Supporting Information

5,7-Bis(2'-arylethenyl)-6*H*-1,4-diazepine-2,3-dicarbonitriles: synthesis, experimental and theoretical evaluation of effect of substituents at 5,6,7-positions on the molecular configuration and spectral properties

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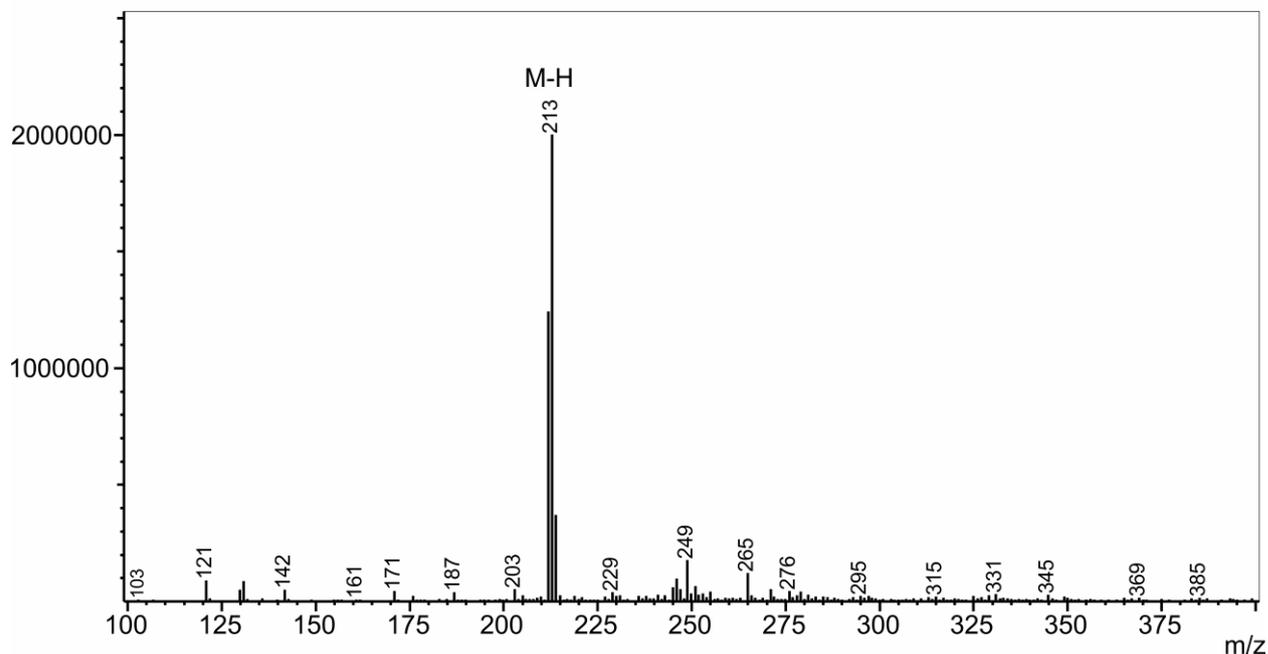
Fig. S1 ESI mass spectrum of **4**.

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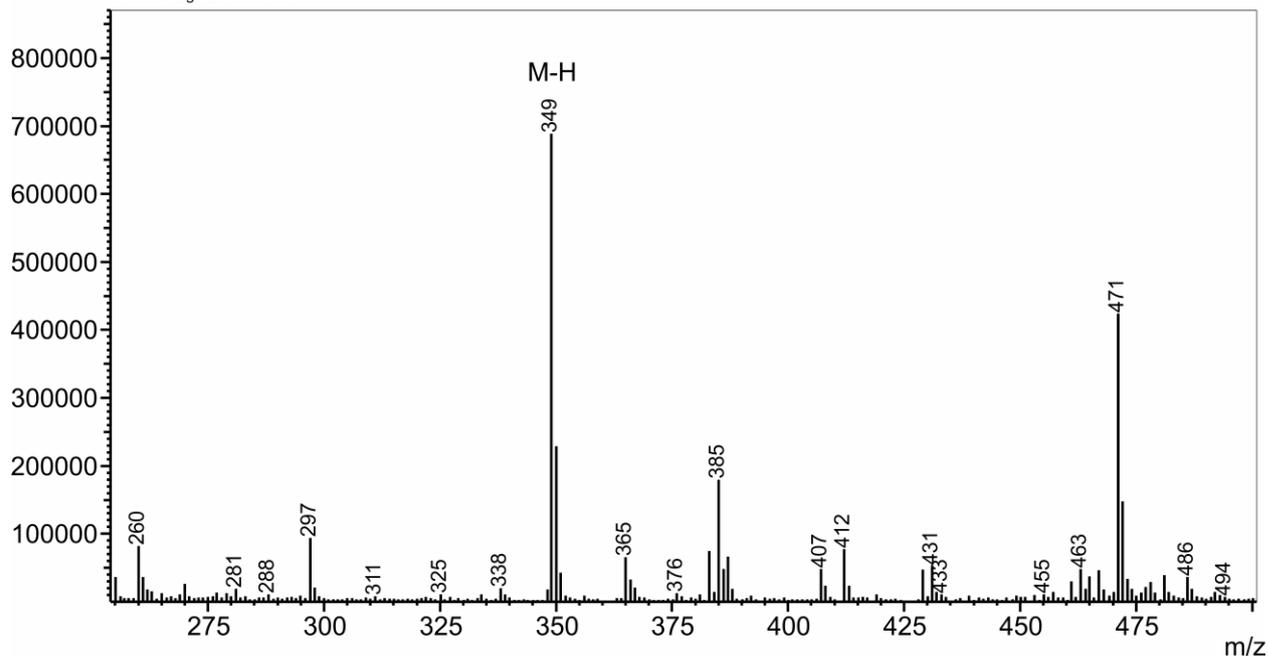
Fig. S2 ESI mass spectrum of **5a**.

