Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Tetracyanobutadiene (TCBD) functionalized benzothiadiazole derivatives: effect of donor strength on the [2+2] cycloaddition-retroelectrocyclization reaction

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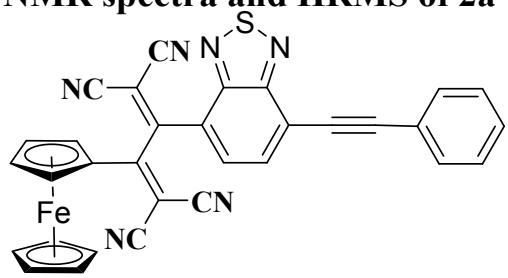
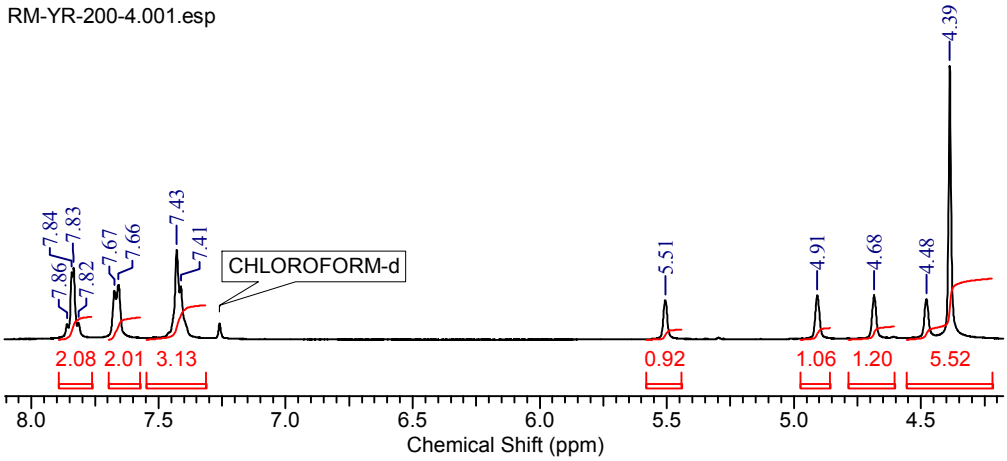




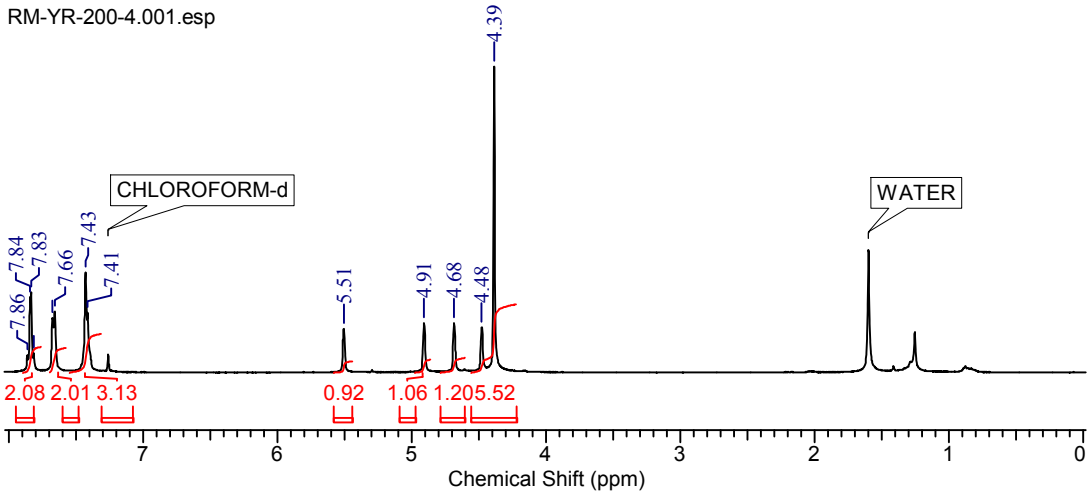


Figure S1. ^{1}H NMR spectrum of **BTD 2a**

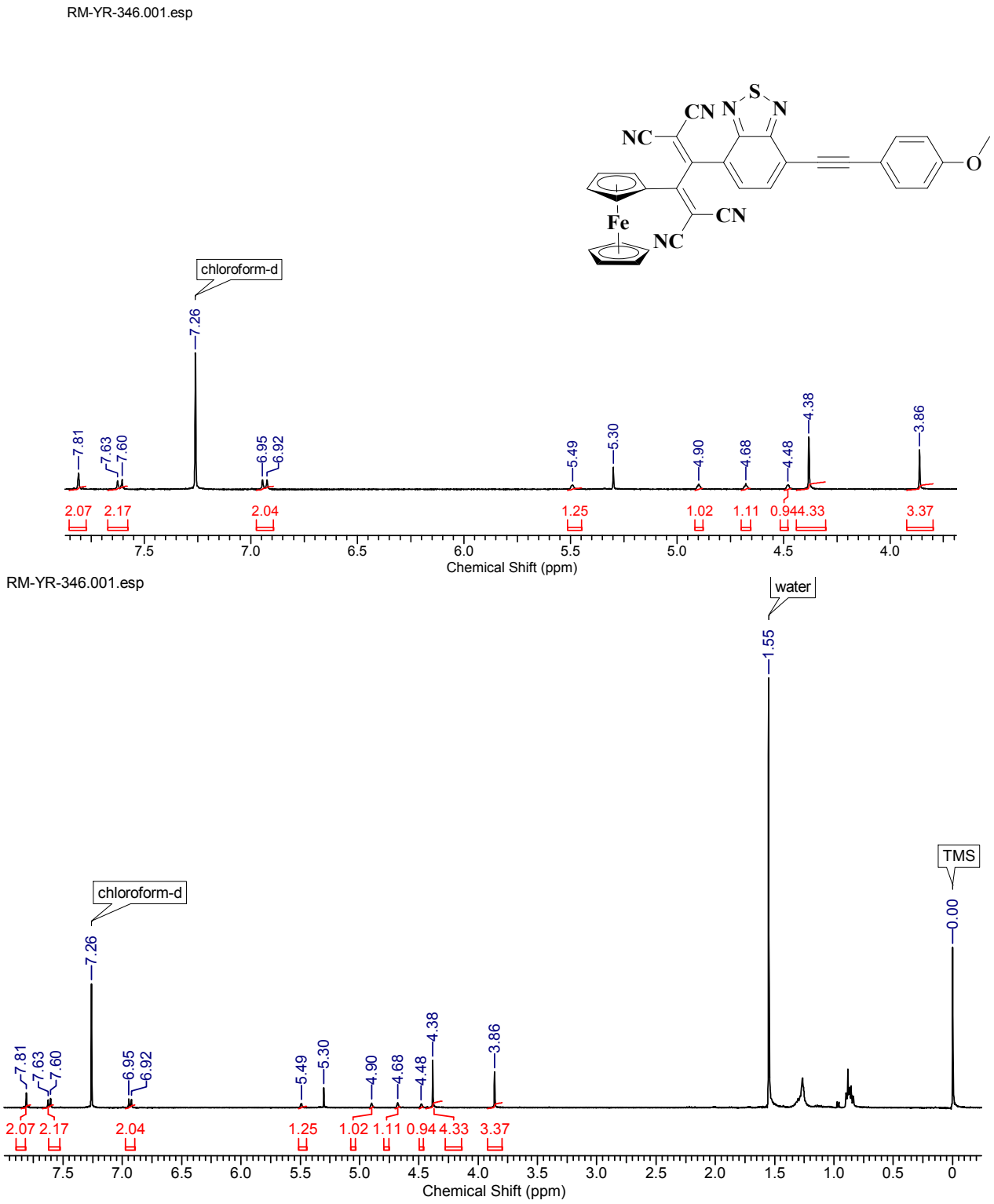


Figure S2. ^{1}H NMR spectrum of **BTD 2b**

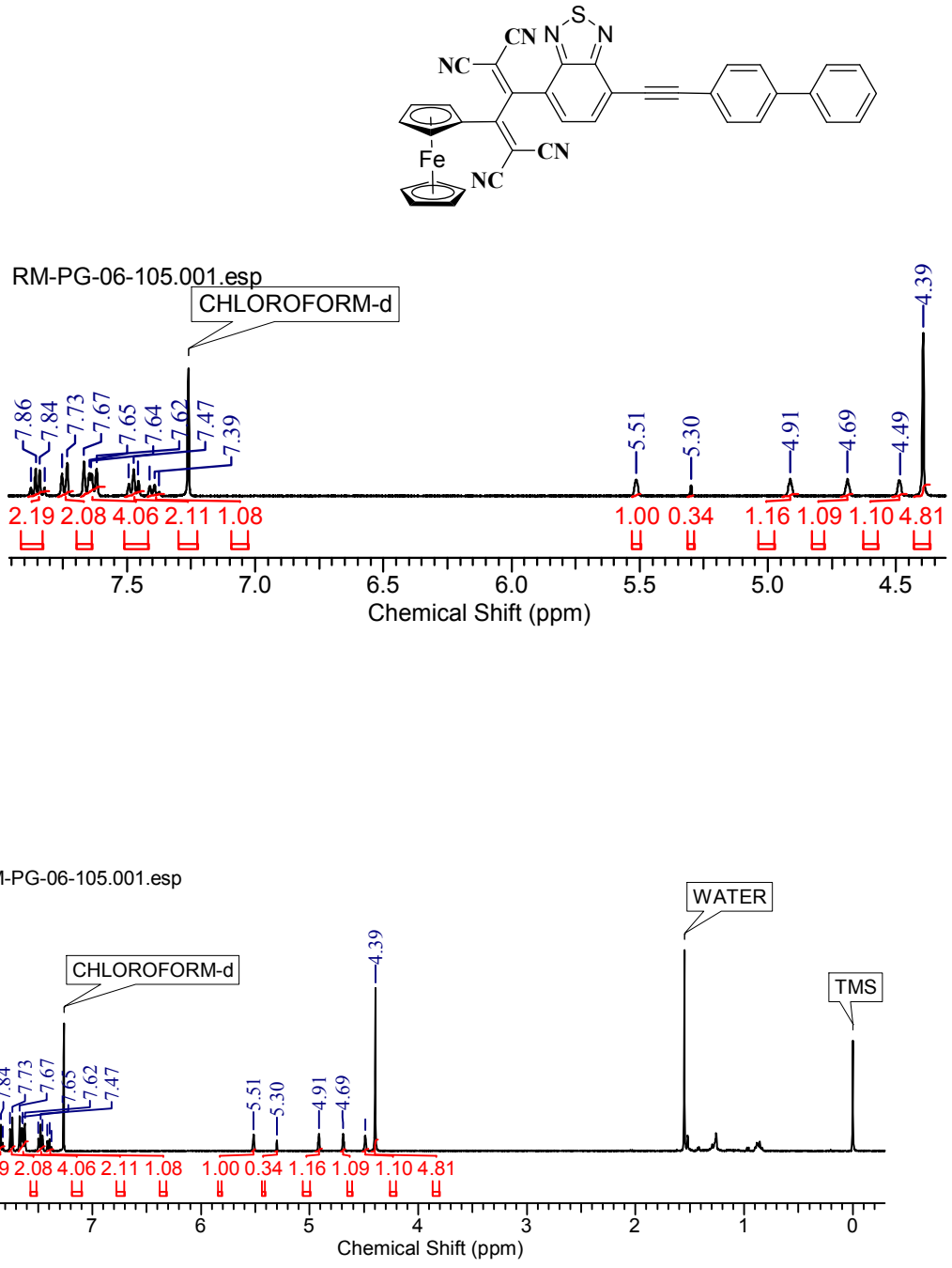
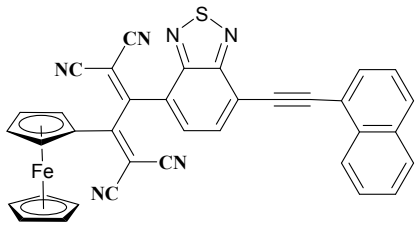
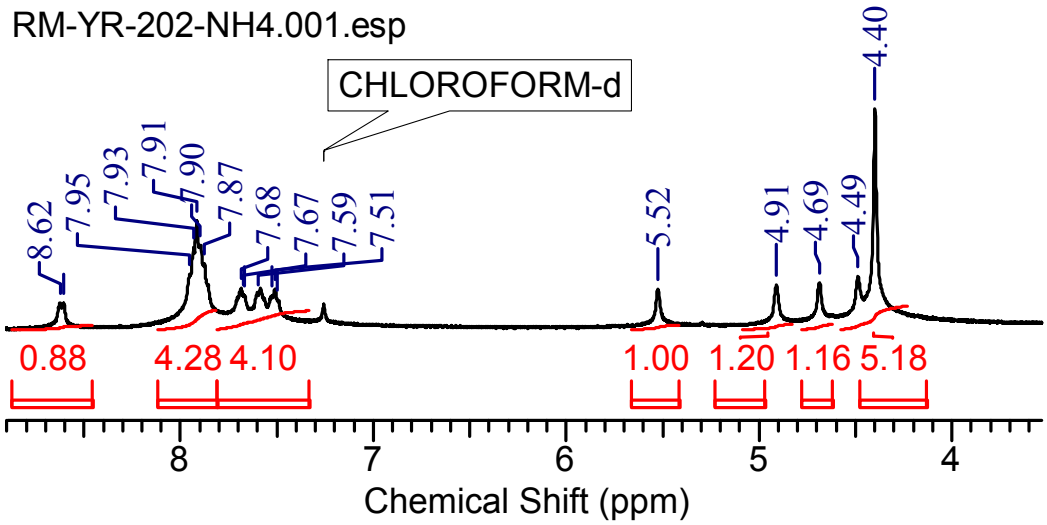


Figure S3. ^{1}H NMR spectrum of **BTD 2c**





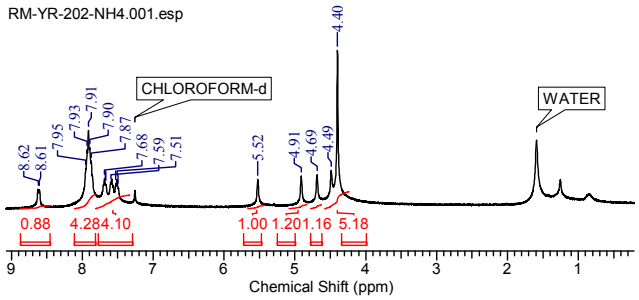
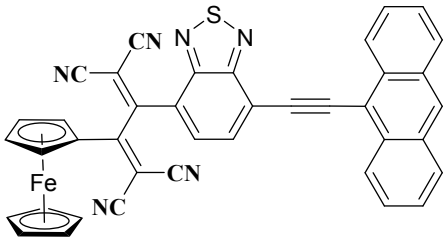
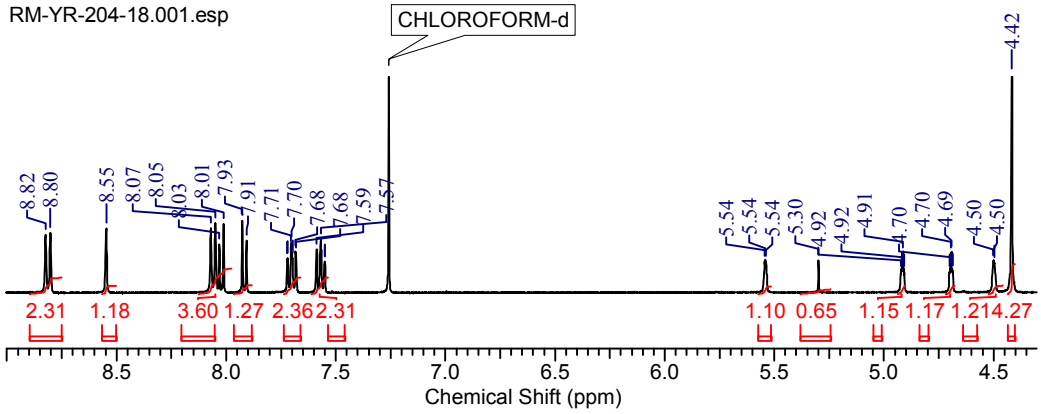


Figure S4. [1]H NMR spectrum of **BTD 2d**





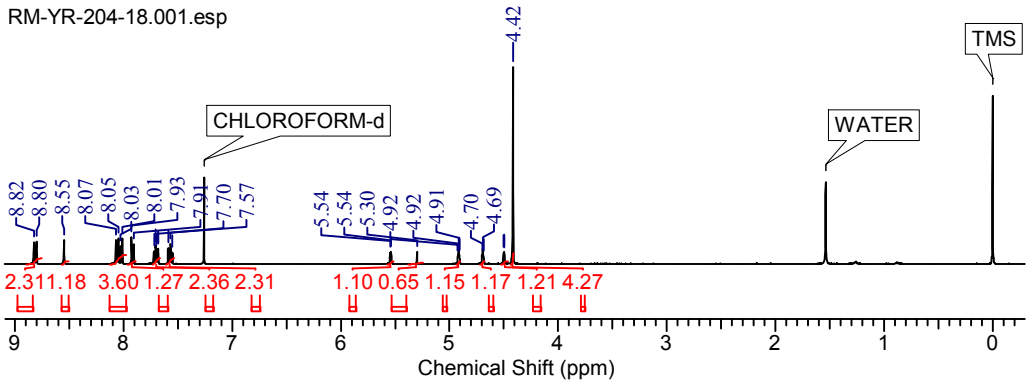
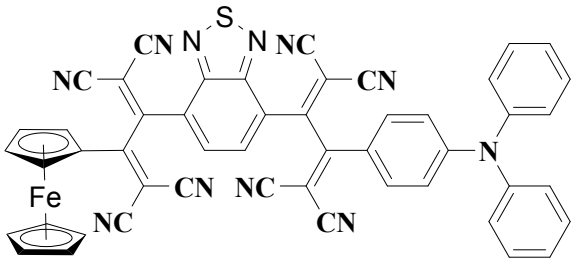


