

Supporting Information

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## Synthesis and Fluorescence Properties of Isoindoline-Benzazole-Based Boron Difluoride Complexes

Xiaoqing Wang,<sup>[a]</sup> Hou-ting Liu,<sup>[a]</sup> Jichun Cui,<sup>[a]</sup> Yanping Wu,<sup>[a]</sup> Hua Lu,\*<sup>[c]</sup> Jing Lu,<sup>[a]</sup> Zhipeng Liu,\*<sup>[a]</sup> and Weijiang He\*<sup>[b]</sup>

<sup>[a]</sup> School of Material Science and Engineering, School of Chemical and Chemistry Engineering, Liaocheng University Hunan Road 1, LiaoCheng, P.R. China, 252000. E-mail: liuzhipeng@lcu.edu.cn; <sup>[b]</sup> State Key Laboratory of Coordination Chemistry, Coordination Chemistry Institute, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, P.R. China. E-mail: hewei69@nju.edu.cn; <sup>[c]</sup> Key Laboratory of Organosilicon Chemistry and Material Technology, Hangzhou Normal University, Hangzhou, P.R. China. 310012, E-mail: hualu@hznu.edu.cn.

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Supporting Information

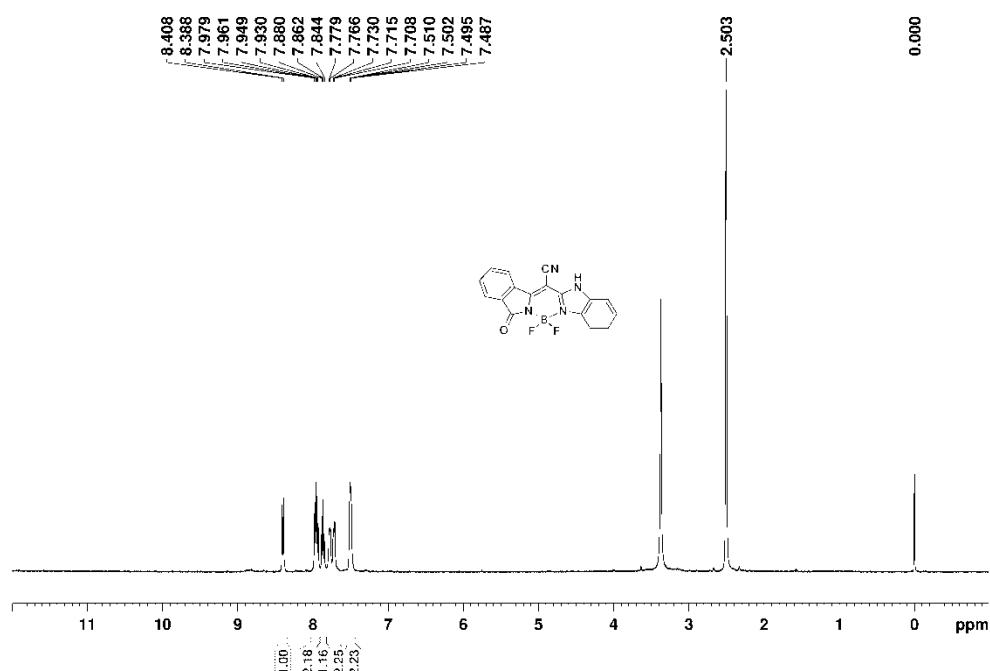


Figure S1  $^1\text{H}$  NMR spectrum of **7** in  $\text{DMSO}-d_6$ .

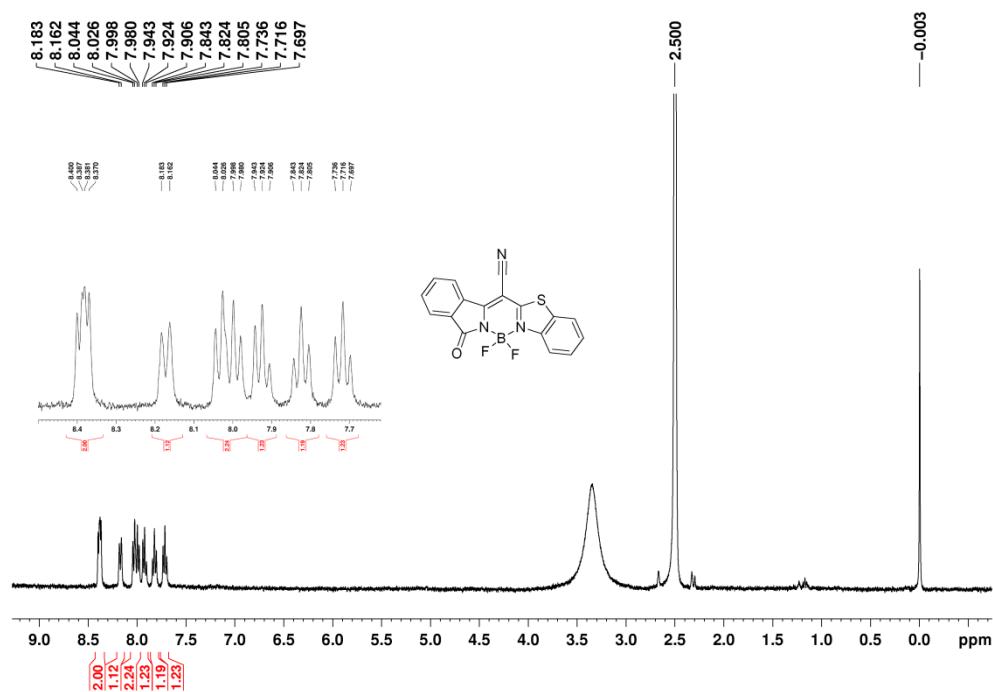
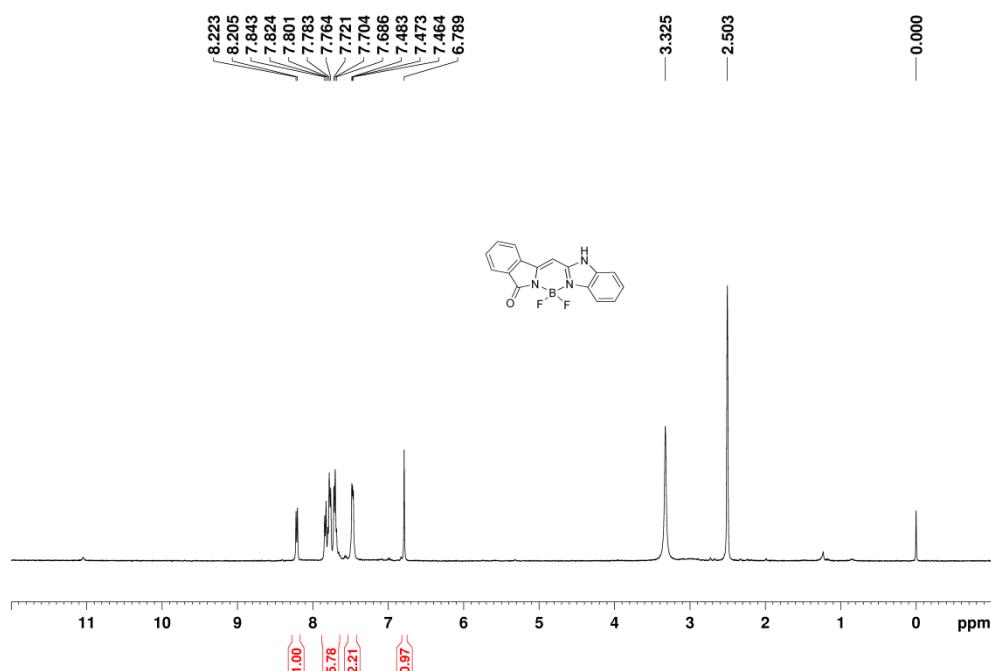
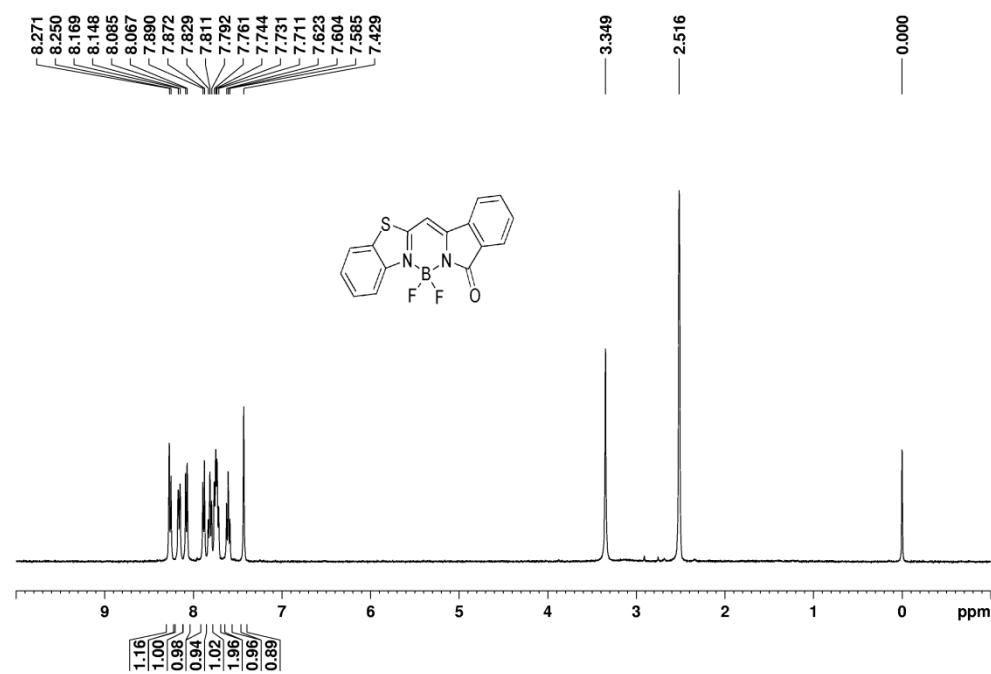


