Electronic Supplementary Information

Study of a carbazole–bromobenzothiadiazole derived fluorescent molecular rotor: crystal structure, redox activity, and solvatofluorochromic effects

Erin T. Chernick,*[a] Maryam F. Abdollahi,[b] Zahra A. Tabasi,[b] Marc J. Junge,[c] and Yuming Zhao*[b]

[a] Department of Chemistry, University of Victoria, Victoria, BC, Canada V8W 2Y2. Tel: +1 250 721 7154; E-mail: erinchernick@uvic.ca

[b]Department of Chemistry, Memorial University of Newfoundland, St. John's, NL, Canada A1B 3X7. Fax: 1 709 864 3702; Tel: +1 709 864 8747; Email: yuming@mun.ca

[c]Institut für Organische Chemie, Universitat Tübingen, 72076 Tübingen, Germany

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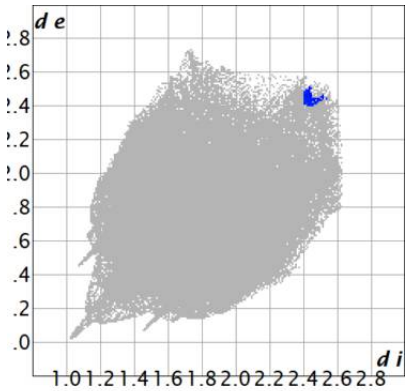
1. 2D Fingerprint Plot of 1



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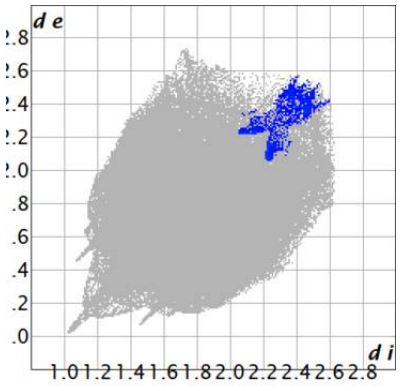

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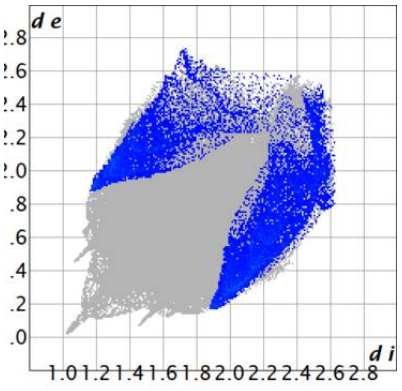

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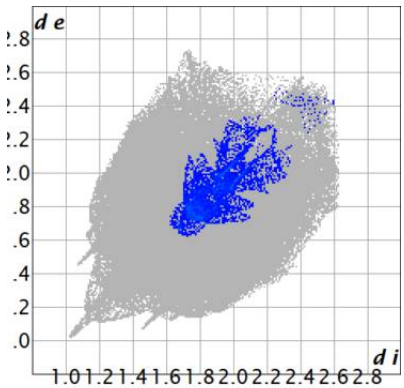

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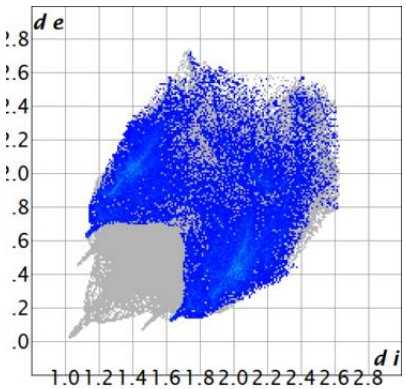

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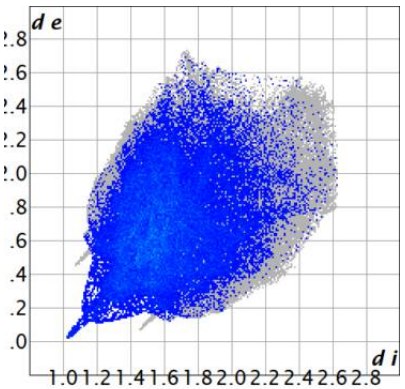

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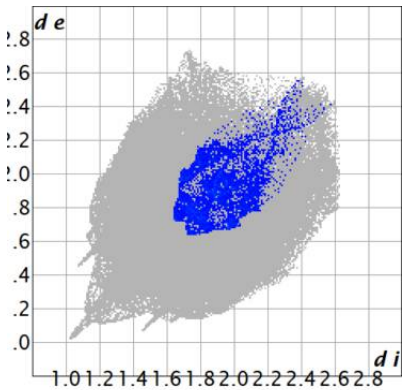

