Supplementary Information

Room temperature cupric halide mediated olefin alkoxylation of BODIPYs with methanol: mechanisms and scope

Ying Yang,[a] Xiangrong Wei,[a] Yuexing Zhang,[d] Xin Chi,[d] Dejian Huang,[c] Fu wang,[b] Haixia Wu*[a,c] and Jialin Ming*[a]

[a]Department of Chemistry, College of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot, China 010021.

[b] School of Environmental Science and Engineering, Shanghai Jiao Tong University, Shanghai, China 200240.

[c] Department of Food Science and Technology, National University of Singapore, 3 Science Drive 3, Singapore 117543.

[d]Ministry of Education Key Laboratory for the Synthesis and Application of Organic Functional Molecules. College of Chemistry and Chemical Engineering, Hubei University, Wuhan, China 430062.

Corresponding author:

E-mail: chmwuhx@imu.edu.cn

E-mail: mingjialin@imu.edu.cn

Experimental Section

Materials and Methods. Otherwise stated, all chemicals and solvents were purchased from commercial suppliers and used without further purification. Anhydrous acetonitrile was distilled from CaH_2 prior to use. Fluorescence emission spectra were carried out on HORIBA Scientific Fluorolog®-3 spectrofluorometer. UV-Vis spectra were obtained on Shimadzu UV-1601 UV-visible spectrophotometer fitted with a quartz cell. ^{1}H NMR and ^{13}C{1H} NMR spectra were recorded on a Bruker AC300 spectrometer (Karlsruhe, Germany) at 300 MHz or 500 MHz, using $CDCl_3$ as solvents. High resolution mass spectra were obtained from the microTOF-Q II 1026 mass spectrometer with an ESI source. Electron spin resonance (ESR) spectra were recorded on a JES-FA200 ESR spectrometer at room temperature. Cyclic voltammetry (CV) was performed in anhydrous and degassed acetonitrile on a CHI 620C electrochemical analyzer with a three-electrode cell, containing 0.1M tetra-n-butylammonium hexafluorophosphate (TBAP) as supporting electrolyte at a scan rate of 0.05 V/s at room temperature. Ag/AgCl (0.01 M $AgNO_3$ in acetonitrile), a gold disk and a Pt wire were used as reference electrode, working electrode and counter electrode, respectively. The oxidation potential was externally calibrated against the ferrocene/ferrocenium (Fc/ Fc^+) redox couple [$E_{1/2}$ (Fc/ Fc^+) = 0.40 V vs. SCE in acetonitrile].[1]

DFT Calculations. The ground state molecular structures were optimized in dichloromethane solvent using the integral equation formalism variant (IEF) of PCM with the B3LYP hybrid exchange-correlation (XC) functional along with the SDD basis set, which includes an effective core potential (ECP) for Cu and the 6-31G(d) basis set for the other atoms. No symmetry constraint was imposed during geometry optimization. At the optimized structures, harmonic vibrational frequencies (all real) were calculated to confirm that all optimized structures correspond to energy minima. All calculations were performed by using the Gaussian 16 program.[2] Ionization potential was calculated as the energy difference between the optimized cation and neutral molecules.

General Alkoxylation Synthesis. BODIPY dyes **1, 2** and **2a** were prepared by our previously work.[3] All alkoxylation products were synthesized by following general method. A solution of cupric halides (1.6 mmol) dissolved in alcohols was added to the solution of substrate (0.16 mmol) in dichloromethane, and the final volume ratio of alcohols and dichloromethane would be 1:10 to achieve the final molar ratio of substrate to Cu^{2+} to 1 to10. The reaction mixture was stirred at room temperature for about 30 min or 1 hour and washed with deionized water three times. The organic solution was dried over anhydrous Na_2SO_4. The solution was then filtered and

the volatiles removed under reduced pressure to give crude product, which was further purified by chromatography on silica gel.

Spectral data for 3-[(1,2-dimethoxyl)-N,N-dimethylaniline]-5-(N,N-dimethylaniline)-1,7-dimethyl-8-nitrobenzene-4,4-difluoroboradiazaindacene (**1a)**: Column separation by dichloromethane and hexanes (v/v, 92:8) gave dark blue solid (19.1 mg, yield 88 %).^{1}H NMR (300 MHz, $CDCl_3$, ppm): 8.13 (d, *J* = 9 Hz, 1H, Ar-H), 7.76-7.61 (m, 3H), 7.53 (d, *J* = 9 Hz, 4H, Ar-H), 7.42 (d, *J* = 9 Hz, 2H, Ar-H), 6.71 (d, *J* = 6 Hz, 4H, Ar-H), 6.59 (s, 1H, Pyrrole-H), 6.29 (s, 1H, Pyrrole-H), 5.00 (d, *J* = 6 Hz, 1H, -$CH_2$$CH_2$-), 4.87 (d, *J* = 6 Hz, 1H, -$CH_2$$CH_2$-), 3.42 (s, 3H, OCH_3), 3.38 (s, 3H, OCH_3), 3.04 (s, 6H, $N(CH_3)_2$), 2.90 (s, 6H, $N(CH_3)_2$), 1.39 (s, 3H, CH_3), 1.34 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm): 149.0, 141.0, 134.0, 131.9, 131.3, 130.4, 129.6, 125.0, 112.3, 54.3, 40.4, 14.3. HRMS (ESI-MS) m/z: $[M+H]^+$ Calcd for $C_{39}H_{43}BF_2N_5O_4$ 694.3379; Found 694.3392.

Spectral data for 3,5-[(1,2-dimethoxyl)-N,N-dimethylaniline]-1,7-dimethyl-8-nitrobenzene-4,4-difluoroboradiazaindacene (**1b)**: Column separation by dichloromethane and hexanes (v/v, 995:5) gave dark purple solid (19.4 mg, yield 80%).^{1}H NMR (500 MHz, $CDCl_3$, ppm): 7.72 (d, *J* = 10 Hz, 1H), 7.66 (d, *J* = 5 Hz, 1H), 7.44-7.39 (m, 6H), 6.74-6.71 (m, 4H), 6.31 (d, *J* = 5 Hz, 1H), 6.29 (s, 1H), 5.00 (d, *J* = 5 Hz, 2H, -$CH_2$$CH_2$-), 4.85 (d, *J* = 5 Hz, 1H, -$CH_2$$CH_2$-), 4.83(d, *J* = 5 Hz, 1H, -$CH_2$$CH_2$-), 3.42 (s, 3H, OCH_3), 3.40 (s, 3H, OCH_3), 3.38 (s, 3H, OCH_3,), 3.36 (s, 3H, OCH_3), 2.93 (s, 6H, $N(CH_3)_2$), 2.92 (s, 6H, $N(CH_3)_2$), 1.32 (s, 6H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm):152.1, 142.9, 141.1, 135.3, 130.5, 124.2, 123.7, 121.0, 116.2, 114.4, 107.2, 55.3, 54.7, 40.5, 14.5. HRMS (ESI-MS) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{48}BF_2N_5O_6Na$ 778.3565; Found 778.3585.

Spectral data for 3,5-[(1,2-dimethoxyl)-N,N-dimethylaniline]-1,7-dimethyl-8-aniline-4,4-difluoroboradiazaindacene (**2b)**: Column separation by dichloromethane and hexanes (v/v, 995:5) gave dark purple solid (20.5 mg, yield 85%).^{1}H NMR (300 MHz, $CDCl_3$, ppm): 7.41 (dd, *J* = 9 Hz, *J* = 3 Hz, 4H, Ar-H), 7.19 (t, *J* = 6 Hz, 1H, Ar-H), 6.91(d, *J* = 6Hz, 1H, Ar-H), 6.81 (d, *J* = 6Hz, 1H, Ar-H), 6.68 (dd, *J* = 9 Hz, *J* = 3 Hz, 5H, Ar-H), 6.31 (s, 2H, Pyrrole-H), 4.98 (d, *J* = 6 Hz, 1H, -$CH_2$$CH_2$-), 4.93 (d, *J* = 9 Hz, 1H, -$CH_2$$CH_2$-), 4.88 (d, *J* = 6 Hz, 1H, -$CH_2$$CH_2$-), 4.84 (d, *J* = 9 Hz, 1H, -$CH_2$$CH_2$-), 3.41 (s, 3H, OCH_3), 3.40 (s, 3H, OCH_3), 3.37 (s, 3H, OCH_3,), 3.36 (s, 3H, OCH_3), 2.91 (s, 12H, $N(CH_3)_2$), 1.52 (s, 6H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm):151.9, 149.8, 143.1, 135.3, 130.2, 124.2, 123.7, 120.5, 116.0, 112.8, 106.9, 55.1, 54.6, 40.9, 14.2. HRMS (ESI-MS) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{50}BF_2N_5O_4Na$ 748.3823; Found 748.3857.

Spectral data for 3-[(1,2-diethoxy)-N,N-dimethylaniline]-5-(N,N-dimethylaniline)-1,7-dimethyl-8-aniline-4,4-difluoroboradiazaindacene (**3)**: Column separation by dichloromethane and hexanes (v/v, 92:8) gave dark blue solid (21.1 mg, yield 90 %).^{1}H NMR (500 MHz, $CDCl_3$, ppm): 7.52 (d, *J* = 10 Hz, 3H, Ar-H), 7.48 (d, *J* = 10 Hz, 2H, Ar-H), 7.23-7.21 (m, 1H, Ar-H), 7.19 (d, *J* = 10 Hz, 1H, Ar-H), 7.04 (d, *J* = 10 Hz, 1H, Ar-H), 6.94 (d, *J* = 10 Hz, 1H, Ar-H), 6.85-6.82 (m, 1H, Ar-H), 6.72 (d, *J* = 10 Hz, 4H, Ar-H),6.57 (s, 1H, Pyrrole-H), 6.40 (s, 1H, Pyrrole-H), 5.00 (d, *J* = 5 Hz, 1H, -$CH_2$$CH_2$-), 4.95 (d, *J* = 5 Hz, 1H, -$CH_2$$CH_2$-), 3,79-3.69 (m, 4H, -$OCH_2$-), 3.04 (s, 6H, $N(CH_3)_2$), 2.91 (s, 6H, $N(CH_3)_2$), 1.57 (s, 6H, CH_3), 1.18 (t, *J* = 5 Hz, 3H, CH_3), 1.14 (t, *J* = 5 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, ppm):154.9, 151.2, 149.7, 144.0, 137.5, 130.5, 130.2, 129.5, 127.5, 125.1, 120.3, 119.1, 117.6, 115.7, 115.1, 112.8, 112.2, 105.0, 62.9, 62.5, 40.9, 40.2, 15.3, 14.0. HRMS (ESI-MS) m/z: $[M+Na]^+$ Calcd for $C_{41}H_{48}BF_2N_5O_4Na$ 714.3768; Found 714.3774.

Spectral data for 1-(1,2-dimethoxy-2-phenylethyl)-4-methoxybenzene (**14)**: Column separation by dichloromethane and hexanes (v/v, 4:6) gave light yellow oil (34.6 mg, yield 80%). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): 7.45-7.28 (m, 7H, Ar-H), 6.95 (d, *J* = 9 Hz, 2H, Ar-H), 5.07 (d, *J* = 9 Hz, 1H, CH_3OCH-), 4.33 (d, *J* = 6 Hz, 1H, CH_3OCH-), 3.81 (s, 3H, Ar-OCH_3), 3.41 (s, 3H, CH_3OCH-), 3.40 (s, 3H, CH_3OCH-); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, ppm): 158.1, 141.5, 133.2, 129.6, 128.6, 128.2, 126.2, 113.7, 106.6, 54.9, 53.9, 53.6. ESI-HRMS: *m/z* calcd for $[M+Na]^+$ $C_{17}H_{20}O_3Na$, 295.1305; found 295.1307.

Spectral data for 4-(1,2-dimethoxy-2-phenylethyl)-N,N-dimethylaniline (**15)**: Column separation by dichloromethane and hexanes (v/v, 9:1) gave yellow waxy (38.4 mg, yield 84%). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): 7.31-7.28 (m, 3H, Ar-H), 7.17 (d, *J* = 9 Hz, 4H, Ar-H), 6.68 (d, *J* = 9 Hz, 2H, Ar-H), 4.94 (d, *J* = 6 Hz, 1H, CH_3OCH-), 4.14 (d, *J* = 6 Hz, 1H, CH_3OCH-), 3.31 (s, 3H, CH_3OCH-), 3.30 (s, 3H, CH_3OCH-), 2.90 (s, 6H, $N(CH_3)_2$); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, ppm): 149.4, 142.1, 129.5, 128.8, 128.4, 126.3, 112.9, 107.0, 54.2, 53.8, 40.8. APCI-HRMS: *m/z* calcd for $[M+H]^+$ $C_{18}H_{24}NO_2$, 286.1802; found 286.1805.

