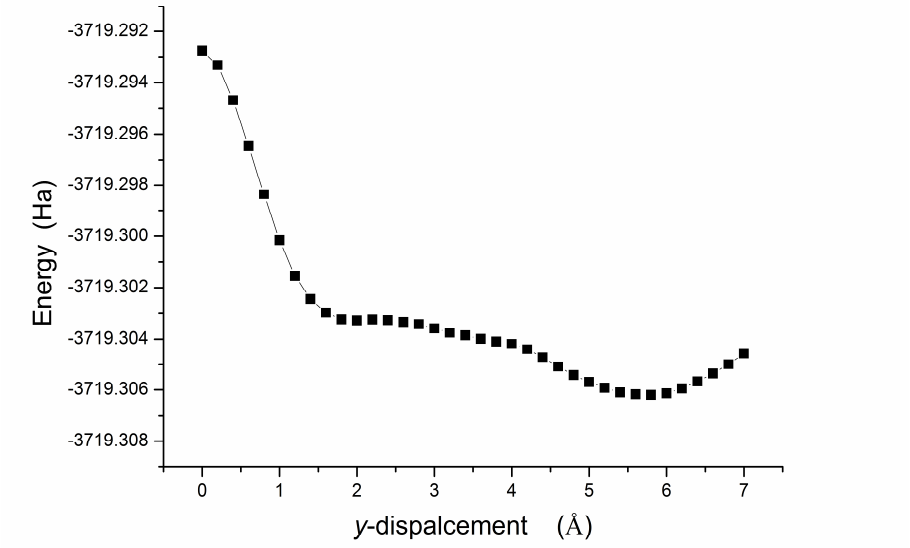

Figure S2 M062x/6-31G** Potential Energy Curve of BTD-1 dimer for the intermolecular displacement along molecular long axis.

Table S1 M062x/6-311+G** monomer Structure of BTD-1. Cartesian Coordinates in Å.

Energy (Ha)	-1859.96453340		
Atom	X	Y	Z
C	0.420814	3.059754	0.000000
C	-0.001151	0.726505	0.000000
N	-1.088265	1.434119	0.000000
N	-0.848498	2.764289	0.000000
S	1.457218	1.659486	0.000000
C	0.001151	-0.726505	0.000000
C	-0.420814	-3.059754	0.000000
N	0.848498	-2.764289	0.000000
N	1.088265	-1.434119	0.000000
S	-1.457218	-1.659486	0.000000
C	0.923889	4.436919	0.000000
C	0.013637	5.492960	0.000000
C	2.293950	4.726233	0.000000
C	0.449413	6.811391	0.000000
H	-1.045963	5.269251	0.000000
C	2.738758	6.033171	0.000000
H	3.022918	3.922689	0.000000
C	1.818694	7.086225	0.000000
H	-0.281146	7.608406	0.000000
H	3.795105	6.270411	0.000000
C	-0.923889	-4.436919	0.000000
C	-0.013637	-5.492960	0.000000
C	-2.293950	-4.726233	0.000000
C	-0.449413	-6.811391	0.000000
H	1.045963	-5.269251	0.000000
C	-2.738758	-6.033171	0.000000
H	-3.022918	-3.922689	0.000000
C	-1.818694	-7.086225	0.000000
H	0.281146	-7.608406	0.000000
H	-3.795105	-6.270411	0.000000
O	-2.347643	-8.330757	0.000000
C	-1.457218	-9.429652	0.000000
H	-0.826832	-9.425011	0.894193
H	-2.080578	10.320510	0.000000
H	-0.826832	-9.425011	-0.894193
O	2.347643	8.330757	0.000000
C	1.457218	9.429652	0.000000
H	2.080578	10.320510	0.000000
H	0.826832	9.425011	-0.894193

	H	0.826832	9.425011	0.894193

Table S2 M062x/6-31G** BTD-1 dimer Structure of minimum 1 (M1). Cartesian Coordinates in Å.