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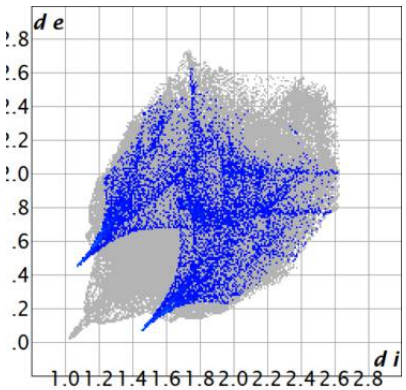

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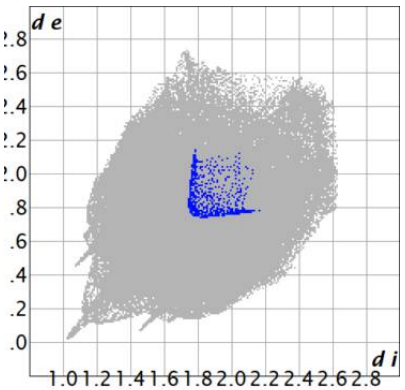

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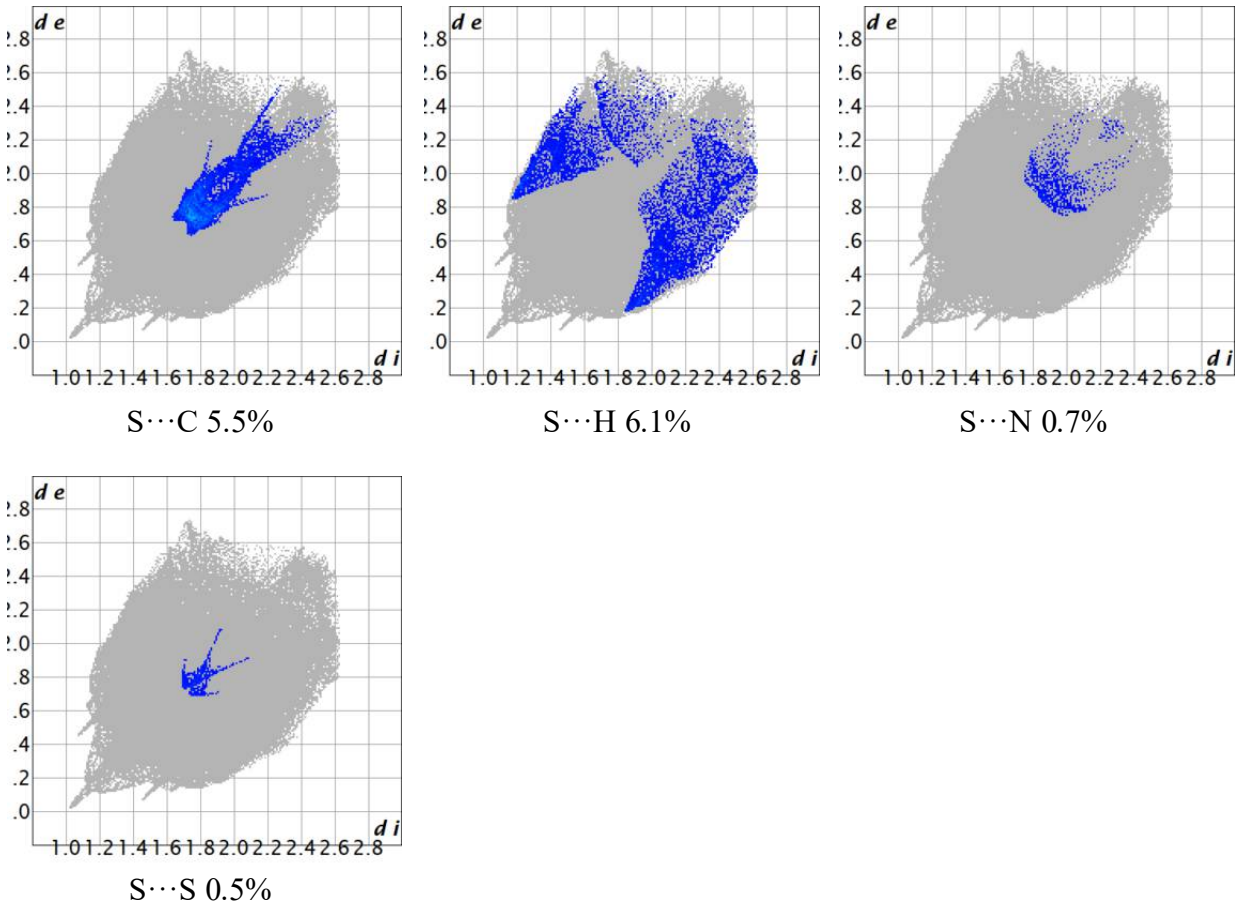

Figure S-1 2D fingerprint plots of **1** showing the contributions of different intermolecular contacts.