==== Shimadzu LabSoluti ons Data Report ====

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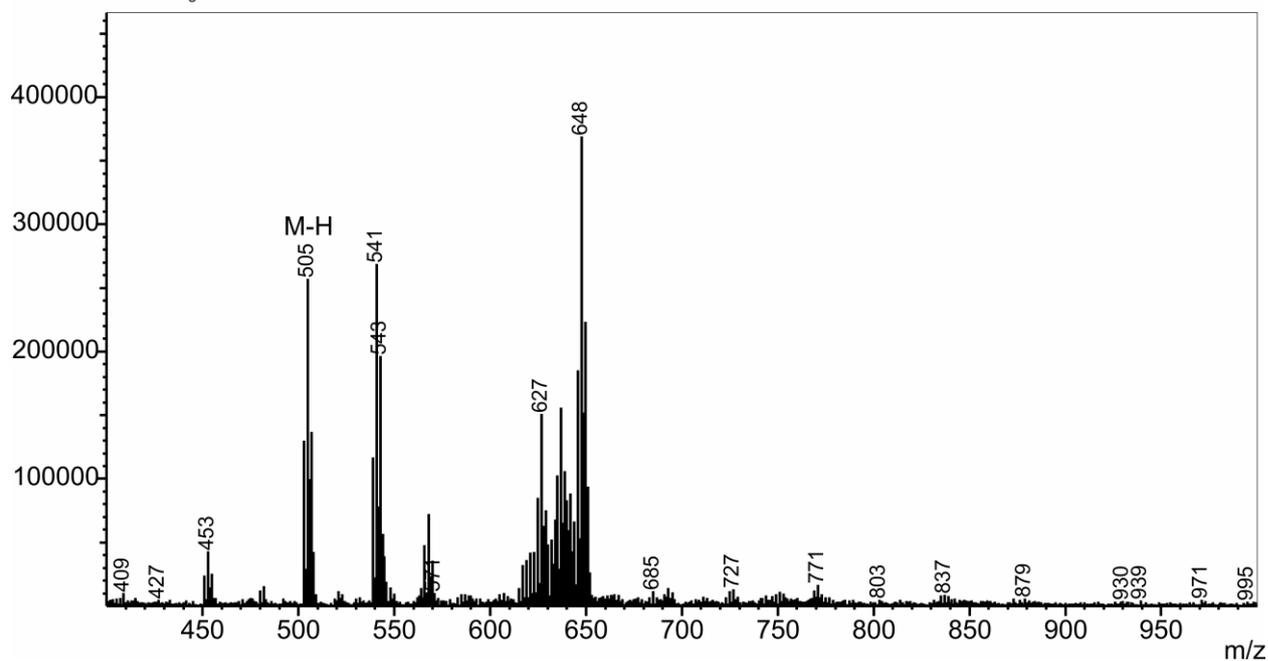
Fig. S3 ESI mass spectrum of 5b.

==== Shimadzu LabSoluti ons Data Report ====

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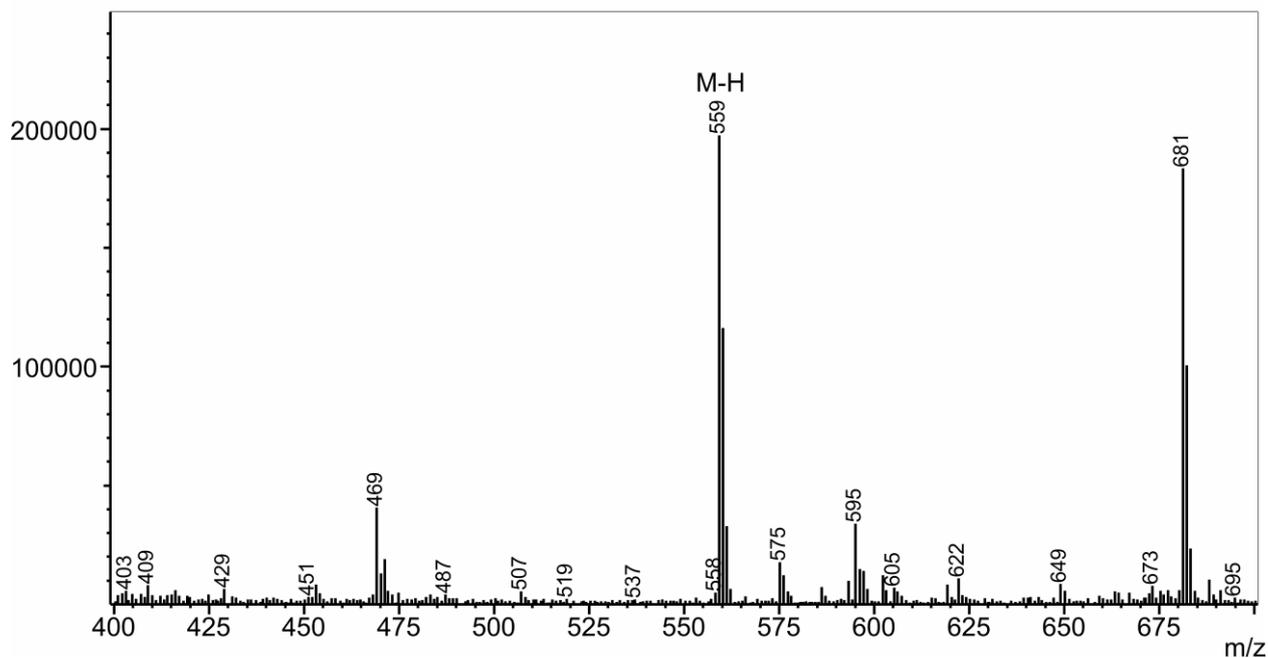
Fig. S4 ESI mass spectrum of 5c.

==== Shimadzu LabSoluti ons Data Report ====

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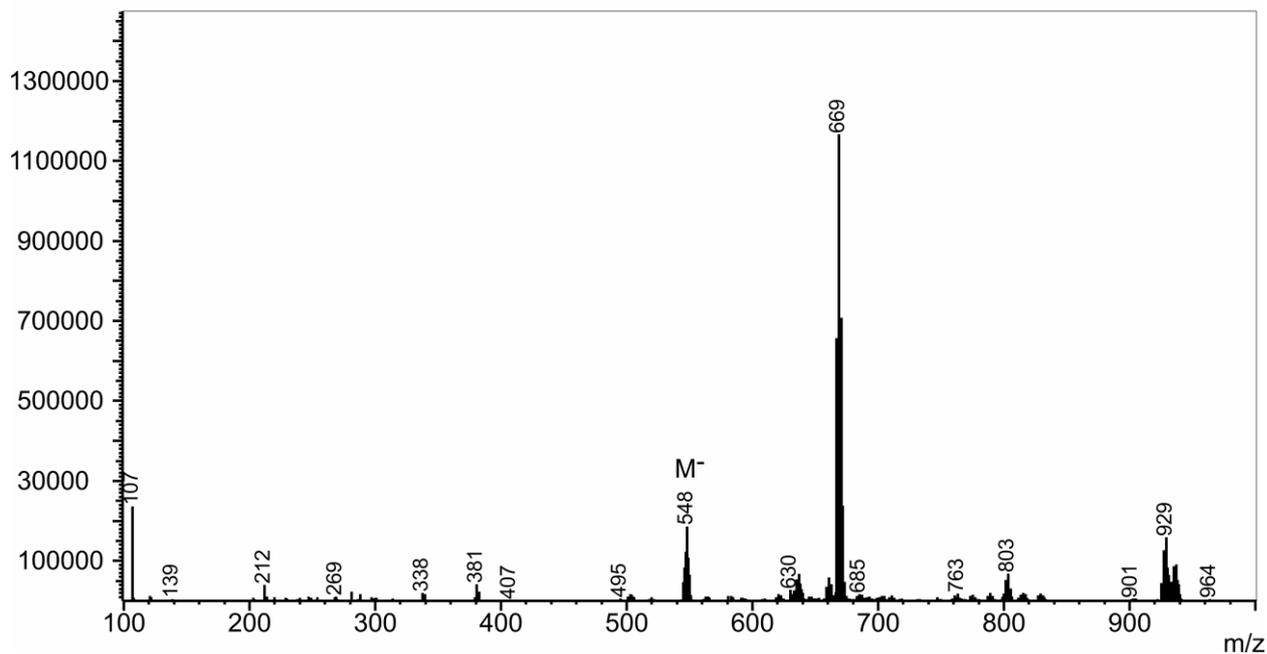
Fig. S5 ESI mass spectrum of **6b**.

