Supporting information

for

Aggregation-induced emission (AIE) of Pyridyl-enamido-based Organoboron luminophores

Xiaoqing Wang,* [a,b] Yanping Wu,[a] Qingsong Liu, [a] Zhenyu Li, [a] Hui Yan, [c,d] Chonglei Ji, [a] Jicheng Duan, [a] and Zhipeng Liu*, [a]

[a] Institution of Functional Organic Molecules and Materials, School of Chemistry and Chemical Engineering, Liaocheng University, No.1 Hunan road, Liaocheng, 252000, P.R. China. E-mail: chliuzp@163.com.

[b] School of Materials and Engineering, Liaocheng University, Liaocheng, 252000, P.R. China. E-mail: wangxiaoqing@lcu.edu.cn.

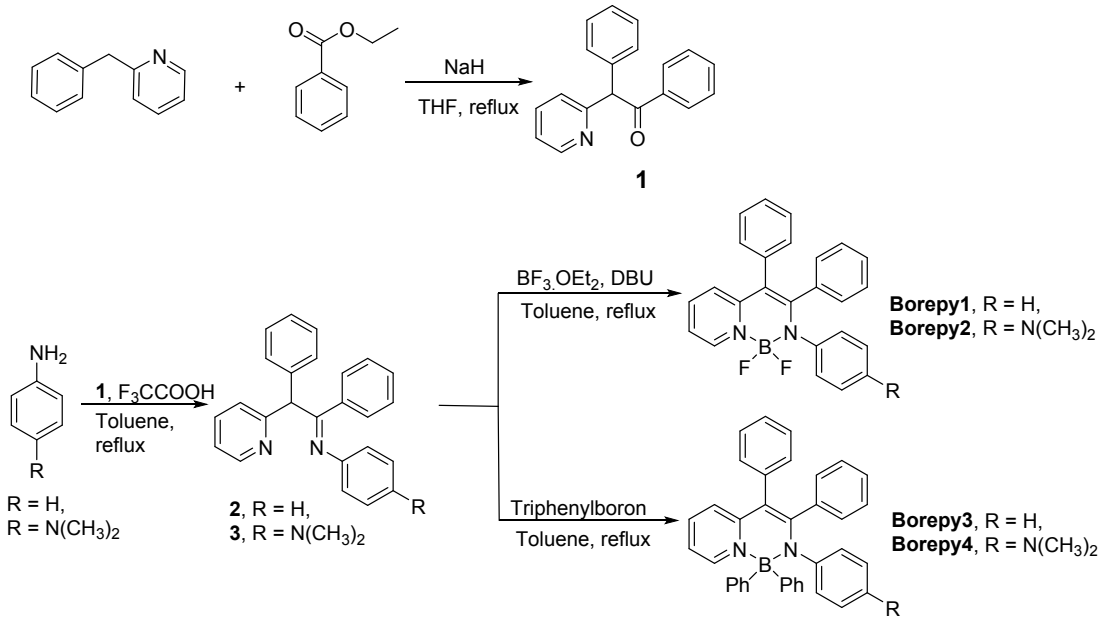
[c] School of Pharmacy, Liaocheng University, Liaocheng, 252000, P.R. China.

[d] School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100, P.R. China.

Contents.

1. Experimental details

General. All reactions and manipulations of air-sensitive compounds were carried out under dry argon by using Schlenk techniques and/or vacuum line techniques. Solvents were dried prior to use by common methods in organometallic chemistry. Chemicals were commercially obtained and used as received. ^{1}H, ^{11}B and ^{13}C NMR spectra were recorded using Varian Mercury-plus 400M spectrometer instrument. Chemical shifts are reported in ppm relative to $Si(CH_3)_4$ (^{1}H, ^{13}C), and coupling constants (*J*) are given in Hz. Mass spectra were obtained on a LCQ (ESI-MS, Thermo Finnigan) mass spectrometer. Thin layer chromatography (TLC) was performed on plates coated with thick silica gel GF254 (Qingdao Haiyang Chemical Co., Ltd). Column chromatography was performed using silica gel (200 mesh, Qingdao Haiyang Chemical Co., Ltd).



Scheme S1. Synthetic routes for **Borepy1-4**.

1,2-diphenyl-2-(pyridin-2-yl)ethan-1-one (1)

2-benzylpyridine (5.00 g, 29.60 mmol) was added to a mixture of THF (15 mL) and NaH (60w% in oil, 2.13 g 88.90 mmol) at room temperature, after stirred for 20 minutes, Ethyl benzoate (4.68 g, 31.20 mmol) was added, and the resulting mixture was heated at reflux for 10 h. After cooling to room temperature, 2 M HCl aq. was slowly added, and the yellow precipitate was filtered and washed with water. After drying, the desire product was obtained as yellow solid. Yield: 98%. (7.928 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.5 Hz, 1H), 8.04 (d, *J* = 7.3 Hz, 2H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.37 (dt, *J* = 20.5, 7.5 Hz, 6H), 7.32 – 7.22 (m, 3H), 7.21 – 7.09 (m, 2H), 6.32 (s, 1H).

(Z)-N,1,2-triphenyl-2-(pyridin-2-yl)ethan-1-imine (2)

Compound **1** (0.69 g, 2.50 mmol), aniline (0.49 g, 5.00 mmol) and toluene (15 mL)

were added to a round bottom flask equipped with a Dean-Stark trap, condenser and magnetic stirring bar, and then 2 drops of trifluoroacetic acid (cat. amount) was added. The resulting solution was heated to reflux for 12 h. After cooling to room temperature, toluene was removed in vacuo. Column chromatography of the residue (EA: P = 1: 10, R_f = 0.6) on silica gel gave desired product as yellow solid. Yield: 67% (0. 59 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 12.75 (s, 1H), 8.56 (d, *J* = 4.7, 1H), 7.92 (s, 1H), 7.56 (d, *J* = 7.8, 2H), 7.40 (dd, *J* = 14.6, 7.2, 3H), 7.11 (dd, *J* = 17.9, 5.8, 8H), 6.84 (d, *J* = 8.3, 1H), 6.77 (s, 1H), 6.61 (d, *J* = 8.0, 2H).

(Z)-4-((1,2-diphenyl-2-(pyridin-2-yl)ethylidene)amino)-N,N-dimethylaniline (3)

Compound **1** (1.21 g, 4.40 mmol), 4-*N*,*N*-dimethylaniline (1.20 g, 8.80 mmol) and toluene (15 mL) were added to a round bottom flask equipped with a Dean-Stark trap, condenser and magnetic stirring bar, and then 2 drops of trifluoroacetic acid (cat. amount) was added. The resulting solution was heated to reflux for 10 h. After cooling to room temperature, toluene was removed in vacuo. Column chromatography of the residue (EA: P = 1: 6, R_f = 0.5) on silica gel gave desired product as yellow solid. Yield: 68.9% (1.19 g). ^{1}H NMR (400 MHz, $CDCl_3$) *δ*/ppm = 12.66 (s, 1H), 8.52 (d, *J* = 4.5, 1H), 7.39 (t, *J* = 7.0, 1H), 7.18–7.03 (m, 7H), 6.99 (d, *J* = 4.6, 3H), 6.93–6.85 (m, 1H), 6.79 (d, *J* = 8.4, 1H), 6.62 (d, *J* = 8.8, 2H), 6.48 (d, *J* = 8.9, 2H), 2.80 (s, 6H).

General procedure for the synthesis of Borepys 1–2.

Corresponding enamide (2–3, 1 eq.) was dissolved in dry toluene. DBU (3 eq.) was added to the solution and stirred for 10 minutes at room temperature. A solution of toluene containing of boron trifluoride diethyl ether complex (5 eq.) was slowly added to the mixture via syringe. The resulting mixture was heated to reflux for 1 h. After cooling to room temperature, the solution was extracted with dichloride methane. The organic layer was washed with water and brine, and dried over anhydrous magnesium sulfate. The dried organic layer was filtrated though a short pad of silica gel. Removing the solvent yielded the **Borepy**s with high purity.