2. DFT and TD-DFT Optimized Geometries of 1

Cartesian coordinates of **1** in the ground state optimized at the B3LYP/6-311+G(2d,p) level

Br	-8.73617700	0.24801400	-0.22221600
S	-4.77535500	2.74105100	1.00511300
S	-1.33606600	-0.03657500	-0.04876700
N	-3.77209900	1.50253100	0.68097400
N	-6.20409300	2.05980100	0.63864000
N	5.38428400	0.15263300	-0.03902000
C	-4.52866000	0.48501600	0.26163200
C	-5.94208400	0.81313900	0.23899500
C	-6.88055000	-0.16130300	-0.18399800
C	-6.41212300	-1.38609200	-0.56797800
H	-7.10762700	-2.14292500	-0.90598100
C	-5.02987800	-1.69459200	-0.55009200
H	-4.73926400	-2.67681200	-0.89836000
C	-4.05310900	-0.80946400	-0.13437100
C	-2.64555600	-1.18666000	-0.10349300
C	-2.13323600	-2.46373000	-0.15050500
H	-2.76029600	-3.34581300	-0.14539800
C	-0.71985500	-2.54532400	-0.15775900
C	-0.13314500	-1.29567400	-0.11115900
C	0.00723500	-3.86288500	-0.15640900
H	0.98816500	-3.78361200	0.31261100
H	-0.56785200	-4.61367600	0.38925800
H	0.15587800	-4.24497400	-1.17122800
C	1.28815800	-0.93057000	-0.08521700
C	2.21867300	-1.57730000	-0.91114600
H	1.88292100	-2.34087200	-1.60034300
C	3.55938700	-1.22155400	-0.89985200

H	4.25835600	-1.71418500	-1.56412200
C	4.01292200	-0.20955600	-0.05446200
C	3.09993100	0.44440000	0.77277000
H	3.44846200	1.21849100	1.44482200
C	1.75919700	0.09193400	0.75203100
H	1.06914300	0.59689100	1.41700500
C	6.45172200	-0.69893300	0.25406500
C	6.43711500	-2.04347900	0.61917100
H	5.50966700	-2.59462200	0.70382500
C	7.65563700	-2.65638900	0.88018700
H	7.67027200	-3.70153200	1.16554300
C	8.86288100	-1.95139400	0.78580700
H	9.79599800	-2.45990200	0.99486100
C	8.87074700	-0.60950600	0.43391900
H	9.80575100	-0.06499900	0.37147100
C	7.66001700	0.03087300	0.16663200
C	7.30636200	1.38425000	-0.19761100
C	8.04800200	2.54062900	-0.44314200
H	9.12839400	2.52893600	-0.35802000
C	7.38540300	3.70510600	-0.80273000
H	7.94944900	4.60946900	-0.99500200
C	5.98971600	3.72200500	-0.92635300
H	5.49192500	4.63936000	-1.21714500
C	5.22786300	2.58581300	-0.68742900
H	4.15124700	2.60746800	-0.79458500
C	5.89751000	1.42231900	-0.31439600

Cartesian coordinates of **1** in the first excited state optimized at the TD-B3LYP/6-311+G(2d,p) level

Br	-8.65956600	0.28888000	0.06979900

S	-4.58226300	2.86334400	0.63236400
S	-1.36047400	-0.10136300	-0.00184500
N	-3.60994200	1.52738800	0.35345600
N	-6.07818400	2.15288500	0.47630600
N	5.32718200	0.14208200	-0.00504200
C	-4.45448800	0.50030100	0.13322300
C	-5.84459900	0.85991100	0.20358200
C	-6.81206500	-0.14756800	-0.01345000
C	-6.42854600	-1.45202400	-0.28738200
H	-7.17992100	-2.21107800	-0.45330400
C	-5.07656400	-1.78365900	-0.35094400
H	-4.81746700	-2.81067900	-0.56919500
C	-4.06305900	-0.83330500	-0.14492600
C	-2.66815400	-1.22872200	-0.21338500
C	-2.15974700	-2.50421000	-0.45192800
H	-2.79468800	-3.36737200	-0.58989100
C	-0.76405500	-2.59579700	-0.48299400
C	-0.15185400	-1.35386900	-0.25400200
C	-0.07592100	-3.91742500	-0.68471200
H	0.76724100	-4.04940300	-0.00438900
H	-0.77790800	-4.73349600	-0.51069500
H	0.30070900	-4.02879400	-1.70651600
C	1.24340700	-0.99753300	-0.19040600
C	2.26139700	-1.77488500	-0.79298500
H	2.00064900	-2.65090800	-1.36581100
C	3.58920900	-1.40778200	-0.72861000
H	4.33576500	-2.00222700	-1.23897400
C	3.97463100	-0.23476900	-0.06517700
C	2.98396700	0.55958200	0.53020700
H	3.26726500	1.44826400	1.07862600