==== Shimadzu LabSoluti ons Data Report ====

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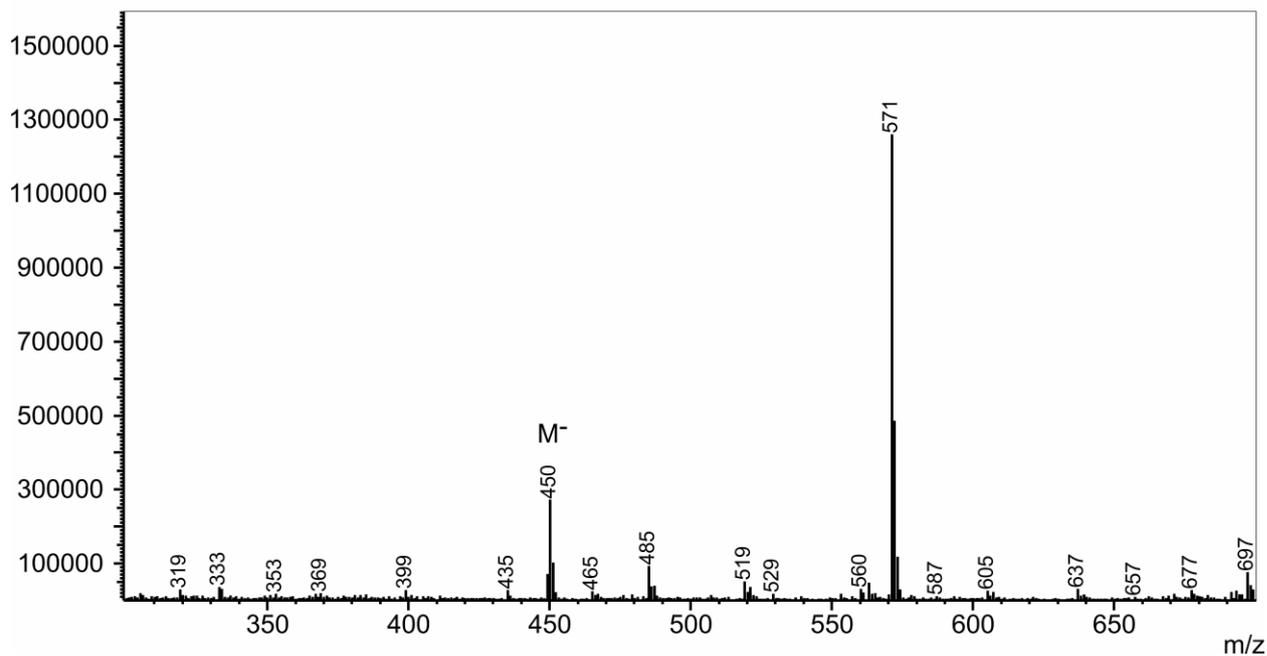
Fig. S6 ESI mass spectrum of **6d**.
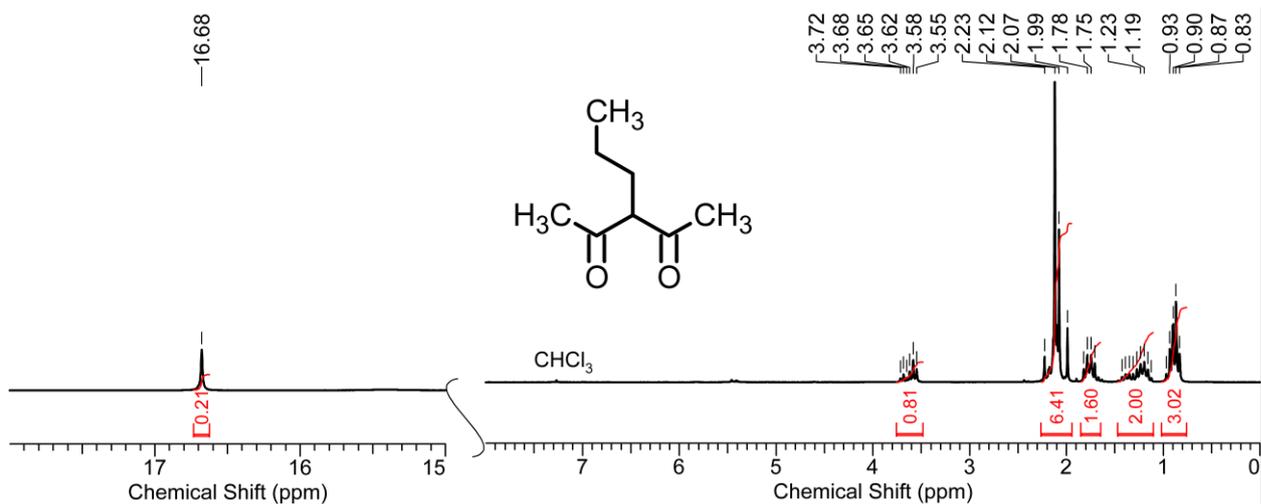
Fig. S7 ^{1}H NMR spectrum of **2** (CDCl$_3$, 293 K).