Borepy1 (P: DCM = 1: 1, R_f = 0.4) Yield: 76 %. ^{1}H NMR (400 MHz, $CDCl_3$) *δ*/ppm = 8.46 (d, *J* = 5.8, 1H), 7.58 (dd, *J* = 15.0, 7.7, 1H), 7.17 (t, *J* = 7.3, 2H), 7.15–7.02 (m, 8H), 7.03–6.94 (m, 1H), 6.96–6.81 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ*/ppm = 156.91, 151.34, 142.73, 138.92, 138.76, 138.66, 137.21, 136.36, 133.20, 130.55, 128.74, 128.39, 128.04, 127.26, 127.03, 126.73, 125.28, 121.59, 117.20, 105.97; ESI-MS: calcd., $[M+Na]^+$ = 419.23, found: $[M+Na]^+$ = 419.40; Elemental analysis (%) calcd for $C_{25}H_{19}BF_2N_2$: C, 75.78; H, 4.83; N, 7.07. Found: C, 75.12; H, 4.97; N, 7.24.

Borepy2 (P: DCM = 1: 1, R_f = 0.4) Yield: 79 %. ^{1}H NMR (400 MHz, $CDCl_3$) *δ*/ppm = 8.41 (d, *J* = 6.0 Hz, 1H), 7.51 (t, *J* = 7.9 Hz, 1H), 7.15 (t, *J* = 7.3 Hz, 2H), 7.07 (dd, *J* = 15.9, 7.0 Hz, 3H), 7.02–6.81 (m, 8H), 6.45 (d, *J* = 8.7 Hz, 2H), 2.81 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ*/ppm = 153.20, 146.58, 143.63, 134.19, 133.52, 132.91, 132.03,

128.63, 127.45, 125.74, 124.51, 123.67, 122.33, 121.89, 116.72, 111.88, 107.56, 100.37, 72.82, 72.51, 72.19, 36.17; ESI-MS: calcd., $[M+Na]^+$ = 462.30, found: $[M+Na]^+$ = 462.75; Elemental analysis (%) calcd for $C_{27}H_{24}BF_2N_3$: C, 73.82; H, 5.51; N, 9.57. Found, C, 73.12; H, 5.85; N, 9.86.

General procedure for the synthesis of Borepys 3–4.

Corresponding enamide (2–3, 1 eq.) was dissolved in dry toluene. Triphenylboron (1 eq.) was added to the solution and the resulting mixture was heated to reflux for 6 h. After cooling to room temperature, toluene was removed in vacuo. Column chromatography of the residue on silica gel gave desired product as yellow solid.

Borepy3 (P: DCM = 1: 10, R_f = 0.5) Yield: 52.3 %. ^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm = ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 6.1 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 7.8 Hz, 4H), 7.17 (dd, *J* = 14.4, 7.7 Hz, 8H), 7.03 (dt, *J* = 24.0, 7.1 Hz, 3H), 6.87 (dd, *J* = 15.2, 7.1 Hz, 5H), 6.71 (q, *J* = 7.8 Hz, 4H), 6.60 (t, *J* = 6.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm = 157.58, 152.77, 147.21, 142.65, 138.33, 138.10, 137.69, 134.87, 133.44, 131.47, 129.51, 127.95, 127.18, 127.01, 126.90, 126.81, 126.28, 125.86, 122.97, 120.25, 117.07, 111.86; ESI-MS: calcd., $[M]^+$ = 513.46, found: $[M]^+$ = 513.75; Elemental analysis (%) calcd for $C_{37}H_{29}BN_2$: C, 86.72; H, 5.70; N, 5.47. Found: C, 86.12; H, 5.93; N, 5.87.

Borepy4 (P: DCM = 1: 10, R_f = 0.4) Yield: 70.8 %. ^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm = 7.77 (d, *J*=5.9, 1H), 7.43 (t, *J*=7.8, 1H), 7.27 (t, *J*=6.2, 4H), 7.15 (dt, *J*=18.0, 8.0, 9H), 7.04 (t, *J*=7.2, 2H), 6.99 (d, *J*=7.1, 1H), 6.89 (t, *J*=7.4, 2H), 6.82 (d, *J*=7.4, 3H), 6.77 (t, *J*=6.6, 1H), 6.59 (d, *J*=8.8, 2H), 6.11 (d, *J*=8.8, 2H), 5.29 (s, 1H), 2.66 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm = 157.95, 152.44, 146.68, 142.39, 138.66, 138.48, 137.49, 137.13, 134.87, 133.49, 131.30, 129.78, 127.85, 126.86, 126.85, 126.05, 125.66, 119.91, 116.33, 111.48, 110.78, 40.93. ESI-MS: calcd., $[M]^+$ = 556.53, found: $[M]^+$ = 556.83; Elemental analysis (%) calcd for $C_{39}H_{34}BN_3$: C, 84.32; H, 6.17; N, 7.56. Found: C, 84.02; H, 6.77; N, 7.81.

2. X-ray crystallographic analysis

Borepy1

Green and prism single crystals of **Borepy1** were grown from a solution of CH_2Cl_2. Intensity data were collected at 298 K on a Gemini A Single Crystal CCD X-ray diffractometer with $Mo_{K\alpha}$ radiation (l = 0.71073 Å) and graphite monochromator. The structure was solved by direct methods (SHELX-97)[1] and refined by the full-matrix least-squares on F_2 (SHELX-97). All the non-hydrogen atoms were refined anisotropically and all the hydrogen atoms were placed by using AFIX instructions. Crystal data: Formula C25H19BF2N2, *M*W = 396.23, Orthorhombic, *P* 21 21 21, *a* = 10.9427(7), *b* = 12.7077(7), *c* = 14.9474(11) Å, α = 90°, β = 90°, γ = 90°, *V* = 2078.5(2) Å^3, *Z* = 4, *D*calc = 1.266 g.cm^{-3}; μ = 0.086 mm^{-1}; R_1 ($I > 2\sigma(I)$) = 0.0506, wR_2 (all data) = 0.0946, GOF = 1.041. Total 14308 reflections were collected, among which 3651

reflections were independent (R_{int} = 0.0683). CCDC-1013247.

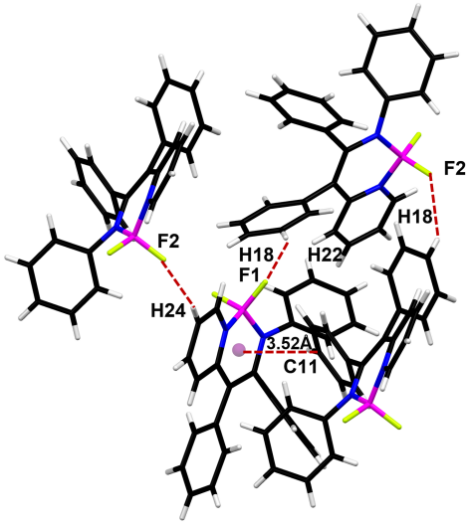


Figure S1. Crystal packing structure of **Borepy1**. The red dotted lines show intermolecular hydrogen-bonds and C–H···π interactions within **Borepy1**.

Borepy2

Yellow and block single crystals of **Borepy2** were grown from a solution of CH_2Cl_2. Intensity data were collected at 298 K on a Gemini A Single Crystal CCD X-ray diffractometer with $Mo_{K\alpha}$ radiation (l = 0.71073 Å) and graphite monochromator. The structure was solved by direct methods (SHELX-97)[1] and refined by the full-matrix least-squares on F_2 (SHELX-97). All the non-hydrogen atoms were refined anisotropically and all the hydrogen atoms were placed by using AFIX instructions. Crystal data: Formula C54H48B2F4N6, *M*W = 878.60, Triclinic, *P* -1, *a* = 12.2723(9), *b* = 14.7050(16), *c* = 14.7883(16) Å, α = 69.664(10)°, β = 67.961(8)°, γ = 82.665(7)°, *V* = 2319.6(4) Å^3, *Z* = 2, *D*calc = 1.258 g.cm^{-3}; μ = 0.085 mm^{-1}; R_1 ($I > 2\sigma(I)$) = 0.0752, wR_2 (all data) = 0.2352, GOF = 1.100. Total 15483 reflections were collected, among which 8180 reflections were independent (R_{int} = 0.0486). CCDC-1013248.

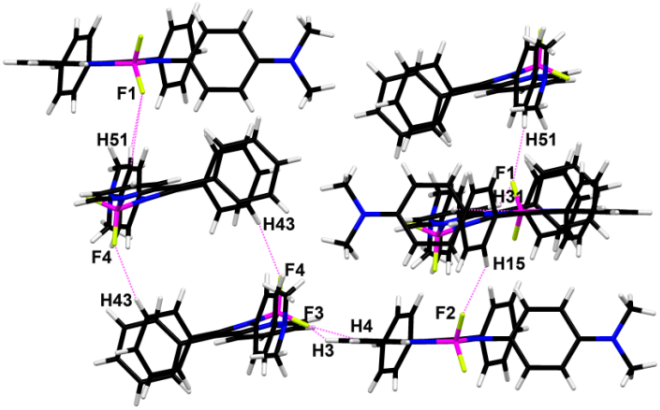


Figure S2. Crystal packing structure of **Borepy2**. The red dotted lines show intermolecular hydrogen-bonds within **Borepy2**.