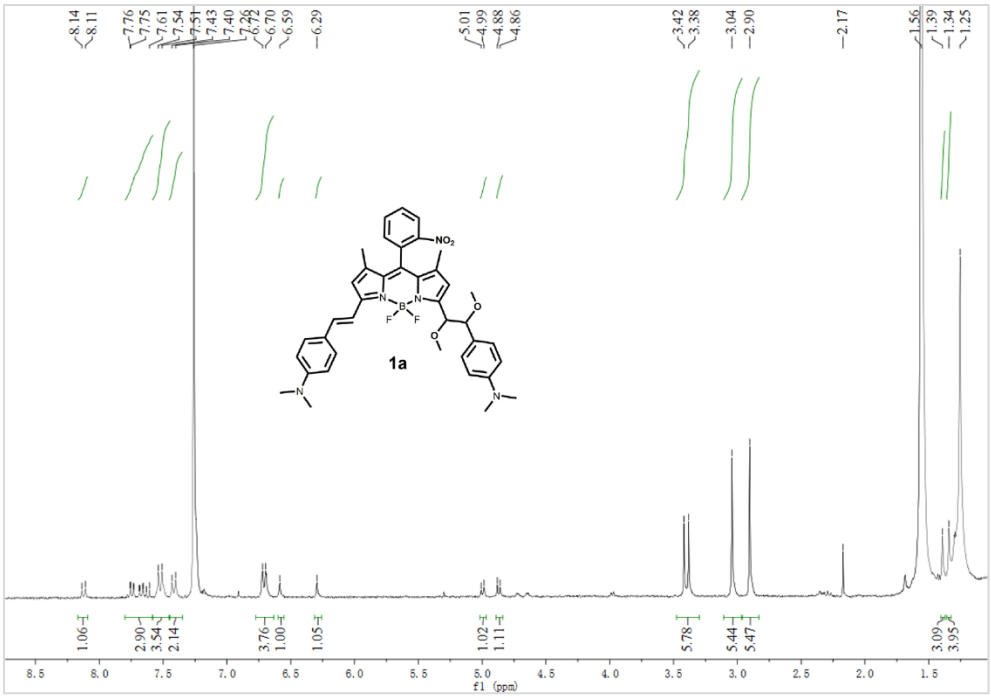
Spectral data for (1-bromo-2-methoxypropan-2-yl) benzene (**17)**: Column separation by hexanes gave colorless oil (24.9 mg, yield 68%). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): 7.43-7.31 (m, 5H, Ar-H), 3.64 (d, *J*=9 Hz, 1H), 3.51 (d, *J* = 12 Hz, 1H), 3.15(s, 3H, CH_3O), 1.71 (s, 3H, CH_3); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, ppm): 141.9, 128.6, 128.0, 126.6, 78.0, 51.2, 43.3, 22.0. APCI-MS: *m/z* calcd for $[M-OCH_3]^+$ $C_9H_{10}Br^+$, 198.1; found 199.0. calcd for $[M-Br]^+$ $C_{10}H_{13}O^+$, 149.1; found 149.1.

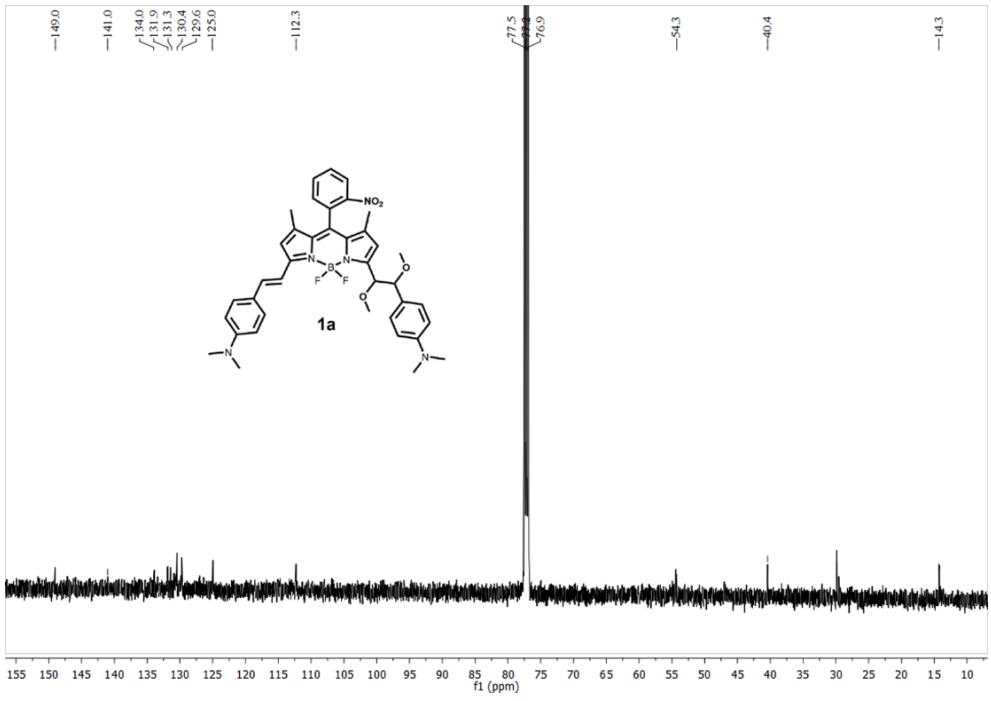
Spectral data for 1-(2-bromo-1-methoxyethyl)-4-methoxybenzene (**19)**: Column separation by dichloromethane and hexanes (v/v, 6:4) gave light yellow oil (29.0 mg, yield 74%). ^{1}H NMR (300 MHz, $CDCl_3$,

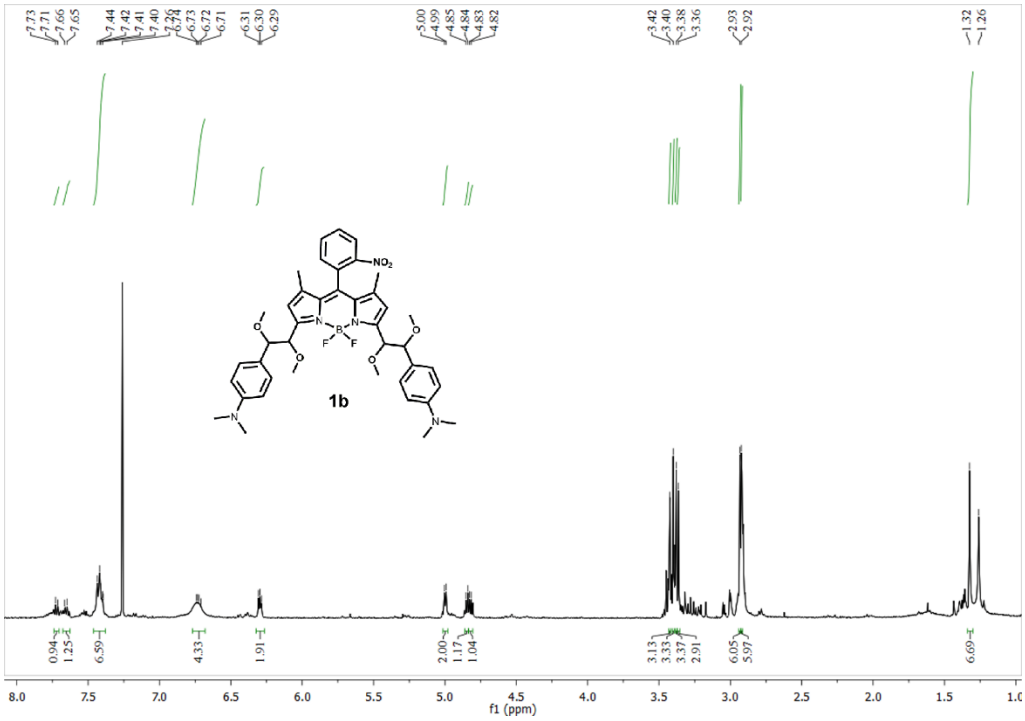
ppm): 7.29 (d, *J* = 9 Hz, 2H, Ar-H), 6.95 (d, *J* = 9 Hz, 2H, Ar-H), 4.38 (dd, *J* = 9 Hz, *J* = 6 Hz, 1H, CH_3OCH-), 3.85 (s, 3H, Ar-OCH_3), 3.57 (dd, *J* = 12 Hz, *J* = 9 Hz, 1H, $BrCH_2$), 3.47 (dd, *J* = 9 Hz, *J* = 3 Hz, 1H, $BrCH_2$), 3.32 (s, 3H, OCH_3) ; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, ppm): 159.8, 131.0, 128.1, 114.1, 83.0, 57.1, 55.3, 36.5. EI-MS: *m/z* $[M\text{-}Br\text{-}CH_2]^+$ $C_9H_{11}O_2^+$, 151.2; found 151.1.

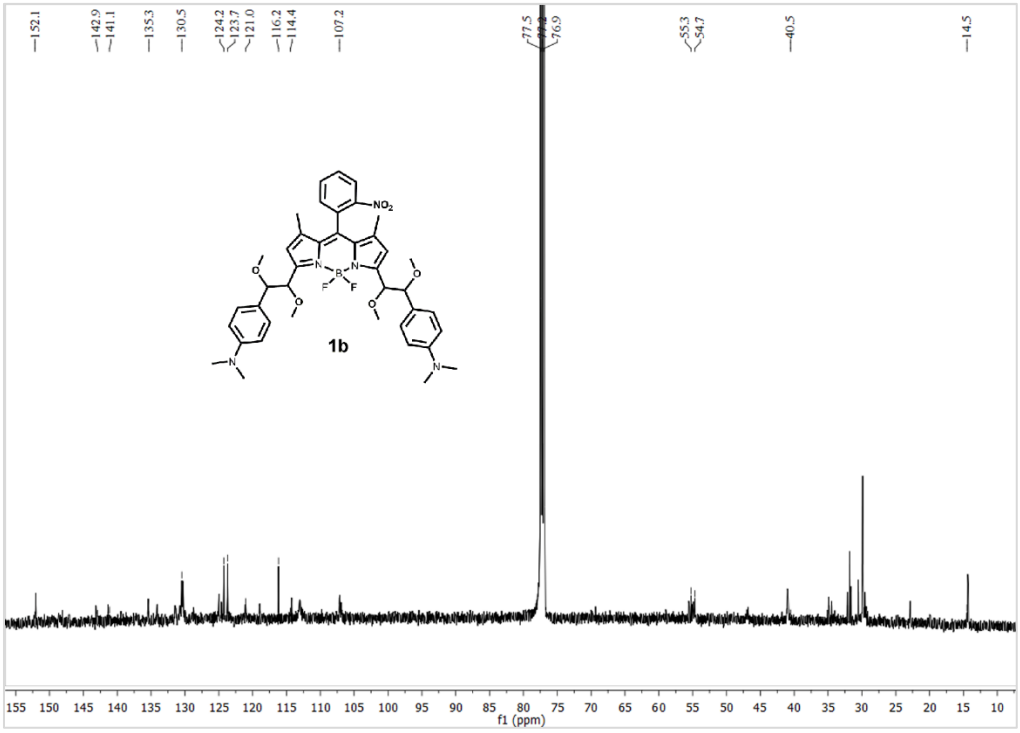
References

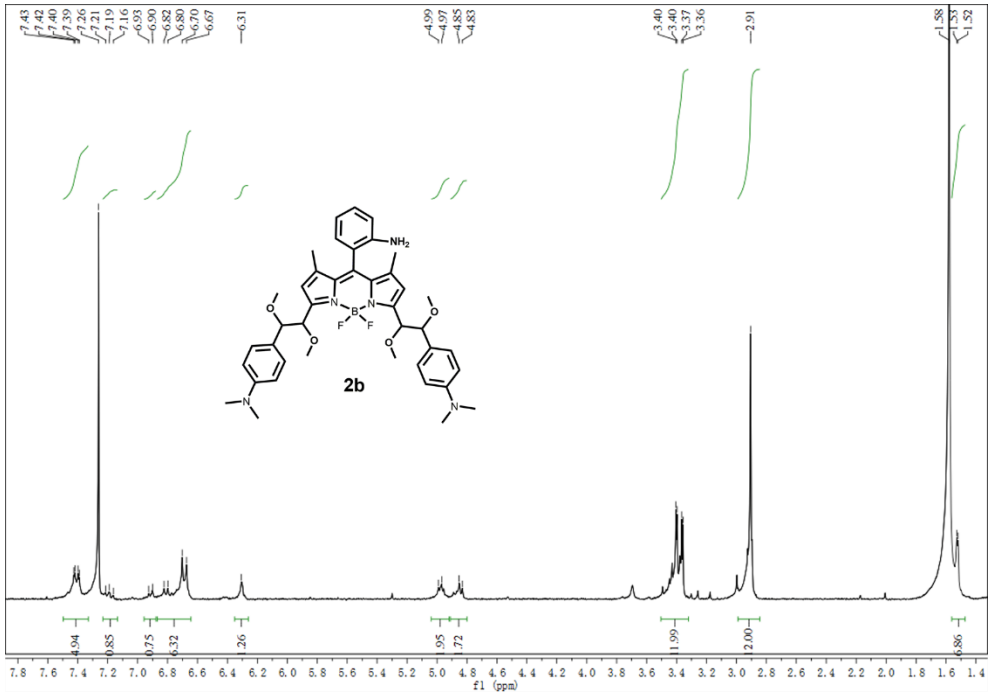
1. M. A. Halcrow and G. Christou, *Chem. Rev.,* 1994, **94**, 2421-2481.
2. M. J. Frisch, et al. Gaussian 16, Revision A.03, Gaussian, Inc., Wallingford CT, 2016.
3. H. X. Wu, S. Krishnakumar, J. Yu, D. Liang, H. Y. Qi,; Z. W. Lee, L. W. Deng and D. J. Huang, *Chem. Asian J.*, 2014, **9**, 3604-3611.