Figure S2  $^1\text{H}$  NMR spectrum of **8** in  $\text{DMSO}-d_6$ .

Supporting Information

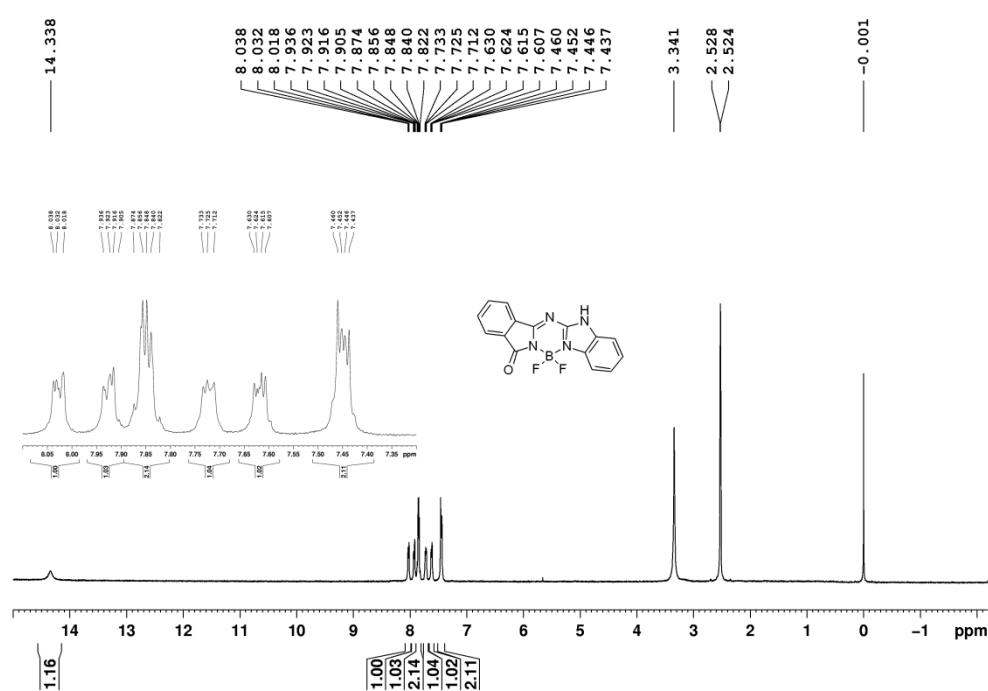


**Figure S3** <sup>1</sup>H NMR spectrum of **9** in DMSO-*d*<sub>6</sub>.

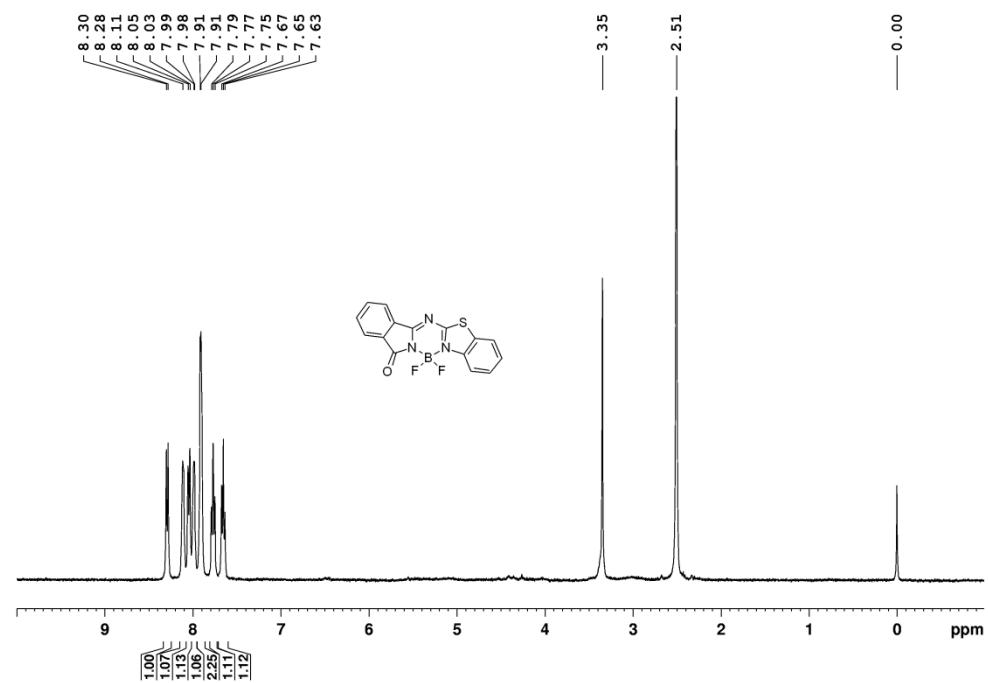


**Figure S4** <sup>1</sup>H NMR spectrum of **10** in DMSO-*d*<sub>6</sub>.

Supporting Information

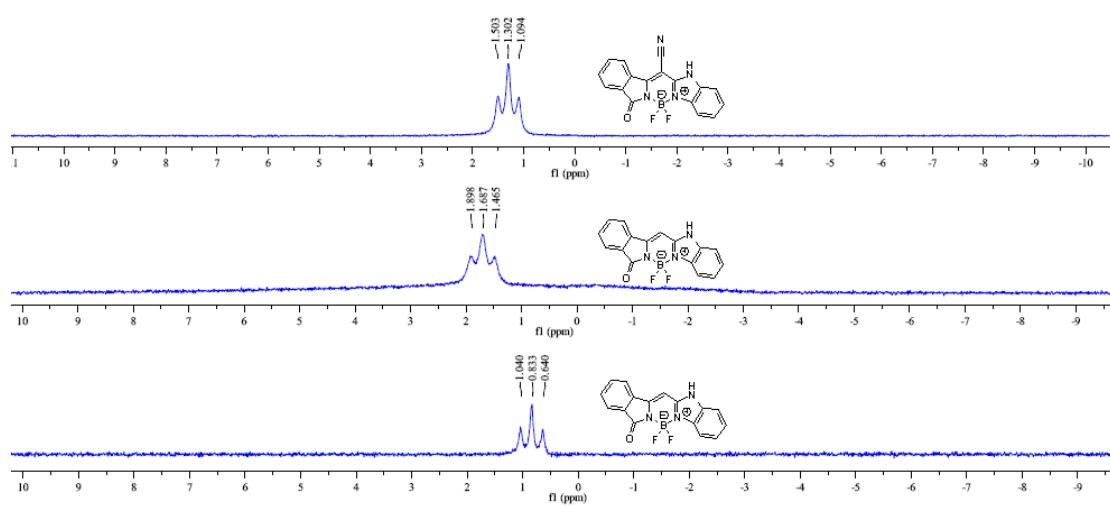


**Figure S5**  $^1\text{H}$  NMR spectrum of **11** in  $\text{DMSO}-d_6$ .

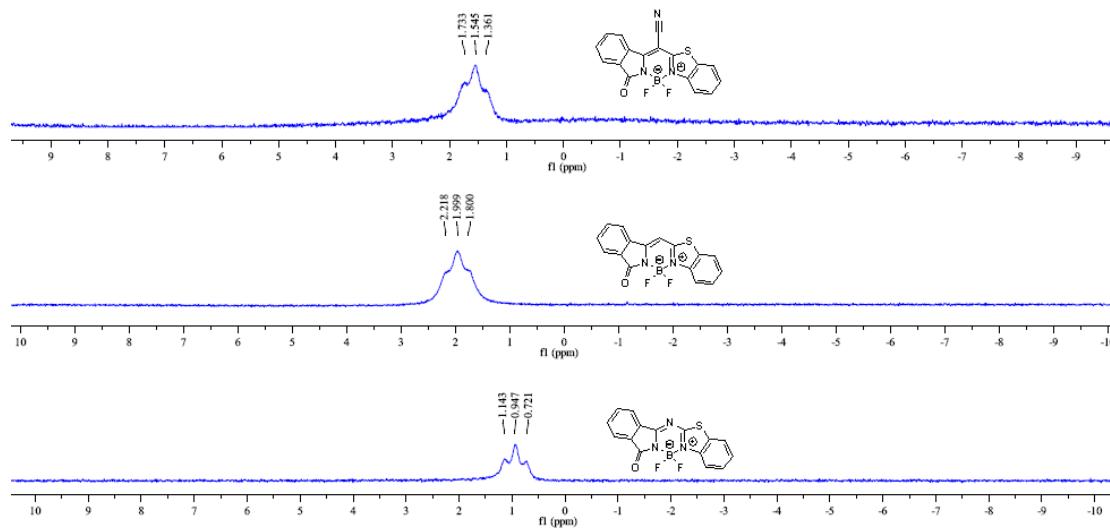