Borepy3

Yellow and prism single crystals of **Borepy3** were grown from a solution of CH_2Cl_2/hexane. Intensity data were collected at 298 K on a Gemini A Single Crystal CCD X-ray diffractometer with $Mo_{K\alpha}$ radiation (l = 0.71073 Å) and graphite monochromator. The structure was solved by direct methods (SHELX-97)[1] and refined by the full-matrix least-squares on F_2 (SHELX-97). All the non-hydrogen atoms were refined anisotropically and all the hydrogen atoms were placed by using AFIX instructions. Crystal data: Formula C37H29BN2, *M*W = 512.43, Monoclinic, P2(1)/n, *a* = 10.9565(8), *b* = 19.2414(16), *c* = 13.7066(11) Å, α = 90°, β = 95.0020(10)°, γ = 90°, *V* = 2878.6(4) Å^3, *Z* = 4, *D*calc = 1.182 g.cm^{-3}; μ = 0.068 mm^{-1}; R_1 ($I > 2\sigma(I)$) = 0.0512, wR_2 (all data) = 0.2325, GOF = 0.758. Total 14281 reflections were collected, among which 5066 reflections were independent (R_{int} = 0.0441). CCDC-1013249.

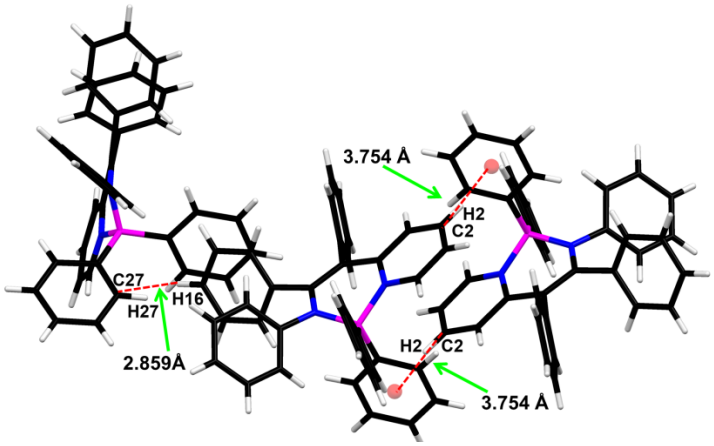


Figure S3. Crystal packing structure of **Borepy3**. The red dotted lines show intermolecular hydrogen-bonds and C–H···π interactions within **Borepy3**.

Borepy4

Red and block single crystals of **Borepy4** were grown from a solution of CH_2Cl_2. Intensity data were collected at 298 K on a Gemini A Single Crystal CCD X-ray diffractometer with $Mo_{K\alpha}$ radiation (l = 0.71073 Å) and graphite monochromator. The structure was solved by direct methods (SHELX-97)[1] and refined by the full-matrix least-squares on F_2 (SHELX-97). All the non-hydrogen atoms were refined anisotropically and all the hydrogen atoms were placed by using AFIX instructions. Crystal data: Formula C39H34BN3, *M*W = 555.50, Orthorhombic, P21 21 21, *a* = 8.6210(9), *b* = 18.3501(19), *c* = 19.690(2) Å, α = 90°, β = 90°, γ = 90°, *V* = 3114.9(6) Å^3, *Z* = 4, *D*calc = 1.185 g.cm^{-3}; μ = 0.069 mm^{-1}; R_1 ($I > 2\sigma(I)$) = 0.0580, wR_2 (all data) = 0.1190, GOF = 0.752. Total 15871 reflections were collected, among which 5499 reflections were independent (R_{int} = 0.1469). CCDC-1013250.

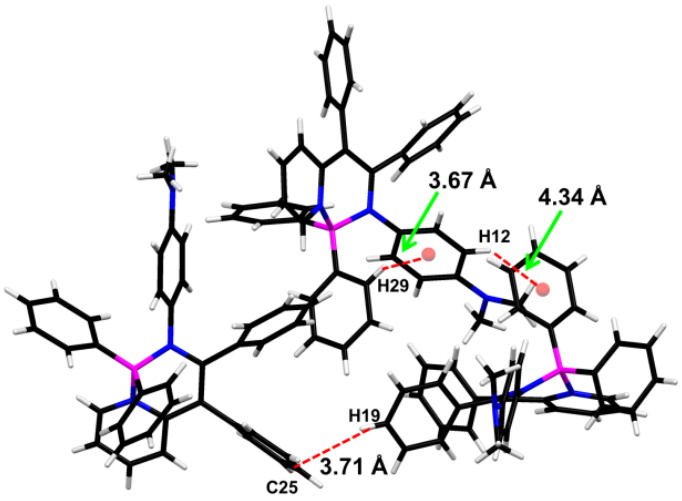
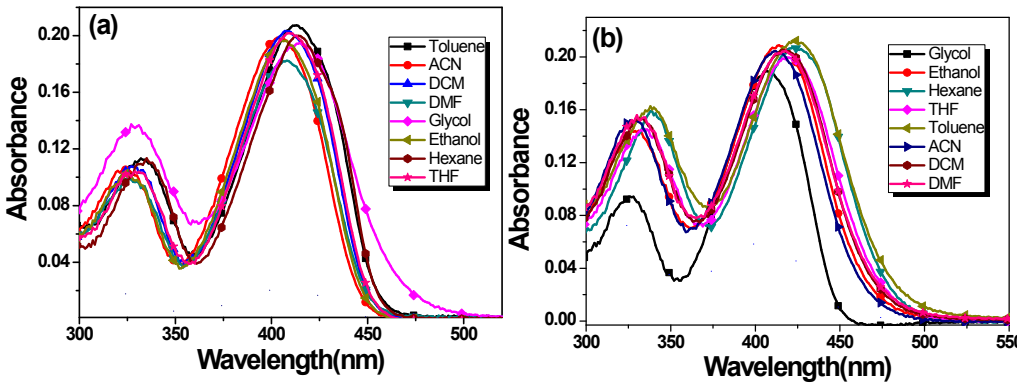


Figure S4. Crystal packing structure of **Borepy4**. The red dotted lines show intermolecular hydrogen-bonds and C–H···π interactions within **Borepy4**.

3. Photophysical properties

UV-vis absorption spectra were recorded on a Shimadzu UV-3600 spectrometer with a resolution of 1.0 nm. A solution of the sample (*ca.* 10^{-5} M) in a 1 cm square quarts cell was used for the measurement. Fluorescence spectra were recorded on a Hitachi F-7000 spectrometer under following conditions: excitation wavelength = 401 nm (**Borepy1-2**), 445 nm (**Borepy3-4**), an excitation slit width of 8 nm, an emission slit width of 8 nm and a PMT voltage of 650 V for **Borepy1** and **Borepy3**, and 775 V for **Borepy2** and **Borepy4.** Powder samples of **Borepy1-4** were used for the absorption and emission spectra recording. The fluorescence lifetimes and the absolute quantum yields (Φ_f) of the powder samples were determined with a Horiba Jobin Yvon Fluorolog-3 spectrofluorimeter. Fluorescence quantum yield of **Borepy1-4** in solution were determined by using 4-methylamino-7-nitro-2,1,3-benzoxadiazole (Φ_f = 0.38 in acetonitrile) as reference.[2]



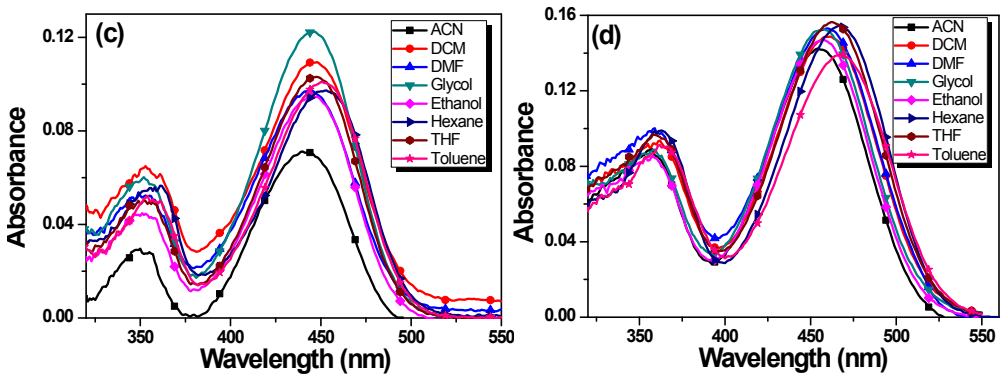


Figure S5. Absorption spectra of **Borepy1 (a)**, **Borepy2 (b)**, **Borepy3 (c)** and **Borepy4 (d)** in various solvents.