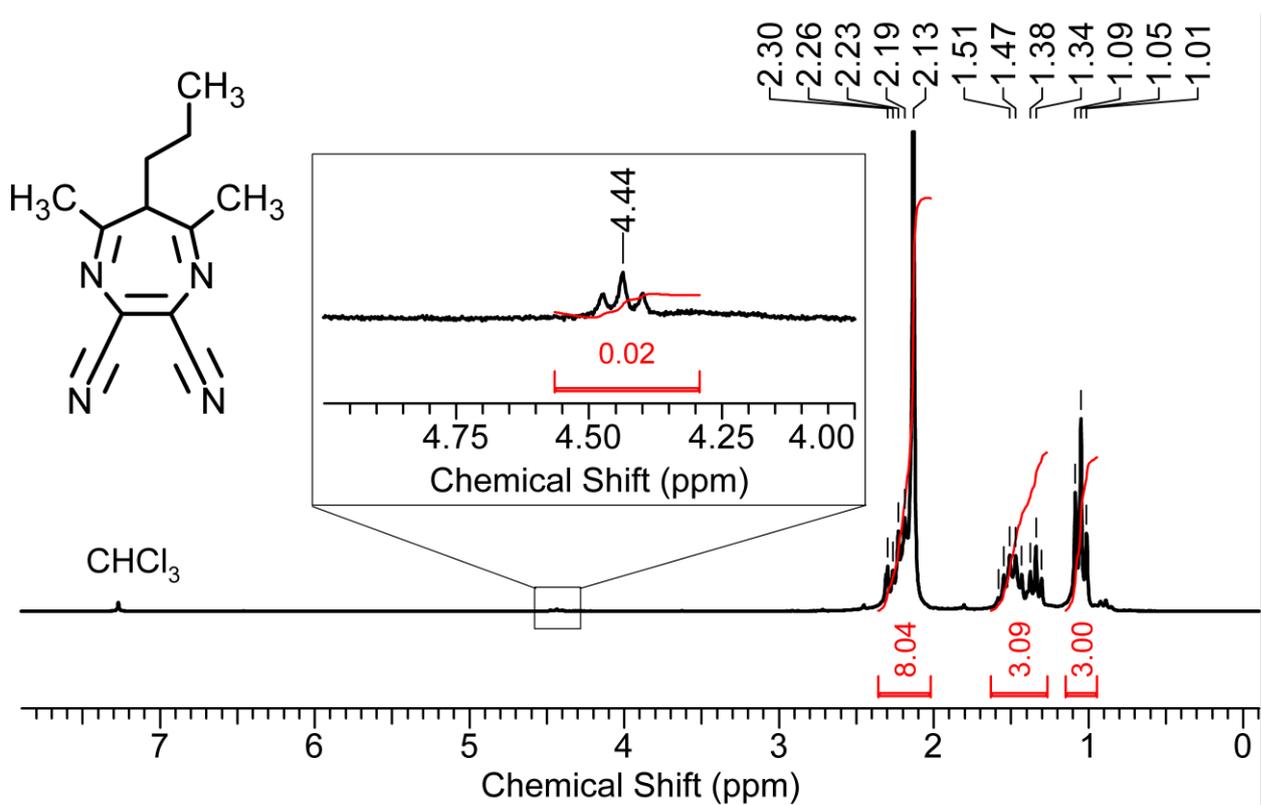
Fig. S8 ^{1}H NMR spectrum of **4** (CDCl$_3$, 293 K).
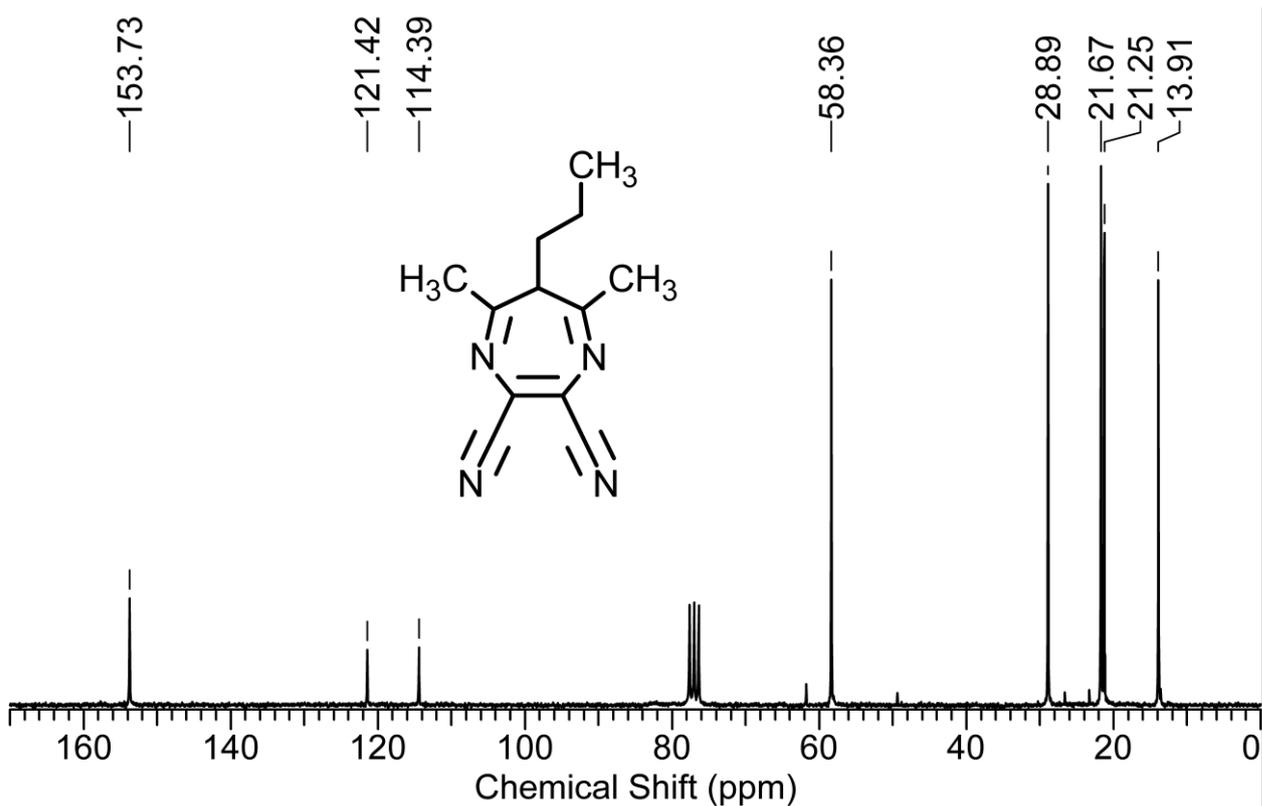
Fig. S9 ^{13}C NMR spectrum of **4** (CDCl$_3$, 293 K).