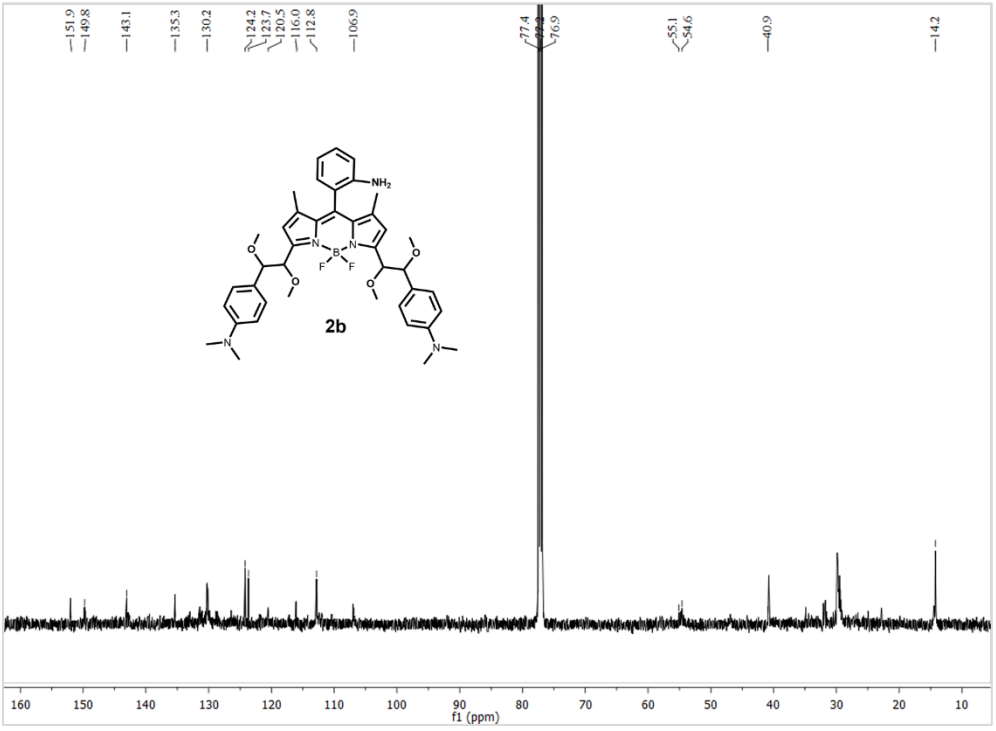

8.14
8.11
7.76
7.75
7.61
7.54
7.51
7.43
7.40
7.28
6.72
6.70
6.59
6.29
5.01
4.99
4.88
4.86
3.42
3.38
3.04
2.90
2.17
1.56
1.39
1.34
1.25
1.06
2.90
3.54
2.14
3.76
1.00
1.05
1.02
1.11
5.78
5.44
5.47
3.09
3.95
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)
NO2
1a

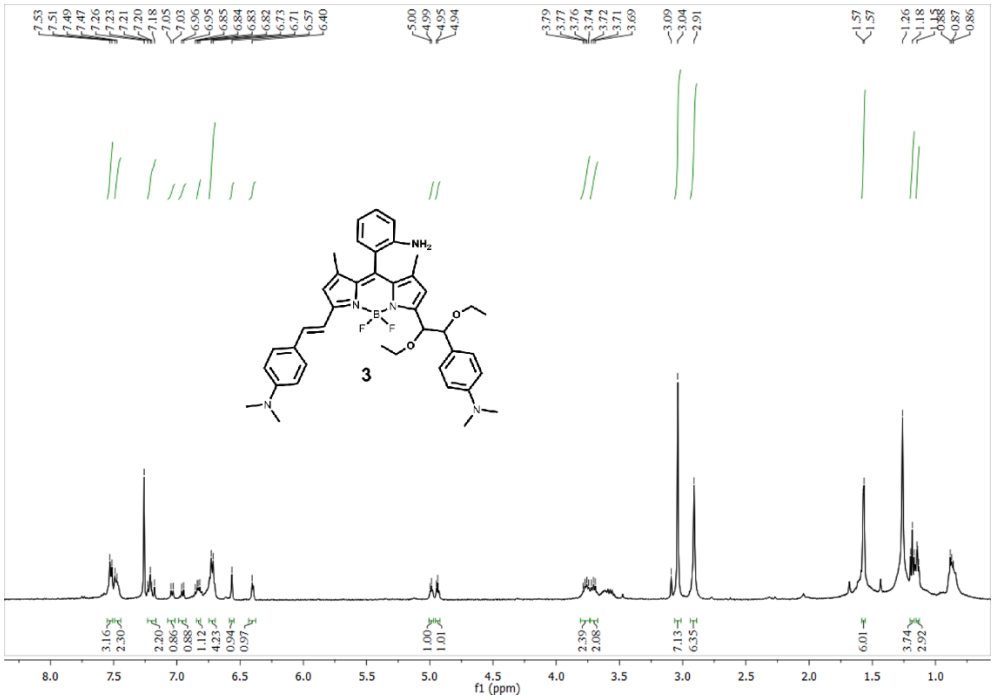

149.0
141.0
134.0
131.9
131.3
130.4
129.6
125.0
112.3
77.5
76.9
54.3
40.4
14.3
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)
NO2
1a

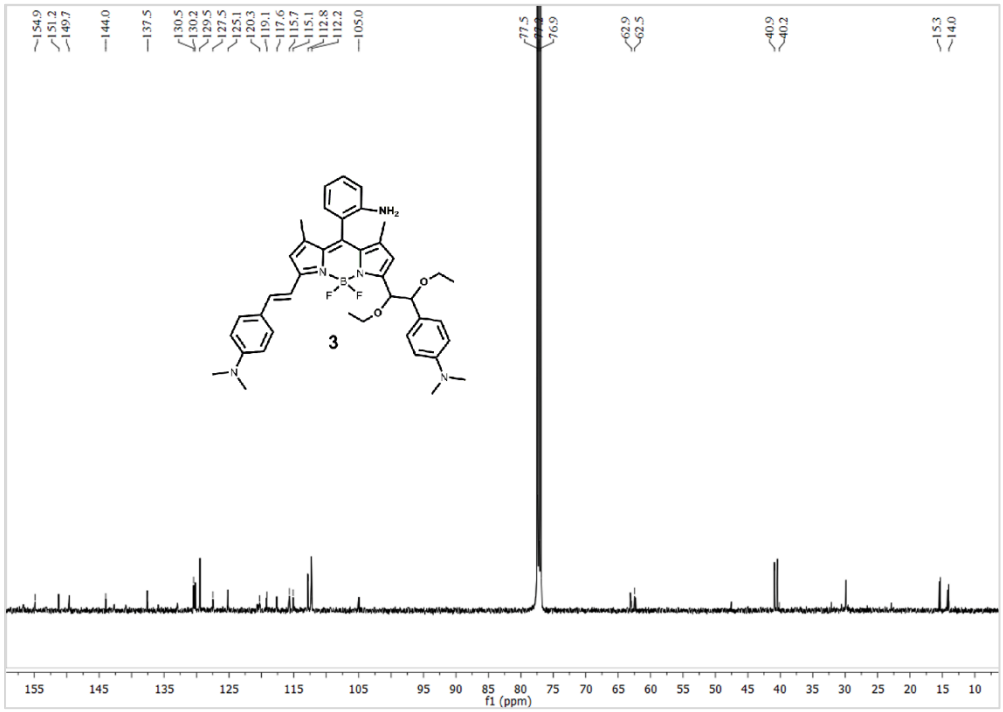

7.73
7.71
7.66
7.65
7.44
7.42
7.41
7.40
7.26
6.74
6.73
6.72
6.71
6.31
6.30
6.29
5.00
4.99
4.85
4.84
4.83
4.82
3.42
3.40
3.38
3.36
2.93
2.92
1.32
1.26
NO2
1b
0.94
1.25
6.59
4.33
1.91
2.00
1.17
1.04
3.13
3.33
3.37
2.91
6.05
5.97
6.69
f1 (ppm)

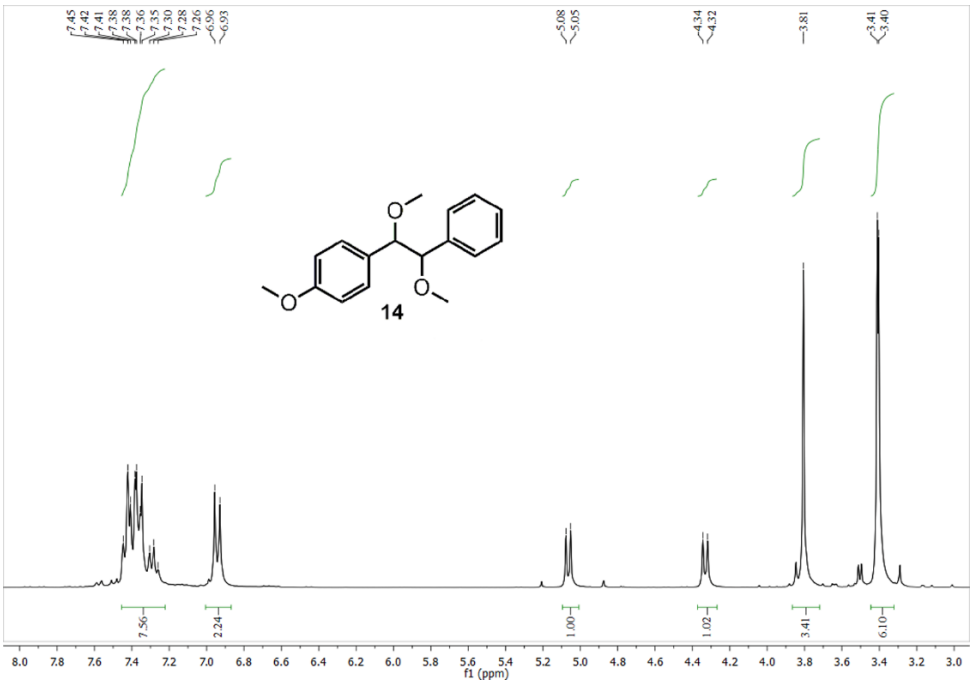

152.1
142.9
141.1
135.3
130.5
124.2
123.7
121.0
116.2
114.4
107.2
77.5
76.9
55.3
54.7
40.5
14.5
NO2
1b
f1 (ppm)

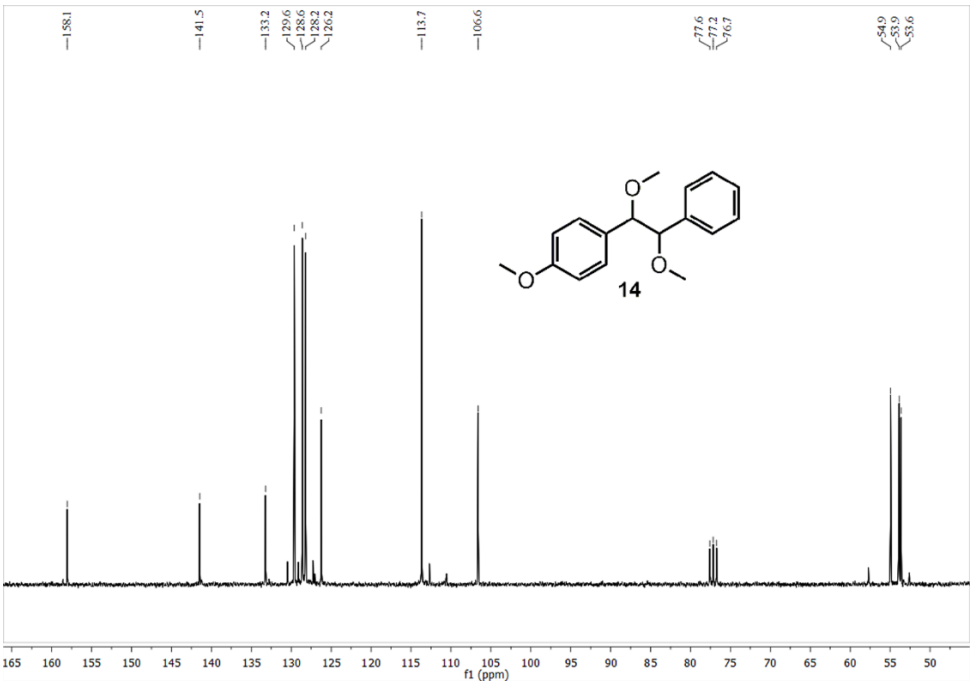

7.43
7.42
7.40
7.39
7.26
7.21
7.19
7.16
6.93
6.90
6.82
6.80
6.70
6.67
6.31
4.99
4.97
4.85
4.83
3.40
3.40
3.37
3.36
2.91
1.58
1.53
1.52
NH2
2b
4.94
0.85
0.75
6.32
2.26
0.95
0.72
1.99
2.00
6.86
f1 (ppm)