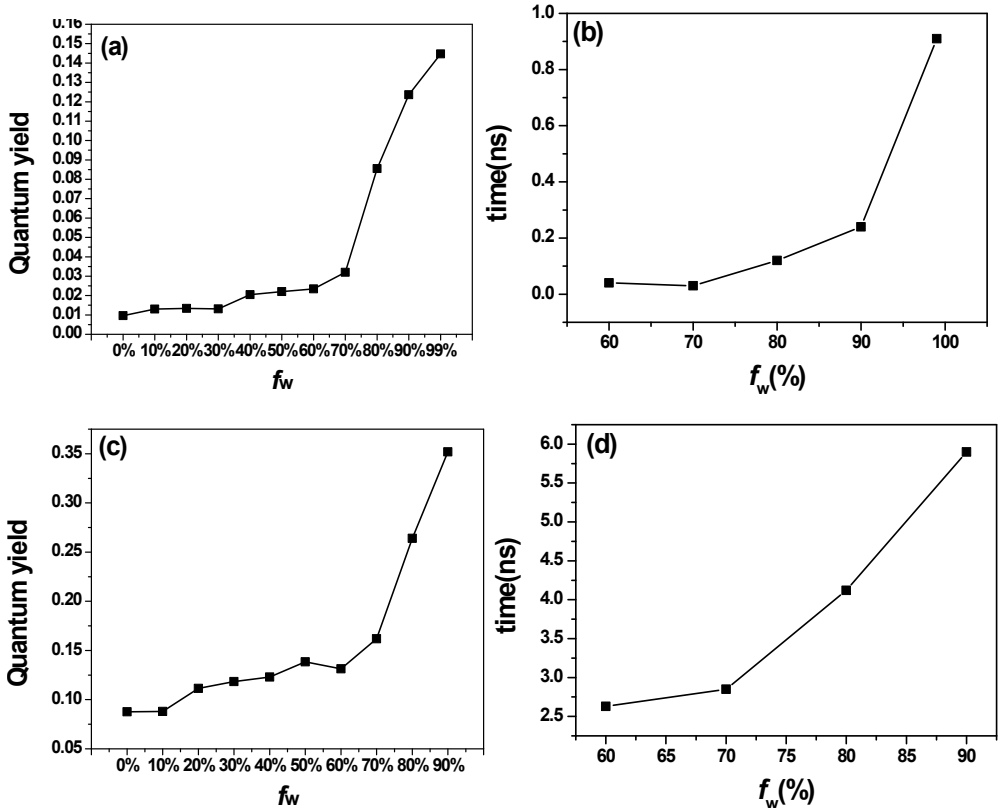


Figure S6. Changes in the quantum yields and lifetimes of **Borepy1 (a, b)** and **Borepy3 (c, d)** in THF/water mixtures (10 μM) with varied volumetric fractions of water (f_w).

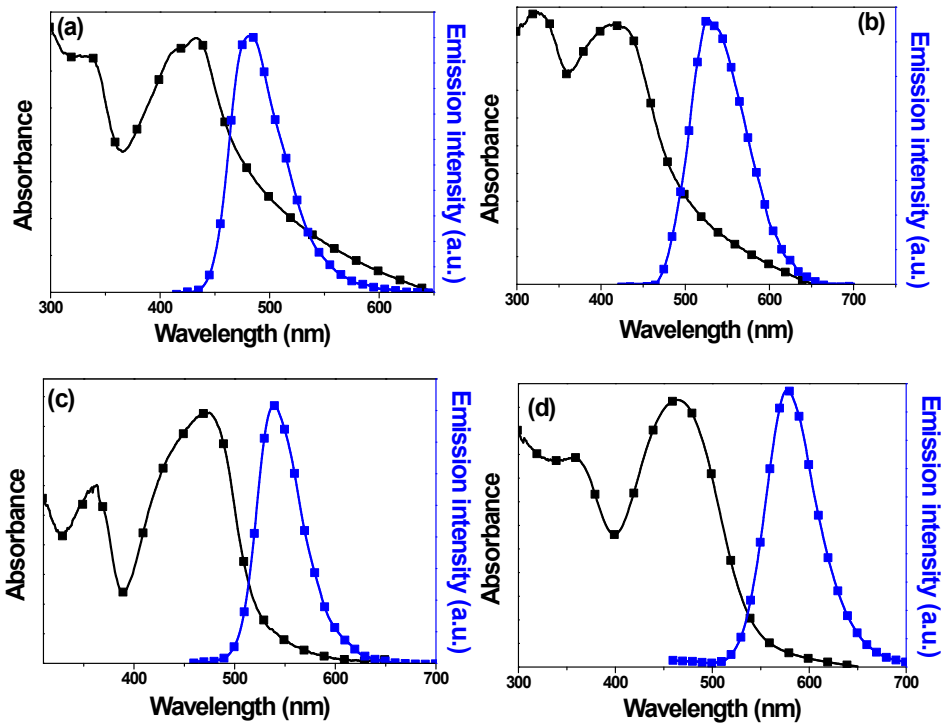


Figure S7. Absorption and emission of **Borepy1 (a)**, **Borepy2 (b)**, **Borepy3 (c)** and **Borepy4 (d)** in the solid state.

Table S1. Photophysical data of **Borepy1-4** in solution and in the solid state.

	CH_2Cl_2 [a]			Glycerol [a]	Solid-state		
	λ_{abs} (nm)	λ_{em} (nm)	SS [b] (cm^{-1})[b]	Φ_f (%)[c]	λ_{abs} (nm)	λ_{em} (nm)	Φ_f (%)[d]
1	330, 407	471	3340	0.4	333, 434	481	12
2	330, 416	464	2490	0.13	325, 423	534	20
3	353, 448	522	3160	0.15	363, 472	538	26
4	353, 461	513	2200	0.38	357, 464	577	10

[a] Measured at a concentration of 10 μM at 25 °C; [b] Frequency units between the longest absorption band and emission band; [c] determined by using 4-methylamino-7-nitro-2,1,3-benzoxadiazole (Φ_f = 0.38 in acetonitrile) as reference [d] Absolute quantum yield determined by calibrated integrating sphere systems.

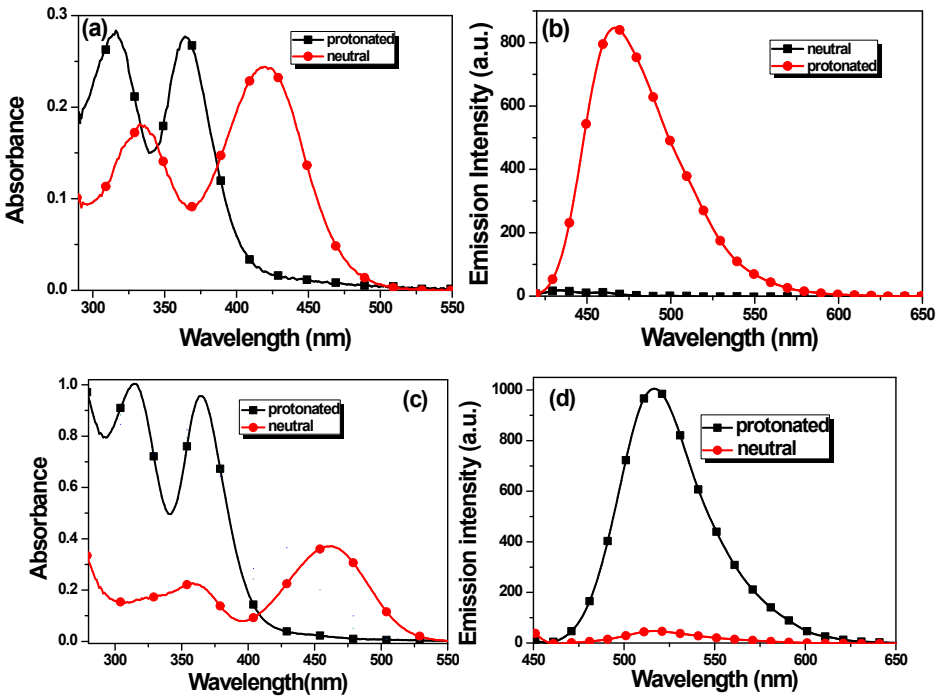


Figure S8. Absorption (1.0×10^{-5} M in THF) and fluorescence spectra of the switching between **Borepy2** (a) and **Borepy4** (c), and their protonated form **Borepy2**-H^+ (b) and **Borepy4**-H^+ (d) in THF (1.0×10^{-5} M), respectively.