Figure S5. ^{1}H NMR spectrum of **BTD 2e**



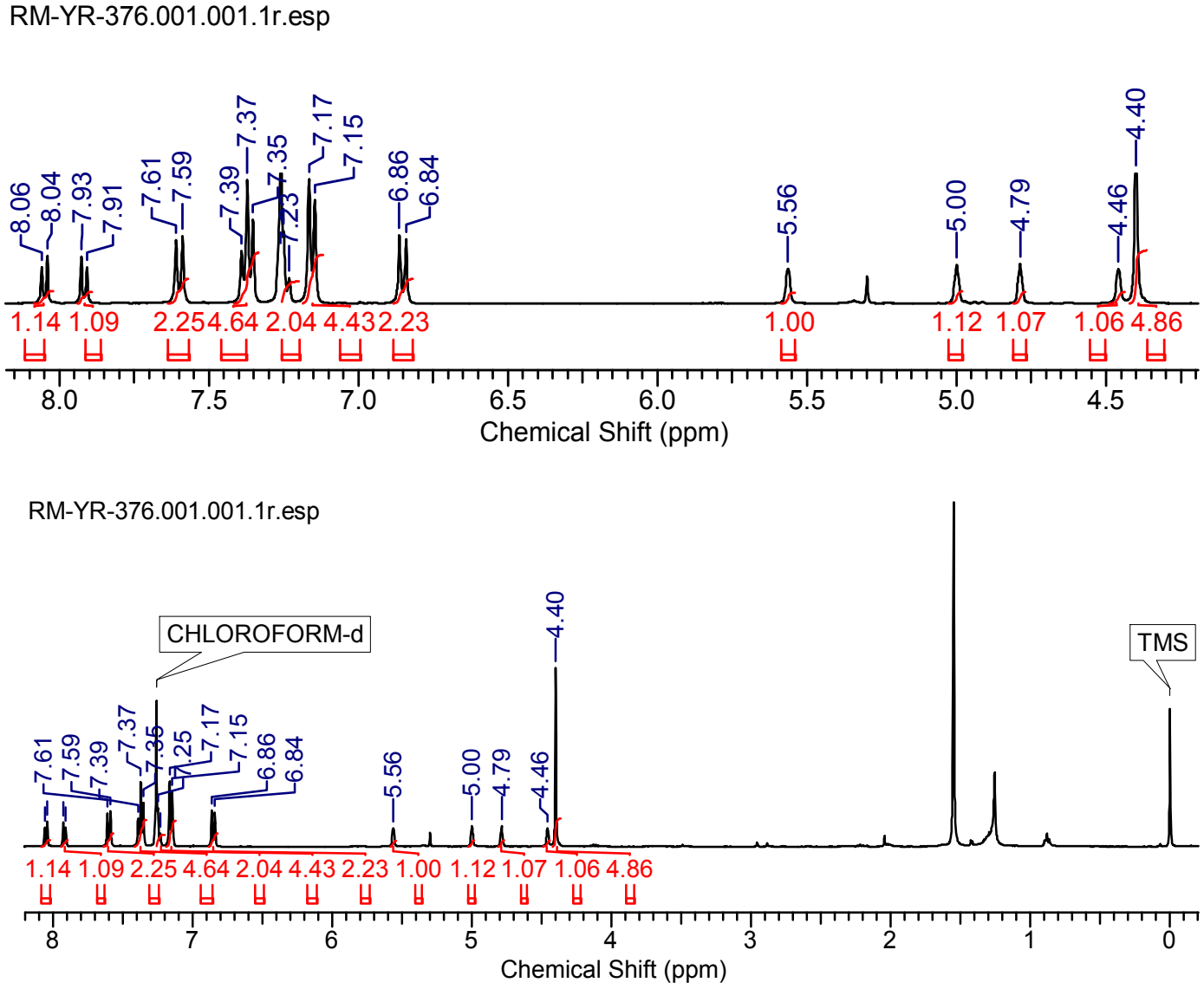
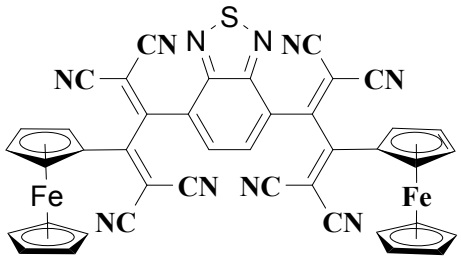
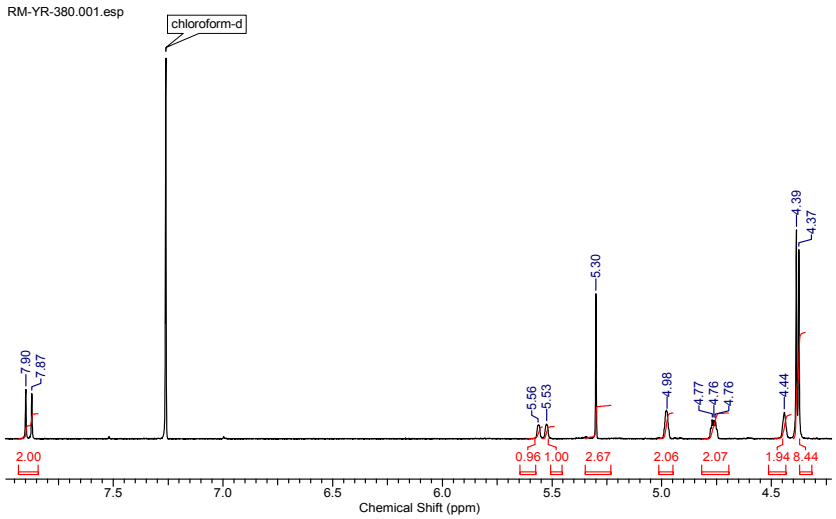


Figure S6. ^{1}H NMR spectrum of **BTD 2f**





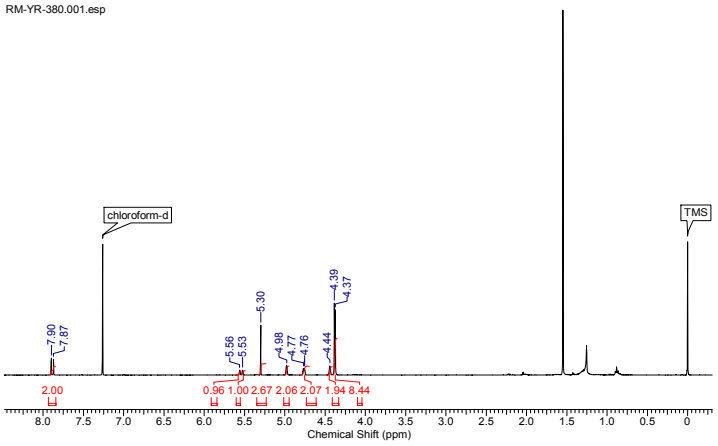
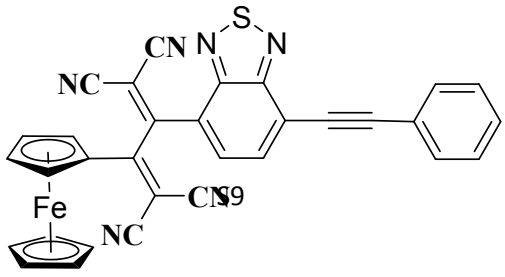


Figure S7. ^{1}H NMR spectrum of **BTD 2g**



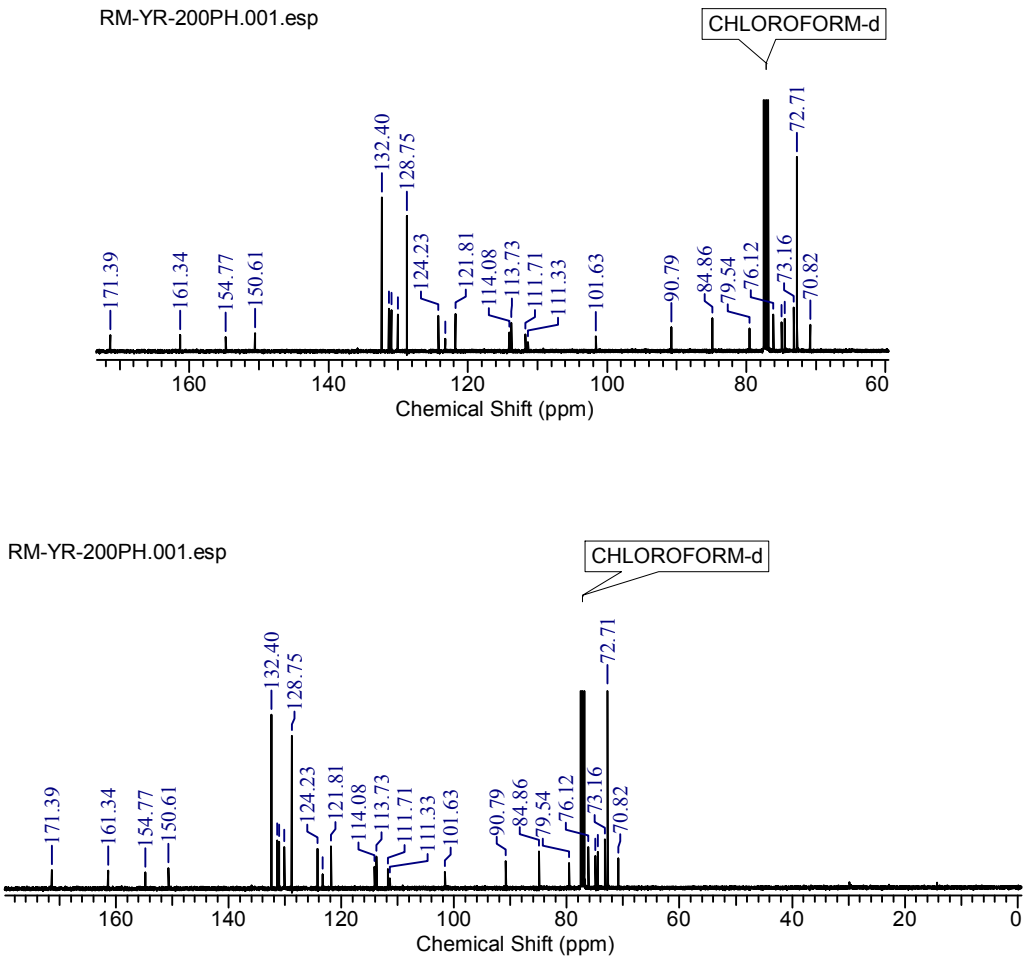


Figure S8. ^{13}C NMR of **2a**

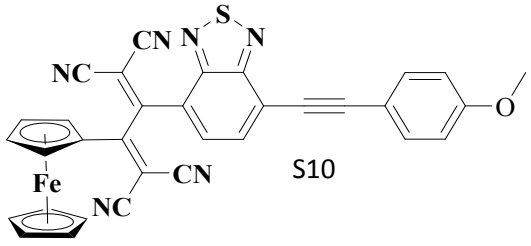
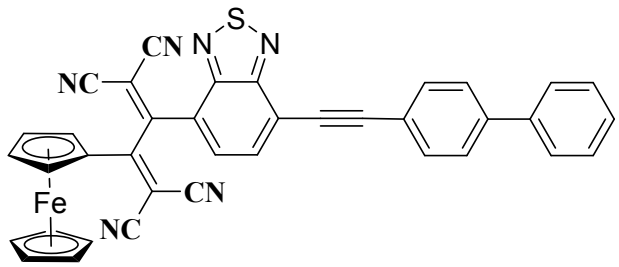