**Figure S6**  $^1\text{H}$  NMR spectrum of **12** in  $\text{DMSO}-d_6$ .

Supporting Information

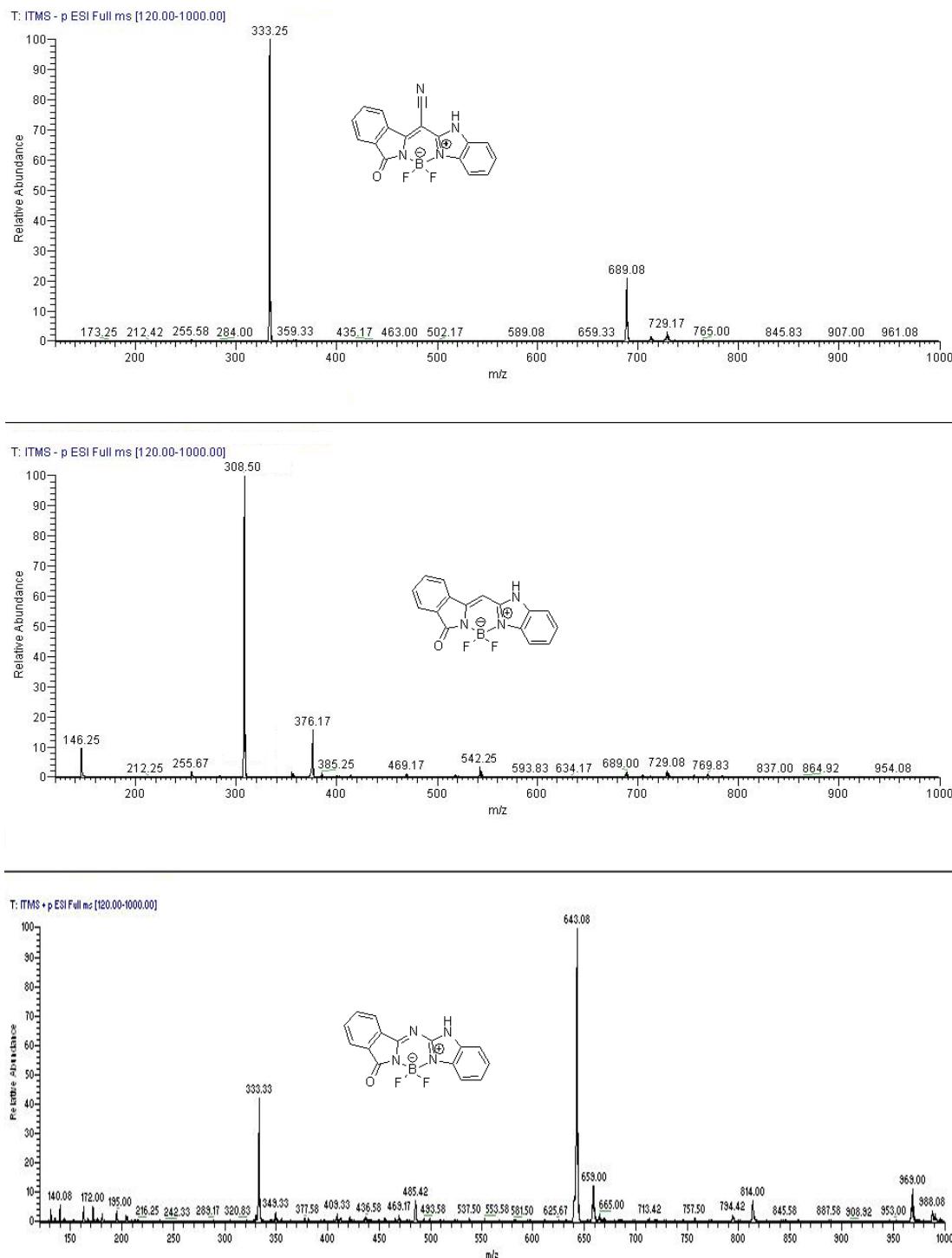


**Figure S7**  $^{11}\text{B}$  NMR spectra of **7, 9, 11** in  $\text{DMSO}-d_6$ .



**Figure S8**  $^{11}\text{B}$  NMR spectra of **8, 10, 12** in  $\text{DMSO}-d_6$ .

Supporting Information



**Figure S9** ESI-MS spectra of **7, 9, 11**.

Supporting Information

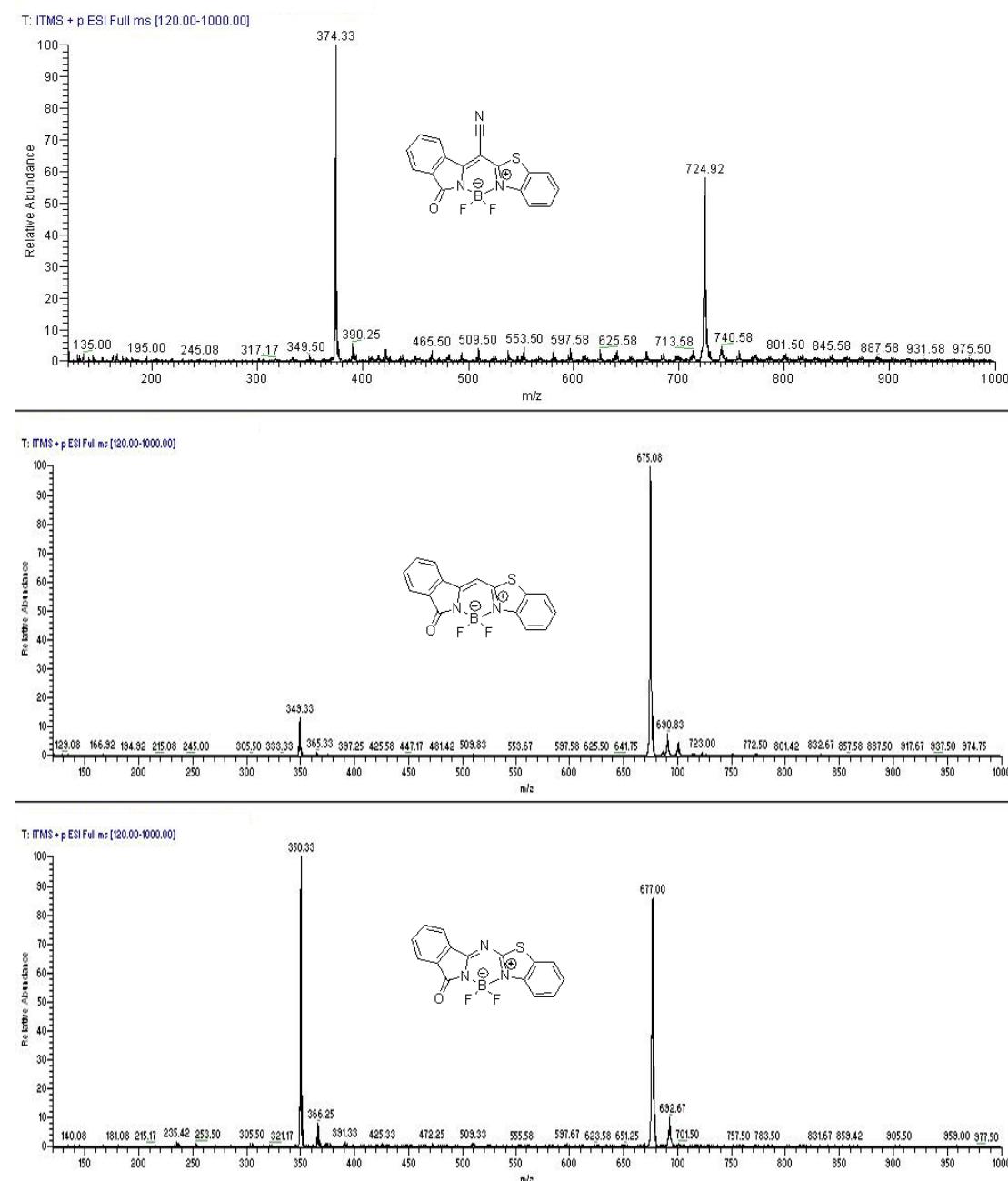


Figure S10 ESI-MS spectra of **8, 10, 12**.