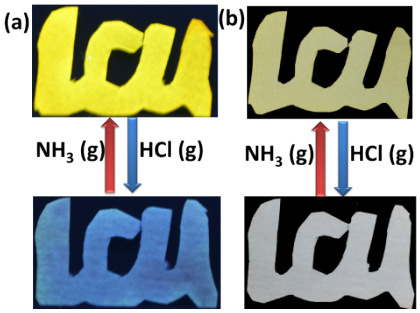


Figure S9. The pictures of **Borepy2** on a filter paper support under ambient (b) and UV light (a)

4. Computational methods

The density functions theory (DFT) calculation at the B3LYP/6-31G(d,p) level were carried out using the crystal structures as model structures. [3] The UV-Vis spectra were calculated using the SWizard program, revision 5.0, using the Gaussian model. The half-bandwidths, $\Delta_{1/2,l,}$ were taken to be equal to cm^{-1}.[4]

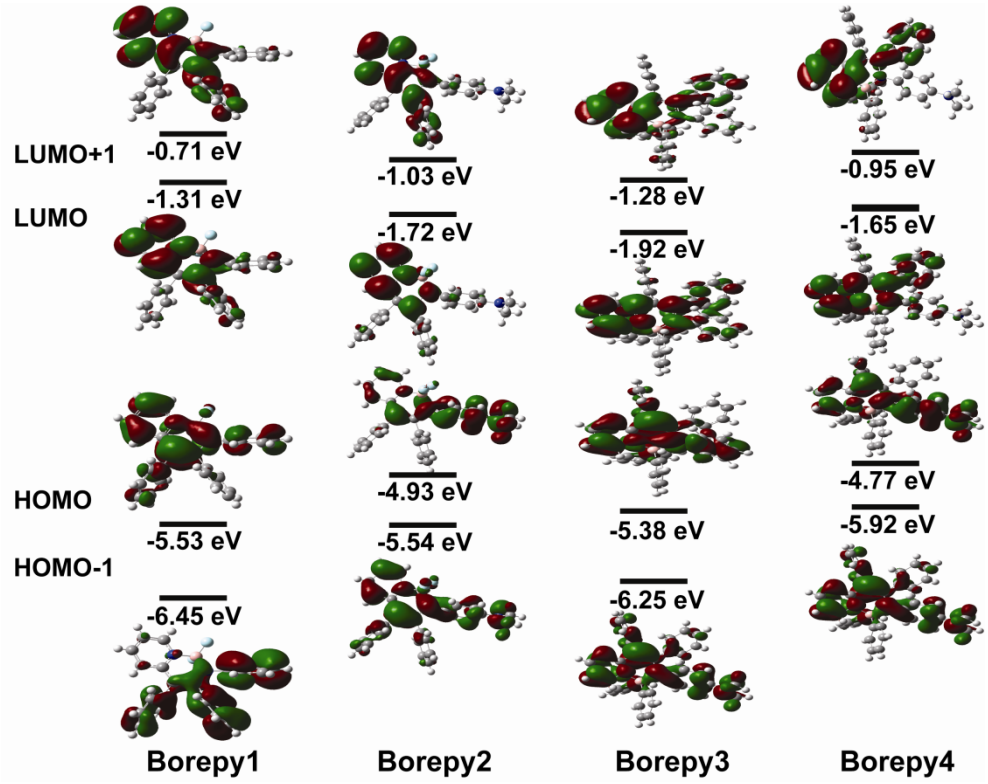


Figure S10. Molecular orbital energy diagram and isodensity surface plots of the HOMOs and LUMOs of **Borepy1**–**4**.

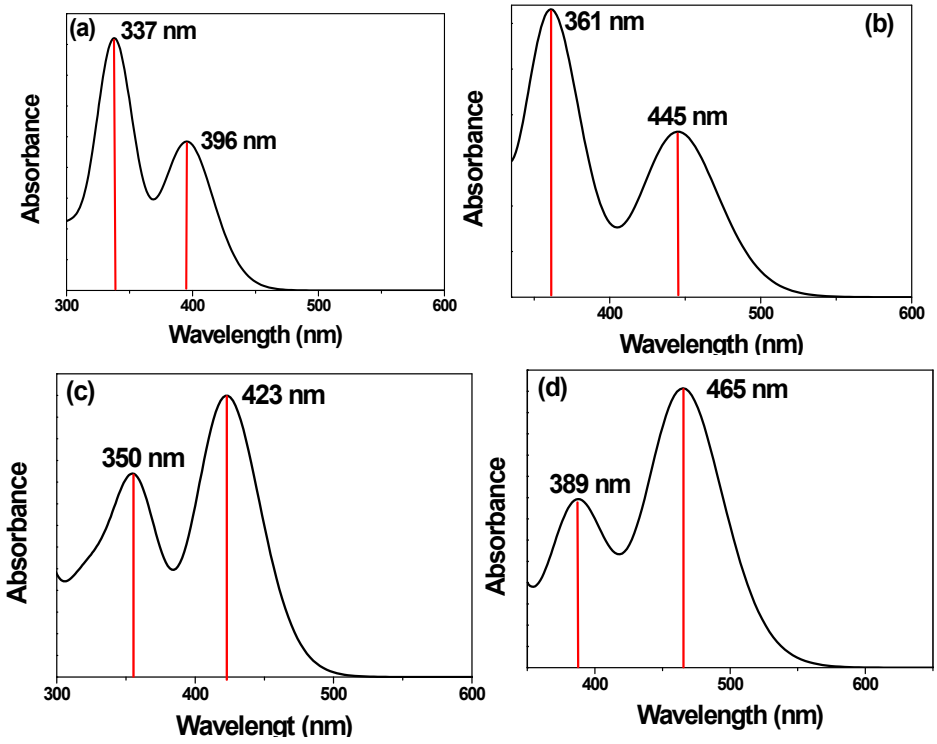


Figure S11. Calculated absorption spectra of **Borepy** (a), **Borepy2** (b), **Borepy3** (c) and **Borepy4** (d)**.**

5. Reference

[1] Sheldrick, G. M. SHELX-97, *Program for the Refinement of Crystal Structures*;University of Göttingen: Göttingen, Germany, **1997**.

[2] Uchiyama, S.; Matsumura, Y.; de Silva, A. P.; Iwai, K. *Anal. Chem.* **2003**, *75*, 5926.

[3] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03, Revision D.01, Gaussian, Inc., Wallingford CT, **2004**.

[4] (a) S. I. Gorelsky, *SWizard program*, http://www.sg-chem.net/, University of Ottawa, Ottawa, Canada, **2013**; (b) S. I. Gorelsky, A. B. P. Lever, *J. Organomet. Chem.* 2001, **635**, 187.