Figure S9. ^{13}C NMR of **2b**



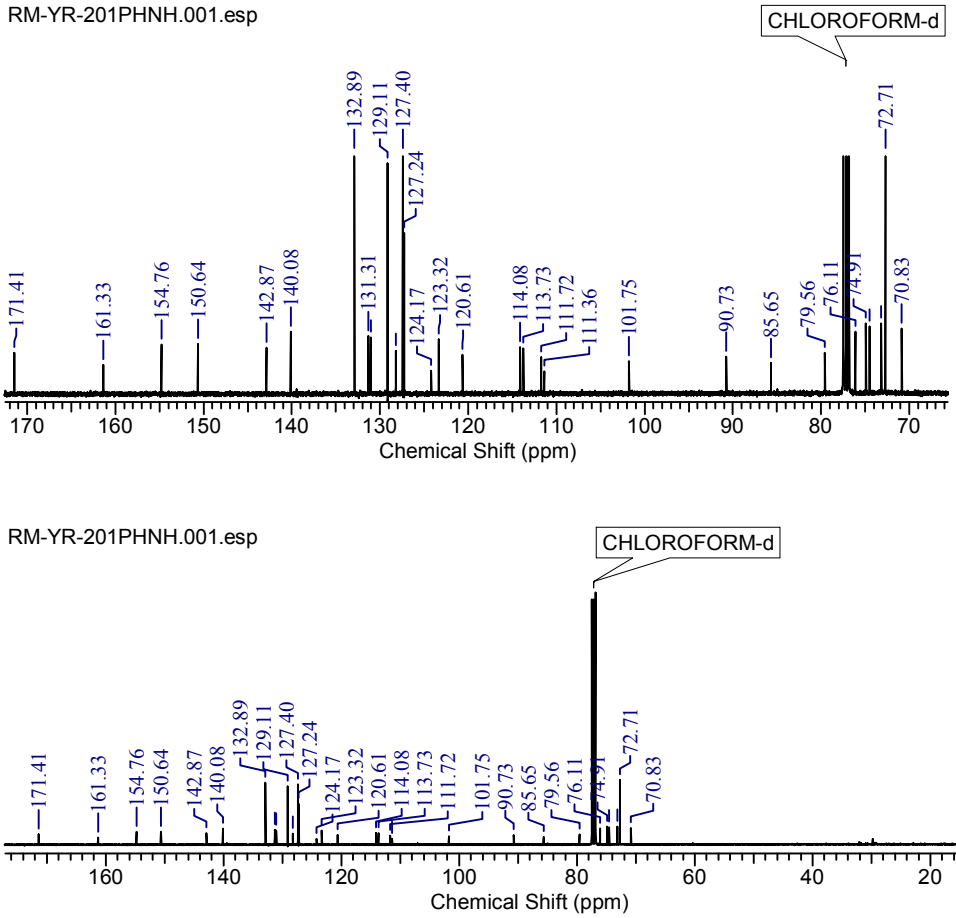


Figure S10. ^{13}C NMR of **2c**

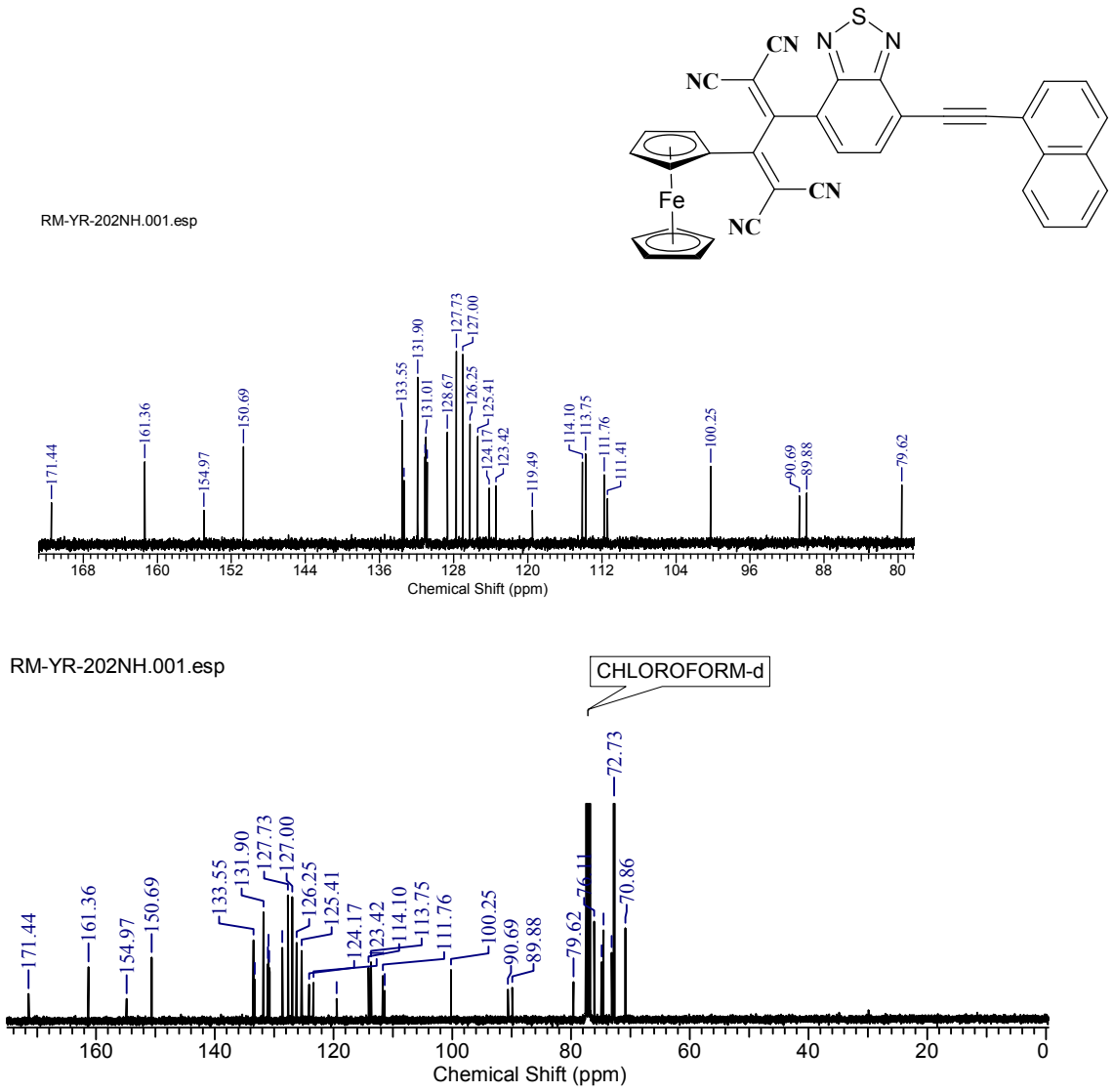
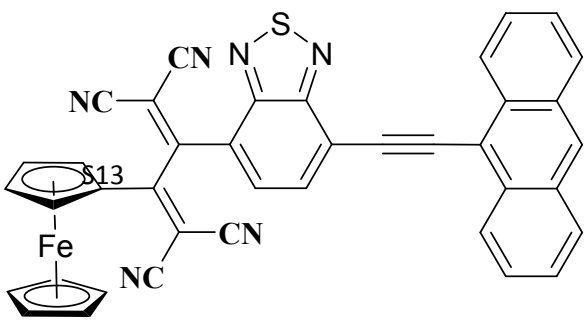
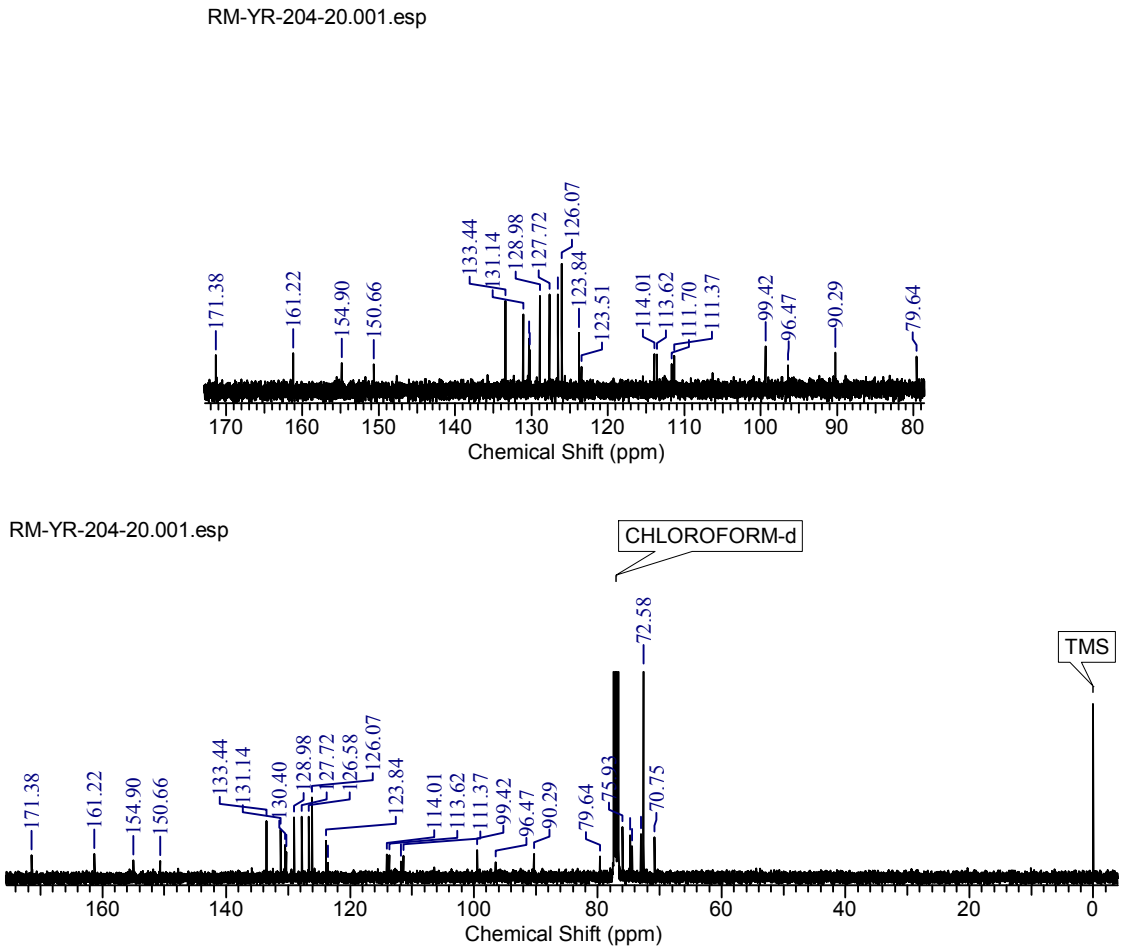


Figure S11. ^{13}C NMR of **2d**





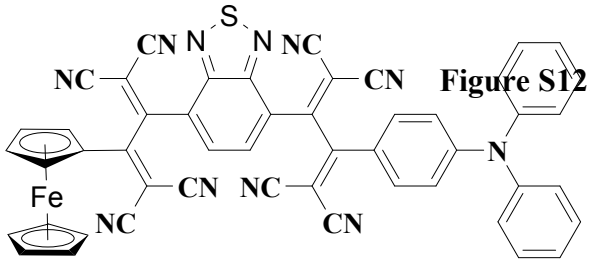


Figure S12. ^{13}C NMR of **2e**

Figure S13. ^{13}C NMR of **2f**

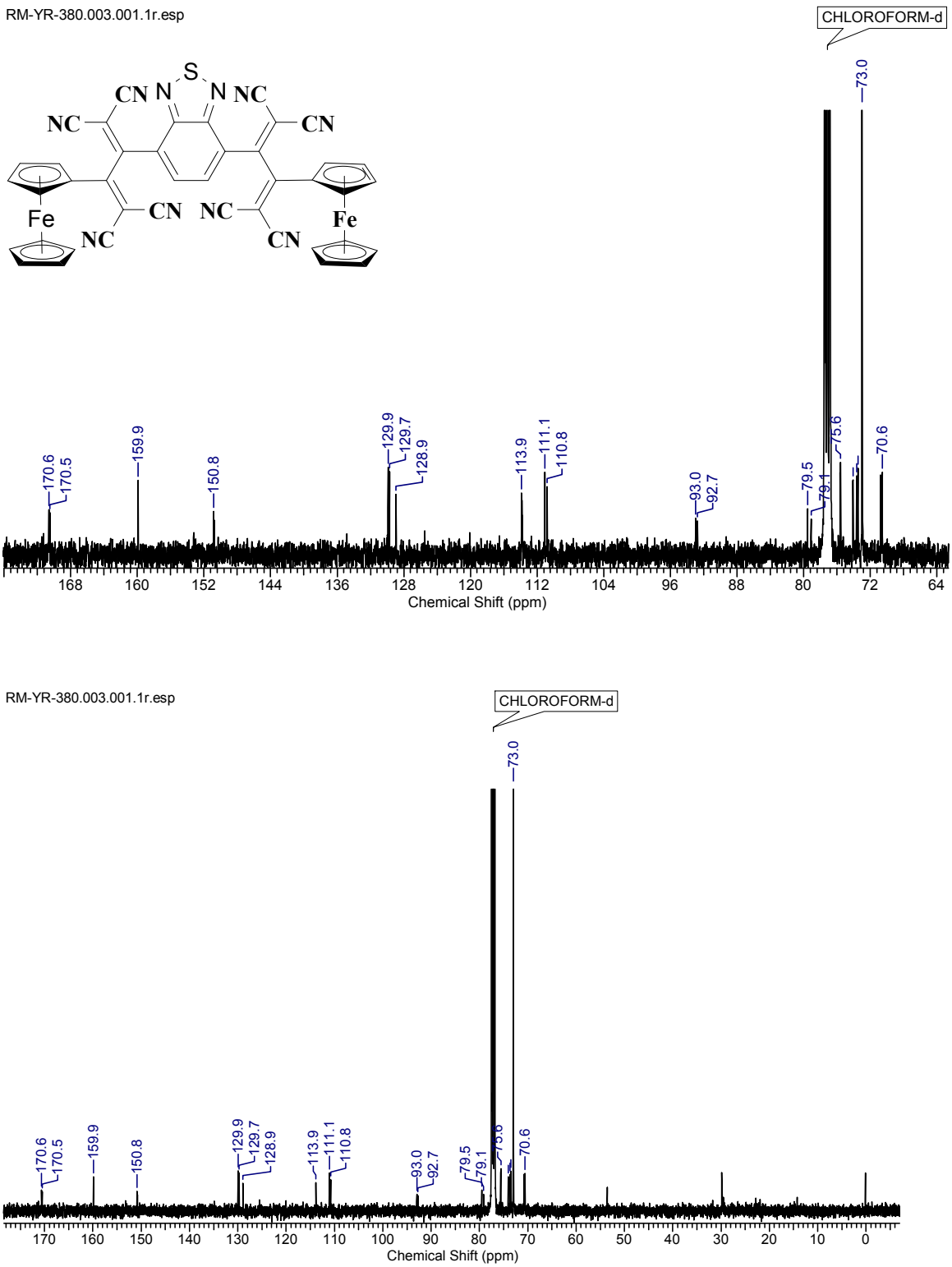
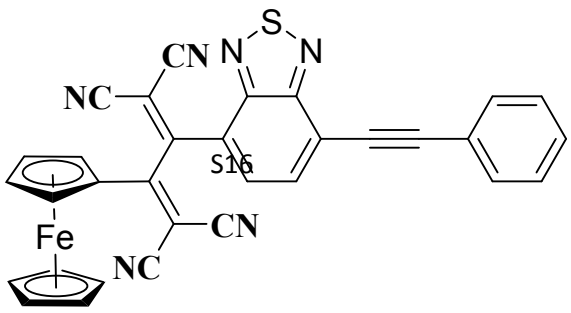


Figure S14. ^{13}C NMR of **2g**



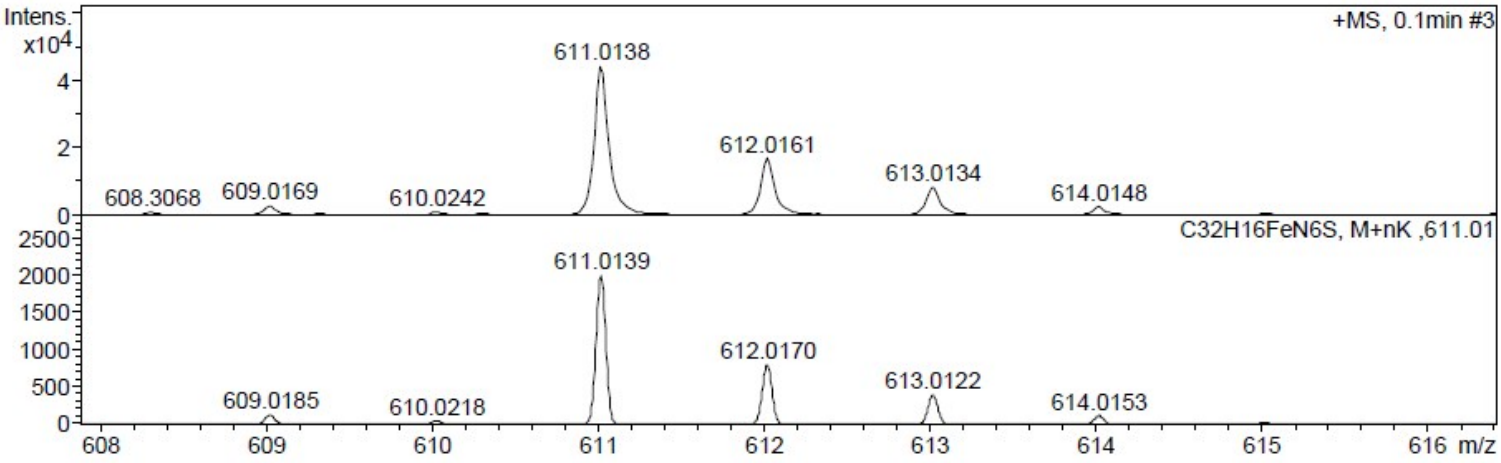
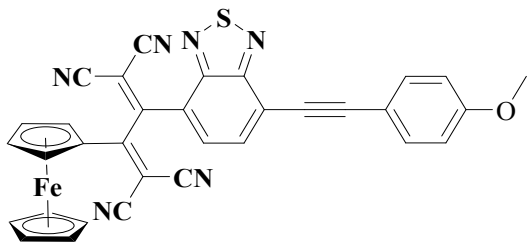


Figure S15. HRMS of **2a**



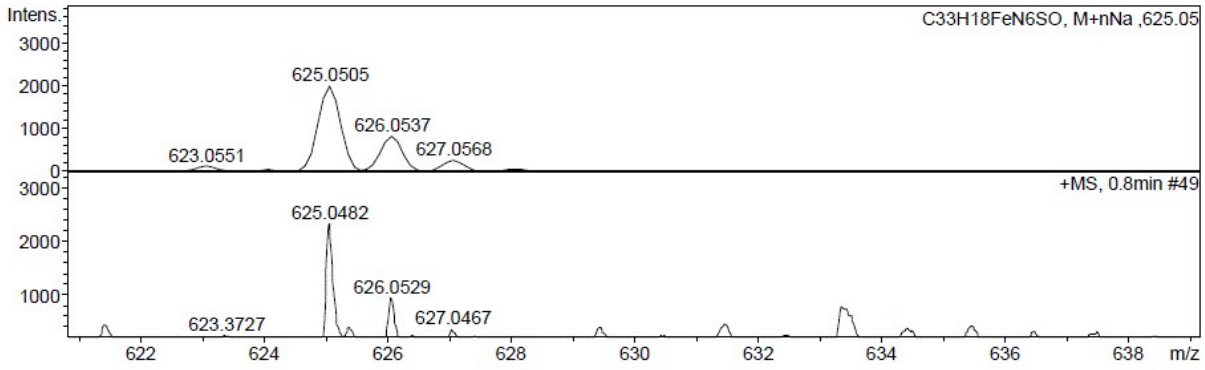
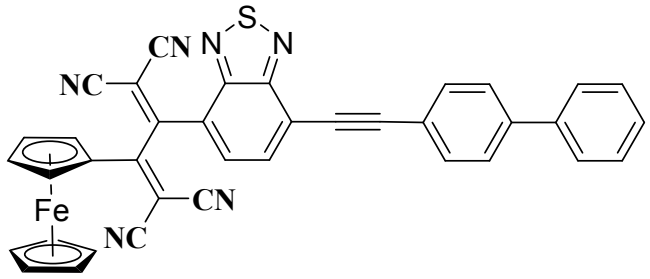


Figure S16. HRMS of **2b**



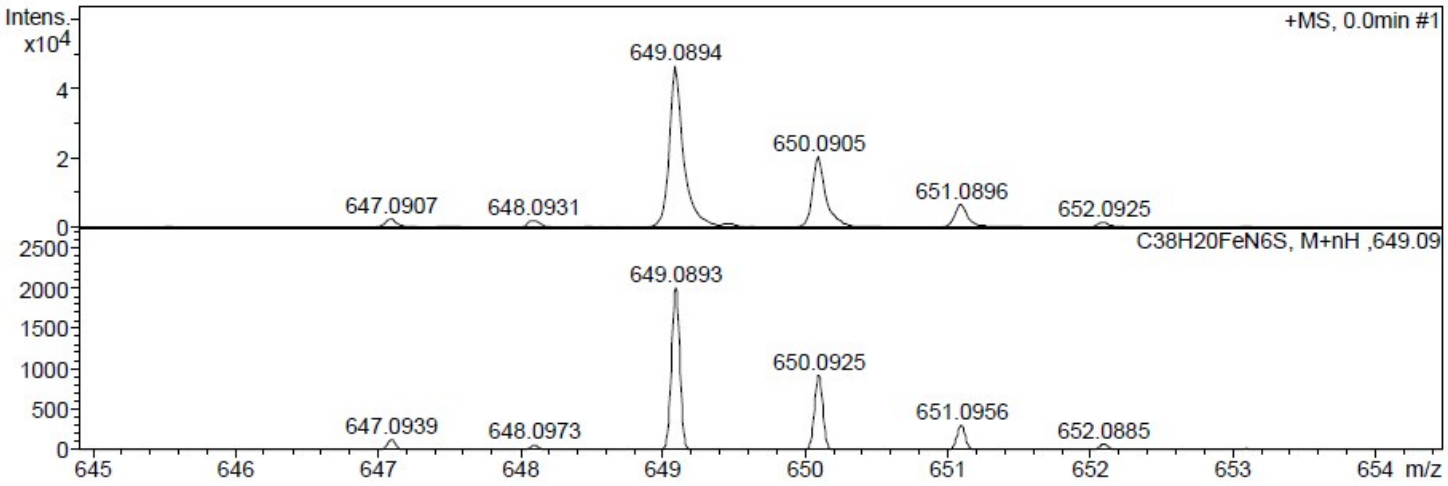
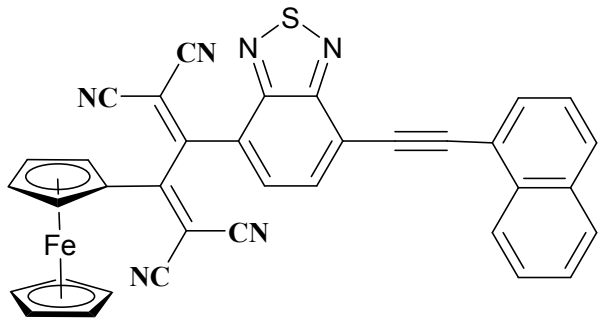