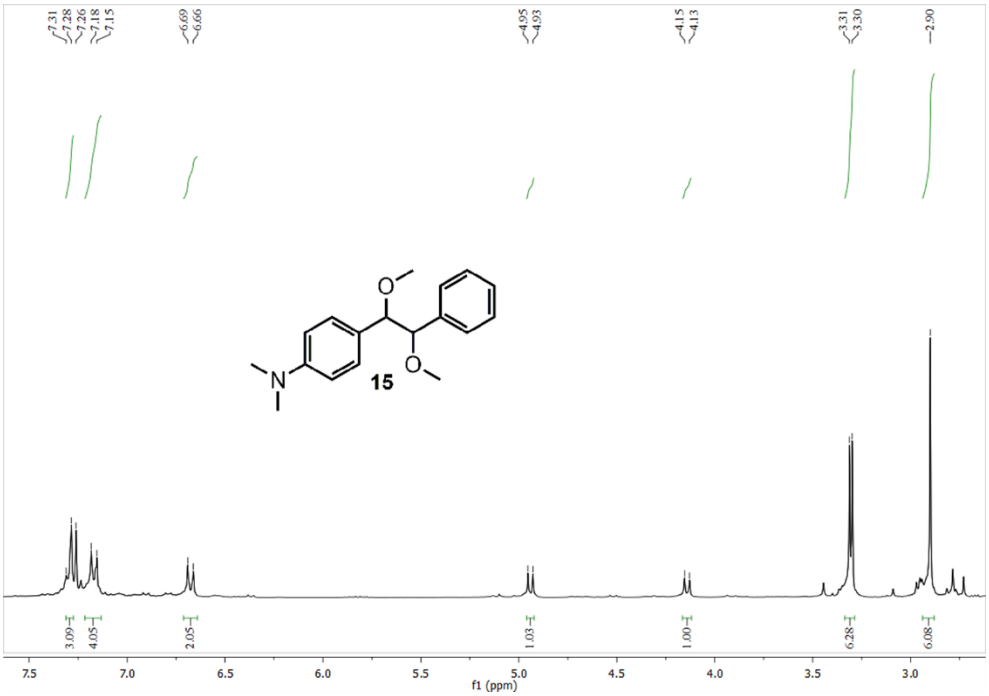

151.9
149.8
143.1
135.3
130.2
124.2
123.7
120.5
116.0
112.8
106.9
77.4
76.9
55.1
54.6
40.9
14.2
NH2
2b
f1 (ppm)


7.53
7.51
7.49
7.47
7.26
7.23
7.21
7.20
7.18
7.05
7.03
6.96
6.95
6.85
6.84
6.83
6.82
6.73
6.71
6.57
6.40
5.00
4.99
4.95
4.94
3.79
3.77
3.76
3.74
3.72
3.71
3.69
3.09
3.04
2.91
1.57
1.57
1.26
1.18
0.88
0.87
0.86
NH2
3
3.16
2.30
2.20
0.86
0.88
1.12
4.23
0.94
0.97
1.00
1.01
2.39
2.08
7.13
6.35
6.01
3.74
2.92
f1 (ppm)

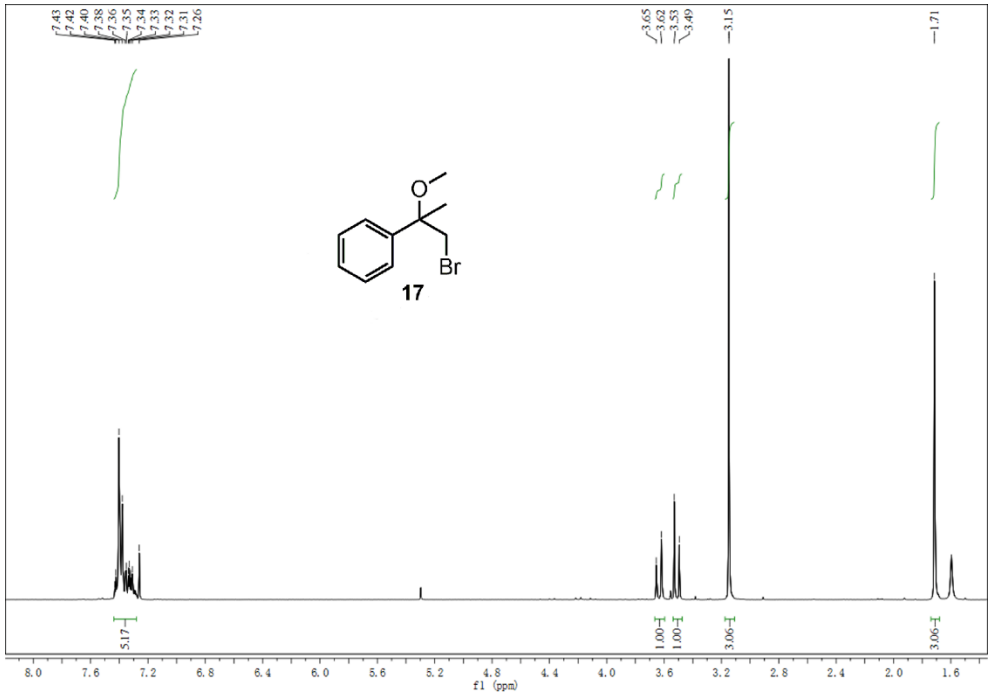

154.9
151.2
149.7
144.0
137.5
130.5
130.2
129.5
127.5
125.1
120.3
119.1
117.6
115.7
115.1
112.8
112.2
105.0
77.5
76.9
62.9
62.5
40.9
40.2
15.3
14.0
NH2
3
f1 (ppm)

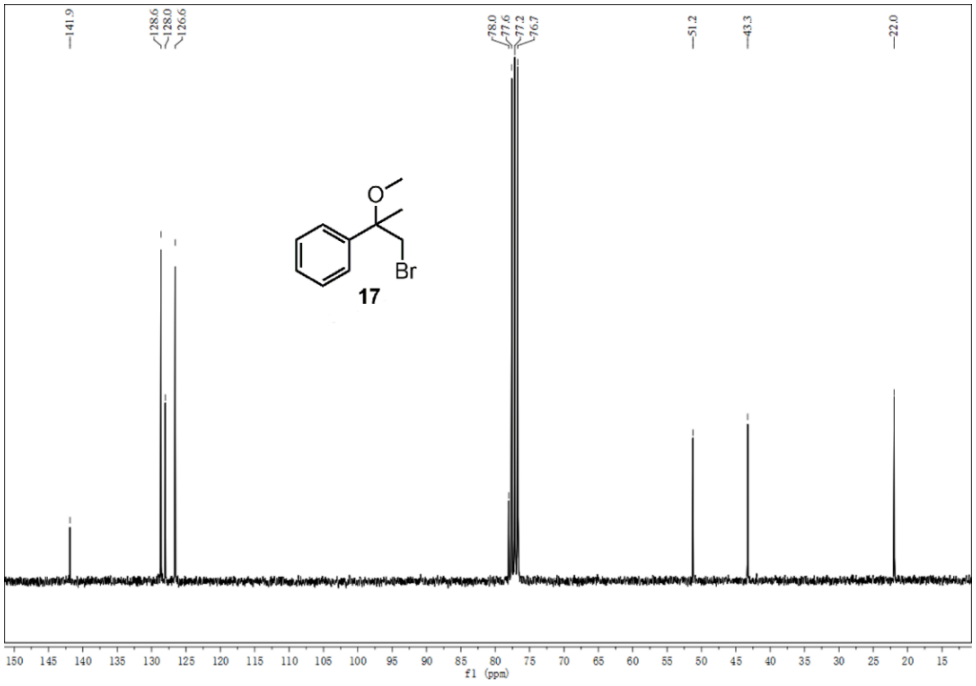

7.45
7.42
7.41
7.38
7.38
7.36
7.35
7.30
7.28
7.26
6.96
6.93
5.08
5.05
4.34
4.32
3.81
3.41
3.40
14
7.56
2.24
1.00
1.02
3.41
6.10
f1 (ppm)


158.1
141.5
133.2
129.6
128.6
128.2
126.2
113.7
106.6
77.6
77.2
76.7
54.9
53.9
53.6
14
f1 (ppm)


7.31
7.28
7.26
7.18
7.15
6.69
6.66
4.95
4.93
4.15
4.13
3.31
3.30
2.90
O
O
N
15
3.09
4.05
2.05
1.03
1.00
6.28
6.08
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f1 (ppm)


149.4
142.1
129.5
128.8
128.4
126.3
112.9
107.0
77.6
77.2
76.7
54.2
53.8
40.8
O
O
N
15
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
f1 (ppm)


7.43
7.42
7.40
7.38
7.36
7.35
7.34
7.33
7.32
7.31
7.26
3.65
3.62
3.53
3.49
3.15
1.71
O
Br
17
5.17
1.00
1.00
3.06
3.06
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
f1 (ppm)


141.9
128.6
128.0
126.6
78.0
77.6
77.2
76.7
51.2
43.3
22.0
O
Br
17
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)

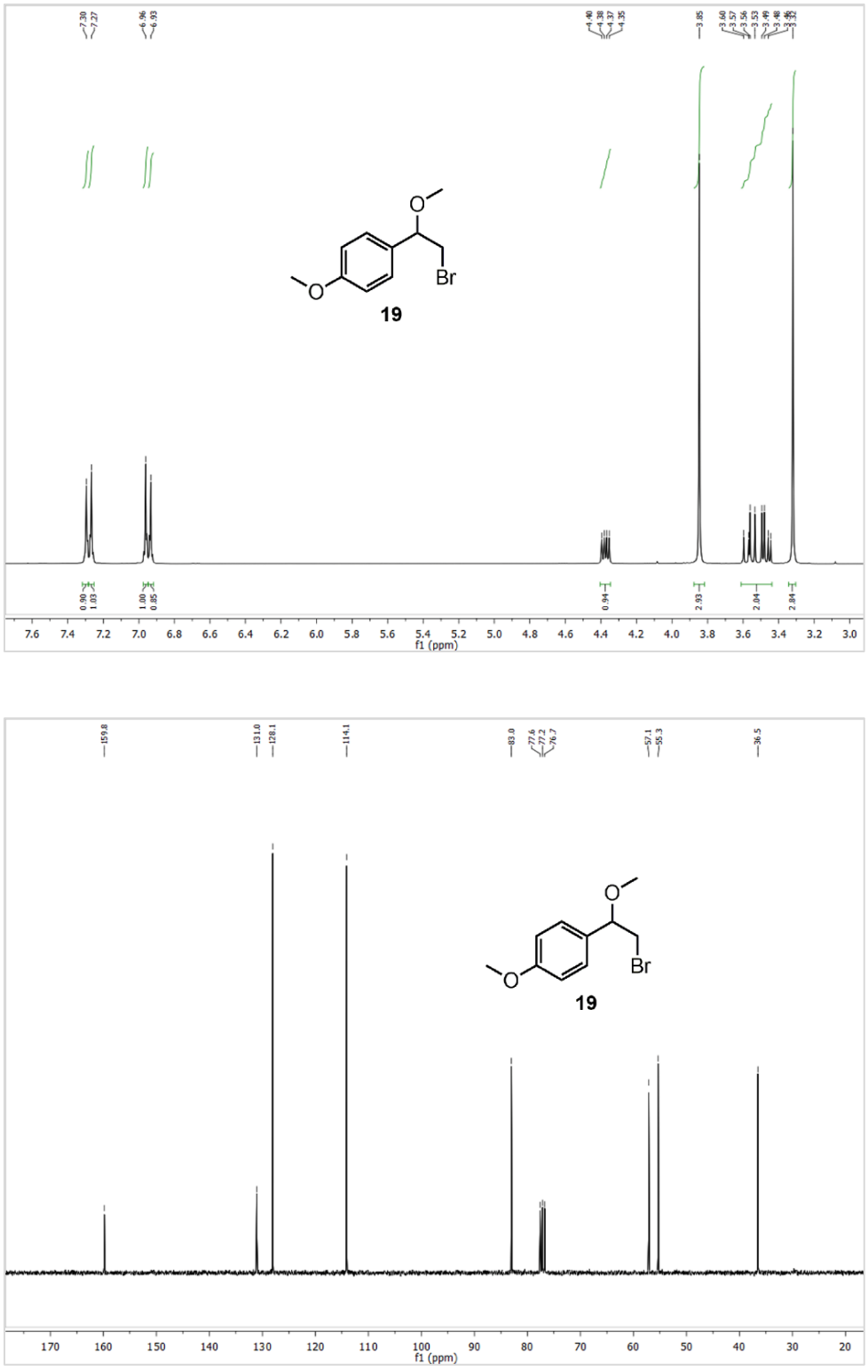


Fig. S1 NMR spectra of alkoxylated products.