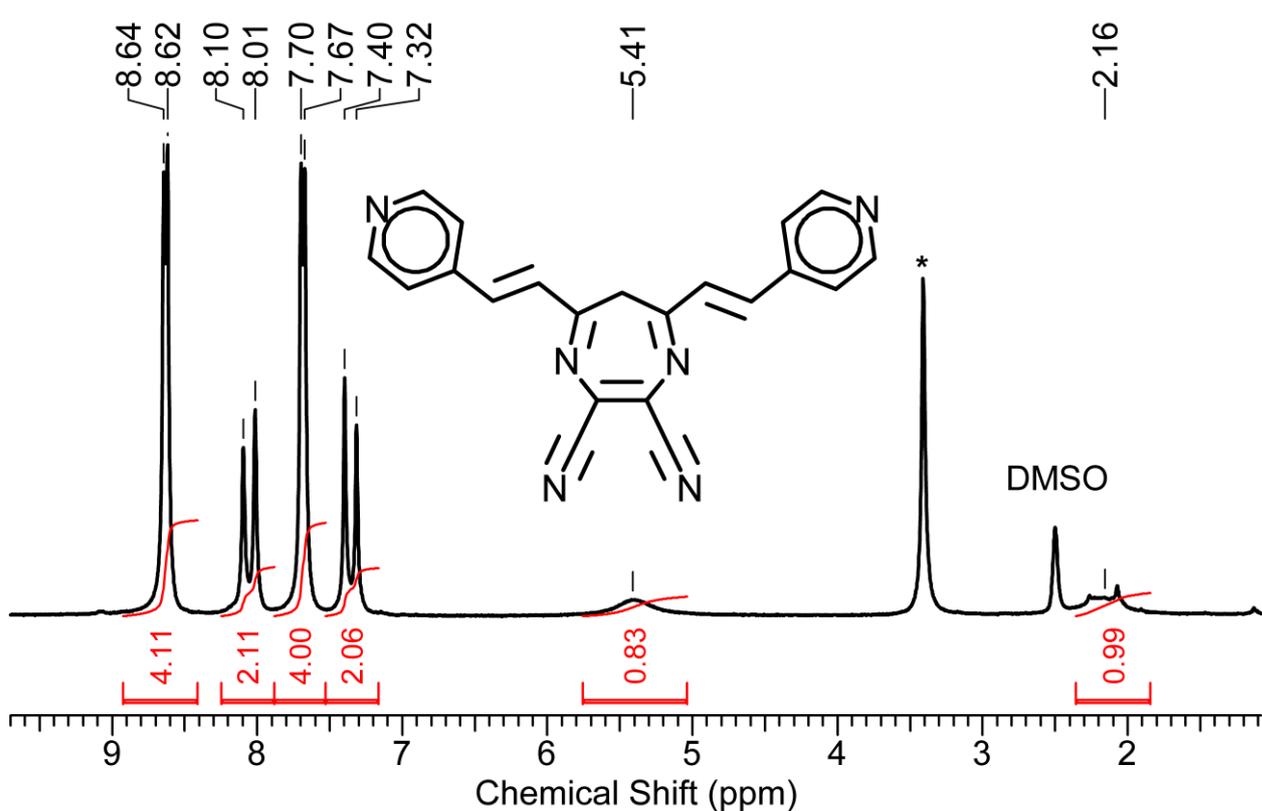
Fig. S10 ^{1}H NMR spectrum of **5a** (DMSO-d_6, 293 K).
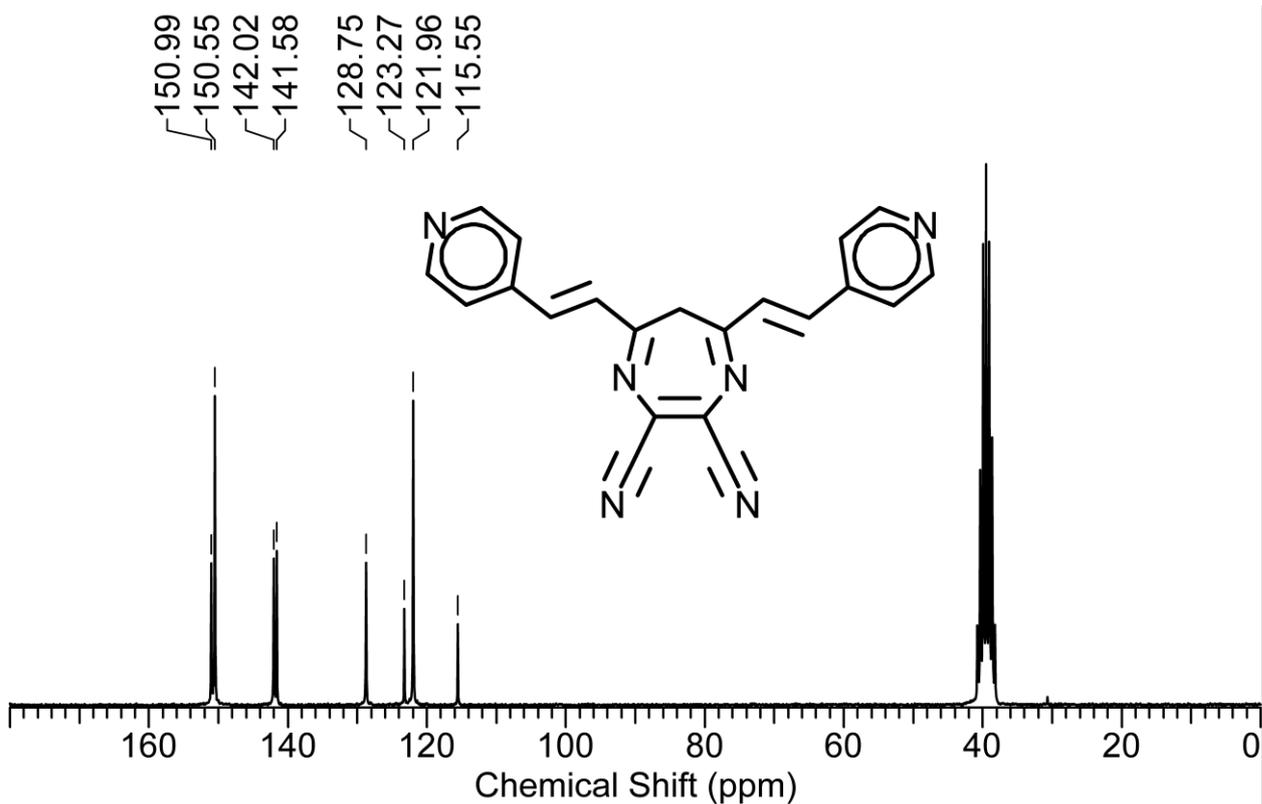
Fig. S11 ^{13}C NMR spectrum of **5a** (DMSO-d_6, 293 K).