Figure S17. HRMS of **2c**



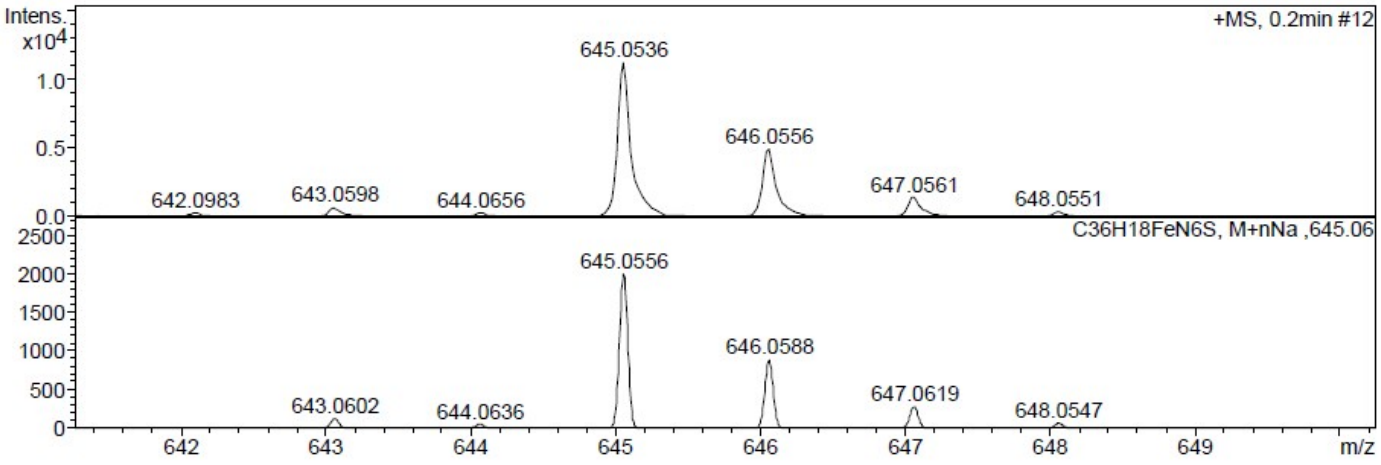
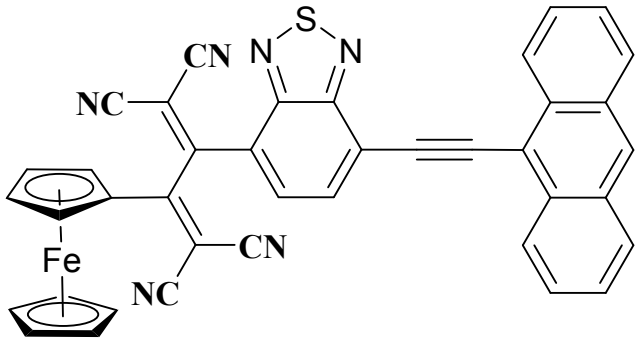


Figure S18. HRMS of **2d**



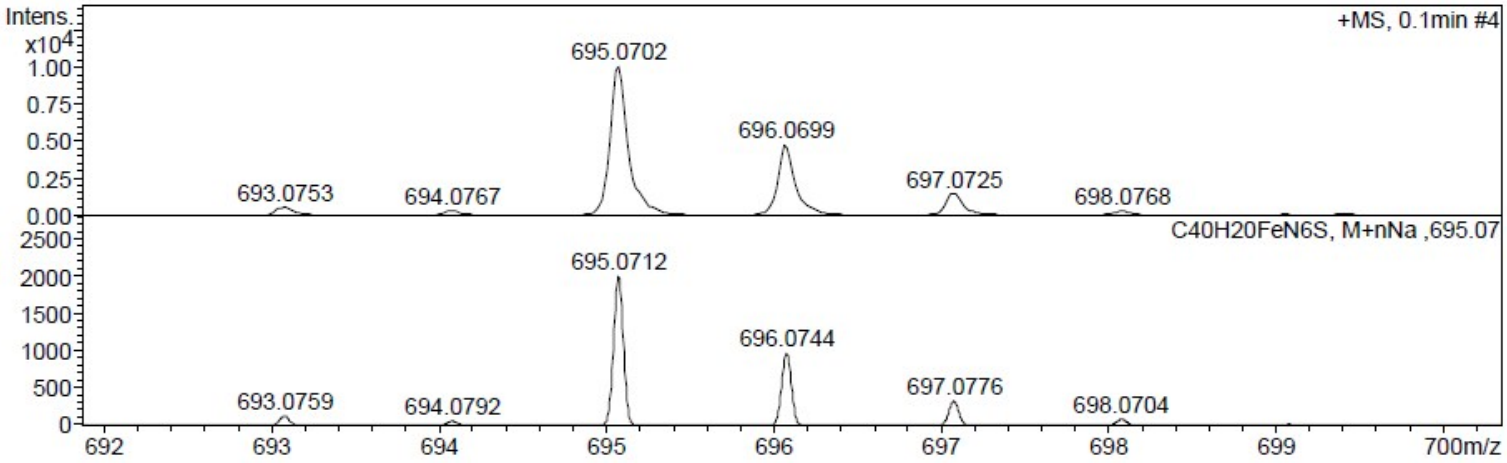


Figure S19. HRMS of **2e**

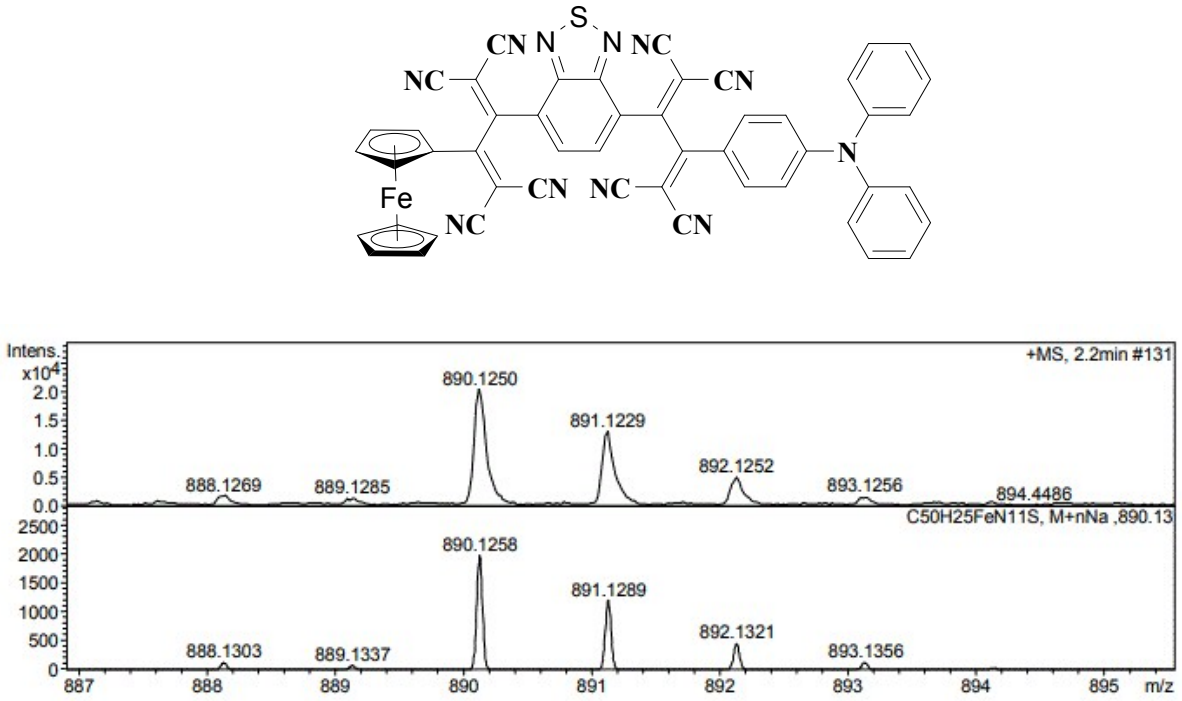
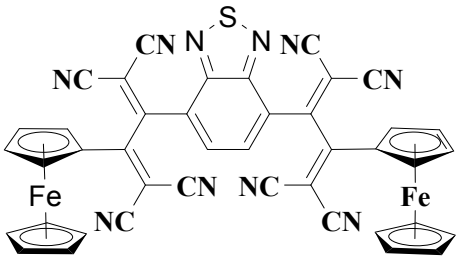


Figure S20. HRMS of **2f**



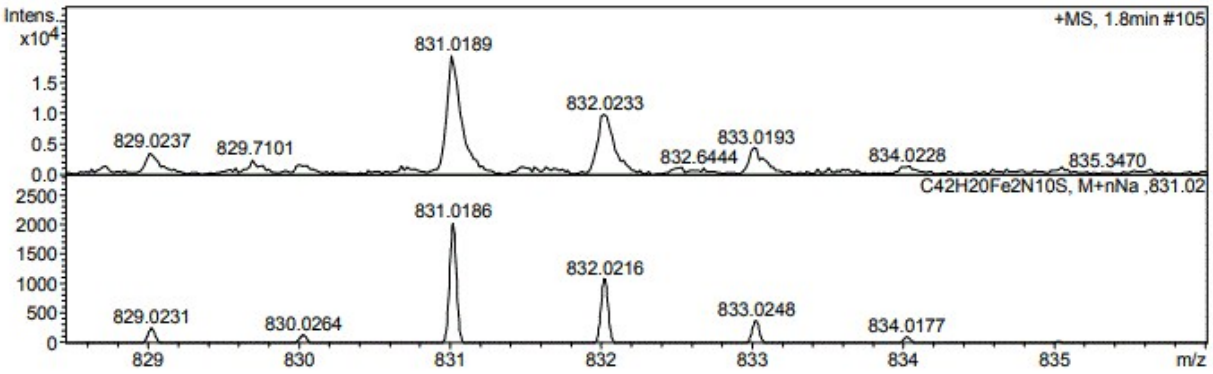


Figure S21. HRMS of **2g**

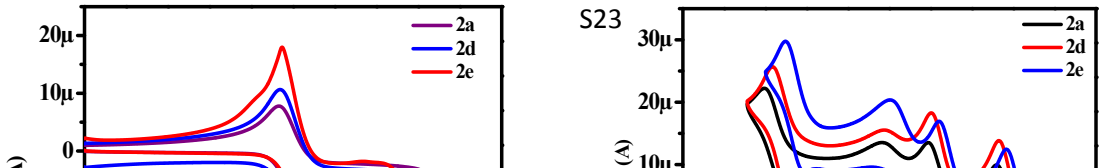


Figure S22. Cyclic voltammograms of BTD **2a**, **2b**, **2d**, **2e**, **2g** and **2f** at 0.1 M concentration of $TBAPF_6$ in dichloromethane recorded at a scan rate of 100 mV s^{-1}.

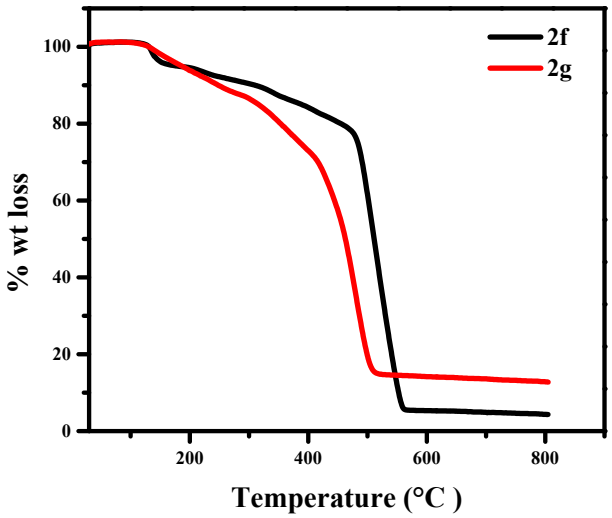


Figure S23. Thermogravimetric analysis (TGA) of benzothiazoles **2f and 2g** measured at a heating rate of 10 ^{o}C min^{-1} under a nitrogen atmosphere.

Table S1. Crystal data and structure refinement for BTD 2c

Identification code	Ligand 1
Empirical formula	$C_{44}H_{34}FeN_6S$
*M*r	734.68
crystal system	Monoclinic
space group	*P* $2_1/c$
a(Å)	18.9402(4)
b(Å)	8.5785(2)
c(Å)	23.1650(6)
α (deg)	90
β (deg)	90.691(2)
γ (deg)	90
Volume (Å$^{3)}$	3763.54(15)
Z	4
Dx (Mg m^{-3})	1.297
F(000)	1528
μ (mm^{-1})	4.037
θ range for data collection(deg)	3.81 to 71.48
Limiting indices	-23<=h<=22, -6<=k<=10, -28<=l<=27
Reflections collected	23712
unique reflections	7236
R(int)	0.0747
Completeness to θ	99.6
Data / restraints / parameters	7236 / 0 / 471
GOF on F^2	0.915

*R*1 and *R*2 [$I>2\sigma(I)$]	R1 = 0.0607, wR2 =0.1706
*R*1 and *R*2 (all data)	R1=0.0770, wR2 =0.1993
Largest diff. peak and hole($e.A^{-3}$)	0.519 and -0.479

Table S2. Selected bond length and bond angle of BTD 2c

Bond lengths [A] and angles [deg]

	Bond Length
Fe(1)-C(30)	2.030(3)
Fe(1)-C(35)	2.035(4)
Fe(1)-C(37)	2.039(4)
Fe(1)-C(36)	2.032(4)
Fe(1)-C(31)	2.045(3)
Fe(1)-C(29)	2.050(3)
Fe(1)-C(33)	2.050(3)
Fe(1)-C(34)	2.057(4)
Fe(1)-C(38)	2.053(4)
Fe(1)-C(32)	2.067(3)

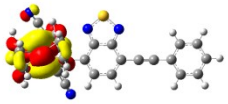
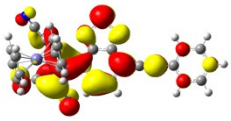
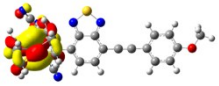
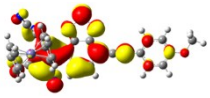
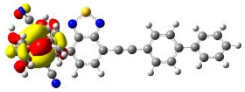
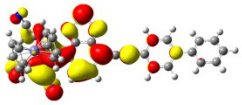
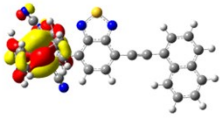
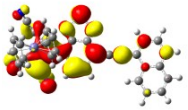
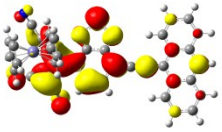
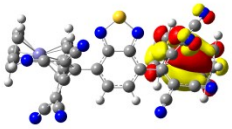
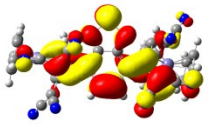
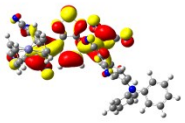
	Bond Angles
C(30)-Fe(1)-C(35)	107.33(17)
C(30)-Fe(1)-C(37)	162.08(17)
C(35)-Fe(1)-C(37)	67.5(2)
C(30)-Fe(1)-C(36)	125.91(19)
C(35)-Fe(1)-C(36)	41.4(2)
C(37)-Fe(1)-C(36)	39.0(2)
C(30)-Fe(1)-C(31)	40.58(13)

C(35)-Fe(1)-C(31)	115.9(2)
C(37)-Fe(1)-C(31)	124.65(16)
C(36)-Fe(1)-C(31)	104.32(16)
C(30)-Fe(1)-C(29)	41.43(12)
C(35)-Fe(1)-C(29)	130.23(18)
C(37)-Fe(1)-C(29)	154.42(17)
C(36)-Fe(1)-C(29)	166.58(18)
C(31)-Fe(1)-C(29)	68.50(13)

Crystallographic data

A single crystal X-ray structural study of BTD **2c** was performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 150(2) K using graphitemonochromated Mo Kα radiation (λα = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on F2. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2Ueq of their parent atoms. The CCDC number 1888906 contains the supplementary crystallographic data for BTD **2c**. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S3. The molecular orbitals of BTDs **2a–2g** estimated from DFT calculation.

BTD	HOMO	LUMO
2a		
2b		
2c		
2d		
2e		
2f		
2g		

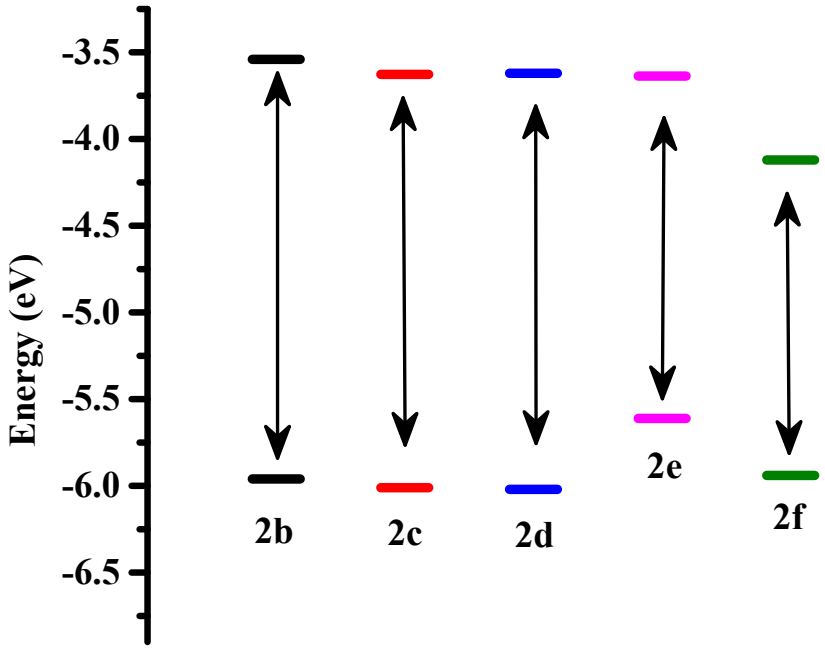
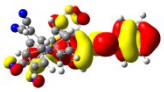
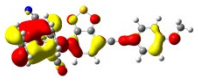
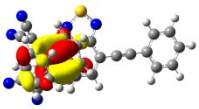
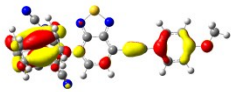
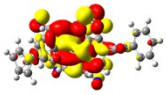
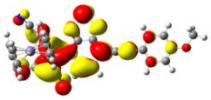
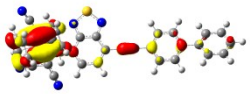
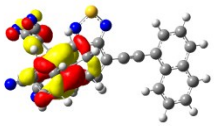
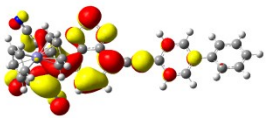
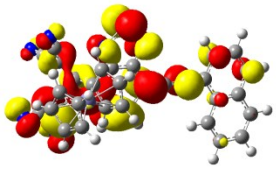
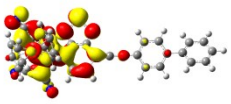
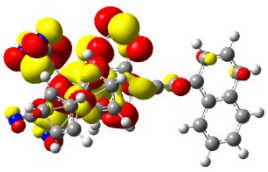
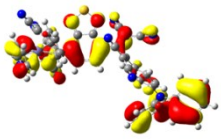
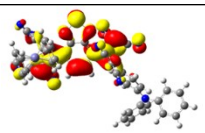
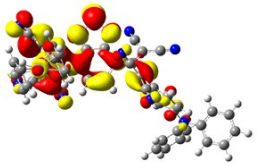
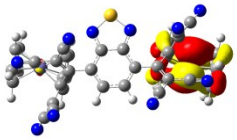
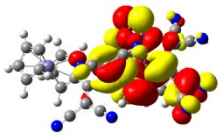


Figure S24. Energy levels diagram of the frontier orbitals of BTDs **2b–2f** estimated by DFT calculations.