Energy (Ha)	-3719.314123731118		
Atom	X	Y	Z
C	-0.03596400	8.67952900	1.50000000
C	0.04519100	6.30982000	1.50000000
N	-1.16700800	6.77145500	1.50000000
N	-1.21404900	8.12224200	1.50000000
S	1.27319600	7.53018900	1.50000000
C	0.35480900	4.89018000	1.50000000
C	0.43596400	2.52047100	1.50000000
N	1.61404900	3.07775800	1.50000000
N	1.56700800	4.42854500	1.50000000
S	-0.87319600	3.66981100	1.50000000
C	0.16440300	10.13194800	1.50000000
C	-0.94864300	10.97153700	1.50000000
C	1.44225800	10.70453500	1.50000000
C	-0.80162800	12.35231500	1.50000000
H	-1.93694100	10.52874500	1.50000000
C	1.60053200	12.07599100	1.50000000
H	2.32470900	10.07338000	1.50000000
C	0.47852800	12.91058500	1.50000000
H	-1.68425300	12.97675200	1.50000000
H	2.58278800	12.53132000	1.50000000
C	0.23559700	1.06805200	1.50000000
C	1.34864300	0.22846300	1.50000000
C	-1.04225800	0.49546500	1.50000000
C	1.20162800	-1.15231500	1.50000000
H	2.33694100	0.67125500	1.50000000
C	-1.20053200	-0.87599100	1.50000000
H	-1.92470900	1.12662000	1.50000000
C	-0.07852800	-1.71058500	1.50000000
H	2.08425300	-1.77675200	1.50000000
H	-2.18278800	-1.33132000	1.50000000
O	-0.33224100	-3.03884600	1.50000000
C	0.77049200	-3.92451400	1.50000000
H	1.38563100	-3.78662700	2.39419300
H	0.34969000	-4.92707600	1.50000000
H	1.38563100	-3.78662700	0.60580700
O	0.73224100	14.23884600	1.50000000
C	-0.37049200	15.12451400	1.50000000
H	0.05031000	16.12707600	1.50000000
H	-0.98563100	14.98662700	0.60580700

H	-0.98563100	14.98662700	2.39419300
C	-0.23596443	3.07952914	-1.90000000
C	-0.15480861	0.70982049	-1.90000000
N	-1.36700839	1.17145469	-1.90000000
N	-1.41404934	2.52224245	-1.90000000
S	1.07319581	1.93018881	-1.90000000
C	0.15480861	-0.70982049	-1.90000000
C	0.23596443	-3.07952914	-1.90000000
N	1.41404934	-2.52224245	-1.90000000
N	1.36700839	-1.17145469	-1.90000000
S	-1.07319581	-1.93018881	-1.90000000
C	-0.03559736	4.53194814	-1.90000000
C	-1.14864325	5.37153742	-1.90000000
C	1.24225774	5.10453530	-1.90000000
C	-1.00162770	6.75231526	-1.90000000
H	-2.13694115	4.92874499	-1.90000000
C	1.40053211	6.47599085	-1.90000000
H	2.12470934	4.47338043	-1.90000000
C	0.27852814	7.31058511	-1.90000000
H	-1.88425316	7.37675233	-1.90000000
H	2.38278830	6.93131993	-1.90000000
C	0.03559736	-4.53194814	-1.90000000
C	1.14864325	-5.37153742	-1.90000000
C	-1.24225774	-5.10453530	-1.90000000
C	1.00162770	-6.75231526	-1.90000000
H	2.13694115	-4.92874499	-1.90000000
C	-1.40053211	-6.47599085	-1.90000000
H	-2.12470934	-4.47338043	-1.90000000
C	-0.27852814	-7.31058511	-1.90000000
H	1.88425316	-7.37675233	-1.90000000
H	-2.38278830	-6.93131993	-1.90000000
O	-0.53224063	-8.63884597	-1.90000000
C	0.57049221	-9.52451362	-1.90000000
H	1.18563064	-9.38662684	-1.00580700
H	0.14968966	-10.52707578	-1.90000000
H	1.18563064	-9.38662684	-2.79419300
O	0.53224063	8.63884597	-1.90000000
C	-0.57049221	9.52451362	-1.90000000
H	-0.14968966	10.52707578	-1.90000000
H	-1.18563064	9.38662684	-2.79419300
H	-1.18563064	9.38662684	-1.00580700

Table S3 M062x/6-31G** BTD-1 dimer Structure of minimum 2 (M2). Cartesian Coordinates in Å.