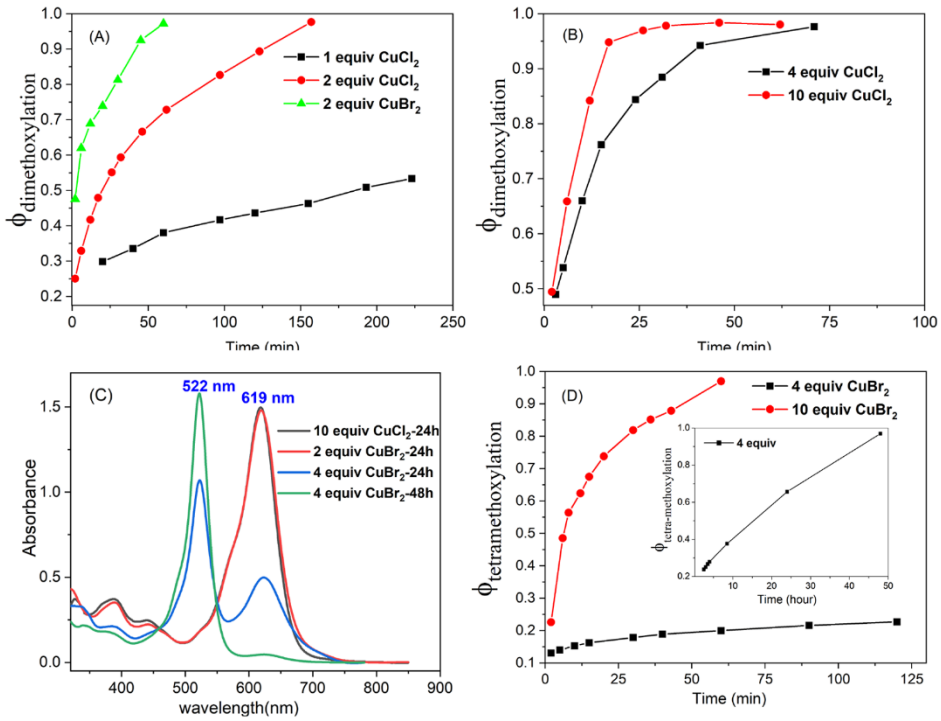


Fig. S2 Kinetics study for dimethoxylated product **2a** and tetramethoxylated product **2b** mediated by $CuCl_2$ and $CuBr_2$, respectively.

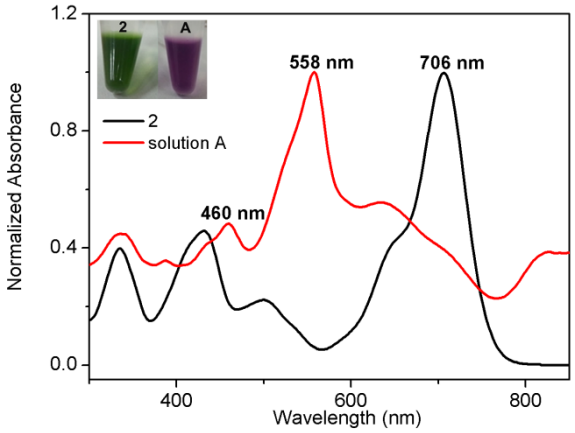


Fig. S3 UV-Vis absorption spectra of **2** and intermediate complex **A** in CH_2Cl_2. The inset shows the photograph of **2** and solution **A** in CH_2Cl_2.

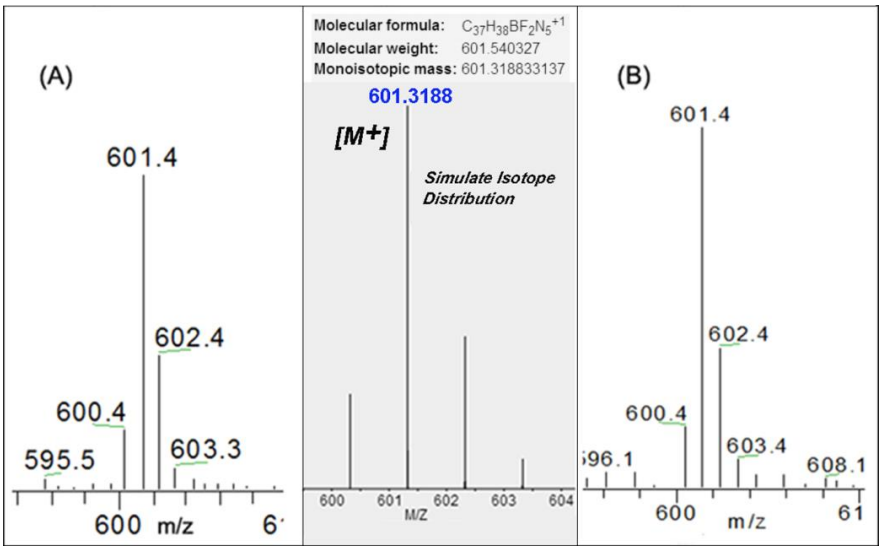


Fig. S4 ESI-MS spectra (positive mode) of radical cation of **2**. (A) Solution A formed by dissolving complex A in CH_2Cl_2. (B) the pink solution of **2** after titrating Cp_2FePF_6.

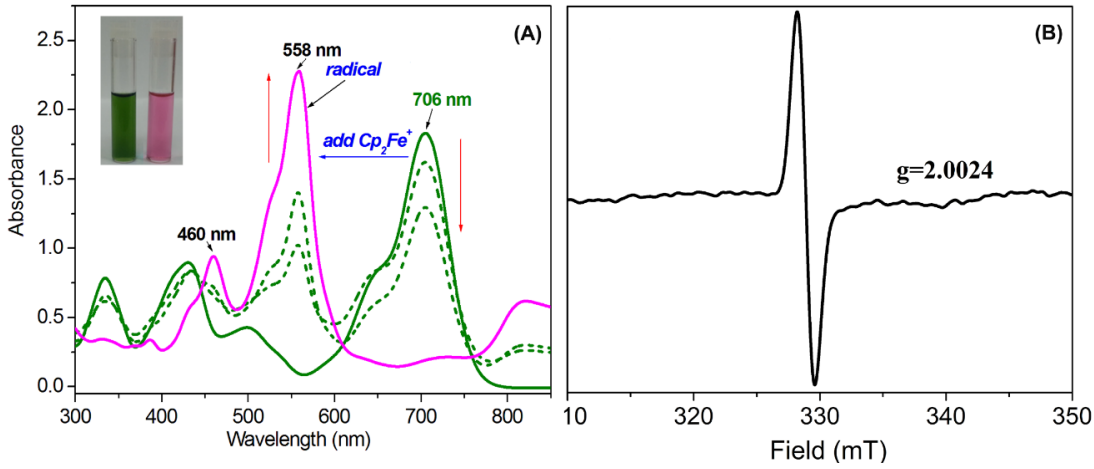


Fig. S5 (A) UV-Vis absorption spectra of radical cation formed by titrating **2** with Cp_2FePF_6 in CH_2Cl_2. The inset shows the photograph of **2** (Left) and its radical cation (Right) in CH_2Cl_2. (B) ESR spectrum of radical cation which was generated by titrating Cp_2FePF_6 to **2** in CH_2Cl_2.

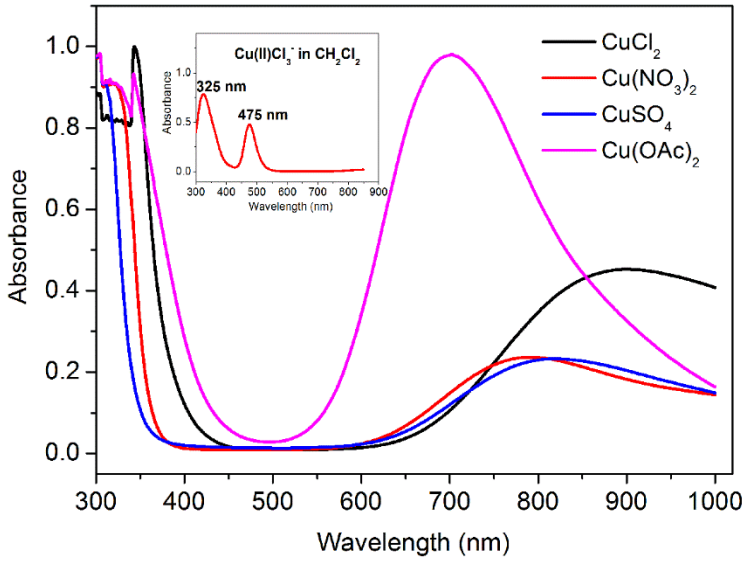


Fig. S6 UV-Vis absorption spectra of different copper salts in MeOH. The inset one was $Cu(II)Cl_3^-$ in CH_2Cl_2 .

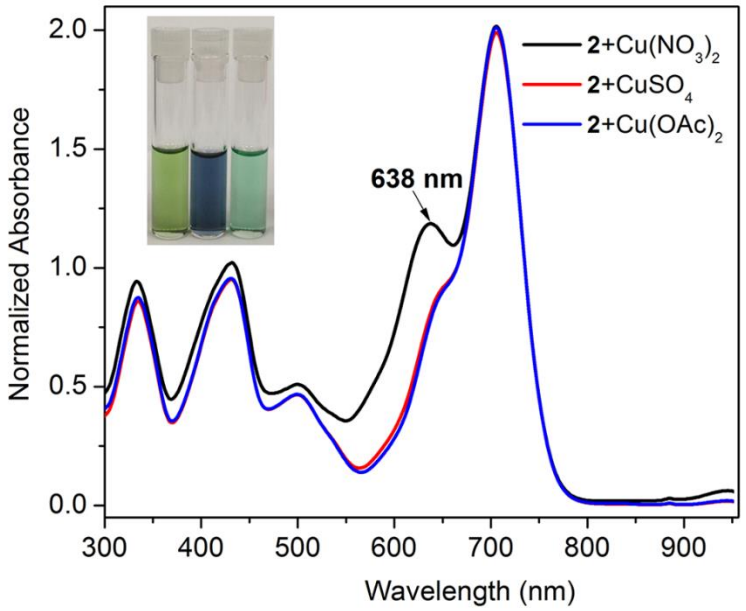


Fig. S7. UV-Vis absorption spectra of samples in CH_2Cl_2. Samples were prepared by **2** mixing with different kinds of 10 equiv. copper salts for 4 hours in a mixture solution of CH_2Cl_2 and MeOH (v/v=10:1), then the mixture solution were washed with deionized water twice. The inset shows the photograph of **2** only, **2** with $Cu(NO_3)_2$ before and after washing with water twice, respectively (from left to right).

Cartesian coordinates, number of imaginary frequencies, computed total energies of optimized structures.

Compound 2, no imaginary frequencies, E(RB3LYP) = -1931.31531888 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.318119	-0.008898	-1.534526
2	6	0	-5.927046	-0.010127	-1.432944
3	6	0	-5.283106	-0.012451	-0.189404
4	6	0	-6.058021	-0.013212	0.993443
5	6	0	-7.461154	-0.009361	0.882909
6	6	0	-8.080890	-0.008168	-0.363029
7	6	0	-3.787907	-0.010152	-0.128144
8	6	0	-3.087064	-1.229025	-0.112656
9	7	0	-1.690474	-1.250809	-0.091924
10	5	0	-0.798331	-0.002234	0.136445
11	7	0	-1.695960	1.242370	-0.095085
12	6	0	-3.092384	1.214276	-0.120452
13	6	0	-3.550513	-2.590684	-0.139933
14	6	0	-2.418851	-3.385666	-0.139098

15	6	0	-1.270420	-2.549952	-0.107137
16	6	0	-1.280580	2.542892	-0.119240
17	6	0	-2.431697	3.373504	-0.163530
18	6	0	-3.560767	2.574053	-0.163484
19	6	0	0.118211	-2.923005	-0.106938
20	6	0	0.556633	-4.207625	-0.007641
21	6	0	1.930484	-4.670606	-0.011417
22	6	0	0.106828	2.921621	-0.114604
23	6	0	0.539580	4.208268	-0.018664
24	6	0	1.911700	4.676846	-0.016710
25	6	0	2.198408	-6.051146	0.105311
26	6	0	3.487124	-6.560692	0.107832
27	6	0	4.609183	-5.700754	-0.009058
28	6	0	4.346720	-4.308254	-0.125667
29	6	0	3.052537	-3.819316	-0.126027
30	6	0	2.173465	6.058789	0.096703
31	6	0	3.460156	6.573479	0.105411
32	6	0	4.586286	5.717625	-0.001551
33	6	0	4.330010	4.323726	-0.114867
34	6	0	3.037754	3.829651	-0.121513
35	7	0	5.893640	-6.189492	-0.009790

36	6	0	7.024851	-5.281026	-0.132299
37	6	0	6.131492	-7.619246	0.125693
38	7	0	5.868825	6.211477	0.003892
39	6	0	7.004435	5.306810	-0.105211
40	6	0	6.100234	7.642242	0.139636
41	6	0	-4.956596	-3.114414	-0.160108
42	6	0	-4.967479	3.096517	-0.207702
43	9	0	-0.294429	0.000977	1.442871
44	9	0	0.272972	-0.000529	-0.773105
45	7	0	-5.453275	-0.084472	2.249003
46	1	0	-7.796887	-0.007191	-2.509072
47	1	0	-5.316384	-0.006966	-2.332323
48	1	0	-8.060517	-0.010239	1.790498
49	1	0	-9.166451	-0.003761	-0.417422
50	1	0	-2.408097	-4.467015	-0.174581
51	1	0	0.829387	-2.110776	-0.202183
52	1	0	-0.186393	-4.998588	0.090225
53	1	0	0.821623	2.111777	-0.202553
54	1	0	-0.207109	4.996683	0.072052
55	1	0	1.363589	-6.742865	0.196492
56	1	0	3.625439	-7.631144	0.200034