Table S4. The molecular orbitals of BTDs **2a–2g** estimated from DFT calculation.

2a		**2b**	
HOMO-2		**HOMO-6**	
HOMO-1		**HOMO-2**	
LUMO+1		**LUMO**	
2c		**2d**	
HOMO-1		**HOMO**	
LUMO		**LUMO**	
LUMO+1		**LUMO+1**	
2e		**2f**	
HOMO		**HOMO-7**	
LUMO		**HOMO**	

		LUMO	
		LUMO+2	

2g	
HOMO-2	
LUMO	
LUMO+1	

TD-DFT Calculation data

BTDs **2a**–**2g**

Calculation method: B3LYP/6-31G (d, p) level

BTD 2a

Excitation energies and oscillator strengths:

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    1.6798 eV  738.10 nm
f=0.0016  <S**2>=0.000
     140 ->142         0.44409
     140 ->143         0.39785
     140 ->144        -0.19297
     140 ->148         0.22057
     140 ->149        -0.11623
     141 ->147        -0.15443
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2078.94447851
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited state symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.7230 eV  719.60 nm
f=0.0107  <S**2>=0.000
     140 ->147         0.13787
     141 ->142         0.54372
     141 ->143         0.30888
     141 ->144        -0.13073
     141 ->148         0.19787
     141 ->149        -0.10810

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    1.9622 eV  631.86 nm
f=0.0021  <S**2>=0.000
     140 ->147        -0.20430
     141 ->142         0.44602
     141 ->143        -0.32393
     141 ->144         0.20131
     141 ->148        -0.23113
     141 ->149         0.12865

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    2.0208 eV  613.53 nm
f=0.0137  <S**2>=0.000
     140 ->142         0.53414
     140 ->143        -0.25037
     140 ->144         0.17243
     140 ->148        -0.18935
     140 ->149         0.10851
     141 ->143        -0.10165
     141 ->147         0.18498

 Excited state symmetry could not be determined.
```

```
 Excited State   5:      Singlet-?Sym    2.3017 eV  538.66 nm
f=0.7272  <S**2>=0.000
     139 ->142         0.70016

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    2.3603 eV  525.30 nm
f=0.0029  <S**2>=0.000
     137 ->142        -0.14749
     137 ->143        -0.25036
     137 ->144         0.15657
     137 ->148        -0.24373
     137 ->149         0.13187
     138 ->142        -0.10635
     138 ->143        -0.16184
     138 ->148        -0.15519
     140 ->146        -0.11683
     140 ->147         0.37917
     141 ->143        -0.12954
     141 ->147        -0.12048

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.4710 eV  501.75 nm
f=0.0004  <S**2>=0.000
     137 ->147        -0.19231
     138 ->147        -0.17166
     140 ->143         0.28008
     140 ->147         0.16507
     141 ->143        -0.12566
     141 ->146        -0.16773
     141 ->147         0.49863

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    2.6288 eV  471.64 nm
f=0.0032  <S**2>=0.000
     137 ->142        -0.11432
     137 ->143        -0.14829
     138 ->142        -0.29131
     138 ->143        -0.12719
     140 ->143         0.13817
     140 ->147        -0.24523
     141 ->143         0.40832
     141 ->147         0.11164
     141 ->148        -0.19173

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    2.7612 eV  449.03 nm
f=0.0181  <S**2>=0.000
     138 ->142         0.61017
     140 ->143         0.13937
     141 ->143         0.17529
     141 ->144         0.10357
```

```
 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    2.7982 eV  443.09 nm
f=0.0186  <S**2>=0.000
     137 ->147         0.25919
     138 ->142        -0.11464
     138 ->147         0.18141
     139 ->143         0.15242
     140 ->143         0.36689
     140 ->144         0.20349
     140 ->146         0.10779
     140 ->148        -0.26693
     140 ->149         0.14175
     141 ->143        -0.15487
     141 ->144        -0.11539
     141 ->148         0.10548

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    2.8277 eV  438.47 nm
f=0.1928  <S**2>=0.000
     139 ->143         0.68042

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    2.9475 eV  420.64 nm
f=0.0029  <S**2>=0.000
     137 ->142         0.59892
     140 ->147         0.16925
     141 ->143         0.11264
     141 ->144         0.24800
     141 ->148        -0.10164

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    3.0318 eV  408.95 nm
f=0.0007  <S**2>=0.000
     136 ->142         0.65753
     136 ->143         0.11960
     137 ->142        -0.12117
     141 ->144         0.13837

 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    3.0752 eV  403.17 nm
f=0.0014  <S**2>=0.000
     136 ->142        -0.20931
     137 ->142        -0.26543
     137 ->143         0.15703
     137 ->144        -0.10566
     138 ->143         0.21023
     140 ->147         0.20338
     141 ->144         0.44407

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    3.2014 eV  387.28 nm
f=0.0005  <S**2>=0.000
```

```
     137 ->147        -0.21288
     138 ->147        -0.13503
     140 ->144         0.58356
     140 ->148         0.16755
     141 ->144        -0.11119
     141 ->147        -0.10129

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    3.2718 eV  378.95 nm
f=0.0023  <S**2>=0.000
     135 ->142         0.70168

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    3.3803 eV  366.78 nm
f=0.0536  <S**2>=0.000
     133 ->142         0.48505
     134 ->142         0.24158
     137 ->143        -0.10591
     138 ->143         0.28173
     139 ->144        -0.27341

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    3.4008 eV  364.57 nm
f=0.0390  <S**2>=0.000
     133 ->142         0.28098
     134 ->142        -0.26371
     138 ->143         0.18788
     139 ->144         0.53958

 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    3.4638 eV  357.94 nm
f=0.0601  <S**2>=0.000
     130 ->142         0.11569
     134 ->142         0.26397
     137 ->143        -0.25156
     138 ->143        -0.14087
     139 ->144         0.15160
     140 ->147        -0.16428
     140 ->148         0.12842
     141 ->144         0.26644
     141 ->146        -0.15384
     141 ->148         0.30406
     141 ->149        -0.16169

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    3.4750 eV  356.79 nm
f=0.0928  <S**2>=0.000
     131 ->142         0.15652
     133 ->142        -0.15514
     134 ->142         0.51649
     138 ->143         0.10860
     139 ->144         0.29174
```

```
     141 ->144        -0.12492
     141 ->148        -0.13749
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

BTD 2b

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      1.6862 eV  735.28 nm  f=0.0027
<S**2>=0.000
     147 ->150         0.43608
     147 ->151         0.39233
     147 ->152        -0.19101
     147 ->156         0.21893
     147 ->157        -0.11694
     148 ->155        -0.15484
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2193.47163012
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      1.7335 eV  715.21 nm  f=0.0123
<S**2>=0.000
     147 ->155         0.14344
     148 ->150         0.52919
     148 ->151         0.31561
     148 ->152        -0.13664
     148 ->156         0.20510
     148 ->157        -0.11283

 Excited State   3:      Singlet-A      1.9909 eV  622.74 nm  f=0.0120
<S**2>=0.000
     147 ->155        -0.20413
     148 ->150         0.46298
     148 ->151        -0.31475
     148 ->152         0.19598
     148 ->156        -0.22468
     148 ->157         0.12507

 Excited State   4:      Singlet-A      2.0331 eV  609.84 nm  f=0.4417
<S**2>=0.000
     147 ->150         0.30697
     147 ->151        -0.19409
     147 ->152         0.13218
     147 ->156        -0.14493
     148 ->155         0.13791
     149 ->150         0.53976
```

```
 Excited State   5:      Singlet-A      2.0727 eV  598.17 nm  f=0.3504
<S**2>=0.000
     147 ->150         0.44836
     147 ->151        -0.15624
     147 ->152         0.10854
     147 ->156        -0.12574
     148 ->155         0.13968
     149 ->150        -0.43969

 Excited State   6:      Singlet-A      2.3630 eV  524.68 nm  f=0.0033
<S**2>=0.000
     144 ->150        -0.15592
     144 ->151        -0.25112
     144 ->152         0.15595
     144 ->154         0.10737
     144 ->156        -0.24163
     144 ->157         0.13279
     146 ->150        -0.10929
     146 ->151        -0.15939
     146 ->156        -0.15043
     147 ->154        -0.14556
     147 ->155         0.36482
     148 ->151        -0.12854
     148 ->155        -0.11331

 Excited State   7:      Singlet-A      2.4773 eV  500.47 nm  f=0.0019
<S**2>=0.000
     144 ->155        -0.19559
     146 ->155        -0.17137
     147 ->151         0.26884
     147 ->155         0.16451
     148 ->151        -0.12206
     148 ->154        -0.20704
     148 ->155         0.47977

 Excited State   8:      Singlet-A      2.5821 eV  480.17 nm  f=0.2078
<S**2>=0.000
     149 ->151         0.69042

 Excited State   9:      Singlet-A      2.6460 eV  468.58 nm  f=0.0034
<S**2>=0.000
     144 ->150        -0.11891
     144 ->151        -0.14645
     146 ->150        -0.29864
     146 ->151        -0.12580
     147 ->151         0.13764
     147 ->154         0.12093
     147 ->155        -0.24193
     148 ->151         0.40839
     148 ->155         0.12525
     148 ->156        -0.17677
```

```
 Excited State  10:      Singlet-A      2.7882 eV  444.68 nm  f=0.0178
<S**2>=0.000
     146 ->150         0.60036
     147 ->151         0.15868
     148 ->151         0.17540

 Excited State  11:      Singlet-A      2.8183 eV  439.93 nm  f=0.0030
<S**2>=0.000
     144 ->154        -0.10460
     144 ->155         0.26140
     146 ->150        -0.13906
     146 ->155         0.18080
     147 ->151         0.36872
     147 ->152         0.18996
     147 ->154         0.12209
     147 ->156        -0.26917
     147 ->157         0.14473
     148 ->151        -0.17119
     148 ->152        -0.12133
     148 ->156         0.10783

 Excited State  12:      Singlet-A      2.9737 eV  416.94 nm  f=0.0029
<S**2>=0.000
     144 ->150         0.58301
     147 ->155         0.17616
     148 ->151         0.12229
     148 ->152         0.26516
     148 ->156        -0.10705

 Excited State  13:      Singlet-A      3.0403 eV  407.80 nm  f=0.0030
<S**2>=0.000
     143 ->150        -0.47258
     145 ->150         0.47955

 Excited State  14:      Singlet-A      3.1004 eV  399.89 nm  f=0.0022
<S**2>=0.000
     144 ->150        -0.30833
     144 ->151         0.15013
     144 ->152        -0.10433
     145 ->150         0.14363
     146 ->150        -0.10058
     146 ->151         0.20348
     147 ->155         0.19313
     148 ->152         0.44296

 Excited State  15:      Singlet-A      3.1277 eV  396.40 nm  f=0.0075
<S**2>=0.000
     143 ->150         0.43419
     145 ->150         0.32792
     149 ->152        -0.41729
```

```
 Excited State  16:      Singlet-A      3.2006 eV  387.37 nm  f=0.1500
<S**2>=0.000
     143 ->150         0.24826
     144 ->155        -0.10670
     145 ->150         0.31389
     147 ->152         0.24568
     149 ->152         0.47620

 Excited State  17:      Singlet-A      3.2347 eV  383.30 nm  f=0.0626
<S**2>=0.000
     144 ->155        -0.17446
     145 ->150        -0.15914
     146 ->155        -0.10953
     147 ->152         0.53720
     147 ->156         0.12234
     149 ->152        -0.25876

 Excited State  18:      Singlet-A      3.4044 eV  364.19 nm  f=0.0088
<S**2>=0.000
     141 ->150        -0.19073
     142 ->150         0.65666
     146 ->151        -0.11533

 Excited State  19:      Singlet-A      3.4075 eV  363.85 nm  f=0.0333
<S**2>=0.000
     139 ->150        -0.14195
     141 ->150         0.52525
     142 ->150         0.24122
     144 ->151        -0.10263
     146 ->151         0.31144

 Excited State  20:      Singlet-A      3.4777 eV  356.51 nm  f=0.0246
<S**2>=0.000
     139 ->150         0.48754
     139 ->151        -0.12333
     144 ->151         0.15414
     146 ->151         0.17362
     147 ->155         0.12964
     148 ->152        -0.21406
     148 ->154         0.13027
     148 ->156        -0.23047
     148 ->157         0.12270
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

BTD 2c

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    1.6722 eV  741.44 nm
f=0.0025  <S**2>=0.000
     159 ->162         0.41813
     159 ->163         0.35732
     159 ->164        -0.17449
     159 ->168         0.18744
     159 ->169        -0.12016
     160 ->162         0.19546
     160 ->163         0.15239
     161 ->167        -0.14902
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2310.00545514
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited state symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.7138 eV  723.44 nm
f=0.0114  <S**2>=0.000
     159 ->167         0.12208
     161 ->162         0.55667
     161 ->163         0.29686
     161 ->164        -0.12569
     161 ->168         0.17881
     161 ->169        -0.12039

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    1.9684 eV  629.87 nm
f=0.0042  <S**2>=0.000
     159 ->167        -0.19379
     161 ->162         0.43012
     161 ->163        -0.33376
     161 ->164         0.20367
     161 ->166         0.11099
     161 ->168        -0.22215
     161 ->169         0.14825

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    2.0221 eV  613.16 nm
f=0.0685  <S**2>=0.000
     159 ->162         0.40946
     159 ->163        -0.23927
     159 ->164         0.16334
     159 ->168        -0.16779
     159 ->169         0.11503
     160 ->162         0.33724
     160 ->163        -0.10259
```

```
     161 ->167         0.18700

 Excited state symmetry could not be determined.
 Excited State   5:      Singlet-?Sym    2.1105 eV  587.48 nm
f=0.8279  <S**2>=0.000
     159 ->162        -0.37650
     160 ->162         0.58579

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    2.3600 eV  525.35 nm
f=0.0035  <S**2>=0.000
     155 ->162        -0.15651
     155 ->163        -0.24688
     155 ->164         0.15490
     155 ->166         0.10936
     155 ->168        -0.22528
     155 ->169         0.14815
     157 ->162        -0.11624
     157 ->163        -0.16072
     157 ->168        -0.14468
     159 ->166        -0.11006
     159 ->167         0.34578
     160 ->167         0.14028
     161 ->163        -0.12765
     161 ->167        -0.11339

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.4717 eV  501.62 nm
f=0.0008  <S**2>=0.000
     155 ->167        -0.18880
     157 ->167        -0.17156
     159 ->163         0.25015
     159 ->167         0.14668
     160 ->163         0.12963
     161 ->163        -0.12641
     161 ->166        -0.17174
     161 ->167         0.49348

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    2.6251 eV  472.30 nm
f=0.0029  <S**2>=0.000
     155 ->162        -0.11109
     155 ->163        -0.13521
     157 ->162        -0.31674
     157 ->163        -0.11813
     159 ->163         0.12645
     159 ->167        -0.23324
     161 ->163         0.39737
     161 ->167         0.11295
     161 ->168        -0.17742

 Excited state symmetry could not be determined.
```

```
 Excited State   9:      Singlet-?Sym    2.6736 eV  463.74 nm
f=0.2126  <S**2>=0.000
     159 ->163        -0.24519
     160 ->163         0.64726

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    2.7527 eV  450.40 nm
f=0.0188  <S**2>=0.000
     155 ->162        -0.10168
     157 ->162         0.56697
     158 ->162         0.18196
     159 ->163         0.12790
     161 ->163         0.20898
     161 ->164         0.11411

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    2.8034 eV  442.27 nm
f=0.0021  <S**2>=0.000
     155 ->167         0.26464
     157 ->167         0.18661
     159 ->163         0.36721
     159 ->164         0.19206
     159 ->166         0.11876
     159 ->168        -0.24529
     159 ->169         0.16008
     161 ->163        -0.14971
     161 ->164        -0.11269
     161 ->168         0.10334

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    2.9385 eV  421.93 nm
f=0.0681  <S**2>=0.000
     154 ->162        -0.17068
     155 ->162         0.18700
     157 ->162        -0.19714
     158 ->162         0.61264

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    2.9463 eV  420.82 nm
f=0.0083  <S**2>=0.000
     155 ->162         0.57228
     158 ->162        -0.17369
     159 ->167         0.15434
     161 ->163         0.11254
     161 ->164         0.23728

 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    3.0407 eV  407.76 nm
f=0.0174  <S**2>=0.000
     154 ->162         0.62537
     154 ->163         0.11165
     155 ->162        -0.12249
```