Energy (Ha)	-3719.310341853164		
Atom	X	Y	Z
C	-0.23596405	3.95594843	1.51367675
C	-0.15480900	1.58891787	1.62631375
N	-1.36700801	2.05003107	1.60437134
N	-1.41404904	3.39929130	1.54016573
S	1.07319597	2.80790753	1.56830716
C	0.15480902	0.17088247	1.69379208
C	0.23596407	-2.19614808	1.80642909
N	1.41404906	-1.63949095	1.77994010
N	1.36700803	-0.29023072	1.71573449
S	-1.07319595	-1.04810718	1.75179868
C	-0.03559708	5.40672578	1.44464036
C	-1.14864310	6.24536579	1.40473303
C	1.24225791	5.97866562	1.41742414
C	-1.00162812	7.62458312	1.33910189
H	-2.13694109	5.80307425	1.42577984
C	1.40053188	7.34857149	1.35223609
H	2.12470892	5.34822402	1.44742418
C	0.27852787	8.18222214	1.31256618
H	-1.88425314	8.24831431	1.30942117
H	2.38278787	7.80338586	1.33059337
C	0.03559710	-3.64692544	1.87546547
C	1.14864311	-4.48556544	1.91537280
C	-1.24225789	-4.21886527	1.90268170
C	1.00162814	-5.86478277	1.98100394
H	2.13694111	-4.04327390	1.89432599
C	-1.40053186	-5.58877114	1.96786975
H	-2.12470890	-3.58842368	1.87268165
C	-0.27852785	-6.42242179	2.00753965
H	1.88425315	-6.48851396	2.01068467
H	-2.38278785	-6.04358551	1.98951246
O	-0.53224082	-7.74918148	2.07067456
C	0.57049220	-8.63384841	2.11277211
H	1.18563121	-8.45361446	2.99940036
H	0.14969022	-9.63527723	2.16042590
H	1.18563118	-8.53862003	1.21303575
O	0.53224084	9.50898183	1.24943128
C	-0.57049218	10.39364875	1.20733372
H	-0.14969020	11.39507758	1.15967994
H	-1.18563119	10.21341481	0.32070547

H	-1.18563116	10.29842038	2.10707008
C	-0.23596407	2.19614808	-1.80642909
C	-0.15480902	-0.17088247	-1.69379208
N	-1.36700803	0.29023072	-1.71573449
N	-1.41404906	1.63949095	-1.77994010
S	1.07319595	1.04810718	-1.75179868
C	0.15480900	-1.58891787	-1.62631375
C	0.23596405	-3.95594843	-1.51367675
N	1.41404904	-3.39929130	-1.54016573
N	1.36700801	-2.05003107	-1.60437134
S	-1.07319597	-2.80790753	-1.56830716
C	-0.03559710	3.64692544	-1.87546547
C	-1.14864311	4.48556544	-1.91537280
C	1.24225789	4.21886527	-1.90268170
C	-1.00162814	5.86478277	-1.98100394
H	-2.13694111	4.04327390	-1.89432599
C	1.40053186	5.58877114	-1.96786975
H	2.12470890	3.58842368	-1.87268165
C	0.27852785	6.42242179	-2.00753965
H	-1.88425315	6.48851396	-2.01068467
H	2.38278785	6.04358551	-1.98951246
C	0.03559708	-5.40672578	-1.44464036
C	1.14864310	-6.24536579	-1.40473303
C	-1.24225791	-5.97866562	-1.41742414
C	1.00162812	-7.62458312	-1.33910189
H	2.13694109	-5.80307425	-1.42577984
C	-1.40053188	-7.34857149	-1.35223609
H	-2.12470892	-5.34822402	-1.44742418
C	-0.27852787	-8.18222214	-1.31256618
H	1.88425314	-8.24831431	-1.30942117
H	-2.38278787	-7.80338586	-1.33059337
O	-0.53224084	-9.50898183	-1.24943128
C	0.57049218	-10.39364875	-1.20733372
H	1.18563119	-10.21341481	-0.32070547
H	0.14969020	-11.39507758	-1.15967994
H	1.18563116	-10.29842038	-2.10707008
O	0.53224082	7.74918148	-2.07067456
C	-0.57049220	8.63384841	-2.11277211
H	-0.14969022	9.63527723	-2.16042590
H	-1.18563121	8.45361446	-2.99940036
H	-1.18563118	8.53862003	-1.21303575