57	1	0	5.166888	-3.606177	-0.215455
58	1	0	2.909558	-2.746355	-0.216757
59	1	0	1.335403	6.747545	0.180383
60	1	0	3.593654	7.644787	0.194836
61	1	0	5.153468	3.624556	-0.196914
62	1	0	2.899591	2.755802	-0.209270
63	1	0	7.063236	-4.563257	0.698343
64	1	0	7.949276	-5.858979	-0.122536
65	1	0	6.989326	-4.713286	-1.071680
66	1	0	5.730630	-8.009970	1.070778
67	1	0	5.676190	-8.186602	-0.697301
68	1	0	7.205586	-7.805977	0.111405
69	1	0	6.977260	4.733114	-1.041194
70	1	0	7.926460	5.888555	-0.093281
71	1	0	7.040347	4.594350	0.730163
72	1	0	5.692897	8.032245	1.082304
73	1	0	7.173620	7.833327	0.130612
74	1	0	5.646939	8.207008	-0.686199
75	1	0	-5.513899	-2.773302	-1.038502
76	1	0	-4.941721	-4.208865	-0.169049
77	1	0	-5.521596	-2.789950	0.720290

78	1	0	-4.952657	4.190875	-0.221987
79	1	0	-5.509582	2.751018	-1.093843
80	1	0	-5.551470	2.778109	0.662484
81	1	0	-6.020047	0.263701	3.013371
82	1	0	-4.507942	0.277832	2.294878
83	1	0	-2.425108	4.454477	-0.210161

Cation of Compound 2 (2^+), no imaginary frequencies, E(UB3LYP) = -1931.15504036 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.246341	0.149227	-1.585076
2	6	0	-5.858940	0.136481	-1.452201
3	6	0	-5.245168	0.062684	-0.194461
4	6	0	-6.046350	-0.000701	0.969204
5	6	0	-7.446607	0.017574	0.825428
6	6	0	-8.035880	0.089857	-0.432372
7	6	0	-3.752392	0.047141	-0.101887
8	6	0	-3.055975	-1.178034	-0.087214

9	7	0	-1.672333	-1.218094	-0.048707
10	5	0	-0.764716	0.013893	0.220015
11	7	0	-1.644385	1.265465	-0.054917
12	6	0	-3.029596	1.256475	-0.089967
13	6	0	-3.549417	-2.545600	-0.144967
14	6	0	-2.439858	-3.351305	-0.143209
15	6	0	-1.267048	-2.528559	-0.083373
16	6	0	-1.209397	2.565902	-0.081641
17	6	0	-2.363135	3.416030	-0.130608
18	6	0	-3.491181	2.636413	-0.134688
19	6	0	0.091314	-2.919336	-0.076331
20	6	0	0.499273	-4.236919	-0.056460
21	6	0	1.841692	-4.718355	-0.047990
22	6	0	0.158022	2.924986	-0.074852
23	6	0	0.597033	4.232127	-0.050958
24	6	0	1.950502	4.682274	-0.040070
25	6	0	2.076617	-6.119589	-0.033182
26	6	0	3.345543	-6.652262	-0.024978
27	6	0	4.491748	-5.802865	-0.029613
28	6	0	4.263923	-4.391532	-0.043132
29	6	0	2.989102	-3.877674	-0.051798

30	6	0	2.217516	6.077625	-0.026069
31	6	0	3.498484	6.580940	-0.015901
32	6	0	4.624766	5.705427	-0.017237
33	6	0	4.364507	4.299782	-0.029112
34	6	0	3.078094	3.815412	-0.039975
35	7	0	5.751430	-6.313256	-0.020528
36	6	0	6.914250	-5.426278	-0.023389
37	6	0	5.964761	-7.759928	-0.004641
38	7	0	5.896004	6.186652	-0.006401
39	6	0	7.037711	5.272786	-0.006362
40	6	0	6.142779	7.627936	0.008138
41	6	0	-4.965149	-3.033338	-0.189953
42	6	0	-4.894337	3.161532	-0.174369
43	9	0	-0.329815	0.013200	1.545551
44	9	0	0.339707	-0.000476	-0.640377
45	7	0	-5.473514	-0.151378	2.231192
46	1	0	-7.702513	0.205140	-2.568544
47	1	0	-5.227726	0.184381	-2.335947
48	1	0	-8.067581	-0.030921	1.716742
49	1	0	-9.119630	0.102473	-0.511727
50	1	0	-2.444566	-4.431443	-0.194325

51	1	0	0.826504	-2.124384	-0.098260
52	1	0	-0.267866	-5.008762	-0.042852
53	1	0	0.873942	2.112810	-0.101437
54	1	0	-0.151320	5.022106	-0.036794
55	1	0	1.223470	-6.793036	-0.028936
56	1	0	3.463892	-7.728159	-0.014351
57	1	0	5.102850	-3.707414	-0.045552
58	1	0	2.868218	-2.799250	-0.059855
59	1	0	1.379945	6.770529	-0.024405
60	1	0	3.641722	7.653799	-0.006404
61	1	0	5.187389	3.596360	-0.028250
62	1	0	2.932615	2.740002	-0.045804
63	1	0	6.922405	-4.778805	0.861147
64	1	0	7.820268	-6.030464	-0.013233
65	1	0	6.931004	-4.795693	-0.919930
66	1	0	5.524829	-8.216265	0.889781
67	1	0	5.528363	-8.235169	-0.890846
68	1	0	7.035137	-7.960815	-0.000574
69	1	0	7.040882	4.640563	-0.901908
70	1	0	7.957677	5.855495	0.004161
71	1	0	7.029502	4.626504	0.879043

72	1	0	5.711915	8.095606	0.901134
73	1	0	7.217550	7.803957	0.014035
74	1	0	5.719220	8.112174	-0.879437
75	1	0	-5.505412	-2.648159	-1.060183
76	1	0	-4.975480	-4.126367	-0.232725
77	1	0	-5.522399	-2.719767	0.698767
78	1	0	-4.877056	4.255009	-0.149909
79	1	0	-5.424918	2.845685	-1.077879
80	1	0	-5.483961	2.809166	0.678062
81	1	0	-6.064489	0.129843	3.004690
82	1	0	-4.532413	0.209076	2.334259
83	1	0	-2.343022	4.496466	-0.171281

Compound 2a, no imaginary frequencies, E(UB3LYP) = -2161.55333025 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.328246	1.084671	1.414756
2	6	0	-5.938854	0.973839	1.367061
3	6	0	-5.260575	0.798649	0.154454

4	6	0	-5.995941	0.731010	-1.051252
5	6	0	-7.397695	0.843046	-0.994022
6	6	0	-8.052833	1.017679	0.221064
7	6	0	-3.769449	0.677086	0.151911
8	6	0	-2.976235	1.823132	0.067031
9	7	0	-1.580887	1.736916	0.114748
10	5	0	-0.765407	0.413157	0.113967
11	7	0	-1.785824	-0.747494	0.269818
12	6	0	-3.176228	-0.606132	0.258232
13	6	0	-3.327469	3.218946	-0.059703
14	6	0	-2.139447	3.916889	-0.076565
15	6	0	-1.060141	2.990993	0.036147
16	6	0	-1.485329	-2.067268	0.374224
17	6	0	-2.682373	-2.798948	0.439976
18	6	0	-3.754123	-1.908082	0.367996
19	6	0	0.349993	3.253868	0.087101
20	6	0	0.890757	4.491625	-0.090306
21	6	0	2.290966	4.853626	-0.047423
22	6	0	-0.060446	-2.568071	0.436657
23	6	0	0.121685	-3.892170	-0.350119
24	6	0	1.529387	-4.444068	-0.248935

25	6	0	2.665718	6.199362	-0.252073
26	6	0	3.986330	6.614598	-0.221774
27	6	0	5.034139	5.688067	0.019924
28	6	0	4.663579	4.329626	0.223967
29	6	0	3.339140	3.935067	0.190346
30	6	0	1.792458	-5.672992	0.363641
31	6	0	3.083466	-6.186859	0.463026
32	6	0	4.190010	-5.475773	-0.056902
33	6	0	3.916913	-4.245201	-0.704951
34	6	0	2.621047	-3.750094	-0.789401
35	7	0	6.347855	6.082964	0.055485
36	6	0	7.403015	5.107115	0.294050
37	6	0	6.697691	7.480354	-0.159423
38	7	0	5.485392	-5.957330	0.065878
39	6	0	6.559292	-5.316009	-0.678377
40	6	0	5.696527	-7.319959	0.530763
41	6	0	-4.685981	3.844408	-0.168857
42	6	0	-5.197935	-2.319610	0.398658
43	9	0	-0.069114	0.279435	-1.095077
44	9	0	0.144316	0.409965	1.175538
45	7	0	-5.349798	0.626455	-2.283645

46	1	0	-7.835048	1.219792	2.365395
47	1	0	-5.357697	1.020166	2.284541
48	1	0	-7.967646	0.794065	-1.919028
49	1	0	-9.136576	1.099075	0.234293
50	1	0	-2.039477	4.991647	-0.147831
51	1	0	0.989035	2.402626	0.291070
52	1	0	0.215383	5.322330	-0.292069
53	1	0	0.582812	-1.829462	-0.044419
54	1	0	1.889895	6.938361	-0.440342
55	1	0	4.209088	7.661714	-0.386531
56	1	0	5.423847	3.580857	0.410157
57	1	0	3.111959	2.885349	0.351936
58	1	0	0.968184	-6.256221	0.770749
59	1	0	3.224151	-7.148756	0.941238
60	1	0	4.721152	-3.670975	-1.149138
61	1	0	2.454710	-2.807103	-1.304465
62	1	0	7.418444	4.328437	-0.480030
63	1	0	8.367675	5.614821	0.282118
64	1	0	7.288499	4.616849	1.269792
65	1	0	6.387895	7.828526	-1.153968
66	1	0	6.232571	8.133282	0.590888

67	1	0	7.779137	7.593999	-0.082395
68	1	0	6.659183	-4.262254	-0.394244
69	1	0	7.501883	-5.811678	-0.440073
70	1	0	6.410659	-5.361983	-1.768916
71	1	0	5.240941	-8.073013	-0.131849
72	1	0	6.768770	-7.515417	0.584933
73	1	0	5.283481	-7.459951	1.536390
74	1	0	-5.304955	3.643104	0.711279
75	1	0	-4.585263	4.928743	-0.276703
76	1	0	-5.234540	3.464332	-1.037099
77	1	0	-5.267483	-3.406108	0.512353
78	1	0	-5.745239	-1.855441	1.225463
79	1	0	-5.725047	-2.044973	-0.521714
80	1	0	-5.920308	0.247515	-3.030400
81	1	0	-4.436374	0.188056	-2.259425
82	1	0	-2.764085	-3.874994	0.520369
83	1	0	-0.579147	-4.652733	0.028891
84	8	0	0.444143	-2.643692	1.772359
85	8	0	-0.239201	-3.553042	-1.691047
86	6	0	-0.233057	-3.506462	2.675704
87	1	0	-0.161373	-4.562164	2.381200

88	1	0	0.266108	-3.382013	3.640195
89	1	0	-1.292083	-3.241010	2.787523
90	6	0	-0.446898	-4.676467	-2.530764
91	1	0	-0.729064	-4.289100	-3.513206
92	1	0	0.460856	-5.286472	-2.631772
93	1	0	-1.258531	-5.315881	-2.150674

Cation of Compound 2a (2a^{+}), no imaginary frequencies, E(UB3LYP) = -2161.38062994 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.294276	1.086328	1.426243
2	6	0	-5.910990	0.930644	1.364081
3	6	0	-5.248675	0.796798	0.136207
4	6	0	-5.990999	0.808292	-1.066916
5	6	0	-7.387867	0.962333	-0.991599
6	6	0	-8.027480	1.102007	0.235404
7	6	0	-3.761698	0.649671	0.120293

8	6	0	-2.939511	1.800566	-0.012480
9	7	0	-1.567159	1.701886	0.050646
10	5	0	-0.749309	0.377734	0.111273
11	7	0	-1.787623	-0.768300	0.309796
12	6	0	-3.180174	-0.609683	0.282615
13	6	0	-3.296041	3.196647	-0.179416
14	6	0	-2.108887	3.889834	-0.205712
15	6	0	-1.031080	2.962091	-0.054955
16	6	0	-1.507484	-2.076514	0.460361
17	6	0	-2.723517	-2.806918	0.542618
18	6	0	-3.777219	-1.924043	0.433058
19	6	0	0.357677	3.208293	0.016217
20	6	0	0.917173	4.464975	-0.134694
21	6	0	2.297135	4.787138	-0.062734
22	6	0	-0.089184	-2.596745	0.552162
23	6	0	0.088283	-3.903495	-0.265017
24	6	0	1.514150	-4.408295	-0.232990
25	6	0	2.701527	6.143142	-0.240825
26	6	0	4.016053	6.527724	-0.176655
27	6	0	5.044973	5.564307	0.074222
28	6	0	4.647448	4.197439	0.249609