C	1.66026100	0.18602600	0.46987800
H	0.92571800	0.79909700	0.97544400
C	6.39828800	-0.69350400	0.34174100
C	6.38377800	-2.02284900	0.75941400
H	5.46179900	-2.58080600	0.84466100
C	7.59968800	-2.61096800	1.08560200
H	7.61578600	-3.64388700	1.41026300
C	8.79727900	-1.89240000	1.01268900
H	9.72844800	-2.37873100	1.27476200
C	8.80184300	-0.55688100	0.62316300
H	9.72998900	0.00080400	0.59124700
C	7.59732200	0.05178200	0.28804500
C	7.23975000	1.39860100	-0.11094900
C	7.98019500	2.54928300	-0.35858900
H	9.05656600	2.55051900	-0.23640800
C	7.31883600	3.69922600	-0.77754500
H	7.88287900	4.60278600	-0.97164500
C	5.93306000	3.69777800	-0.96616500
H	5.43995000	4.59805500	-1.31076200
C	5.17303300	2.55915000	-0.72886800
H	4.10604000	2.56422400	-0.90216200
C	5.83750600	1.41895100	-0.28111600

3. TD-DFT Calculated Results for 1

Table S-1 Summary of TD-DFT calculated results of 1 at CAM-B3LYP/6-311+G(2d,p) level

λ (nm)	*f*	MO Contributions
413.8	0.5364	H-1→L (51%), H→L (44%)
310.0	0.2116	H-4→L (10%), H-1→L (24%), H→L (29%), H→L+1 (26%)
292.7	0.1663	H-3→L (34%), H-1→L+1 (14%), H→L (12%), H→L+1 (11%)
290.6	0.1216	H-3→L (18%), H-1→L+2 (16%), H→L+2 (49%)
289.7	0.1432	H-3→L (28%), H-1→L+1 (11%), H→L+1 (20%), H→L+2 (14%)
276.2	0.2567	H-7→L (53%), H→L+1 (10%)
273.6	0.0156	H-7→L (17%), H-4→L (45%)
270.9	0.0001	H-2→L (95%)
265.8	0.0428	H-2→L+2 (23%), H→L+3 (51%)
264.2	0.0051	H-12→L (35%), H-10→L (32%)

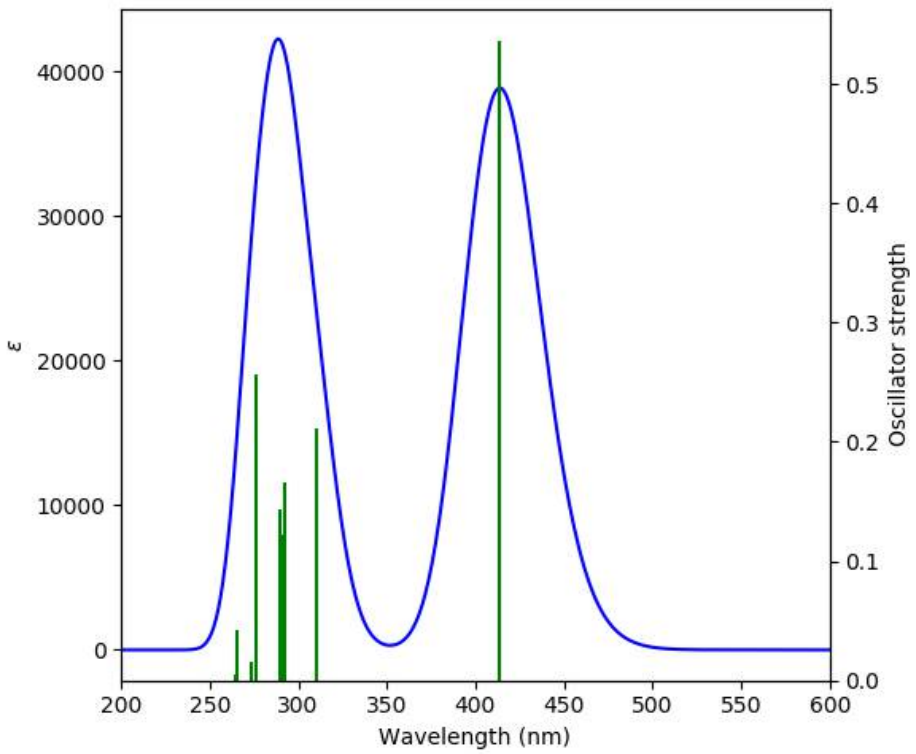

Figure S-2 TD-DFT calculated UV-Vis absorption spectrum of **1**. Simulation done with the GaussSum 3.0 software package.