```
     158 ->162         0.17512
     161 ->164         0.15006

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    3.0827 eV  402.19 nm
f=0.0010  <S**2>=0.000
     154 ->162        -0.22575
     155 ->162        -0.24827
     155 ->163         0.15731
     155 ->164        -0.10383
     157 ->163         0.21325
     159 ->167         0.19123
     161 ->164         0.44110

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    3.1478 eV  393.88 nm
f=0.0003  <S**2>=0.000
     156 ->162         0.70456

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    3.2101 eV  386.23 nm
f=0.0057  <S**2>=0.000
     155 ->167        -0.20650
     157 ->167        -0.13127
     159 ->164         0.47793
     159 ->168         0.13818
     159 ->169        -0.10241
     160 ->164         0.34274
     161 ->164        -0.10398
     161 ->167        -0.10177

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    3.2963 eV  376.13 nm
f=0.1639  <S**2>=0.000
     158 ->164         0.10772
     159 ->164        -0.35962
     160 ->164         0.57480

 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    3.3064 eV  374.99 nm
f=0.0031  <S**2>=0.000
     153 ->162         0.69974

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    3.3790 eV  366.93 nm
f=0.0293  <S**2>=0.000
     152 ->162         0.57974
     155 ->163        -0.11954
     157 ->163         0.30719
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

BTD 2d

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    1.6768 eV  739.40 nm
f=0.0027  <S**2>=0.000
     152 ->155         0.44455
     152 ->156         0.39113
     152 ->157        -0.18989
     152 ->159        -0.10593
     152 ->161        -0.15826
     152 ->162         0.14280
     153 ->160        -0.14754
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2232.58943843
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited state symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.7209 eV  720.45 nm
f=0.0115  <S**2>=0.000
     152 ->160         0.13235
     153 ->155         0.54600
     153 ->156         0.30620
     153 ->157        -0.12981
     153 ->161        -0.13858
     153 ->162         0.13538

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    1.9677 eV  630.09 nm
f=0.0278  <S**2>=0.000
     152 ->160        -0.19674
     153 ->155         0.43903
     153 ->156        -0.32525
     153 ->157         0.19883
     153 ->159         0.10825
     153 ->161         0.17187
     153 ->162        -0.15052
     154 ->155         0.12361

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    1.9937 eV  621.89 nm
f=0.5038  <S**2>=0.000
     152 ->155         0.18111
     152 ->156        -0.15004
     152 ->157         0.10018
     154 ->155         0.63121
```

```
 Excited state symmetry could not be determined.
 Excited State   5:      Singlet-?Sym    2.0371 eV  608.62 nm
f=0.1155  <S**2>=0.000
     152 ->155         0.50680
     152 ->156        -0.21043
     152 ->157         0.14304
     152 ->161         0.11287
     152 ->162        -0.11249
     153 ->156        -0.10020
     153 ->160         0.16047
     154 ->155        -0.27743

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    2.3616 eV  525.00 nm
f=0.0034  <S**2>=0.000
     148 ->155        -0.14994
     148 ->156        -0.24605
     148 ->157         0.15445
     148 ->159         0.11065
     148 ->161         0.17549
     148 ->162        -0.15916
     150 ->155        -0.11298
     150 ->156        -0.16504
     150 ->161         0.11795
     150 ->162        -0.10145
     152 ->159        -0.11807
     152 ->160         0.36496
     153 ->156        -0.13160
     153 ->160        -0.11216

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.4712 eV  501.72 nm
f=0.0014  <S**2>=0.000
     148 ->160        -0.18077
     150 ->160        -0.16706
     152 ->156         0.27561
     152 ->160         0.15788
     153 ->156        -0.12348
     153 ->159        -0.17019
     153 ->160         0.48009

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    2.5642 eV  483.52 nm
f=0.1257  <S**2>=0.000
     154 ->156         0.68842

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    2.6233 eV  472.62 nm
f=0.0059  <S**2>=0.000
     148 ->155        -0.11058
     148 ->156        -0.14264
     150 ->155        -0.28838
```

```
     150 ->156        -0.12625
     152 ->156         0.13188
     152 ->159         0.10012
     152 ->160        -0.23603
     153 ->156         0.40915
     153 ->160         0.11236
     153 ->161         0.15672
     153 ->162        -0.10741

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    2.7569 eV  449.72 nm
f=0.0250  <S**2>=0.000
     150 ->155         0.56505
     151 ->155         0.22298
     152 ->156         0.14107
     153 ->156         0.17960
     153 ->157         0.10788

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    2.7978 eV  443.15 nm
f=0.0022  <S**2>=0.000
     148 ->160         0.25643
     150 ->155        -0.10669
     150 ->160         0.18601
     152 ->156         0.36811
     152 ->157         0.20979
     152 ->159         0.12675
     152 ->161         0.19936
     152 ->162        -0.18762
     152 ->163         0.10394
     153 ->156        -0.15558
     153 ->157        -0.11813

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    2.8707 eV  431.89 nm
f=0.1849  <S**2>=0.000
     150 ->155        -0.23253
     151 ->155         0.64657

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    2.9516 eV  420.06 nm
f=0.0032  <S**2>=0.000
     148 ->155         0.59703
     152 ->160         0.17052
     153 ->156         0.10913
     153 ->157         0.24792

 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    3.0353 eV  408.48 nm
f=0.0060  <S**2>=0.000
     149 ->155         0.69427
```

```
 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    3.0444 eV  407.25 nm
f=0.0140  <S**2>=0.000
     147 ->155         0.63075
     147 ->156         0.11853
     148 ->155        -0.13532
     153 ->157         0.16286

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    3.0816 eV  402.34 nm
f=0.0010  <S**2>=0.000
     147 ->155        -0.24993
     148 ->155        -0.26119
     148 ->156         0.15370
     148 ->157        -0.10271
     150 ->156         0.21309
     152 ->160         0.19516
     153 ->157         0.42699

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    3.1850 eV  389.28 nm
f=0.1093  <S**2>=0.000
     148 ->160        -0.11000
     152 ->157         0.22998
     154 ->157         0.61849

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    3.2207 eV  384.96 nm
f=0.0445  <S**2>=0.000
     148 ->160        -0.17478
     150 ->160        -0.11494
     152 ->157         0.53630
     152 ->162         0.10679
     154 ->157        -0.29675

 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    3.3837 eV  366.41 nm
f=0.0388  <S**2>=0.000
     146 ->155         0.56561
     148 ->156        -0.12913
     150 ->156         0.33329

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    3.4339 eV  361.06 nm
f=0.0379  <S**2>=0.000
     151 ->156         0.67531
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

BTD 2e

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    1.8587 eV  667.06 nm
f=0.0002  <S**2>=0.000
     165 ->169         0.28582
     165 ->171        -0.20109
     165 ->172        -0.11092
     165 ->176         0.21803
     165 ->177         0.39477
     166 ->175         0.28241
     166 ->176         0.18234
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2385.11548561
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited state symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.8774 eV  660.40 nm
f=0.0052  <S**2>=0.000
     165 ->175        -0.29721
     165 ->176        -0.19186
     166 ->169         0.27074
     166 ->171        -0.18827
     166 ->172        -0.10560
     166 ->176         0.21458
     166 ->177         0.38587

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    2.2296 eV  556.07 nm
f=1.0321  <S**2>=0.000
     164 ->168        -0.17424
     167 ->168         0.65164
     167 ->169        -0.15333

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    2.4011 eV  516.35 nm
f=0.0028  <S**2>=0.000
     158 ->169        -0.13701
     158 ->171         0.10462
     158 ->176        -0.11694
     158 ->177        -0.23082
     159 ->169        -0.12787
     159 ->176        -0.13141
     159 ->177        -0.23488
     165 ->175         0.34123
     165 ->176         0.27242
     166 ->169         0.13662
     166 ->175        -0.12905
     166 ->177         0.14620

 Excited state symmetry could not be determined.
```

```
 Excited State   5:      Singlet-?Sym    2.4719 eV  501.57 nm
f=0.0002  <S**2>=0.000
     158 ->175         0.16695
     158 ->176         0.11046
     159 ->175         0.24395
     159 ->176         0.17144
     162 ->175         0.13766
     162 ->176         0.10362
     165 ->169        -0.16263
     165 ->171         0.10133
     165 ->175         0.14189
     165 ->177        -0.15566
     166 ->175         0.37628
     166 ->176         0.29717

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    3.0818 eV  402.32 nm
f=0.0172  <S**2>=0.000
     158 ->169         0.10144
     158 ->177         0.15607
     159 ->169         0.15120
     159 ->171        -0.11081
     159 ->177         0.19470
     165 ->175         0.19793
     165 ->176         0.14473
     166 ->168         0.43126
     166 ->169         0.28279

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    3.2120 eV  386.00 nm
f=0.0119  <S**2>=0.000
     164 ->168        -0.27952
     164 ->169        -0.10764
     165 ->168         0.22568
     165 ->169         0.13973
     167 ->169         0.44113
     167 ->170         0.29413

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    3.2441 eV  382.19 nm
f=0.0106  <S**2>=0.000
     158 ->175         0.14184
     158 ->176         0.13350
     159 ->175         0.15235
     159 ->176         0.14587
     164 ->168         0.15128
     165 ->168         0.34938
     165 ->169         0.26976
     165 ->177        -0.10609
     166 ->168        -0.21556
     166 ->175        -0.12471
     167 ->169        -0.19752
```

```
     167 ->170        -0.14968

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    3.2743 eV  378.66 nm
f=0.0204  <S**2>=0.000
     158 ->177        -0.11472
     159 ->169        -0.13414
     159 ->175         0.11898
     159 ->177        -0.13724
     162 ->168        -0.21979
     162 ->169        -0.15323
     165 ->168         0.21119
     165 ->175        -0.18274
     165 ->176        -0.17496
     166 ->168         0.36711
     166 ->171         0.13780
     166 ->177        -0.14638

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    3.4486 eV  359.52 nm
f=0.1909  <S**2>=0.000
     164 ->168         0.55234
     164 ->169        -0.18357
     167 ->168         0.22543
     167 ->169         0.27308

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    3.4753 eV  356.76 nm
f=0.0624  <S**2>=0.000
     164 ->168         0.12060
     164 ->169         0.17733
     167 ->169        -0.26214
     167 ->170         0.59432
     167 ->171        -0.10007

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    3.5424 eV  350.01 nm
f=0.0039  <S**2>=0.000
     158 ->175        -0.23178
     158 ->176        -0.17244
     159 ->175        -0.24809
     159 ->176        -0.18099
     164 ->168         0.10655
     165 ->168         0.38877
     165 ->171         0.14929
     165 ->177        -0.16242
     166 ->175         0.20390
     166 ->176         0.13906

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    3.6698 eV  337.85 nm
f=0.0559  <S**2>=0.000
```

```
     158 ->168        -0.12127
     162 ->168         0.56637
     162 ->169         0.23779
     166 ->168         0.19821
     166 ->177        -0.11221

 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    3.8058 eV  325.78 nm
f=0.0525  <S**2>=0.000
     163 ->168         0.46445
     163 ->169        -0.20218
     163 ->170        -0.35764
     167 ->173        -0.31057

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    3.8801 eV  319.54 nm
f=0.1584  <S**2>=0.000
     162 ->169        -0.19974
     166 ->168        -0.21347
     166 ->169         0.46284
     166 ->171        -0.12950
     166 ->176        -0.18756
     166 ->177        -0.26658

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    3.9504 eV  313.85 nm
f=0.0133  <S**2>=0.000
     165 ->168        -0.28888
     165 ->169         0.41432
     165 ->171        -0.16075
     165 ->176        -0.18323
     165 ->177        -0.31228
     166 ->175         0.10054

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    3.9974 eV  310.16 nm
f=0.0973  <S**2>=0.000
     157 ->168         0.20320
     164 ->171        -0.27353
     167 ->171         0.57509

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    4.1031 eV  302.17 nm
f=0.0082  <S**2>=0.000
     154 ->168         0.16616
     154 ->169        -0.10298
     155 ->168         0.27425
     156 ->168         0.12241
     161 ->168         0.43729
     161 ->169         0.30257
     162 ->169         0.12698
```

```
 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    4.1152 eV  301.28 nm
f=0.0315  <S**2>=0.000
     154 ->168        -0.25875
     155 ->168        -0.30038
     155 ->169         0.14781
     157 ->168         0.37363
     161 ->168         0.25865
     161 ->169         0.19756

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    4.1323 eV  300.04 nm
f=0.0714  <S**2>=0.000
     154 ->168         0.26522
     154 ->169        -0.10592
     155 ->168         0.21800
     157 ->168         0.49370
     161 ->168        -0.11584
     167 ->171        -0.16092

 Excited state symmetry could not be determined.
 Excited State  21:      Singlet-?Sym    4.2384 eV  292.52 nm
f=0.1325  <S**2>=0.000
     159 ->168        -0.10663
     162 ->168        -0.21421
     162 ->169         0.49389
     162 ->171        -0.22299
     166 ->169         0.11935
     166 ->177        -0.14688

 Excited state symmetry could not be determined.
 Excited State  22:      Singlet-?Sym    4.3163 eV  287.25 nm
f=0.0933  <S**2>=0.000
     154 ->168        -0.13002
     155 ->168         0.14089
     161 ->168         0.10039
     164 ->169         0.53088
     167 ->169         0.24945

 Excited state symmetry could not be determined.
 Excited State  23:      Singlet-?Sym    4.3873 eV  282.60 nm
f=0.0688  <S**2>=0.000
     160 ->168        -0.35459
     160 ->169         0.14354
     160 ->170         0.21581
     163 ->168         0.40222
     163 ->170         0.19886
     167 ->173         0.28089

 Excited state symmetry could not be determined.
 Excited State  24:      Singlet-?Sym    4.4669 eV  277.56 nm
f=0.0165  <S**2>=0.000
```

```
     158 ->168         0.48579
     158 ->169         0.32140
     159 ->168         0.23235
     159 ->177        -0.17247

 Excited state symmetry could not be determined.
 Excited State  25:      Singlet-?Sym    4.5201 eV  274.30 nm
f=0.0018  <S**2>=0.000
     160 ->168         0.45853
     160 ->169        -0.16328
     160 ->170        -0.21545
     163 ->168         0.29774
     163 ->170         0.22103
     167 ->173         0.24165