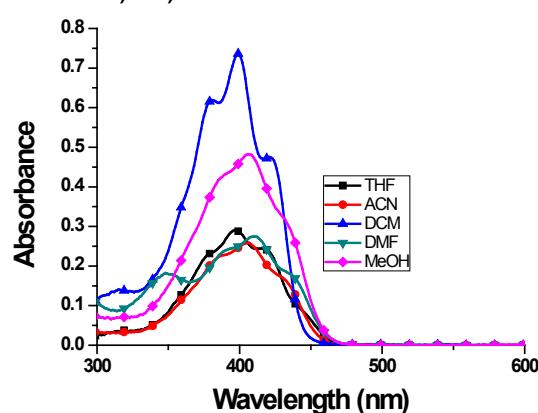
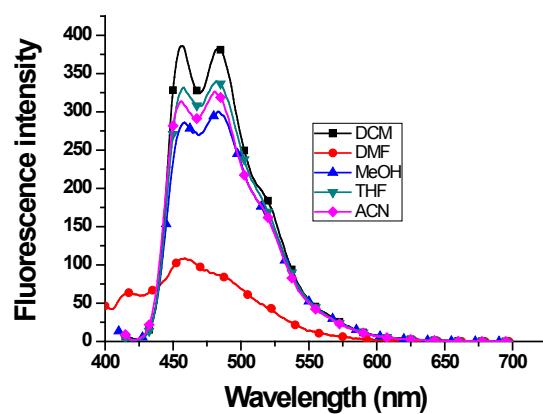
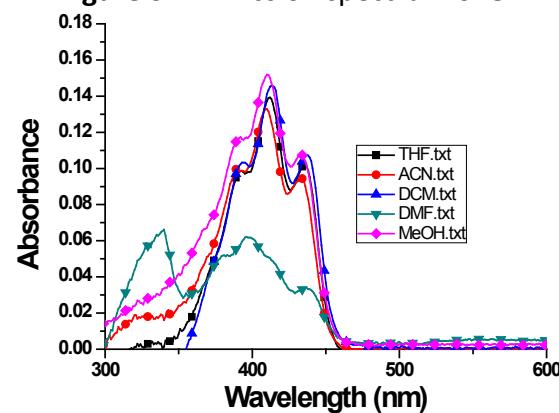


Figure S11 Absorption spectrum of **7**.

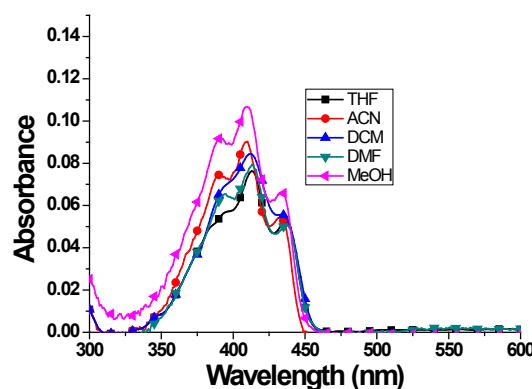
Supporting Information



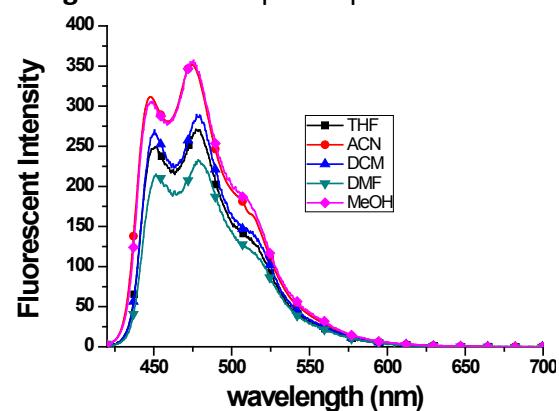
**Figure S12** Emission spectrum of **8**.



**Figure S13** Absorption spectrum of **8**.



**Figure S14** Absorption spectrum of **9**.



**Figure S15** Emission spectrum of **10**.

Supporting Information

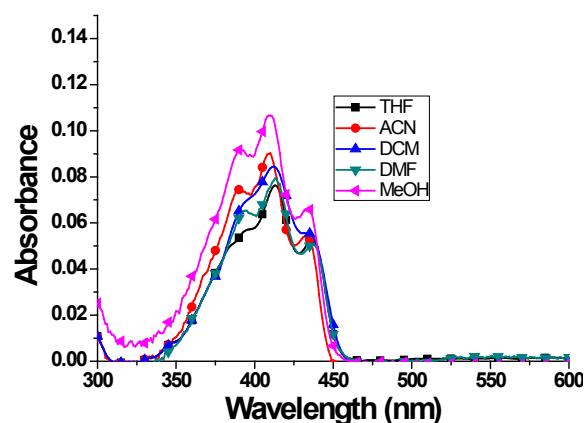


Figure S16 Absorption spectrum of **10**.

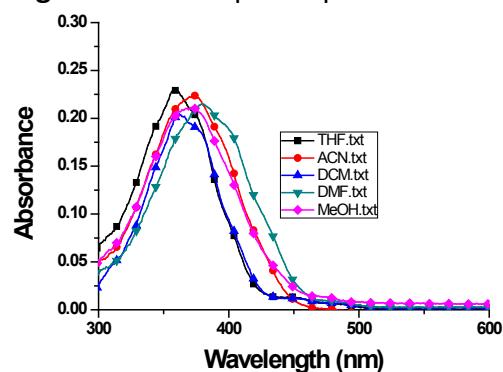


Figure S17 Absorption spectrum of **11**.

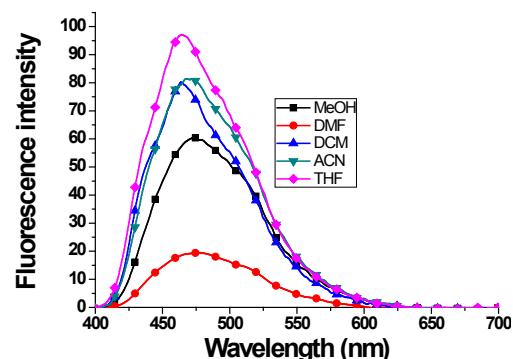


Figure S18 Emission spectrum of **12**.

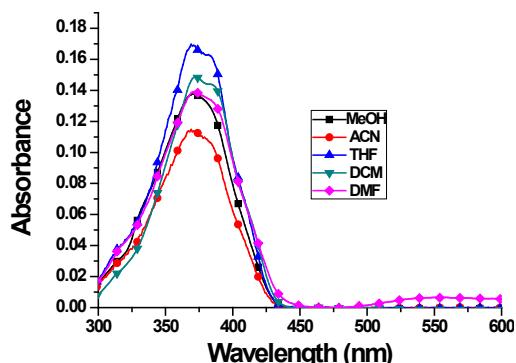


Figure S19 Absorption spectrum of **12**.

Supporting Information

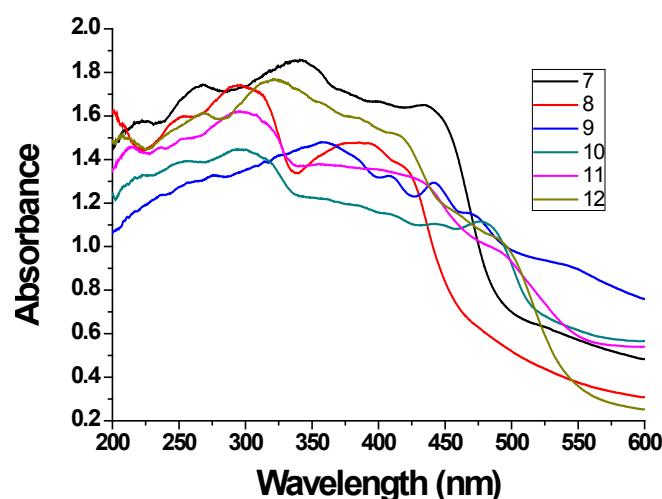


Figure S20 Absorption spectra of **7-12** in the solid state.