6. Z-matrix and total energy of Borepy1-4.

Borepy1

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	1	B4	4	A3	2	D2	0
C	4	B5	1	A4	5	D3	0
C	6	B6	4	A5	1	D4	0
H	7	B7	6	A6	4	D5	0

C	7	B8	6	A7	4	D6	0
H	9	B9	7	A8	6	D7	0
C	9	B10	7	A9	6	D8	0
H	11	B11	9	A10	7	D9	0
C	11	B12	9	A11	7	D10	0
H	13	B13	11	A12	9	D11	0
C	13	B14	11	A13	9	D12	0
H	15	B15	13	A14	11	D13	0
C	4	B16	1	A15	5	D14	0
C	17	B17	4	A16	1	D15	0
C	18	B18	17	A17	4	D16	0
H	19	B19	18	A18	17	D17	0
C	19	B20	18	A19	17	D18	0
H	21	B21	19	A20	18	D19	0
C	21	B22	19	A21	18	D20	0
H	23	B23	21	A22	19	D21	0
C	23	B24	21	A23	19	D22	0
H	25	B25	23	A24	21	D23	0
C	18	B26	17	A25	4	D24	0
H	27	B27	18	A26	17	D25	0
C	17	B28	4	A27	1	D26	0
C	29	B29	17	A28	4	D27	0
C	30	B30	29	A29	17	D28	0
H	31	B31	30	A30	29	D29	0
C	31	B32	30	A31	29	D30	0
H	33	B33	31	A32	30	D31	0
C	33	B34	31	A33	30	D32	0
H	35	B35	33	A34	31	D33	0
C	35	B36	33	A35	31	D34	0
H	37	B37	35	A36	33	D35	0

C	37	B38	35	A37	33	D36	0
H	39	B39	37	A38	35	D37	0
C	5	B40	1	A39	4	D38	0
C	41	B41	5	A40	1	D39	0
H	42	B42	41	A41	5	D40	0
C	42	B43	41	A42	5	D41	0
H	44	B44	42	A43	41	D42	0
C	44	B45	42	A44	41	D43	0
H	46	B46	44	A45	42	D44	0
C	46	B47	44	A46	42	D45	0
H	48	B48	46	A47	44	D46	0

Variables:

B1	1.39136
B2	1.39976
B3	1.51124
B4	1.55621
B5	1.43557
B6	1.37519
B7	0.92964
B8	1.38571
B9	0.93034
B10	1.37187
B11	0.92973
B12	1.37303
B13	0.92947
B14	1.38863
B15	0.93
B16	1.36148
B17	1.48872
B18	1.38357

B19	0.9301
B20	1.39215
B21	0.93057
B22	1.37107
B23	0.92963
B24	1.36263
B25	0.92994
B26	1.37573
B27	0.9298
B28	1.37669
B29	1.49555
B30	1.38381
B31	0.92988
B32	1.37415
B33	0.92999
B34	1.37415
B35	0.93011
B36	1.36562
B37	0.9299
B38	1.38522
B39	0.92996
B40	1.35244
B41	1.40805
B42	0.92938
B43	1.36504
B44	0.93093
B45	1.37319
B46	0.92953
B47	1.35136
B48	0.92986

A1	108.29387
A2	111.51851
A3	108.89387
A4	117.35308
A5	119.05062
A6	119.44799
A7	120.97009
A8	120.13754
A9	119.76389
A10	119.89559
A11	120.2105
A12	120.00582
A13	119.98519
A14	119.9046
A15	120.56829
A16	118.21136
A17	121.16134
A18	120.25463
A19	119.47453
A20	120.21512
A21	119.70977
A22	119.40924
A23	121.20607
A24	120.46492
A25	119.38274
A26	119.50173
A27	122.17027
A28	120.01492
A29	119.66409
A30	119.13254

A31	121.77411
A32	119.82433
A33	120.30939
A34	120.39776
A35	119.22174
A36	119.52643
A37	120.78423
A38	119.5679
A39	122.0614
A40	118.56226
A41	119.90904
A42	120.12321
A43	119.74021
A44	120.33247
A45	120.7986
A46	118.30098
A47	118.61874
D1	123.80433
D2	-119.92882
D3	-155.4619
D4	-49.98434
D5	-1.83906
D6	178.09886
D7	179.76042
D8	-0.13134
D9	-178.80956
D10	1.13127
D11	177.88388
D12	-2.10188
D13	-177.82034

D14	27.42477
D15	170.06878
D16	-59.83755
D17	-1.6622
D18	178.39247
D19	177.96352
D20	-1.95352
D21	-177.72357
D22	2.32716
D23	179.05546
D24	118.10087
D25	2.94615
D26	-11.52667
D27	170.72798
D28	-65.26852
D29	-1.7996
D30	178.19164
D31	179.75253
D32	-0.21053
D33	179.69892
D34	-0.3645
D35	-179.49044
D36	0.51042
D37	179.9436
D38	-27.88682
D39	-170.2647
D40	176.58765
D41	-3.38332
D42	-178.63646
D43	1.34556

D44	-178.78639
D45	1.18593
D46	178.21799

SCF Done: E(RB+HF-LYP) = -1297.98577735 a.u.

Number of Imaginary frequencies: n.a.

Borepy2

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	1	B4	4	A3	3	D2	0
N	5	B5	1	A4	4	D3	0
C	4	B6	1	A5	5	D4	0
H	7	B7	4	A6	1	D5	0
C	7	B8	4	A7	1	D6	0
H	9	B9	7	A8	4	D7	0
C	9	B10	7	A9	4	D8	0
H	11	B11	9	A10	7	D9	0
C	11	B12	9	A11	7	D10	0
H	13	B13	11	A12	9	D11	0
C	4	B14	1	A13	5	D12	0
C	15	B15	4	A14	1	D13	0
C	16	B16	15	A15	4	D14	0
C	17	B17	16	A16	15	D15	0
H	18	B18	17	A17	16	D16	0
C	18	B19	17	A18	16	D17	0
H	20	B20	18	A19	17	D18	0

C	20	B21	18	A20	17	D19	0
H	22	B22	20	A21	18	D20	0
C	22	B23	20	A22	18	D21	0
H	24	B24	22	A23	20	D22	0
C	17	B25	16	A24	15	D23	0
H	26	B26	17	A25	16	D24	0
C	5	B27	1	A26	4	D25	0
C	28	B28	5	A27	1	D26	0
C	29	B29	28	A28	5	D27	0
H	30	B30	29	A29	28	D28	0
C	30	B31	29	A30	28	D29	0
H	32	B32	30	A31	29	D30	0
C	32	B33	30	A32	29	D31	0
H	34	B34	32	A33	30	D32	0
C	34	B35	32	A34	30	D33	0
H	36	B36	34	A35	32	D34	0
C	36	B37	34	A36	32	D35	0
H	38	B38	36	A37	34	D36	0
C	5	B39	1	A38	4	D37	0
C	40	B40	5	A39	1	D38	0
H	41	B41	40	A40	5	D39	0
C	41	B42	40	A41	5	D40	0
H	43	B43	41	A42	40	D41	0
C	43	B44	41	A43	40	D42	0
C	45	B45	43	A44	41	D43	0
H	46	B46	45	A45	43	D44	0
C	40	B47	5	A46	1	D45	0
H	48	B48	40	A47	5	D46	0
C	6	B49	5	A48	1	D47	0
H	50	B50	6	A49	5	D48	0

H	50	B51	6	A50	5	D49	0
H	50	B52	6	A51	5	D50	0
C	6	B53	5	A52	1	D51	0
H	54	B54	6	A53	5	D52	0
H	54	B55	6	A54	5	D53	0
H	54	B56	6	A55	5	D54	0

Variables:

B1	1.34636
B2	1.38395
B3	1.55021
B4	1.51298
B5	5.64779
B6	1.35287
B7	0.92932
B8	1.34925
B9	0.92934
B10	1.38105
B11	0.92998
B12	1.36642
B13	0.93068
B14	1.36292
B15	1.43255
B16	1.48778
B17	1.37625
B18	0.9303
B19	1.37646
B20	0.93013
B21	1.35741
B22	0.92921
B23	1.3553

B24	0.92982
B25	1.37336
B26	0.9301
B27	1.35352
B28	1.49527
B29	1.3817
B30	0.93057
B31	1.38684
B32	0.93026
B33	1.36236
B34	0.92882
B35	1.35379
B36	0.93045
B37	1.37749
B38	0.931
B39	1.43697
B40	1.38165
B41	0.92986
B42	1.39062
B43	0.92965
B44	1.39409
B45	1.37502
B46	0.93013
B47	1.3769
B48	0.93096
B49	1.43565
B50	0.95871
B51	0.96103
B52	0.9602
B53	1.44782

B54	0.96039
B55	0.96002
B56	0.9604
A1	109.16504
A2	108.62445
A3	109.65813
A4	112.17555
A5	116.82275
A6	118.67574
A7	122.70667
A8	120.78836
A9	118.64525
A10	120.34334
A11	119.37333
A12	119.43605
A13	122.86012
A14	118.92406
A15	118.30109
A16	121.38953
A17	119.61187
A18	120.90621
A19	119.38432
A20	121.2882
A21	120.55546
A22	118.80635
A23	119.77864
A24	121.27693
A25	119.29665
A26	122.34491
A27	119.44506

A28	121.02873
A29	119.91922
A30	120.14183
A31	119.76438
A32	120.37564
A33	119.73488
A34	120.42459
A35	120.32623
A36	119.42522
A37	119.08273
A38	115.42552
A39	119.32212
A40	119.73346
A41	120.53511
A42	119.51866
A43	120.85259
A44	117.65594
A45	119.18009
A46	121.93707
A47	119.5144
A48	119.6306
A49	109.47129
A50	109.39635
A51	109.38781
A52	118.77232
A53	109.44875
A54	109.48744
A55	109.49088
D1	115.44936
D2	120.17039