29	6	0	3.329203	3.831520	0.182817
30	6	0	1.858746	-5.597094	0.418819
31	6	0	3.171130	-6.057918	0.462281
32	6	0	4.217045	-5.333209	-0.158747
33	6	0	3.859802	-4.143064	-0.842585
34	6	0	2.543971	-3.699067	-0.868405
35	7	0	6.344609	5.928066	0.143134
36	6	0	7.390593	4.931653	0.396906
37	6	0	6.739475	7.328971	-0.036136
38	7	0	5.529404	-5.764755	-0.100696
39	6	0	6.544118	-5.099325	-0.904393
40	6	0	5.833574	-7.071829	0.462264
41	6	0	-4.653408	3.815618	-0.316443
42	6	0	-5.224040	-2.308277	0.458803
43	9	0	-0.056257	0.189970	-1.083334
44	9	0	0.141160	0.418033	1.180417
45	7	0	-5.355899	0.740284	-2.305935
46	1	0	-7.790430	1.193822	2.385605
47	1	0	-5.323029	0.915891	2.278058
48	1	0	-7.965611	0.973770	-1.912571
49	1	0	-9.107412	1.219124	0.261341

50	1	0	-2.005967	4.961509	-0.306417
51	1	0	0.994116	2.354856	0.215856
52	1	0	0.250826	5.302669	-0.328220
53	1	0	0.573216	-1.855828	0.103066
54	1	0	1.939647	6.893109	-0.433424
55	1	0	4.267979	7.570390	-0.318619
56	1	0	5.393124	3.436578	0.439213
57	1	0	3.076681	2.786010	0.321838
58	1	0	1.083776	-6.190015	0.900934
59	1	0	3.378189	-6.990015	0.973879
60	1	0	4.614231	-3.562859	-1.360201
61	1	0	2.308604	-2.788092	-1.413257
62	1	0	7.405562	4.171684	-0.391090
63	1	0	8.357470	5.430893	0.413646
64	1	0	7.235424	4.440932	1.363212
65	1	0	6.459551	7.689098	-1.031686
66	1	0	6.268629	7.966231	0.719405
67	1	0	7.819654	7.408404	0.069774
68	1	0	6.628406	-4.039300	-0.636653
69	1	0	7.511338	-5.566666	-0.714425
70	1	0	6.336951	-5.162615	-1.983599

71	1	0	5.366477	-7.894320	-0.101004
72	1	0	6.914144	-7.221129	0.452554
73	1	0	5.497533	-7.140193	1.503702
74	1	0	-5.292778	3.599756	0.544824
75	1	0	-4.553238	4.900815	-0.408939
76	1	0	-5.171117	3.442439	-1.205948
77	1	0	-5.314193	-3.395871	0.529085
78	1	0	-5.748855	-1.863101	1.310203
79	1	0	-5.749101	-1.976998	-0.442921
80	1	0	-5.956112	0.468805	-3.075991
81	1	0	-4.479417	0.232397	-2.328142
82	1	0	-2.805504	-3.879248	0.655055
83	1	0	-0.574465	-4.688097	0.132122
84	8	0	0.362750	-2.697615	1.898122
85	8	0	-0.347188	-3.539846	-1.575560
86	6	0	-0.333415	-3.582413	2.771169
87	1	0	-0.292906	-4.625003	2.432424
88	1	0	0.178584	-3.509517	3.733337
89	1	0	-1.382557	-3.291014	2.906743
90	6	0	-0.551740	-4.645512	-2.444028
91	1	0	-0.899902	-4.237050	-3.395773

92	1	0	0.375340	-5.208820	-2.610100
93	1	0	-1.314627	-5.330248	-2.044607

Compound $CuCl_2$, no imaginary frequencies, E(UB3LYP) = -2560.73931250 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-4.590832	2.443035	-5.145324
2	17	0	-4.007866	4.426708	-5.423401
3	17	0	-5.174027	0.459195	-4.868924

Anion of Compound $CuCl_2$ $[CuCl_2]^-$, no imaginary frequencies, E(UB3LYP) = -2560.90842624 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-4.590858	2.443019	-5.145524
2	17	0	-4.001077	4.449767	-5.426513

3	17	0	-5.180790	0.436152	-4.865613

Compound $CuBr_2$, no imaginary frequencies, E(UB3LYP) = -6783.76650207 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.202909	0.000000
2	35	0	2.219468	-0.084133	0.000000
3	35	0	-2.219468	-0.083992	0.000000

Anion of Compound $CuBr_2$ $[CuBr_2]^-$, no imaginary frequencies, E(UB3LYP) = -6783.96244993 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000056	0.000163	0.000020
2	35	0	2.182587	-0.019610	0.221515

3	35	0	-2.182634	0.019474	-0.221531

Compound 2a·CuCl, no imaginary frequencies, E(UB3LYP) = -2819.16575721 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.520701	1.174073	-1.567122
2	6	0	6.139241	1.041337	-1.427438
3	6	0	5.540240	0.922512	-0.166494
4	6	0	6.349114	0.934633	0.993124
5	6	0	7.742184	1.068025	0.842845
6	6	0	8.318138	1.186643	-0.418441
7	6	0	4.055061	0.773878	-0.069694
8	6	0	3.241953	1.898933	0.022734
9	7	0	1.844911	1.783851	0.056233
10	5	0	1.083603	0.462019	-0.175355
11	7	0	2.098466	-0.692465	-0.018649
12	6	0	3.482883	-0.531636	-0.075235
13	6	0	3.568017	3.306417	0.126618

14	6	0	2.370775	3.977247	0.209452
15	6	0	1.301258	3.029448	0.155364
16	6	0	1.822373	-2.029639	0.017568
17	6	0	3.026268	-2.739608	-0.015077
18	6	0	4.082891	-1.822879	-0.074670
19	6	0	-0.108172	3.272171	0.188083
20	6	0	-0.648538	4.525103	0.261790
21	6	0	-2.047240	4.875553	0.287552
22	6	0	0.415653	-2.553286	0.089221
23	6	0	0.306988	-4.036193	0.519038
24	6	0	-1.124246	-4.534857	0.487733
25	6	0	-2.418165	6.231540	0.437078
26	6	0	-3.740268	6.637254	0.475471
27	6	0	-4.793889	5.690580	0.360753
28	6	0	-4.425913	4.324279	0.199587
29	6	0	-3.100553	3.937025	0.165554
30	6	0	-1.549319	-5.482214	-0.448579
31	6	0	-2.870078	-5.921743	-0.501781
32	6	0	-3.836604	-5.434402	0.410459
33	6	0	-3.400790	-4.474657	1.359011
34	6	0	-2.078322	-4.046679	1.391899

35	7	0	-6.108788	6.074310	0.399102
36	6	0	-7.169534	5.083855	0.258248
37	6	0	-6.457716	7.482300	0.538706
38	7	0	-5.146238	-5.889340	0.392490
39	6	0	-6.153539	-5.187494	1.176212
40	6	0	-5.601343	-6.697298	-0.729891
41	6	0	4.918132	3.955653	0.175055
42	6	0	5.534129	-2.209741	-0.100348
43	9	0	0.032146	0.312856	0.748464
44	9	0	0.526535	0.451297	-1.479053
45	7	0	5.782456	0.887015	2.267563
46	1	0	7.965588	1.265450	-2.553244
47	1	0	5.502342	1.026333	-2.308153
48	1	0	8.368426	1.080745	1.731895
49	1	0	9.397025	1.286568	-0.503410
50	1	0	2.253860	5.047698	0.308940
51	1	0	-0.754146	2.402886	0.160310
52	1	0	0.031707	5.374273	0.312541
53	1	0	-0.148932	-1.961961	0.809618
54	1	0	-1.637303	6.983488	0.527448
55	1	0	-3.961548	7.690948	0.593035

56	1	0	-5.189812	3.563978	0.092606
57	1	0	-2.880267	2.882971	0.022617
58	1	0	-0.835929	-5.889418	-1.162796
59	1	0	-3.143795	-6.652023	-1.253557
60	1	0	-4.096904	-4.060932	2.078525
61	1	0	-1.781998	-3.320772	2.145240
62	1	0	-7.121445	4.327292	1.051724
63	1	0	-8.135536	5.584470	0.326388
64	1	0	-7.118685	4.568817	-0.710095
65	1	0	-6.064085	7.903926	1.472668
66	1	0	-6.071393	8.081015	-0.296949
67	1	0	-7.543179	7.581431	0.554150
68	1	0	-6.265917	-4.133200	0.878068
69	1	0	-7.115607	-5.685718	1.045658
70	1	0	-5.909948	-5.214494	2.244346
71	1	0	-5.019073	-7.622436	-0.808808
72	1	0	-6.643398	-6.977390	-0.566987
73	1	0	-5.531520	-6.166897	-1.692840
74	1	0	5.511417	3.735909	-0.718153
75	1	0	4.803589	5.040923	0.254932
76	1	0	5.497022	3.607835	1.037251

77	1	0	5.622674	-3.299832	-0.146447
78	1	0	6.061718	-1.788132	-0.961717
79	1	0	6.066856	-1.870164	0.795119
80	1	0	6.406642	0.564753	2.997821
81	1	0	4.878473	0.432932	2.327000
82	1	0	3.129672	-3.815057	0.029767
83	1	0	0.914321	-4.664440	-0.151925
84	8	0	-0.312839	-2.348359	-1.165575
85	8	0	0.870912	-4.055703	1.827933
86	6	0	0.373853	-2.713383	-2.381833
87	1	0	0.809195	-3.711261	-2.288134
88	1	0	-0.384495	-2.719451	-3.165266
89	1	0	1.150856	-1.981927	-2.615904
90	6	0	1.125383	-5.361695	2.323205
91	1	0	1.566832	-5.240848	3.315333
92	1	0	0.204155	-5.952683	2.406413
93	1	0	1.833894	-5.901856	1.677145
94	29	0	-1.688340	-0.936141	-1.275894
95	17	0	-3.419524	0.314084	-1.458221

Cation of Compound 2a·CuCl [2a·CuCl]$^{+}$, no imaginary frequencies, E(UB3LYP) = -2818.98957040 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.566909	0.752925	-1.559431
2	6	0	6.183496	0.665107	-1.417332
3	6	0	5.580018	0.685099	-0.151655
4	6	0	6.383352	0.780377	1.008262
5	6	0	7.779889	0.861267	0.852159
6	6	0	8.360675	0.851224	-0.411628
7	6	0	4.092219	0.595964	-0.056463
8	6	0	3.313010	1.773260	0.060914
9	7	0	1.933225	1.712936	0.075621
10	5	0	1.103453	0.437148	-0.206858
11	7	0	2.071074	-0.767229	-0.063730
12	6	0	3.465831	-0.658361	-0.100267
13	6	0	3.714011	3.161515	0.177531
14	6	0	2.548354	3.888676	0.253105
15	6	0	1.438972	2.991020	0.180594

16	6	0	1.747718	-2.082029	-0.035846
17	6	0	2.929811	-2.853343	-0.058050
18	6	0	4.015975	-1.994743	-0.099632
19	6	0	0.054812	3.278503	0.194814
20	6	0	-0.454544	4.563478	0.281391
21	6	0	-1.826851	4.920355	0.280293
22	6	0	0.315977	-2.554075	0.033146
23	6	0	0.154987	-4.043282	0.419967
24	6	0	-1.299515	-4.465032	0.432124
25	6	0	-2.184176	6.294483	0.434748
26	6	0	-3.489681	6.709600	0.451570
27	6	0	-4.556156	5.761818	0.307025
28	6	0	-4.203769	4.380463	0.138614
29	6	0	-2.894556	3.981622	0.126430
30	6	0	-1.813343	-5.344070	-0.526970
31	6	0	-3.156338	-5.710201	-0.541364
32	6	0	-4.056557	-5.215973	0.434510
33	6	0	-3.530133	-4.325703	1.405713
34	6	0	-2.186776	-3.969066	1.398713
35	7	0	-5.847040	6.154380	0.323828
36	6	0	-6.933023	5.175342	0.189612

37	6	0	-6.199253	7.571371	0.473262
38	7	0	-5.385511	-5.598258	0.452249
39	6	0	-6.315853	-4.917895	1.342284
40	6	0	-5.929210	-6.349885	-0.670047
41	6	0	5.093067	3.742884	0.235561
42	6	0	5.448484	-2.431472	-0.101627
43	9	0	0.045900	0.317650	0.706009
44	9	0	0.580827	0.490294	-1.510601
45	7	0	5.811708	0.861306	2.276847
46	1	0	8.017002	0.745138	-2.547029
47	1	0	5.549734	0.586557	-2.296688
48	1	0	8.404417	0.934636	1.739143
49	1	0	9.441669	0.915622	-0.500175
50	1	0	2.480434	4.962760	0.355804
51	1	0	-0.622783	2.435275	0.144544
52	1	0	0.246676	5.390727	0.363788
53	1	0	-0.200311	-1.964705	0.791129
54	1	0	-1.392883	7.030020	0.547591
55	1	0	-3.708182	7.761765	0.577855
56	1	0	-4.976261	3.633980	0.008986
57	1	0	-2.683995	2.927975	-0.025196