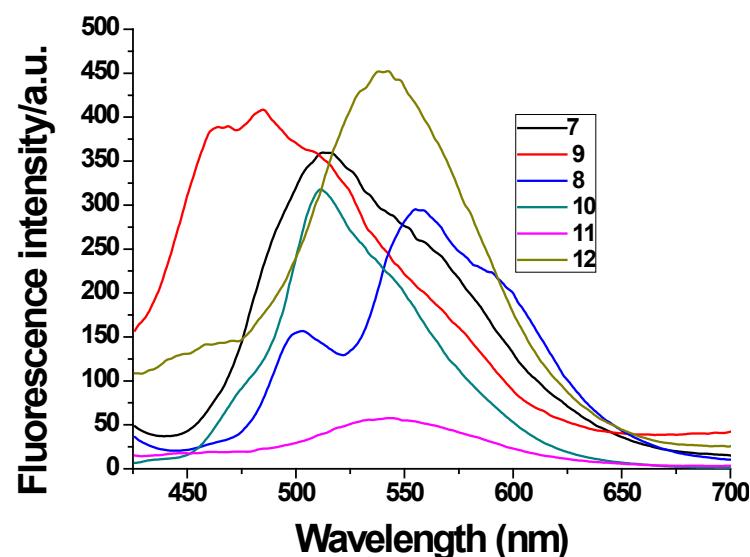


Figure S21 Emission spectra of **7-12** in the solid state.

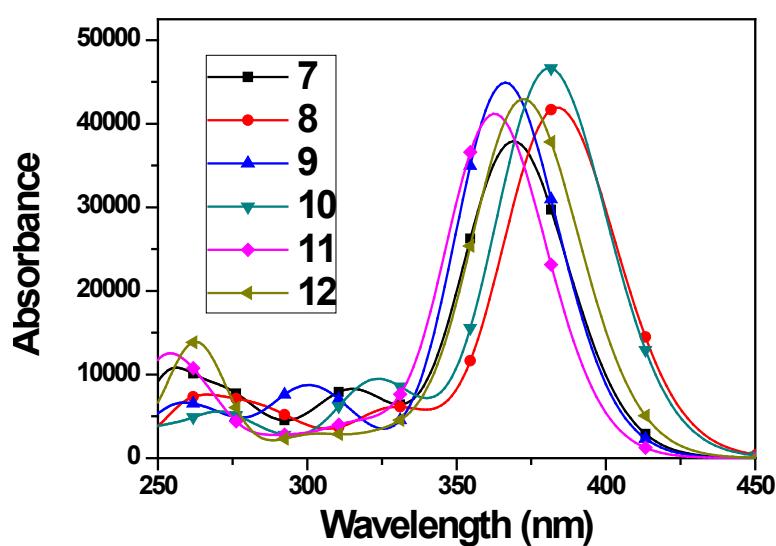


Figure S22 Calculated absorption spectra of **7-12**.



**Supporting Information**

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B4	1.56444
B5	2.20326
B6	1.55704
B7	2.32604
B8	1.20445
B9	1.48118
B10	1.38676
B11	1.38635
B12	1.38618
B13	1.37977
B14	1.38201
B15	1.36634
B16	1.36177
B17	1.13833
B18	1.33291
B19	1.38771
B20	1.38824
B21	1.38613
B22	1.39629
B23	1.3811
B24	1.38342
B25	0.8594
B26	0.92992
B27	0.92942
B28	0.92921
B29	0.93
B30	0.93047
B31	0.93014
B32	0.92946
B33	0.93029
A1	110.93081
A2	118.57607
A3	51.68164
A4	159.867
A5	104.77086
A6	97.82523
A7	30.31696
A8	130.11979
A9	128.84085
A10	117.32933
A11	120.42232
A12	122.39089
A13	117.33335
A14	126.64603

**Supporting Information**

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A15	121.7638
A16	4.80686
A17	34.58602
A18	73.37814
A19	130.90419
A20	116.13404
A21	121.57665
A22	122.16775
A23	106.77589
A24	160.5425
A25	121.33814
A26	119.76418
A27	118.77918
A28	121.3382
A29	121.92432
A30	119.20577
A31	118.86916
A32	121.94113
D1	-176.86047
D2	-93.52394
D3	-0.7513
D4	7.16715
D5	173.18886
D6	176.01955
D7	-179.28006
D8	1.2104
D9	-179.83839
D10	0.53626
D11	-0.82255
D12	0.14242
D13	-8.31708
D14	6.01241
D15	-35.67578
D16	-1.41465
D17	179.54452
D18	-179.70966
D19	179.89399
D20	-2.05926
D21	1.81213
D22	-0.84689
D23	1.20708
D24	0.08501
D25	-179.45279
D26	179.19767

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D27	-179.85669
D28	-0.09283
D29	177.92895
D30	-178.23029
D31	179.47997

SCF Done: E(RB+HF-LYP) = -1172.0723292 a.u.

Number of Imaginary frequencies: n.a.

**Compound 8**

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Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

S

B	1	B1	
F	2	B2	1 A1
F	2	B3	1 A2 3 D1 0
N	2	B4	1 A3 4 D2 0
N	2	B5	1 A4 5 D3 0
N	1	B6	5 A5 2 D4 0
O	6	B7	2 A6 1 D5 0
C	5	B8	2 A7 1 D6 0
C	9	B9	5 A8 2 D7 0
C	10	B10	9 A9 5 D8 0
C	11	B11	10 A10 9 D9 0
C	12	B12	11 A11 10 D10 0
C	13	B13	12 A12 11 D11 0
C	5	B14	2 A13 1 D12 0
C	15	B15	5 A14 2 D13 0
C	6	B16	2 A15 1 D14 0
C	17	B17	6 A16 2 D15 0
C	18	B18	17 A17 6 D16 0
C	8	B19	6 A18 2 D17 0
C	19	B20	18 A19 17 D18 0
C	18	B21	17 A20 6 D19 0
C	21	B22	19 A21 18 D20 0
C	22	B23	18 A22 17 D21 0
C	7	B24	1 A23 15 D22 0

Variables:

B1	4.10757
B2	1.39535
B3	1.37537
B4	1.5821
B5	1.54278

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B6	3.59997
B7	2.32251
B8	1.40677
B9	1.39437
B10	1.38068
B11	1.43154
B12	1.37868
B13	1.40173
B14	1.31813
B15	1.44938
B16	1.36124
B17	1.48509
B18	1.38855
B19	1.20327
B20	1.39131
B21	1.38441
B22	1.39146
B23	1.40361
B24	1.13865
A1	115.10608
A2	113.34607
A3	11.28361
A4	94.68719
A5	99.06747
A6	98.11174
A7	123.18749
A8	126.69482
A9	117.59513
A10	121.19887
A11	120.96375
A12	117.63429
A13	124.75226
A14	122.4012
A15	126.22535
A16	108.91717
A17	106.50629
A18	30.6821
A19	121.67841
A20	130.95225
A21	116.8792
A22	116.40509
A23	52.03274
D1	-127.35933
D2	67.53925

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D3	175.60843
D4	-3.10027
D5	-177.41303
D6	-177.93113
D7	1.42498
D8	179.34605
D9	0.19529
D10	-0.22961
D11	-0.82457
D12	0.77036
D13	0.91454
D14	3.24157
D15	178.69587
D16	-0.04485
D17	-178.42322
D18	179.08366
D19	177.27642
D20	-2.17487
D21	-177.04353
D22	4.80846

SCF Done: E(RB+HF-LYP) = -1509.6114307 a.u.