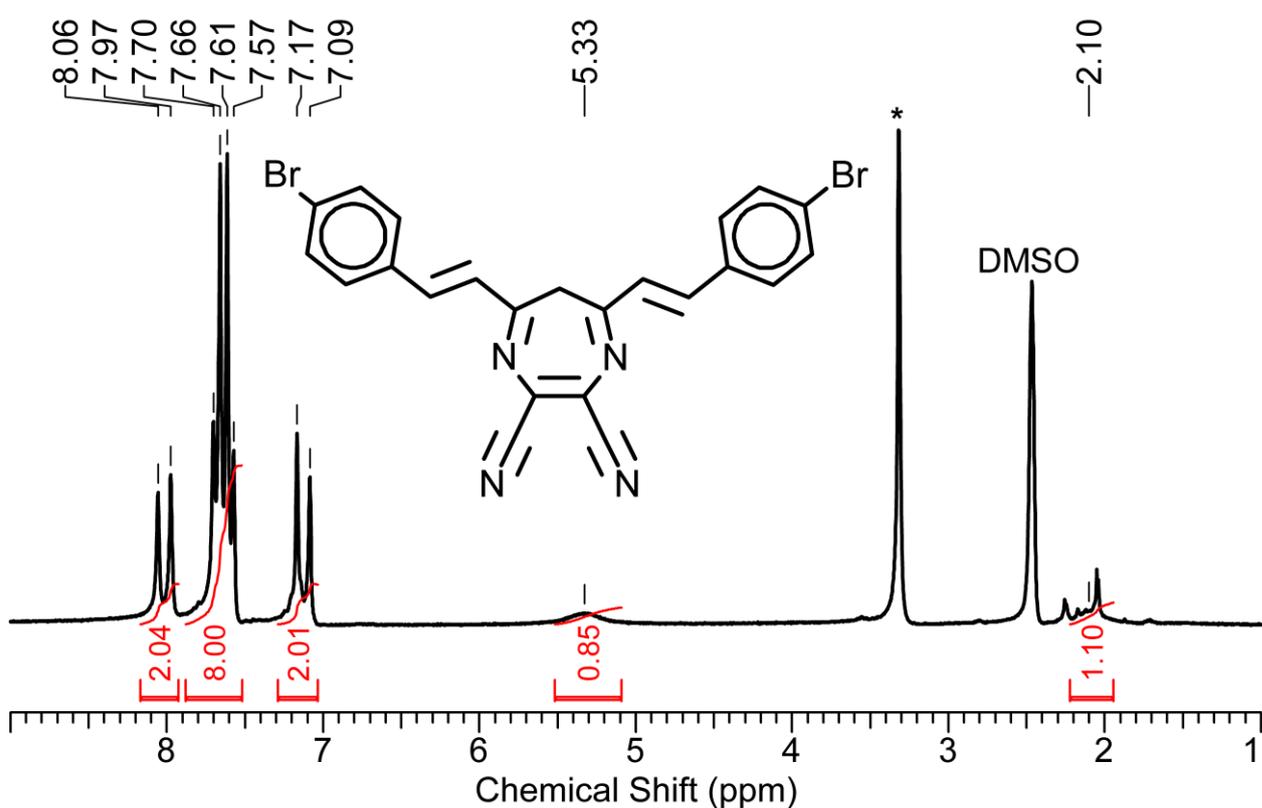
Fig. S12 ^{1}H NMR spectrum of **5b** (DMSO-d_6, 293 K).
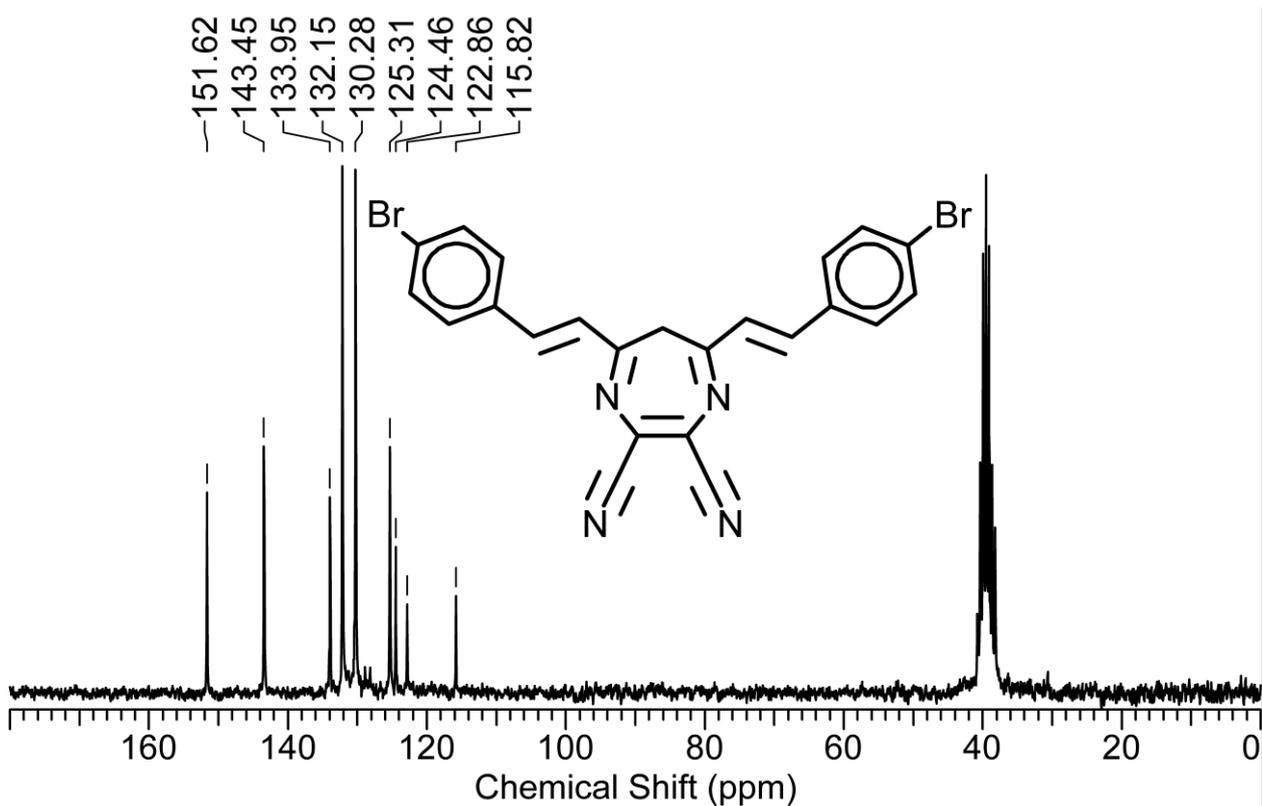
Fig. S13 ^{13}C NMR spectrum of **5b** (DMSO-d_6, 293 K).