58	1	0	-1.153269	-5.755749	-1.288116
59	1	0	-3.500665	-6.390573	-1.310607
60	1	0	-4.172070	-3.912485	2.174075
61	1	0	-1.820060	-3.297335	2.171167
62	1	0	-6.877953	4.425150	0.984249
63	1	0	-7.886601	5.693768	0.267233
64	1	0	-6.886141	4.672670	-0.781844
65	1	0	-5.844196	7.961108	1.432797
66	1	0	-5.766714	8.165804	-0.337495
67	1	0	-7.282135	7.671704	0.437003
68	1	0	-6.394553	-3.840629	1.128724
69	1	0	-7.305523	-5.362965	1.229685
70	1	0	-6.016649	-5.036065	2.390181
71	1	0	-5.406100	-7.305173	-0.794917
72	1	0	-6.979370	-6.571734	-0.474615
73	1	0	-5.863419	-5.797629	-1.620328
74	1	0	5.695554	3.454630	-0.631123
75	1	0	5.030311	4.834323	0.266163
76	1	0	5.625594	3.404083	1.130256
77	1	0	5.499986	-3.522721	-0.052381
78	1	0	5.975780	-2.100551	-1.001955

79	1	0	5.997815	-2.023922	0.753647
80	1	0	6.441487	0.648747	3.041592
81	1	0	4.919478	0.396478	2.395327
82	1	0	2.977125	-3.931675	-0.015973
83	1	0	0.703394	-4.678812	-0.293403
84	8	0	-0.407120	-2.262660	-1.194488
85	8	0	0.774117	-4.118995	1.700572
86	6	0	0.230312	-2.634177	-2.439446
87	1	0	0.620360	-3.652478	-2.376668
88	1	0	-0.548001	-2.588569	-3.200858
89	1	0	1.030770	-1.930262	-2.678699
90	6	0	0.976676	-5.447725	2.165839
91	1	0	1.472445	-5.366806	3.135669
92	1	0	0.026698	-5.982716	2.286457
93	1	0	1.618980	-6.016196	1.477229
94	29	0	-1.790475	-0.858137	-1.214291
95	17	0	-3.466530	0.469467	-1.274417

Compound 2a·CuBr, no imaginary frequencies, E(UB3LYP) = -4930.38135066 A.U.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-7.721582	-1.192402	-1.629708
2	6	0	-6.340281	-1.066818	-1.481712
3	6	0	-5.750048	-0.920323	-0.220540
4	6	0	-6.570201	-0.898203	0.930307
5	6	0	-7.962003	-1.024189	0.773421
6	6	0	-8.528548	-1.169303	-0.489137
7	6	0	-4.265586	-0.774631	-0.108464
8	6	0	-3.458764	-1.899227	0.031328
9	7	0	-2.064496	-1.787648	0.076062
10	5	0	-1.289220	-0.471987	-0.192395
11	7	0	-2.310362	0.688798	-0.048753
12	6	0	-3.691532	0.530659	-0.135314
13	6	0	-3.791450	-3.303525	0.174652
14	6	0	-2.597398	-3.973300	0.284333
15	6	0	-1.524263	-3.027736	0.209245
16	6	0	-2.029671	2.022136	-0.016763
17	6	0	-3.230420	2.737089	-0.088577
18	6	0	-4.287963	1.824047	-0.165227
19	6	0	-0.115013	-3.264229	0.242105

20	6	0	0.438016	-4.508599	0.333518
21	6	0	1.845013	-4.829795	0.336113
22	6	0	-0.623218	2.538059	0.121311
23	6	0	-0.527192	4.053726	0.423777
24	6	0	0.908410	4.537627	0.432095
25	6	0	2.256375	-6.168200	0.514241
26	6	0	3.591682	-6.534867	0.523304
27	6	0	4.609402	-5.562344	0.347727
28	6	0	4.199775	-4.216021	0.155667
29	6	0	2.864346	-3.866041	0.152440
30	6	0	1.395896	5.401084	-0.551612
31	6	0	2.728724	5.803611	-0.580244
32	6	0	3.641721	5.359930	0.403251
33	6	0	3.140041	4.496194	1.406673
34	6	0	1.807872	4.103025	1.415120
35	7	0	5.942634	-5.907432	0.358989
36	6	0	6.960221	-4.896011	0.113437
37	6	0	6.334147	-7.300680	0.487134
38	7	0	4.971584	5.766212	0.398489
39	6	0	5.923875	5.061426	1.244456
40	6	0	5.493929	6.441686	-0.777964

41	6	0	-5.145866	-3.942846	0.240435
42	6	0	-5.737294	2.214523	-0.232135
43	9	0	-0.250644	-0.304831	0.736896
44	9	0	-0.754476	-0.493605	-1.489046
45	7	0	-6.009287	-0.821404	2.205634
46	1	0	-8.159247	-1.305469	-2.616862
47	1	0	-5.694801	-1.078277	-2.356258
48	1	0	-8.596113	-1.013334	1.657448
49	1	0	-9.607457	-1.263469	-0.580945
50	1	0	-2.481551	-5.040631	0.415634
51	1	0	0.524826	-2.392138	0.187980
52	1	0	-0.228875	-5.367014	0.413386
53	1	0	-0.133861	2.009695	0.940166
54	1	0	1.500518	-6.939205	0.650523
55	1	0	3.847392	-7.578318	0.663609
56	1	0	4.928556	-3.430783	-0.004029
57	1	0	2.621941	-2.820995	-0.015723
58	1	0	0.724503	5.766251	-1.327217
59	1	0	3.054216	6.464158	-1.374708
60	1	0	3.795113	4.116928	2.181166
61	1	0	1.460931	3.441502	2.204915

62	1	0	6.909738	-4.088975	0.855187
63	1	0	7.946583	-5.357372	0.184642
64	1	0	6.862620	-4.445860	-0.884434
65	1	0	5.970124	-7.736278	1.427400
66	1	0	5.953002	-7.915583	-0.341450
67	1	0	7.423152	-7.369123	0.486455
68	1	0	5.985629	3.986115	1.014061
69	1	0	6.913740	5.501840	1.107438
70	1	0	5.661345	5.169215	2.303096
71	1	0	4.954582	7.378023	-0.962534
72	1	0	6.541756	6.696876	-0.606260
73	1	0	5.432060	5.825786	-1.690152
74	1	0	-5.741341	-3.743503	-0.656154
75	1	0	-5.038568	-5.026990	0.347672
76	1	0	-5.720808	-3.570465	1.095323
77	1	0	-5.821322	3.304183	-0.301181
78	1	0	-6.248587	1.779214	-1.096580
79	1	0	-6.295355	1.895448	0.655823
80	1	0	-6.625770	-0.472140	2.928362
81	1	0	-5.087398	-0.404637	2.253355
82	1	0	-3.329874	3.812613	-0.044615

83	1	0	-1.086670	4.620907	-0.339734
84	8	0	0.205198	2.215015	-1.035213
85	8	0	-1.171453	4.197620	1.686156
86	6	0	-0.362313	2.460677	-2.334295
87	1	0	-0.804577	3.460714	-2.375884
88	1	0	0.468020	2.401294	-3.039239
89	1	0	-1.108531	1.700298	-2.573099
90	6	0	-1.395440	5.542325	2.067351
91	1	0	-1.899595	5.513403	3.036641
92	1	0	-0.456387	6.103261	2.162682
93	1	0	-2.042573	6.062945	1.342641
94	29	0	1.722694	0.934595	-0.871918
95	35	0	3.639489	-0.223128	-0.793217

Cation of Compound 2a·CuBr [2a·CuBr]$^{+}$, no imaginary frequencies, E(UB3LYP) = -4930.20630267 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-7.679001	-0.998168	-1.606016
2	6	0	-6.301091	-0.864556	-1.446596
3	6	0	-5.715781	-0.839993	-0.172582
4	6	0	-6.532308	-0.936800	0.977820
5	6	0	-7.923102	-1.065697	0.804085
6	6	0	-8.485713	-1.098979	-0.467519
7	6	0	-4.232825	-0.702915	-0.058610
8	6	0	-3.419159	-1.854159	0.079181
9	7	0	-2.041873	-1.752354	0.106932
10	5	0	-1.247128	-0.451861	-0.168839
11	7	0	-2.255410	0.722428	-0.045183
12	6	0	-3.645344	0.569694	-0.103574
13	6	0	-3.780444	-3.251889	0.210046
14	6	0	-2.594926	-3.942909	0.307994
15	6	0	-1.511472	-3.013969	0.233501
16	6	0	-1.974554	2.046989	-0.022283
17	6	0	-3.179772	2.780600	-0.071366
18	6	0	-4.237373	1.887912	-0.124011
19	6	0	-0.120092	-3.263549	0.260068
20	6	0	0.421508	-4.533441	0.373604
21	6	0	1.801997	-4.856688	0.379814

22	6	0	-0.559775	2.563806	0.066726
23	6	0	-0.450169	4.058009	0.451803
24	6	0	0.991182	4.521261	0.492246
25	6	0	2.194192	-6.216838	0.569516
26	6	0	3.509941	-6.597990	0.594516
27	6	0	4.552092	-5.628167	0.420630
28	6	0	4.164195	-4.261587	0.214903
29	6	0	2.845364	-3.896595	0.197091
30	6	0	1.500603	5.407934	-0.462199
31	6	0	2.832728	5.811757	-0.450717
32	6	0	3.725195	5.350046	0.547937
33	6	0	3.203305	4.451786	1.514207
34	6	0	1.870990	4.057089	1.481159
35	7	0	5.852487	-5.987573	0.444266
36	6	0	6.912579	-4.985183	0.278670
37	6	0	6.240906	-7.389896	0.636779
38	7	0	5.042106	5.770270	0.591369
39	6	0	5.972519	5.120161	1.503725
40	6	0	5.588169	6.529561	-0.524622
41	6	0	-5.142189	-3.873574	0.260514
42	6	0	-5.682773	2.278782	-0.154404

43	9	0	-0.208734	-0.296911	0.759919
44	9	0	-0.702854	-0.491767	-1.463624
45	7	0	-5.977167	-0.973174	2.255842
46	1	0	-8.114843	-1.023698	-2.599693
47	1	0	-5.657341	-0.783188	-2.318408
48	1	0	-8.557610	-1.141945	1.683745
49	1	0	-9.562757	-1.199478	-0.569577
50	1	0	-2.497116	-5.013149	0.425547
51	1	0	0.535945	-2.404199	0.196473
52	1	0	-0.258972	-5.375799	0.474311
53	1	0	-0.036758	1.991617	0.833297
54	1	0	1.422216	-6.969145	0.703353
55	1	0	3.755078	-7.640480	0.748722
56	1	0	4.915555	-3.498264	0.060389
57	1	0	2.610100	-2.852941	0.015453
58	1	0	0.845802	5.795187	-1.240505
59	1	0	3.174361	6.495981	-1.217722
60	1	0	3.840007	4.062027	2.299013
61	1	0	1.506790	3.380347	2.250424
62	1	0	6.847183	-4.220305	1.058534
63	1	0	7.879465	-5.478376	0.356244

64	1	0	6.843110	-4.504039	-0.702210
65	1	0	5.900751	-7.757417	1.610458
66	1	0	5.819231	-8.020560	-0.152051
67	1	0	7.325755	-7.464430	0.597123
68	1	0	6.084520	4.044324	1.297980
69	1	0	6.951827	5.591379	1.408211
70	1	0	5.649337	5.235744	2.544759
71	1	0	5.039708	7.467756	-0.668502
72	1	0	6.626586	6.784303	-0.307673
73	1	0	5.560152	5.968753	-1.471790
74	1	0	-5.741450	-3.618379	-0.618668
75	1	0	-5.046825	-4.961948	0.310521
76	1	0	-5.697029	-3.536511	1.142178
77	1	0	-5.769569	3.368610	-0.127417
78	1	0	-6.186572	1.913422	-1.054807
79	1	0	-6.230691	1.871090	0.701789
80	1	0	-6.624028	-0.761201	3.006376
81	1	0	-5.100357	-0.480262	2.376109
82	1	0	-3.261770	3.857257	-0.039811
83	1	0	-1.001022	4.674574	-0.276010
84	8	0	0.188700	2.292940	-1.149800

85	8	0	-1.097916	4.121010	1.718709
86	6	0	-0.441824	2.641228	-2.404433
87	1	0	-0.855846	3.650842	-2.354211
88	1	0	0.346403	2.607790	-3.156226
89	1	0	-1.222961	1.917515	-2.648648
90	6	0	-1.347628	5.445245	2.173821
91	1	0	-1.862717	5.353997	3.132607
92	1	0	-0.415792	6.006848	2.313485
93	1	0	-1.989702	5.993323	1.468619
94	29	0	1.640040	0.951272	-1.141837
95	35	0	3.480070	-0.343290	-1.171239