Number of Imaginary frequencies: n.a.

**Compound 9**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

B

F	1	B1					
F	1	B2	2	A1			
N	1	B3	2	A2	3	D1	0
N	4	B4	1	A3	2	D2	0
N	1	B5	4	A4	5	D3	0
O	6	B6	1	A5	4	D4	0
C	7	B7	6	A6	1	D5	0
C	8	B8	7	A7	6	D6	0
C	9	B9	8	A8	7	D7	0
C	10	B10	9	A9	8	D8	0
C	11	B11	10	A10	9	D9	0
C	12	B12	11	A11	10	D10	0
C	13	B13	12	A12	11	D11	0
C	6	B14	1	A13	4	D12	0
C	5	B15	4	A14	1	D13	0
C	5	B16	4	A15	1	D14	0

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C	17	B17	5	A16	4	D15	0
C	18	B18	17	A17	5	D16	0
C	19	B19	18	A18	17	D17	0
C	20	B20	19	A19	18	D18	0
C	17	B21	5	A20	4	D19	0
H	5	B22	4	A21	1	D20	0
H	10	B23	9	A22	8	D21	0
H	11	B24	10	A23	9	D22	0
H	12	B25	11	A24	10	D23	0
H	13	B26	12	A25	11	D24	0
H	18	B27	17	A26	5	D25	0
H	19	B28	18	A27	17	D26	0
H	20	B29	19	A28	18	D27	0
H	21	B30	20	A29	19	D28	0
C	15	B31	6	A30	1	D29	0
H	32	B32	15	A31	6	D30	0

Variables:

B1	1.37438
B2	1.37993
B3	1.56444
B4	2.20326
B5	1.55704
B6	2.32604
B7	1.20445
B8	1.48118
B9	1.38676
B10	1.38635
B11	1.38618
B12	1.37977
B13	1.38201
B14	1.36634
B15	1.33291
B16	1.38771
B17	1.38824
B18	1.38613
B19	1.39629
B20	1.3811
B21	1.38342
B22	0.8594
B23	0.92992
B24	0.92942
B25	0.92921
B26	0.93
B27	0.93047

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B28	0.93014
B29	0.92946
B30	0.93029
B31	1.36177
B32	1.07
A1	110.93082
A2	109.81148
A3	159.867
A4	104.77085
A5	97.82522
A6	30.31693
A7	130.11975
A8	128.84089
A9	117.32937
A10	120.42231
A11	122.39086
A12	117.33336
A13	126.64604
A14	34.58601
A15	73.37815
A16	130.90417
A17	116.13401
A18	121.57666
A19	122.16774
A20	106.77586
A21	160.54245
A22	121.3381
A23	119.76423
A24	118.77923
A25	121.33817
A26	121.92437
A27	119.20576
A28	118.86919
A29	121.94114
A30	121.76377
A31	117.93415
D1	-120.5186
D2	-112.05543
D3	7.16723
D4	173.18885
D5	176.0195
D6	-179.2801
D7	1.21044
D8	-179.83842

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D9	0.53626
D10	-0.82257
D11	0.14245
D12	-8.31712
D13	-1.41467
D14	179.54448
D15	-179.70967
D16	179.89394
D17	-2.05917
D18	1.81201
D19	-0.84688
D20	1.20693
D21	0.08494
D22	-179.45281
D23	179.19765
D24	-179.8567
D25	-0.09283
D26	177.92893
D27	-178.23034
D28	179.47999
D29	6.01244
D30	179.9429

SCF Done: E(RB+HF-LYP) = -1079.8280242 a.u.

Number of Imaginary frequencies: n.a.

**Compound 10**

--

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

S

F	1	B1					
F	2	B2	1	A1			
N	1	B3	3	A2	2	D1	0
N	4	B4	1	A3	3	D2	0
O	4	B5	1	A4	5	D3	0
B	4	B6	1	A5	5	D4	0
C	1	B7	5	A6	4	D5	0
C	8	B8	1	A7	5	D6	0
C	9	B9	8	A8	1	D7	0
C	10	B10	9	A9	8	D8	0
C	11	B11	10	A10	9	D9	0
C	12	B12	11	A11	10	D10	0
C	5	B13	4	A12	1	D11	0

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C	14	B14	5	A13	4	D12	0
C	15	B15	14	A14	5	D13	0
C	16	B16	15	A15	14	D14	0
C	17	B17	16	A16	15	D15	0
C	18	B18	17	A17	16	D16	0
C	19	B19	18	A18	17	D17	0
C	20	B20	19	A19	18	D18	0
C	21	B21	20	A20	19	D19	0
C	6	B22	4	A21	1	D20	0
H	9	B23	8	A22	1	D21	0
H	10	B24	9	A23	8	D22	0
H	11	B25	10	A24	9	D23	0
H	12	B26	11	A25	10	D24	0
H	15	B27	14	A26	5	D25	0
H	18	B28	17	A27	16	D26	0
H	19	B29	18	A28	17	D27	0
H	20	B30	19	A29	18	D28	0
H	21	B31	20	A30	19	D29	0

Variables:

B1	4.8276
B2	2.25105
B3	4.49273
B4	2.48315
B5	2.32135
B6	1.51644
B7	1.73551
B8	1.37509
B9	1.38301
B10	1.38611
B11	1.37222
B12	1.39261
B13	1.33647
B14	1.42203
B15	1.33981
B16	1.47183
B17	1.37023
B18	1.37368
B19	1.39895
B20	1.38071
B21	1.37902
B22	1.22189
B23	0.93057
B24	0.92966
B25	0.92921

**Supporting Information**

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B26	0.9301
B27	0.93079
B28	0.93046
B29	0.92998
B30	0.93013
B31	0.93027
A1	76.12801
A2	29.66228
A3	27.5187
A4	164.11813
A5	64.95426
A6	62.08393
A7	128.21891
A8	118.07466
A9	120.46848
A10	121.92497
A11	117.77368
A12	88.21502
A13	122.20569
A14	119.49591
A15	129.35677
A16	131.79103
A17	117.23652
A18	122.01507
A19	120.51441
A20	117.38611
A21	30.34214
A22	120.94501
A23	119.82633
A24	118.97635
A25	121.09036
A26	120.33181
A27	121.39798
A28	119.0665
A29	119.73201
A30	121.33836
D1	64.8096
D2	-28.45629
D3	5.63641
D4	0.03334
D5	178.44008
D6	178.85463
D7	-178.6222
D8	-0.41466

**Supporting Information**

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D9	0.3584
D10	-0.3235
D11	-1.18939
D12	-2.28374
D13	2.90162
D14	177.23172
D15	-0.26212
D16	-178.84901
D17	-0.53258
D18	0.57858
D19	-0.37995
D20	176.35946
D21	1.30512
D22	179.52604
D23	-179.53103
D24	179.57525
D25	-177.07448
D26	1.12812
D27	179.50315
D28	-179.53218
D29	179.72871

SCF Done: E(RB+HF-LYP) = -1422.654554 a.u.