D3	159.44584
D4	-166.67233
D5	8.68005
D6	-171.44783
D7	179.92919
D8	-0.12368
D9	178.22012
D10	-1.73288
D11	-179.2753
D12	18.98785
D13	-9.61781
D14	177.31423
D15	-106.10253
D16	0.4316
D17	-179.49806
D18	179.6741
D19	-0.25691
D20	179.96734
D21	0.02198
D22	179.95782
D23	73.8181
D24	-0.5841
D25	-17.57762
D26	-172.06894
D27	72.59402
D28	-4.14899
D29	175.82131
D30	-178.70588
D31	1.3025
D32	179.29016

D33	-0.59189
D34	179.59547
D35	-0.44316
D36	-179.19534
D37	160.48148
D38	58.7945
D39	5.21216
D40	-174.90163
D41	179.14423
D42	-0.80628
D43	1.47436
D44	179.05949
D45	-115.47975
D46	-4.78822
D47	78.4988
D48	-60.42757
D49	179.58166
D50	59.65737
D51	-131.96506
D52	-64.51568
D53	175.49491
D54	55.47787

SCF Done: E(RB+HF-LYP) = -1431.88784509 a.u.
Number of Imaginary frequencies: n.a.

Borepy3

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N

N 1 B1

B	1	B2	2	A1			
C	1	B3	3	A2	2	D1	0
C	4	B4	1	A3	3	D2	0
C	2	B5	1	A4	4	D3	0
C	6	B6	2	A5	1	D4	0
H	7	B7	6	A6	2	D5	0
C	7	B8	6	A7	2	D6	0
H	9	B9	7	A8	6	D7	0
C	9	B10	7	A9	6	D8	0
H	11	B11	9	A10	7	D9	0
C	2	B12	1	A11	4	D10	0
H	13	B13	2	A12	1	D11	0
C	1	B14	4	A13	5	D12	0
C	15	B15	1	A14	4	D13	0
H	16	B16	15	A15	1	D14	0
C	16	B17	15	A16	1	D15	0
H	18	B18	16	A17	15	D16	0
C	18	B19	16	A18	15	D17	0
C	20	B20	18	A19	16	D18	0
H	21	B21	20	A20	18	D19	0
C	21	B22	20	A21	18	D20	0
H	23	B23	21	A22	20	D21	0
C	4	B24	1	A23	15	D22	0
C	25	B25	4	A24	1	D23	0
H	26	B26	25	A25	4	D24	0
C	26	B27	25	A26	4	D25	0
H	28	B28	26	A27	25	D26	0
C	28	B29	26	A28	25	D27	0
H	30	B30	28	A29	26	D28	0
C	30	B31	28	A30	26	D29	0

H	32	B32	30	A31	28	D30	0
C	32	B33	30	A32	28	D31	0
H	34	B34	32	A33	30	D32	0
C	5	B35	4	A34	1	D33	0
C	36	B36	5	A35	4	D34	0
H	37	B37	36	A36	5	D35	0
C	37	B38	36	A37	5	D36	0
H	39	B39	37	A38	36	D37	0
C	39	B40	37	A39	36	D38	0
H	41	B41	39	A40	37	D39	0
C	41	B42	39	A41	37	D40	0
H	43	B43	41	A42	39	D41	0
C	43	B44	41	A43	39	D42	0
H	45	B45	43	A44	41	D43	0
C	3	B46	1	A45	4	D44	0
C	47	B47	3	A46	1	D45	0
H	48	B48	47	A47	3	D46	0
C	48	B49	47	A48	3	D47	0
H	50	B50	48	A49	47	D48	0
C	50	B51	48	A50	47	D49	0
H	52	B52	50	A51	48	D50	0
C	52	B53	50	A52	48	D51	0
H	54	B54	52	A53	50	D52	0
C	54	B55	52	A54	50	D53	0
H	56	B56	54	A55	52	D54	0
C	3	B57	1	A56	4	D55	0
C	58	B58	3	A57	1	D56	0
H	59	B59	58	A58	3	D57	0
C	59	B60	58	A59	3	D58	0
H	61	B61	59	A60	58	D59	0

C	61	B62	59	A61	58	D60	0
H	63	B63	61	A62	59	D61	0
C	63	B64	61	A63	59	D62	0
H	65	B65	63	A64	61	D63	0
C	65	B66	63	A65	61	D64	0
H	67	B67	65	A66	63	D65	0
H	20	B68	18	A67	16	D66	0

Variables:

B1	2.51658
B2	1.58146
B3	1.3657
B4	1.39695
B5	1.37549
B6	1.41963
B7	1.08135
B8	1.3801
B9	1.08613
B10	1.40487
B11	1.0836
B12	1.35568
B13	1.08173
B14	1.43289
B15	1.40179
B16	1.08376
B17	1.39546
B18	1.08627
B19	1.39752
B20	1.3972
B21	1.08645
B22	1.39545

B23	1.08518
B24	1.50073
B25	1.40331
B26	1.08436
B27	1.39545
B28	1.08621
B29	1.39725
B30	1.08619
B31	1.39737
B32	1.08624
B33	1.39542
B34	1.0849
B35	1.50016
B36	1.4043
B37	1.08609
B38	1.39752
B39	1.08641
B40	1.39685
B41	1.08624
B42	1.39792
B43	1.08663
B44	1.39673
B45	1.0872
B46	1.62775
B47	1.41131
B48	1.08787
B49	1.3957
B50	1.08712
B51	1.39927
B52	1.08675

B53	1.39553
B54	1.08715
B55	1.40065
B56	1.08615
B57	1.63799
B58	1.40697
B59	1.08642
B60	1.39875
B61	1.0874
B62	1.39691
B63	1.08659
B64	1.39726
B65	1.08725
B66	1.39837
B67	1.08775
B68	1.08596
A1	38.86017
A2	117.67916
A3	121.22307
A4	88.97664
A5	118.07647
A6	118.63397
A7	120.95014
A8	119.94533
A9	119.49791
A10	122.14482
A11	147.17722
A12	115.24791
A13	119.36245
A14	120.75847

A15	119.68692
A16	120.42494
A17	119.34657
A18	120.51811
A19	119.30762
A20	120.19687
A21	120.27289
A22	120.01225
A23	118.80486
A24	119.9065
A25	119.49546
A26	120.71812
A27	119.64426
A28	120.17948
A29	120.22054
A30	119.56808
A31	120.1595
A32	120.15052
A33	119.7146
A34	121.07901
A35	119.51973
A36	118.99549
A37	120.98113
A38	119.64478
A39	120.23492
A40	120.29339
A41	119.4836
A42	120.137
A43	120.0989
A44	119.54288

A45	112.36972
A46	121.37786
A47	119.40205
A48	122.21718
A49	119.91693
A50	119.98441
A51	120.34691
A52	119.19644
A53	120.08419
A54	120.16557
A55	118.71552
A56	111.04601
A57	121.69985
A58	119.22395
A59	122.43337
A60	119.87021
A61	120.06511
A62	120.50956
A63	118.99746
A64	120.04619
A65	120.14403
A66	117.95194
A67	120.33916
D1	-46.02994
D2	20.42277
D3	-1.54703
D4	-169.59668
D5	-176.76813
D6	3.97408
D7	179.71724

D8	-0.11583
D9	179.72519
D10	-156.24836
D11	-28.90063
D12	-156.1774
D13	-129.52941
D14	0.19033
D15	-179.23146
D16	179.96503
D17	0.00293
D18	0.54624
D19	179.25005
D20	-0.17056
D21	178.69332
D22	25.19895
D23	57.62017
D24	-0.58199
D25	178.81755
D26	-179.47636
D27	0.70874
D28	179.61905
D29	-0.28906
D30	179.72363
D31	-0.33877
D32	179.90724
D33	-167.38387
D34	75.91862
D35	-0.17965
D36	179.82995
D37	179.64325

D38	-0.53322
D39	-179.93818
D40	0.12521
D41	179.69153
D42	0.2259
D43	179.04447
D44	-163.60475
D45	55.15182
D46	-1.5447
D47	178.95456
D48	179.73486
D49	0.08471
D50	179.85203
D51	-0.10437
D52	-179.98584
D53	-0.07735
D54	-179.78895
D55	67.74099
D56	33.92621
D57	-3.48397
D58	176.54647
D59	179.99217
D60	0.09074
D61	179.84083
D62	-0.12804
D63	179.92192
D64	0.04278
D65	-179.9778
D66	-179.9265

SCF Done: E(RB+HF-LYP) = -1561.91743804 a.u.