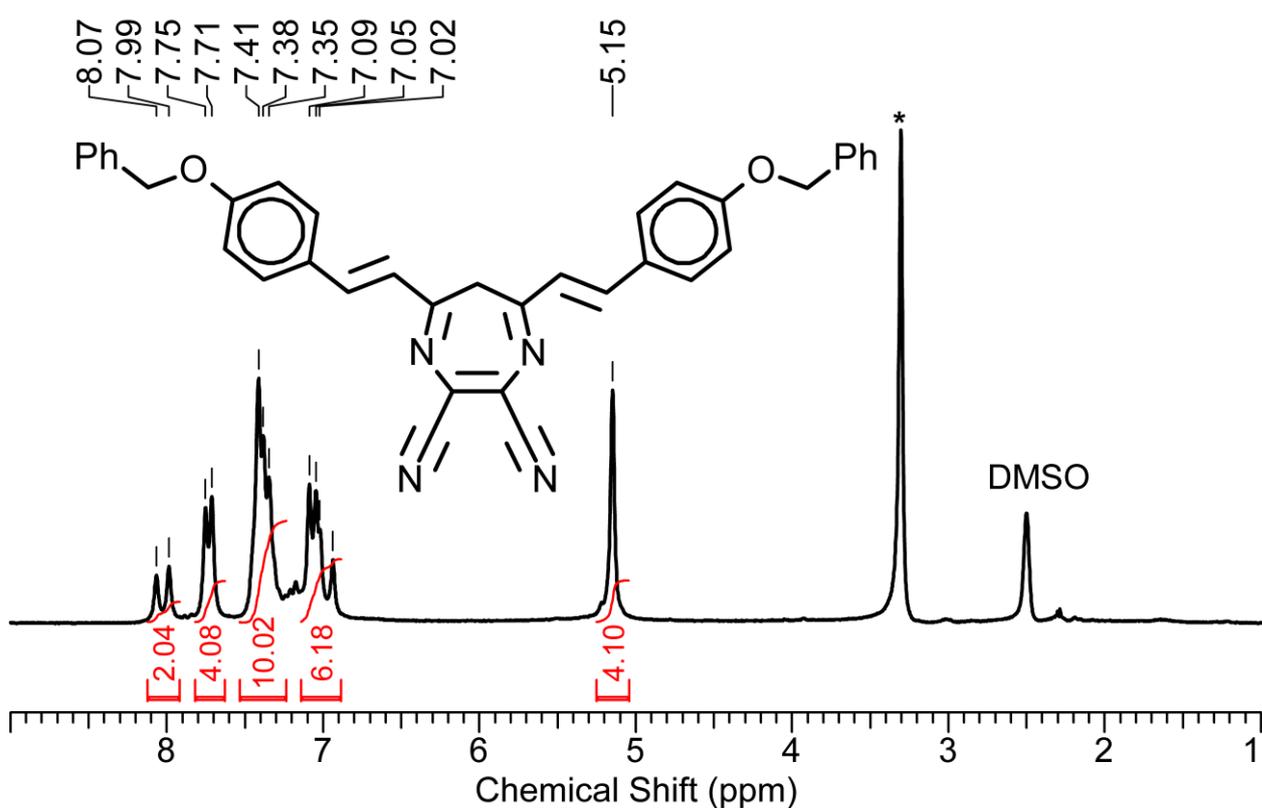
Fig. S14 ^{1}H NMR spectrum of **5c** (DMSO-d_6, 293 K).
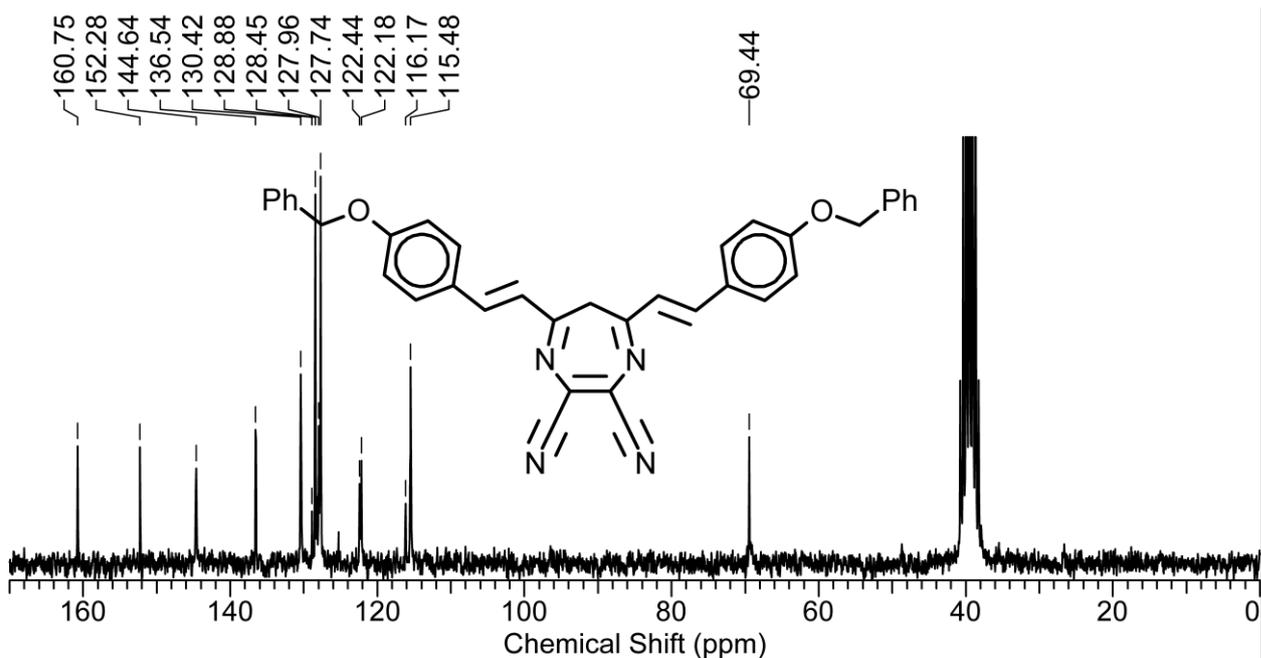
Fig. S15 ^{13}C NMR spectrum of **5c** (DMSO-d_6, 293 K).
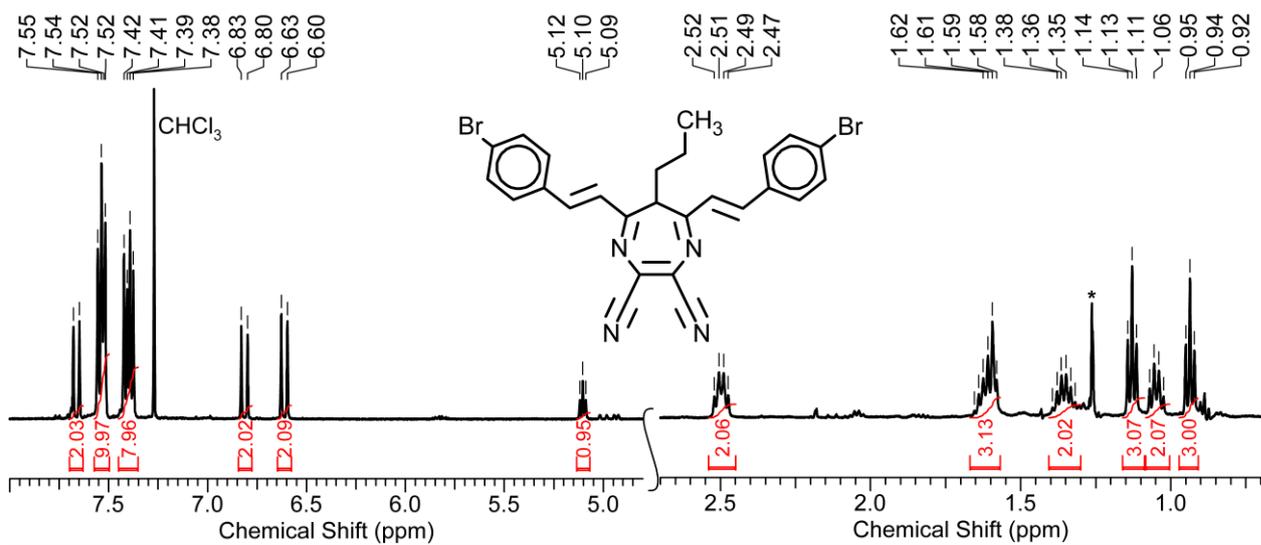
Fig. S16 ^{1}H NMR spectrum of **6b** (CDCl$_3$, 293 K).