Number of Imaginary frequencies: n.a.

**Compound 11**

BIN-E

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Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

B

F	1	B1					
F	1	B2	2	A1			
N	1	B3	3	A2	2	D1	0
N	4	B4	1	A3	3	D2	0
N	1	B5	4	A4	5	D3	0
O	6	B6	1	A5	4	D4	0
C	7	B7	6	A6	1	D5	0
C	8	B8	7	A7	6	D6	0
C	9	B9	8	A8	7	D7	0
C	10	B10	9	A9	8	D8	0
C	11	B11	10	A10	9	D9	0
C	12	B12	11	A11	10	D10	0
C	13	B13	12	A12	11	D11	0

**Supporting Information**

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C	6	B14	1	A13	4	D12	0
C	4	B15	1	A14	6	D13	0
C	5	B16	4	A15	1	D14	0
C	17	B17	5	A16	4	D15	0
C	18	B18	17	A17	5	D16	0
C	19	B19	18	A18	17	D17	0
C	20	B20	19	A19	18	D18	0
C	4	B21	1	A20	6	D19	0
H	5	B22	4	A21	1	D20	0
H	10	B23	9	A22	8	D21	0
H	11	B24	10	A23	9	D22	0
H	12	B25	11	A24	10	D23	0
H	13	B26	12	A25	11	D24	0
H	18	B27	17	A26	5	D25	0
H	19	B28	18	A27	17	D26	0
H	20	B29	19	A28	18	D27	0
H	21	B30	20	A29	19	D28	0
N	15	B31	6	A30	1	D29	0

Variables:

B1	1.38609
B2	1.38606
B3	1.58372
B4	2.21259
B5	1.56464
B6	2.34666
B7	1.21012
B8	1.49568
B9	1.38771
B10	1.40236
B11	1.40273
B12	1.40145
B13	1.39048
B14	1.36541
B15	1.3432
B16	1.3917
B17	1.3943
B18	1.39537
B19	1.40878
B20	1.39416
B21	1.39446
B22	1.00916
B23	1.08527
B24	1.08584
B25	1.08584

**Supporting Information**

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B26	1.0849
B27	1.08521
B28	1.08537
B29	1.08526
B30	1.08364
B31	1.31403
A1	112.20707
A2	108.89577
A3	158.85317
A4	102.74405
A5	100.57715
A6	29.6559
A7	128.43594
A8	130.63124
A9	117.40151
A10	121.05517
A11	121.14722
A12	117.2921
A13	124.80563
A14	123.47797
A15	74.02257
A16	132.41391
A17	116.72035
A18	121.52856
A19	121.63504
A20	128.6426
A21	157.9128
A22	120.90288
A23	119.60607
A24	119.34104
A25	121.54632
A26	121.81939
A27	119.15062
A28	119.16124
A29	122.13161
A30	126.46346
D1	120.61089
D2	118.77438
D3	0.09511
D4	180.
D5	-179.93441
D6	-179.99239
D7	-0.00673
D8	-179.99702

**Supporting Information**

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D9	0.
D10	0.
D11	0.
D12	0.04189
D13	0.01295
D14	179.88442
D15	179.98986
D16	-179.99632
D17	0.
D18	0.
D19	179.94663
D20	-0.21482
D21	0.
D22	180.
D23	180.
D24	-179.99638
D25	0.00811
D26	180.
D27	-180.
D28	-179.99666
D29	-0.06167

SCF Done: E(RB+HF-LYP) = -1096.0857339 a.u.

Number of Imaginary frequencies: n.a.

Compound 12

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Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

S	
F	1 B1
F	2 B2 1 A1
N	1 B3 2 A2 3 D1 0
N	4 B4 1 A3 2 D2 0
O	4 B5 1 A4 5 D3 0
B	4 B6 1 A5 5 D4 0
C	1 B7 5 A6 4 D5 0
C	8 B8 1 A7 5 D6 0
C	9 B9 8 A8 1 D7 0
C	10 B10 9 A9 8 D8 0
C	11 B11 10 A10 9 D9 0
C	5 B12 4 A11 1 D10 0
C	5 B13 4 A12 1 D11 0
C	4 B14 1 A13 14 D12 0
C	15 B15 4 A14 1 D13 0

Supporting Information

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C	16	B16	15	A15	4	D14	0
C	17	B17	16	A16	15	D15	0
C	18	B18	17	A17	16	D16	0
C	19	B19	18	A18	17	D17	0
C	20	B20	19	A19	18	D18	0
C	6	B21	4	A20	1	D19	0
H	9	B22	8	A21	1	D20	0
H	10	B23	9	A22	8	D21	0
H	11	B24	10	A23	9	D22	0
H	12	B25	11	A24	10	D23	0
H	17	B26	16	A25	15	D24	0
H	18	B27	17	A26	16	D25	0
H	19	B28	18	A27	17	D26	0
H	20	B29	19	A28	18	D27	0
N	15	B30	4	A29	1	D28	0

Variables:

B1	4.86163
B2	2.30107
B3	4.46699
B4	2.47913
B5	2.34731
B6	1.55366
B7	1.75866
B8	1.39671
B9	1.39357
B10	1.40598
B11	1.39138
B12	1.39819
B13	1.33504
B14	1.36115
B15	1.47243
B16	1.3903
B17	1.4016
B18	1.4026
B19	1.40261
B20	1.38755
B21	1.2094
B22	1.08508
B23	1.08543
B24	1.08531
B25	1.08301
B26	1.08487
B27	1.08578
B28	1.08581

**Supporting Information**

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B29	1.08527
B30	1.3153
A1	76.32781
A2	29.91128
A3	28.91368
A4	168.76752
A5	67.84702
A6	61.70014
A7	128.5374
A8	118.0063
A9	120.85582
A10	121.32069
A11	161.47078
A12	85.26415
A13	56.51967
A14	109.48036
A15	131.45842
A16	117.23401
A17	121.16708
A18	121.08929
A19	117.36855
A20	29.78558
A21	121.01834
A22	119.40347
A23	119.49287
A24	121.64161
A25	121.14839
A26	119.49624
A27	119.33199
A28	121.68509
A29	126.20345
D1	-64.94471
D2	28.36042
D3	0.02555
D4	-0.02192
D5	179.99336
D6	180.
D7	-179.99723
D8	0.
D9	0.
D10	179.97917
D11	-0.00764
D12	-0.51533
D13	-179.99049

**Supporting Information**

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D14	179.99664
D15	-180.
D16	0.
D17	0.
D18	0.
D19	179.97729
D20	0.00438
D21	-180.
D22	180.
D23	-180.
D24	0.00327
D25	-180.
D26	180.
D27	180.
D28	0.00574

SCF Done: E(RB+HF-LYP) = -1438.9028817 a.u.

Number of Imaginary frequencies: n.a.