 Excited state symmetry could not be determined.
 Excited State  26:      Singlet-?Sym    4.5556 eV  272.16 nm
f=0.0310  <S**2>=0.000
     153 ->168         0.12275
     158 ->168        -0.14307
     158 ->169        -0.17223
     159 ->168         0.49439
     159 ->169         0.27419
     162 ->168        -0.17324
     164 ->169         0.12190
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   26
LETran=     478.
```

BTD 2f

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      1.2700 eV  976.26 nm  f=0.0277
<S**2>=0.000
     217 -> 218        0.70314
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3043.99173642
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      1.4925 eV  830.71 nm  f=0.0024
<S**2>=0.000
     216 -> 218        0.67377
     216 -> 219       -0.16064

 Excited State   3:      Singlet-A      1.5336 eV  808.44 nm  f=0.0028
<S**2>=0.000
     215 -> 218        0.60162
     215 -> 219       -0.23648
     215 -> 220       -0.18648
```

```
 Excited State   4:      Singlet-A      1.7556 eV  706.22 nm  f=0.0005
<S**2>=0.000
     215 -> 218        0.30762
     215 -> 219        0.26444
     215 -> 220        0.33846
     215 -> 221        0.18831
     215 -> 222       -0.15954
     215 -> 227       -0.20625
     215 -> 229       -0.11341
     216 -> 220       -0.11204
     216 -> 226       -0.15652

 Excited State   5:      Singlet-A      1.8086 eV  685.53 nm  f=0.0145
<S**2>=0.000
     215 -> 218        0.17210
     215 -> 226        0.17541
     216 -> 218        0.14992
     216 -> 219        0.32395
     216 -> 220        0.34580
     216 -> 221        0.17309
     216 -> 222       -0.14483
     216 -> 227       -0.22400
     216 -> 229       -0.13725
     216 -> 230        0.11664

 Excited State   6:      Singlet-A      1.9471 eV  636.75 nm  f=0.2056
<S**2>=0.000
     217 -> 219        0.70266

 Excited State   7:      Singlet-A      2.2586 eV  548.95 nm  f=0.0010
<S**2>=0.000
     215 -> 226       -0.23559
     215 -> 227       -0.12007
     216 -> 219        0.56932
     216 -> 220       -0.14148
     216 -> 221       -0.12308
     216 -> 222        0.10114
     216 -> 227        0.12581

 Excited State   8:      Singlet-A      2.2909 eV  541.20 nm  f=0.1949
<S**2>=0.000
     217 -> 220        0.70212

 Excited State   9:      Singlet-A      2.3141 eV  535.78 nm  f=0.0001
<S**2>=0.000
     215 -> 219        0.53467
     215 -> 221       -0.10934
     215 -> 229        0.10699
     216 -> 226        0.27329
     216 -> 227        0.12618
```

```
 Excited State  10:      Singlet-A      2.3435 eV  529.05 nm  f=0.0026
<S**2>=0.000
     211 -> 218        0.12026
     211 -> 219       -0.15375
     211 -> 220       -0.18167
     211 -> 221       -0.12233
     211 -> 227        0.14198
     211 -> 229        0.11597
     214 -> 218        0.28717
     214 -> 219       -0.14226
     214 -> 220       -0.13032
     215 -> 219        0.17738
     215 -> 226        0.22043
     215 -> 227        0.16114
     216 -> 219        0.15132
     216 -> 220       -0.13878

 Excited State  11:      Singlet-A      2.4100 eV  514.45 nm  f=0.0170
<S**2>=0.000
     214 -> 218        0.61754
     215 -> 226       -0.17711
     216 -> 220        0.11703

 Excited State  12:      Singlet-A      2.4806 eV  499.81 nm  f=0.0001
<S**2>=0.000
     211 -> 226       -0.13627
     214 -> 226       -0.13316
     215 -> 219       -0.21132
     215 -> 220        0.34446
     215 -> 226        0.12814
     216 -> 220       -0.21406
     216 -> 225       -0.10728
     216 -> 226        0.37947
     216 -> 227        0.14611

 Excited State  13:      Singlet-A      2.5665 eV  483.09 nm  f=0.0039
<S**2>=0.000
     211 -> 218        0.22297
     211 -> 219       -0.10478
     214 -> 218       -0.10345
     215 -> 220        0.20723
     215 -> 226       -0.16457
     216 -> 220        0.45823
     216 -> 221       -0.12498
     216 -> 227        0.18605

 Excited State  14:      Singlet-A      2.6211 eV  473.03 nm  f=0.0669
<S**2>=0.000
     212 -> 218        0.17148
     213 -> 218        0.66087
```

```
 Excited State  15:      Singlet-A      2.6523 eV  467.45 nm  f=0.0017
<S**2>=0.000
     211 -> 218        0.56851
     212 -> 218       -0.26738
     215 -> 220       -0.14523

 Excited State  16:      Singlet-A      2.6941 eV  460.20 nm  f=0.0828
<S**2>=0.000
     209 -> 218       -0.43667
     211 -> 218        0.22034
     212 -> 218        0.47087

 Excited State  17:      Singlet-A      2.7187 eV  456.05 nm  f=0.0014
<S**2>=0.000
     211 -> 226        0.21779
     211 -> 227        0.11389
     214 -> 226        0.17204
     215 -> 220        0.36916
     215 -> 221       -0.23041
     215 -> 222        0.12762
     215 -> 225        0.10335
     215 -> 227        0.15239
     215 -> 229        0.13713
     215 -> 230       -0.10974
     216 -> 220       -0.14076
     216 -> 221        0.11867
     216 -> 226       -0.13451
     216 -> 227       -0.14691

 Excited State  18:      Singlet-A      2.7991 eV  442.95 nm  f=0.1689
<S**2>=0.000
     208 -> 218        0.17275
     209 -> 218        0.45611
     210 -> 218       -0.30000
     211 -> 218        0.15528
     212 -> 218        0.34354
     213 -> 218       -0.10397

 Excited State  19:      Singlet-A      2.8316 eV  437.86 nm  f=0.0387
<S**2>=0.000
     205 -> 218       -0.11390
     209 -> 218        0.24183
     210 -> 218        0.61318
     212 -> 218        0.14604

 Excited State  20:      Singlet-A      2.8588 eV  433.70 nm  f=0.3086
<S**2>=0.000
     208 -> 218        0.41064
     212 -> 218       -0.10998
     213 -> 218        0.15178
     217 -> 221        0.40883
     217 -> 222        0.31834
```

```
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

BTDg

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      1.6030 eV  773.45 nm  f=0.0035
<S**2>=0.000
     195 ->196         0.65148
     195 ->197        -0.16699
     195 ->198        -0.13680
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2804.80069686
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      1.6200 eV  765.32 nm  f=0.0017
<S**2>=0.000
     193 ->196         0.51363
     193 ->197        -0.24739
     193 ->198        -0.28241
     193 ->200        -0.15697
     193 ->206        -0.10558

 Excited State   3:      Singlet-A      1.6664 eV  744.04 nm  f=0.0005
<S**2>=0.000
     192 ->197         0.42726
     192 ->198        -0.28825
     192 ->199        -0.22106
     192 ->200         0.14788
     192 ->205        -0.15570
     192 ->207        -0.15801
     194 ->196         0.19174
     194 ->203         0.15200

 Excited State   4:      Singlet-A      1.7081 eV  725.85 nm  f=0.0022
<S**2>=0.000
     192 ->196        -0.11141
     192 ->197        -0.14534
     194 ->196         0.61471
     194 ->197         0.23219

 Excited State   5:      Singlet-A      1.7529 eV  707.32 nm  f=0.0075
<S**2>=0.000
```

```
     192 ->196         0.32683
     192 ->203         0.16545
     194 ->196         0.25757
     194 ->197        -0.31029
     194 ->198         0.24515
     194 ->199         0.17998
     194 ->200        -0.12750
     194 ->205         0.15010
     194 ->207         0.16121

 Excited State   6:      Singlet-A      1.8015 eV  688.24 nm  f=0.0013
<S**2>=0.000
     193 ->196         0.33097
     193 ->197         0.14950
     193 ->198         0.26423
     193 ->200         0.18781
     193 ->205         0.17602
     193 ->206         0.12233
     195 ->196         0.19374
     195 ->197         0.14240
     195 ->198         0.22308
     195 ->200         0.15490
     195 ->204        -0.16155
     195 ->208         0.11074

 Excited State   7:      Singlet-A      1.8279 eV  678.30 nm  f=0.0101
<S**2>=0.000
     192 ->196         0.59785
     194 ->197         0.21088
     194 ->198        -0.14324

 Excited State   8:      Singlet-A      1.8459 eV  671.68 nm  f=0.0130
<S**2>=0.000
     193 ->196         0.32960
     193 ->198         0.16226
     193 ->200         0.12494
     193 ->204        -0.17631
     195 ->196        -0.14701
     195 ->197        -0.21030
     195 ->198        -0.30285
     195 ->200        -0.18429
     195 ->205        -0.18865
     195 ->206        -0.15158
     195 ->208        -0.11545

 Excited State   9:      Singlet-A      2.3168 eV  535.16 nm  f=0.0043
<S**2>=0.000
     190 ->197        -0.11688
     192 ->202         0.11160
     192 ->203         0.38668
     192 ->207        -0.11233
     194 ->197         0.34446
```

```
     194 ->199         0.10577
     194 ->203         0.11858

 Excited State  10:      Singlet-A      2.3299 eV  532.14 nm  f=0.0029
<S**2>=0.000
     189 ->198         0.13767
     189 ->200         0.11100
     191 ->198         0.10185
     193 ->204        -0.34578
     193 ->205        -0.19571
     195 ->197         0.39416

 Excited State  11:      Singlet-A      2.3717 eV  522.77 nm  f=0.0002
<S**2>=0.000
     189 ->198        -0.10353
     192 ->197         0.20261
     193 ->197         0.20937
     194 ->197         0.13293
     194 ->203        -0.19693
     195 ->197         0.34302
     195 ->204         0.22848

 Excited State  12:      Singlet-A      2.3719 eV  522.71 nm  f=0.0003
<S**2>=0.000
     192 ->197         0.29246
     193 ->197        -0.13523
     194 ->197         0.21368
     194 ->202        -0.11278
     194 ->203        -0.28081
     194 ->207         0.13182
     195 ->197        -0.23343
     195 ->204        -0.15752

 Excited State  13:      Singlet-A      2.3870 eV  519.42 nm  f=0.0004
<S**2>=0.000
     188 ->197         0.12240
     190 ->197         0.12891
     192 ->197        -0.23686
     192 ->203        -0.12459
     194 ->197         0.31841
     194 ->198         0.15142
     194 ->199         0.15087
     194 ->203         0.20166

 Excited State  14:      Singlet-A      2.3997 eV  516.67 nm  f=0.0004
<S**2>=0.000
     193 ->197         0.41057
     193 ->205        -0.15901
     193 ->206        -0.10132
     195 ->197        -0.24993
     195 ->198         0.14527
     195 ->204         0.23478
```

```
     195 ->205         0.18228

 Excited State  15:      Singlet-A      2.4961 eV  496.72 nm  f=0.0003
<S**2>=0.000
     193 ->197         0.38964
     193 ->198        -0.31980
     193 ->204         0.11793
     195 ->198        -0.23761
     195 ->204        -0.27436
     195 ->205        -0.10926

 Excited State  16:      Singlet-A      2.5158 eV  492.82 nm  f=0.0149
<S**2>=0.000
     191 ->196         0.57992
     193 ->197         0.11809
     193 ->198        -0.13427
     193 ->204        -0.12763
     195 ->198         0.23943
     195 ->205        -0.11153

 Excited State  17:      Singlet-A      2.5492 eV  486.37 nm  f=0.0004
<S**2>=0.000
     188 ->203         0.12144
     190 ->203         0.15902
     192 ->197         0.31128
     192 ->198         0.33232
     192 ->199         0.14906
     192 ->200        -0.10330
     192 ->203        -0.10508
     194 ->198         0.21968
     194 ->203         0.27279
     194 ->207        -0.10615

 Excited State  18:      Singlet-A      2.5716 eV  482.12 nm  f=0.0068
<S**2>=0.000
     189 ->196         0.10582
     189 ->198        -0.10574
     191 ->196        -0.35355
     193 ->198        -0.20142
     195 ->198         0.39817
     195 ->200        -0.13291
     195 ->205        -0.14870
     195 ->206        -0.10396

 Excited State  19:      Singlet-A      2.5912 eV  478.47 nm  f=0.0046
<S**2>=0.000
     190 ->196        -0.22429
     190 ->197        -0.13481
     192 ->198        -0.15854
     192 ->203        -0.14024
     194 ->198         0.53102
     194 ->199        -0.11440
```

```
     194 ->203        -0.13424

 Excited State  20:      Singlet-A      2.6206 eV  473.11 nm  f=0.0054
<S**2>=0.000
     190 ->196         0.64435
     192 ->198        -0.13002
     194 ->198         0.17215
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   20
LETran=     370.
```

Theoretical calculation:

Calculation method: B3LYP/6-31G** for C, H, N, S with Gaussian 09.

BTD 2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.732727	0.385889	3.025903
2	7	0	2.973401	0.185978	1.973918
3	7	0	0.533511	0.783219	1.977448
4	6	0	2.480370	0.425927	0.757218
5	6	0	1.070293	0.768926	0.753833
6	6	0	0.393038	1.078780	-0.480606
7	6	0	1.165535	0.999554	-1.634258
8	1	0	0.702975	1.185449	-2.596055
9	6	0	2.535517	0.655617	-1.636056
10	1	0	3.058801	0.611031	-2.584632
11	6	0	3.234085	0.366835	-0.469392
12	6	0	4.602617	0.027561	-0.462687
13	6	0	5.785147	-0.263321	-0.447834
14	6	0	7.164295	-0.602375	-0.404687
15	6	0	7.924971	-0.675038	-1.590059
16	6	0	7.788143	-0.869156	0.832313
17	6	0	9.275120	-1.006450	-1.534302
18	6	0	9.138904	-1.199270	0.875855
19	6	0	9.884975	-1.269011	-0.304265
20	1	0	10.939161	-1.526854	-0.265450
21	1	0	9.612367	-1.402448	1.831688
22	1	0	7.200769	-0.811691	1.742759
23	1	0	9.854388	-1.059804	-2.451177
24	1	0	7.445471	-0.468896	-2.541409
25	6	0	-1.032292	1.431145	-0.512427

26	6	0	-1.959523	0.739744	0.446405
27	6	0	-1.569417	2.325517	-1.409347
28	6	0	-2.560149	1.486015	1.431698
29	6	0	-2.096573	-0.698669	0.258869
30	6	0	-2.985425	2.526159	-1.524347
31	6	0	-0.794867	3.129795	-2.308752
32	6	0	-2.247276	2.868448	1.638681
33	6	0	-3.505826	0.944827	2.358461
34	6	0	-1.821449	-1.393322	-0.979315
35	6	0	-2.481723	-1.703661	1.225859
36	7	0	-4.127950	2.694456	-1.666161
37	7	0	-0.211811	3.803138	-3.057566
38	7	0	-2.006492	3.988835	1.840529
39	7	0	-4.286830	0.534715	3.117987
40	6	0	-2.009802	-2.782334	-0.764381
41	1	0	-1.540605	-0.929409	-1.913783
42	6	0	-2.407330	-2.972133	0.594313
43	1	0	-2.762290	-1.523968	2.251688
44	1	0	-1.907078	-3.557397	-1.511014
45	1	0	-2.649394	-3.918131	1.058466
46	26	0	-3.783685	-1.740463	-0.383609
47	6	0	-5.616908	-2.708002	-0.286153
48	6	0	-5.715131	-1.420951	0.325551
49	6	0	-5.232932	-2.522601	-1.648857
50	1	0	-5.768538	-3.658970	0.206096
51	6	0	-5.396634	-0.442062	-0.661855
52	1	0	-5.945062	-1.220243	1.362599
53	6	0	-5.095052	-1.120173	-1.880239
54	1	0	-5.048034	-3.308107	-2.368932
55	1	0	-5.349925	0.627591	-0.513046
56	1	0	-4.795820	-0.650629	-2.806903

E(HF)= -2078.98809911 Hartree

BTD 2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.103305	0.260862	3.026985
2	7	0	2.351105	0.208271	1.965052
3	7	0	-0.113062	0.693689	2.011944
4	6	0	1.847191	0.530097	0.772286
5	6	0	0.422777	0.808889	0.793442
6	6	0	-0.269241	1.192271	-0.412417
7	6	0	0.508013	1.245874	-1.566266
8	1	0	0.037098	1.490164	-2.510630
9	6	0	1.890337	0.966212	-1.593152
10	1	0	2.414361	1.025494	-2.540496

11	6	0	2.604021	0.610807	-0.452189
12	6	0	3.984188	0.336473	-0.471004
13	6	0	5.180771	0.102734	-0.484335
14	6	0	6.570788	-0.169188	-0.482830
15	6	0	7.330774	-0.085664	-1.673230
16	6	0	7.229332	-0.527992	0.709506
17	6	0	8.687873	-0.350291	-1.664423
18	6	0	8.594403	-0.795329	0.724257
19	6	0	9.332786	-0.707433	-0.466081
20	1	0	9.071841	-1.067912	1.657574
21	1	0	6.656391	-0.594133	1.628602
22	1	0	9.280767	-0.288616	-2.570691
23	1	0	6.837288	0.190652	-2.599211
24	6	0	-1.706783	1.480501	-0.419859
25	6	0	-2.598333	0.692261	0.497978
26	6	0	-2.292821	2.401744	-1.259625
27	6	0	-3.233009	1.353229	1.522330
28	6	0	-2.670132	-0.738485	0.230797
29	6	0	-3.717166	2.536782	-1.361403
30	6	0	-1.565640	3.300143	-2.107395
31	6	0	-2.983084	2.734138	1.809751
32	6	0	-4.154033	0.718679	2.413933
33	6	0	-2.357577	-1.351921	-1.040608
34	6	0	-3.015948	-1.810502	1.138852
35	7	0	-4.867196	2.656243	-1.492987
36	7	0	-1.022454	4.049839	-2.812629
37	7	0	-2.793448	3.850112	2.079383
38	7	0	-4.916425	0.232536	3.147110
39	6	0	-2.485633	-2.757599	-0.902901
40	1	0	-2.090565	-0.826312	-1.946009
41	6	0	-2.881775	-3.038413	0.440416
42	1	0	-3.310988	-1.699609	2.170290
43	1	0	-2.345658	-3.485483	-1.689850
44	1	0	-3.085010	-4.017800	0.850810
45	26	0	-4.305928	-1.817900	-0.480177
46	6	0	-6.093560	-2.870845	-0.449757
47	6	0	-6.253399	-1.624887	0.230143
48	6	0	-5.711310	-2.594277	-1.797378
49	1	0	-6.205171	-3.853025	-0.010952
50	6	0	-5.974257	-0.580040	-0.699916
51	1	0	-6.498450	-1.492119	1.274738
52	6	0	-5.636296	-1.176496	-1.951140
53	1	0	-5.485980	-3.329966	-2.557400
54	1	0	-5.975140	0.480968	-0.493109
55	1	0	-5.354764	-0.644118	-2.848993
56	8	0	10.664217	-0.945438	-0.566784
57	6	0	11.384284	-1.308008	0.605433
58	1	0	12.418997	-1.444787	0.289582
59	1	0	11.338589	-0.518289	1.365151
60	1	0	11.009044	-2.245599	1.033341

E(HF)= - 2193.5139139 Hartree

BTD 2c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.057727	1.043086	2.979360
2	7	0	1.329991	0.837072	1.966689
3	7	0	-1.153342	1.206758	1.882742
4	6	0	0.839450	0.890025	0.726844
5	6	0	-0.595594	1.100432	0.673201
6	6	0	-1.276748	1.199481	-0.593588
7	6	0	-0.478439	1.063469	-1.724895
8	1	0	-0.938483	1.092543	-2.705201
9	6	0	0.916378	0.851076	-1.676923
10	1	0	1.458564	0.746726	-2.610052
11	6	0	1.617520	0.759694	-0.479185
12	6	0	3.008711	0.542579	-0.427466
13	6	0	4.211450	0.351801	-0.384718
14	6	0	-2.728763	1.397382	-0.676731
15	6	0	-3.598887	0.740404	0.356847
16	6	0	-3.338812	2.111007	-1.683411
17	6	0	-4.305432	1.540540	1.223097
18	6	0	-3.570962	-0.716262	0.370120
19	6	0	-4.765082	2.140264	-1.835430
20	6	0	-2.635374	2.877058	-2.670011
21	6	0	-4.149997	2.964347	1.246207
22	6	0	-5.214577	1.027169	2.200803
23	6	0	-3.162846	-1.539790	-0.746464
24	6	0	-3.885551	-1.614692	1.459520
25	7	0	-5.915591	2.161937	-2.007950
26	7	0	-2.111437	3.512515	-3.492139
27	7	0	-4.037421	4.121225	1.300962
28	7	0	-5.970089	0.638729	2.996692
29	6	0	-3.203574	-2.897674	-0.339340
30	1	0	-2.889810	-1.180650	-1.728091
31	6	0	-3.641255	-2.941258	1.019621
32	1	0	-4.233999	-1.328185	2.439122
33	1	0	-2.979339	-3.751814	-0.962869
34	1	0	-3.800454	-3.834847	1.607008
35	26	0	-5.098609	-2.029896	-0.167769