Number of Imaginary frequencies: n.a.

Borepy4

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N							
N	1	B1					
N	1	B2	2	A1			
B	1	B3	2	A2	3	D1	0
C	1	B4	4	A3	2	D2	0
C	5	B5	1	A4	4	D3	0
C	2	B6	1	A5	5	D4	0
C	7	B7	2	A6	1	D5	0
H	8	B8	7	A7	2	D6	0
C	8	B9	7	A8	2	D7	0
H	10	B10	8	A9	7	D8	0
C	10	B11	8	A10	7	D9	0
H	12	B12	10	A11	8	D10	0
C	2	B13	1	A12	5	D11	0
H	14	B14	2	A13	1	D12	0
C	1	B15	5	A14	6	D13	0
C	16	B16	1	A15	5	D14	0
H	17	B17	16	A16	1	D15	0
C	17	B18	16	A17	1	D16	0
H	19	B19	17	A18	16	D17	0
C	19	B20	17	A19	16	D18	0
C	21	B21	19	A20	17	D19	0
H	22	B22	21	A21	19	D20	0
C	16	B23	1	A22	5	D21	0
H	24	B24	16	A23	1	D22	0

C	3	B25	1	A24	5	D23	0
H	26	B26	3	A25	1	D24	0
H	26	B27	3	A26	1	D25	0
H	26	B28	3	A27	1	D26	0
C	3	B29	1	A28	5	D27	0
H	30	B30	3	A29	1	D28	0
H	30	B31	3	A30	1	D29	0
H	30	B32	3	A31	1	D30	0
C	5	B33	1	A32	16	D31	0
C	34	B34	5	A33	1	D32	0
H	35	B35	34	A34	5	D33	0
C	35	B36	34	A35	5	D34	0
H	37	B37	35	A36	34	D35	0
C	37	B38	35	A37	34	D36	0
H	39	B39	37	A38	35	D37	0
C	39	B40	37	A39	35	D38	0
H	41	B41	39	A40	37	D39	0
C	41	B42	39	A41	37	D40	0
H	43	B43	41	A42	39	D41	0
C	6	B44	5	A43	1	D42	0
C	45	B45	6	A44	5	D43	0
H	46	B46	45	A45	6	D44	0
C	46	B47	45	A46	6	D45	0
H	48	B48	46	A47	45	D46	0
C	48	B49	46	A48	45	D47	0
H	50	B50	48	A49	46	D48	0
C	50	B51	48	A50	46	D49	0
H	52	B52	50	A51	48	D50	0
C	52	B53	50	A52	48	D51	0
H	54	B54	52	A53	50	D52	0

C	4	B55	1	A54	5	D53	0
C	56	B56	4	A55	1	D54	0
H	57	B57	56	A56	4	D55	0
C	57	B58	56	A57	4	D56	0
H	59	B59	57	A58	56	D57	0
C	59	B60	57	A59	56	D58	0
H	61	B61	59	A60	57	D59	0
C	61	B62	59	A61	57	D60	0
H	63	B63	61	A62	59	D61	0
C	56	B64	4	A63	1	D62	0
H	65	B65	56	A64	4	D63	0
C	4	B66	1	A65	5	D64	0
C	67	B67	4	A66	1	D65	0
H	68	B68	67	A67	4	D66	0
C	68	B69	67	A68	4	D67	0
H	70	B70	68	A69	67	D68	0
C	70	B71	68	A70	67	D69	0
H	72	B72	70	A71	68	D70	0
C	72	B73	70	A72	68	D71	0
H	74	B74	72	A73	70	D72	0
C	67	B75	4	A74	1	D73	0
H	76	B76	67	A75	4	D74	0

Variables:

B1	2.50417
B2	5.6577
B3	1.56855
B4	1.36979
B5	1.40708
B6	1.38033
B7	1.41852

B8	0.9308
B9	1.34796
B10	0.93015
B11	1.396
B12	0.93048
B13	1.34705
B14	0.92829
B15	1.4444
B16	1.39131
B17	0.92843
B18	1.38694
B19	0.9298
B20	1.35607
B21	1.41924
B22	0.93081
B23	1.36474
B24	0.93012
B25	1.44787
B26	0.95873
B27	0.96174
B28	0.96093
B29	1.44264
B30	0.95891
B31	0.96034
B32	0.961
B33	1.47748
B34	1.38734
B35	0.93081
B36	1.38466
B37	0.93056

B38	1.3514
B39	0.92935
B40	1.38693
B41	0.93139
B42	1.38592
B43	0.92992
B44	1.47771
B45	1.36624
B46	0.92921
B47	1.37033
B48	0.92931
B49	1.38756
B50	0.92939
B51	1.3764
B52	0.92941
B53	1.3734
B54	0.93148
B55	1.60209
B56	1.39681
B57	0.92854
B58	1.39497
B59	0.92926
B60	1.38669
B61	0.92992
B62	1.36018
B63	0.93081
B64	1.38683
B65	0.92959
B66	1.64416
B67	1.39551

B68	0.92888
B69	1.37323
B70	0.92986
B71	1.36198
B72	0.93075
B73	1.36396
B74	0.9299
B75	1.39726
B76	0.9292
A1	145.8448
A2	39.32324
A3	119.07391
A4	120.10943
A5	89.16334
A6	117.06624
A7	119.88802
A8	120.1363
A9	119.14688
A10	121.79016
A11	121.57546
A12	146.908
A13	118.55398
A14	119.97992
A15	119.32586
A16	119.44174
A17	121.19211
A18	119.48392
A19	121.02774
A20	118.51515
A21	120.29231

A22	122.82303
A23	119.10317
A24	120.28302
A25	109.58007
A26	109.43274
A27	109.43393
A28	119.10095
A29	109.50191
A30	109.43522
A31	109.43433
A32	119.31239
A33	121.38912
A34	119.41704
A35	121.15311
A36	119.957
A37	120.03536
A38	119.43785
A39	121.07661
A40	120.64344
A41	118.66641
A42	119.34283
A43	120.41499
A44	119.75526
A45	118.63284
A46	122.66132
A47	119.97381
A48	119.87346
A49	120.57306
A50	118.97417
A51	119.97227

A52	119.98911
A53	119.20664
A54	113.4549
A55	121.04074
A56	118.68755
A57	122.43216
A58	120.21825
A59	119.49569
A60	120.07938
A61	119.80423
A62	120.13436
A63	123.31287
A64	118.59184
A65	109.61031
A66	123.53031
A67	118.75626
A68	122.58737
A69	119.543
A70	120.9057
A71	120.24418
A72	119.46843
A73	120.23114
A74	121.55583
A75	118.84613
D1	66.73001
D2	-44.96966
D3	16.87701
D4	2.61954
D5	-173.12085
D6	-174.01067

D7	5.9376
D8	179.95356
D9	-0.06662
D10	175.88849
D11	-153.91415
D12	-23.90163
D13	-170.25042
D14	-121.95825
D15	-0.56329
D16	179.47024
D17	-179.26956
D18	0.69831
D19	0.54808
D20	178.14514
D21	58.2174
D22	-0.58788
D23	-113.92787
D24	46.05612
D25	-73.88772
D26	166.22007
D27	80.67126
D28	-73.14486
D29	166.74011
D30	46.89327
D31	10.98004
D32	52.31804
D33	-0.73756
D34	179.40678
D35	-177.68505
D36	2.23576

D37	179.55579
D38	-0.57725
D39	178.80396
D40	-0.92684
D41	-179.02682
D42	-164.79927
D43	66.92274
D44	-0.98397
D45	179.00319
D46	178.00903
D47	-2.08647
D48	-177.32169
D49	2.7754
D50	178.95726
D51	-1.01214
D52	178.60829
D53	-161.83506
D54	43.69483
D55	-2.16102
D56	177.84039
D57	179.96169
D58	-0.12971
D59	179.24682
D60	-0.7268
D61	-178.87895
D62	-139.33054
D63	2.58963
D64	66.73602
D65	21.73817
D66	-4.15446

D67	175.80971
D68	-179.6067
D69	0.39215
D70	-178.37539
D71	1.7048
D72	179.1046
D73	-159.55018
D74	4.93172

SCF Done: E(RB+HF-LYP) = -1695.17489366 a.u.

Number of Imaginary frequencies: n.a.