36	6	0	-6.811222	-3.183677	0.026265
37	6	0	-7.083875	-1.840144	0.427571
38	6	0	-6.388151	-3.161157	-1.337414
39	1	0	-6.872612	-4.059928	0.657033
40	6	0	-6.834022	-0.990149	-0.690478
41	1	0	-7.383492	-1.514553	1.413989
42	6	0	-6.401095	-1.803277	-1.779768
43	1	0	-6.080242	-4.017884	-1.921290
44	1	0	-6.916799	0.087662	-0.707840
45	1	0	-6.115714	-1.447768	-2.760063
46	6	0	5.610327	0.127289	-0.316798
47	6	0	6.258117	0.018399	0.931746
48	6	0	6.382438	0.006334	-1.490939
49	6	0	7.626361	-0.205725	0.996172
50	1	0	5.671315	0.101552	1.840633
51	6	0	7.750248	-0.216040	-1.413525
52	1	0	5.897356	0.099857	-2.457158
53	6	0	8.403300	-0.328551	-0.171456
54	1	0	8.100993	-0.314866	1.966223
55	1	0	8.330570	-0.277811	-2.328700
56	6	0	9.864275	-0.570164	-0.096236
57	6	0	10.643529	0.023388	0.912363
58	6	0	10.506794	-1.399947	-1.032007
59	6	0	12.016828	-0.204110	0.981712
60	1	0	10.173587	0.690348	1.629014
61	6	0	11.879774	-1.628472	-0.961131
62	1	0	9.920521	-1.891614	-1.802606
63	6	0	12.640841	-1.031237	0.045654
64	1	0	12.601713	0.272305	1.763226
65	1	0	12.354417	-2.280874	-1.688425
66	1	0	13.710829	-1.208790	0.100363

E(HF)= -2310.0476121 Hartree

BTD 2d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.640702	2.411671	2.429734
2	7	0	1.984774	1.748421	1.765734
3	7	0	-0.462028	2.033748	1.273395
4	6	0	1.606079	1.205288	0.607267
5	6	0	0.192846	1.364929	0.319788

6	6	0	-0.370642	0.850944	-0.903230
7	6	0	0.514708	0.195497	-1.752542
8	1	0	0.142254	-0.241481	-2.671288
9	6	0	1.888230	0.027773	-1.471427
10	1	0	2.502317	-0.508464	-2.186262
11	6	0	2.477948	0.514138	-0.309420
12	6	0	3.844922	0.345259	-0.013474
13	6	0	5.022571	0.208885	0.270750
14	6	0	-1.800673	0.982337	-1.208721
15	6	0	-2.782200	0.863026	-0.077730
16	6	0	-2.288895	1.151113	-2.484079
17	6	0	-3.530192	1.964365	0.263291
18	6	0	-2.806864	-0.429056	0.595932
19	6	0	-3.693798	1.102225	-2.770489
20	6	0	-1.466993	1.378052	-3.636661
21	6	0	-3.327531	3.243995	-0.347774
22	6	0	-4.535375	1.944175	1.280712
23	6	0	-2.346522	-1.668251	0.009917
24	6	0	-3.222074	-0.734533	1.947844
25	7	0	-4.823335	1.037399	-3.042053
26	7	0	-0.842644	1.563340	-4.601007
27	7	0	-3.180271	4.299571	-0.814711
28	7	0	-5.367300	1.953291	2.094892
29	6	0	-2.453458	-2.691763	0.985739
30	1	0	-1.999316	-1.794673	-1.005228
31	6	0	-2.984191	-2.114084	2.179440
32	1	0	-3.628989	-0.035078	2.661056
33	1	0	-2.211572	-3.734816	0.837117
34	1	0	-3.207613	-2.642889	3.095634
35	26	0	-4.330514	-1.852996	0.603222
36	6	0	-6.104148	-2.753418	1.191655
37	6	0	-6.343547	-1.386563	0.854041
38	6	0	-5.580563	-3.409975	0.036756
39	1	0	-6.253276	-3.202714	2.163975
40	6	0	-5.973807	-1.201831	-0.511853
41	1	0	-6.698001	-0.614688	1.522848
42	6	0	-5.499815	-2.448890	-1.016693
43	1	0	-5.269802	-4.444304	-0.019983
44	1	0	-6.004421	-0.273354	-1.065095
45	1	0	-5.125336	-2.625791	-2.015345
46	6	0	6.384502	0.073023	0.641925
47	6	0	7.306543	-0.678592	-0.170842
48	6	0	6.827809	0.678909	1.816545
49	6	0	6.918746	-1.318839	-1.374441
50	6	0	8.668658	-0.782479	0.259449
51	6	0	8.170603	0.569106	2.224133
52	1	0	6.119204	1.240627	2.416102
53	6	0	7.833302	-2.030506	-2.120367
54	1	0	5.886457	-1.238202	-1.699061
55	6	0	9.585994	-1.524235	-0.533273
56	6	0	9.071287	-0.145771	1.463375
57	1	0	8.490614	1.051424	3.142483

58	6	0	9.179657	-2.135708	-1.697291
59	1	0	7.520397	-2.514676	-3.040760
60	1	0	10.618116	-1.599629	-0.201417
61	1	0	10.108234	-0.232087	1.777091
62	1	0	9.889764	-2.699700	-2.294621

E(HF)=-2232.6322885 Hartree

BTD 2e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.368168	-2.684197	1.405716
2	7	0	1.631626	-1.731470	0.972566
3	7	0	-0.832809	-1.565092	1.420541
4	6	0	1.144197	-0.498569	0.824826
5	6	0	-0.280731	-0.397126	1.079440
6	6	0	-0.956818	0.873528	0.979376
7	6	0	-0.160803	1.955037	0.607564
8	1	0	-0.617951	2.928120	0.477038
9	6	0	1.222392	1.859827	0.352605
10	1	0	1.759084	2.755452	0.060327
11	6	0	1.920398	0.658820	0.452390
12	6	0	3.298548	0.541520	0.204518
13	6	0	4.492799	0.389146	-0.000462
14	6	0	-2.395251	1.004611	1.227234
15	6	0	-3.291837	-0.140749	0.848553
16	6	0	-2.980079	2.140066	1.744890
17	6	0	-3.938487	-0.825032	1.849810
18	6	0	-3.351145	-0.450353	-0.574114
19	6	0	-4.404330	2.294189	1.813221
20	6	0	-2.252857	3.265131	2.253970
21	6	0	-3.697187	-0.556215	3.236017
22	6	0	-4.861821	-1.889224	1.603214
23	6	0	-3.023870	0.480824	-1.630615
24	6	0	-3.686402	-1.705137	-1.211131
25	7	0	-5.554260	2.467184	1.858083
26	7	0	-1.708709	4.202341	2.678433
27	7	0	-3.513621	-0.373318	4.370444
28	7	0	-5.625716	-2.750880	1.432563
29	6	0	-3.132418	-0.195223	-2.872540
30	1	0	-2.758600	1.519449	-1.495324

31	6	0	-3.531427	-1.541747	-2.612057
32	1	0	-3.986982	-2.611743	-0.710299
33	1	0	-2.977116	0.244436	-3.847798
34	1	0	-3.722151	-2.302677	-3.356182
35	26	0	-4.968121	-0.218829	-1.869765
36	6	0	-6.745112	-0.676979	-2.837647
37	6	0	-6.919643	-0.791307	-1.424537
38	6	0	-6.360934	0.666971	-3.129370
39	1	0	-6.847149	-1.477898	-3.557240
40	6	0	-6.648233	0.483899	-0.845634
41	1	0	-7.167210	-1.692265	-0.880607
42	6	0	-6.299767	1.384365	-1.895933
43	1	0	-6.125636	1.061909	-4.108239
44	1	0	-6.660099	0.726177	0.207821
45	1	0	-6.020112	2.421317	-1.772181
46	6	0	5.867715	0.169243	-0.232977
47	6	0	6.720457	1.261967	-0.568371
48	6	0	6.387794	-1.156204	-0.130164
49	6	0	6.244991	2.600485	-0.675565
50	6	0	8.118786	1.012376	-0.807651
51	6	0	7.790032	-1.378009	-0.376158
52	6	0	5.572211	-2.275570	0.207118
53	6	0	7.095797	3.628425	-0.999132
54	1	0	5.193280	2.793699	-0.493494
55	6	0	8.971934	2.108877	-1.143101
56	6	0	8.612735	-0.294146	-0.706945
57	6	0	8.311273	-2.705087	-0.276457
58	1	0	4.515407	-2.118943	0.397732
59	6	0	6.112525	-3.535350	0.293367
60	6	0	8.476811	3.382934	-1.236778
61	1	0	6.713271	4.642089	-1.074205
62	1	0	10.024925	1.908105	-1.321468
63	1	0	9.669836	-0.472606	-0.890589
64	6	0	7.496323	-3.757026	0.049020
65	1	0	9.370314	-2.859757	-0.464608
66	1	0	5.475811	-4.376099	0.552758
67	1	0	9.133469	4.209345	-1.491193
68	1	0	7.901105	-4.761883	0.122994

E(HF)= -2386.2721504 Hartree

BTD 2f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.621648	-2.687974	2.919183

2	7	0	-1.086791	-2.564675	2.374667
3	7	0	-3.246039	-1.294008	2.328539
4	6	0	-1.005467	-1.409777	1.710548
5	6	0	-2.258888	-0.679607	1.669539
6	6	0	-2.359854	0.568896	0.963390
7	6	0	-1.217639	0.994837	0.304606
8	1	0	-1.243588	1.906508	-0.279845
9	6	0	-0.001494	0.268712	0.324734
10	1	0	0.836407	0.668269	-0.237209
11	6	0	0.157180	-0.910845	1.031875
12	6	0	-3.627807	1.322781	0.901408
13	6	0	-4.906153	0.553535	0.745768
14	6	0	-3.671174	2.693900	0.926567
15	6	0	-5.833736	0.613122	1.760207
16	6	0	-5.016715	-0.240716	-0.468985
17	6	0	-4.888283	3.421394	0.701877
18	6	0	-2.527006	3.528036	1.160000
19	6	0	-5.573105	1.287722	2.996315
20	6	0	-7.113235	-0.021518	1.688134
21	6	0	-4.259708	-0.004271	-1.679414
22	6	0	-5.838069	-1.407411	-0.711424
23	7	0	-5.847061	4.044158	0.488221
24	7	0	-1.627605	4.243339	1.340387
25	7	0	-5.385933	1.819594	4.014258
26	7	0	-8.167698	-0.513321	1.653104
27	6	0	-4.589631	-1.014835	-2.617380
28	1	0	-3.574332	0.814004	-1.846174
29	6	0	-5.553626	-1.880305	-2.017425
30	1	0	-6.532299	-1.852511	-0.016495
31	1	0	-4.204627	-1.093818	-3.624212
32	1	0	-6.019354	-2.734361	-2.488965
33	26	0	-6.293563	0.077514	-2.083092
34	6	0	-8.035154	0.005758	-3.207220
35	6	0	-8.315558	0.545039	-1.914621
36	6	0	-7.076815	0.852173	-3.842582
37	1	0	-8.444606	-0.907282	-3.617261
38	6	0	-7.533535	1.727837	-1.755651
39	1	0	-8.968515	0.114249	-1.168468
40	6	0	-6.765666	1.917008	-2.943279
41	1	0	-6.638501	0.694337	-4.818521
42	1	0	-7.496984	2.357786	-0.877323
43	1	0	-6.058221	2.715355	-3.119344
44	6	0	1.450558	-1.622294	1.013844
45	6	0	2.187530	-1.689010	-0.294248
46	6	0	2.017314	-2.177582	2.131677
47	6	0	3.503161	-1.066770	-0.364805
48	6	0	1.539517	-2.314914	-1.346414
49	6	0	3.225123	-2.950445	2.064703
50	6	0	1.510882	-1.991245	3.459811
51	6	0	3.830454	0.008093	0.498243
52	6	0	4.507318	-1.490248	-1.267875
53	6	0	0.290772	-2.989873	-1.162429

54	6	0	2.014335	-2.322941	-2.694974
55	7	0	4.191862	-3.597025	2.052484
56	7	0	1.179791	-1.812534	4.560172
57	6	0	5.058175	0.638234	0.449116
58	1	0	3.102285	0.360448	1.221750
59	6	0	5.746267	-0.882621	-1.308385
60	1	0	4.326977	-2.326565	-1.930882
61	7	0	-0.729893	-3.536781	-1.036890
62	7	0	2.347980	-2.336587	-3.810695
63	6	0	6.056607	0.203675	-0.454829
64	1	0	5.265673	1.457909	1.125884
65	1	0	6.491538	-1.246051	-2.004947
66	7	0	7.304841	0.813754	-0.494845
67	6	0	8.457804	0.116579	-0.986072
68	6	0	7.492448	2.152657	-0.018707
69	6	0	9.275588	0.718432	-1.950896
70	6	0	8.789054	-1.149284	-0.483287
71	6	0	8.505333	2.428176	0.908927
72	6	0	6.687130	3.194486	-0.499395
73	6	0	10.412891	0.055359	-2.409681
74	1	0	9.016169	1.699996	-2.333987
75	6	0	9.920694	-1.810923	-0.958518
76	1	0	8.161587	-1.607549	0.274589
77	6	0	8.705692	3.734716	1.352165
78	1	0	9.128445	1.619020	1.275587
79	6	0	6.885303	4.495900	-0.039807
80	1	0	5.914274	2.980046	-1.230707
81	6	0	10.737519	-1.211600	-1.919895
82	1	0	11.041051	0.527687	-3.159067
83	1	0	10.170029	-2.791717	-0.564809
84	6	0	7.895327	4.771588	0.884595
85	1	0	9.491847	3.939896	2.072620
86	1	0	6.257055	5.297549	-0.416558
87	1	0	11.621414	-1.727026	-2.282732
88	1	0	8.051165	5.786979	1.235634

E(HF)= - 3044.0076903 Hartree

BTD 2g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.165395	1.532582	-3.200047
2	7	0	-1.132480	1.526429	-2.202156

3	7	0	1.371602	1.556538	-2.093548
4	6	0	-0.656250	1.562829	-0.953683
5	6	0	0.792923	1.564305	-0.888671
6	6	0	1.469710	1.575616	0.380542
7	6	0	0.663814	1.550649	1.505319
8	1	0	1.117082	1.528096	2.489227
9	6	0	-0.754696	1.531941	1.440356
10	1	0	-1.304538	1.519769	2.375271
11	6	0	-1.444627	1.565787	0.244482
12	6	0	2.945433	1.571097	0.469332
13	6	0	3.707959	0.674782	-0.461612
14	6	0	3.628392	2.305988	1.402658
15	6	0	4.518944	1.250391	-1.410556
16	6	0	3.463396	-0.751876	-0.293616
17	6	0	5.048183	2.178270	1.576267
18	6	0	3.008209	3.243914	2.294322
19	6	0	4.585318	2.668525	-1.599761
20	6	0	5.331929	0.490457	-2.309313
21	6	0	2.972062	-1.364536	0.921415
22	6	0	3.620095	-1.814005	-1.264060
23	7	0	6.190988	2.071812	1.763622
24	7	0	2.549675	4.008035	3.041643
25	7	0	4.654826	3.815603	-1.781761
26	7	0	6.011316	-0.102698	-3.045102
27	6	0	2.810939	-2.754220	0.687984
28	1	0	2.781866	-0.853750	1.854384
29	6	0	3.202041	-3.027052	-0.658486
30	1	0	3.979066	-1.703187	-2.275065
31	1	0	2.487389	-3.484210	1.416662
32	1	0	3.216662	-3.999681	-1.130376
33	26	0	4.803703	-2.191044	0.393313
34	6	0	6.333825	-3.591809	0.342699
35	6	0	6.781401	-2.364257	-0.234092
36	6	0	5.951463	-3.333221	1.693858
37	1	0	6.260540	-4.543037	-0.166559
38	6	0	6.679923	-1.350131	0.763902
39	1	0	7.098128	-2.214732	-1.256637
40	6	0	6.164702	-1.945373	1.953645
41	1	0	5.542587	-4.055316	2.387468
42	1	0	6.915462	-0.302394	0.638921
43	1	0	5.955357	-1.428838	2.880036
44	6	0	-2.926806	1.575845	0.217432
45	6	0	-3.611987	0.494063	0.999176
46	6	0	-3.646928	2.499916	-0.481934
47	6	0	-4.213377	0.835656	2.190828
48	6	0	-3.488036	-0.843938	0.444618
49	6	0	-3.043731	3.600479	-1.177119
50	6	0	-5.080175	2.448734	-0.548125
51	6	0	-4.171183	2.173470	2.702142
52	6	0	-4.916495	-0.101656	3.011845
53	6	0	-3.156682	-1.123541	-0.937163
54	6	0	-3.637970	-2.123348	1.108851

55	7	0	-2.586806	4.515224	-1.729857
56	7	0	-6.239392	2.415497	-0.631898
57	7	0	-4.126935	3.247740	3.148033
58	7	0	-5.500537	-0.845218	3.690594
59	6	0	-3.077204	-2.529232	-1.098138
60	1	0	-3.001391	-0.384248	-1.710450
61	6	0	-3.364149	-3.141519	0.160033
62	1	0	-3.897850	-2.279993	2.143679
63	1	0	-2.875106	-3.047565	-2.024997
64	1	0	-3.409344	-4.204373	0.353268
65	26	0	-4.991460	-1.978149	-0.447081
66	6	0	-6.593494	-3.285116	-0.605869
67	6	0	-6.905860	-2.248122	0.325802
68	6	0	-6.330207	-2.678481	-1.871272
69	1	0	-6.529096	-4.341311	-0.382848
70	6	0	-6.840919	-1.003815	-0.367839
71	1	0	-7.116392	-2.375696	1.378539
72	6	0	-6.480704	-1.266389	-1.722914
73	1	0	-6.035294	-3.195750	-2.774075
74	1	0	-6.998854	-0.023091	0.058393
75	1	0	-6.331800	-0.522218	-2.492830

E(HF)= - 2804.8308431 Hartree