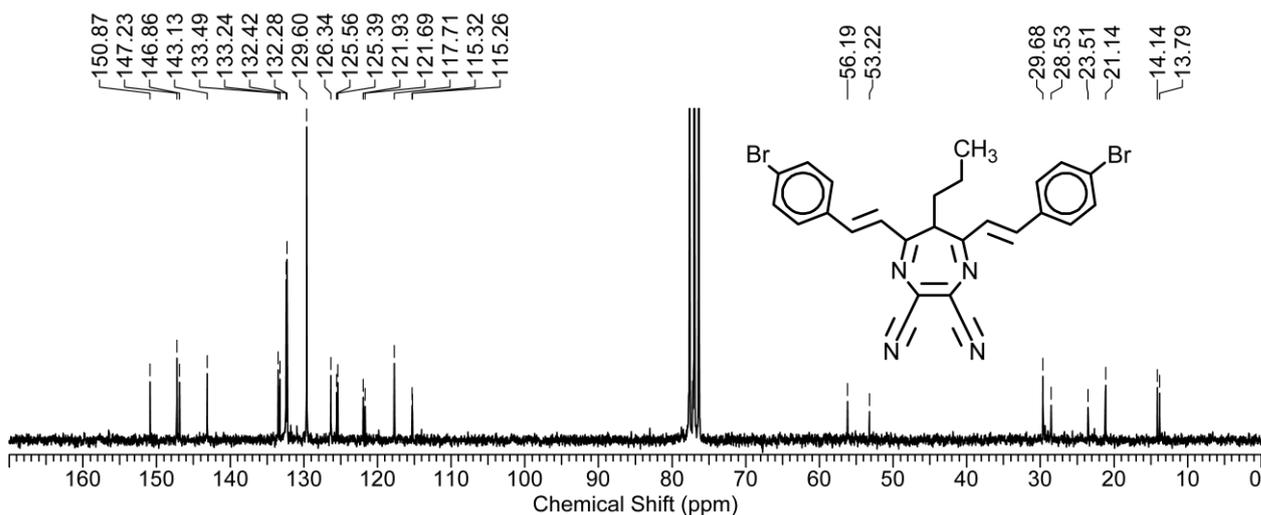
Fig. S17 ^{13}C NMR spectrum of **6b** (CDCl$_3$, 293 K).
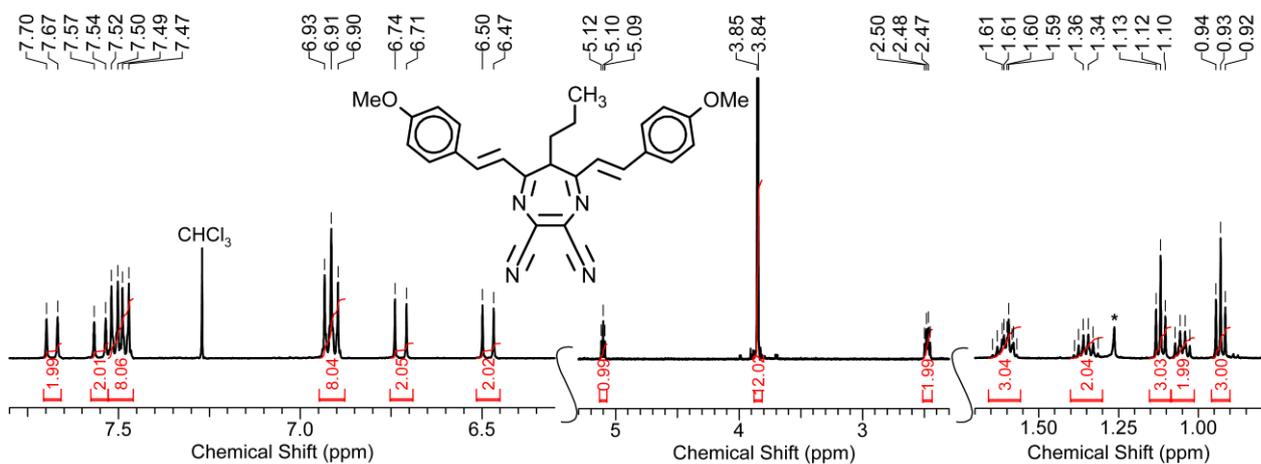
Fig. S18 ^{1}H NMR spectrum of **6d** (CDCl$_3$, 293 K).
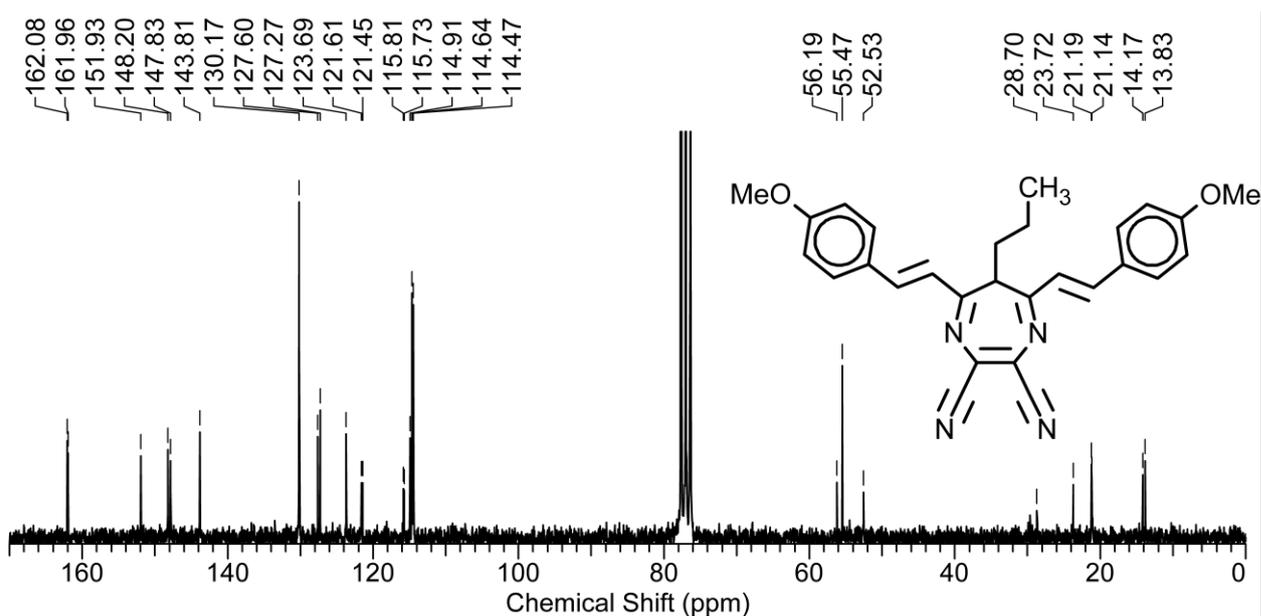
Fig. S19 ^{13}C NMR spectrum of **6d** (CDCl$_3$, 293 K).
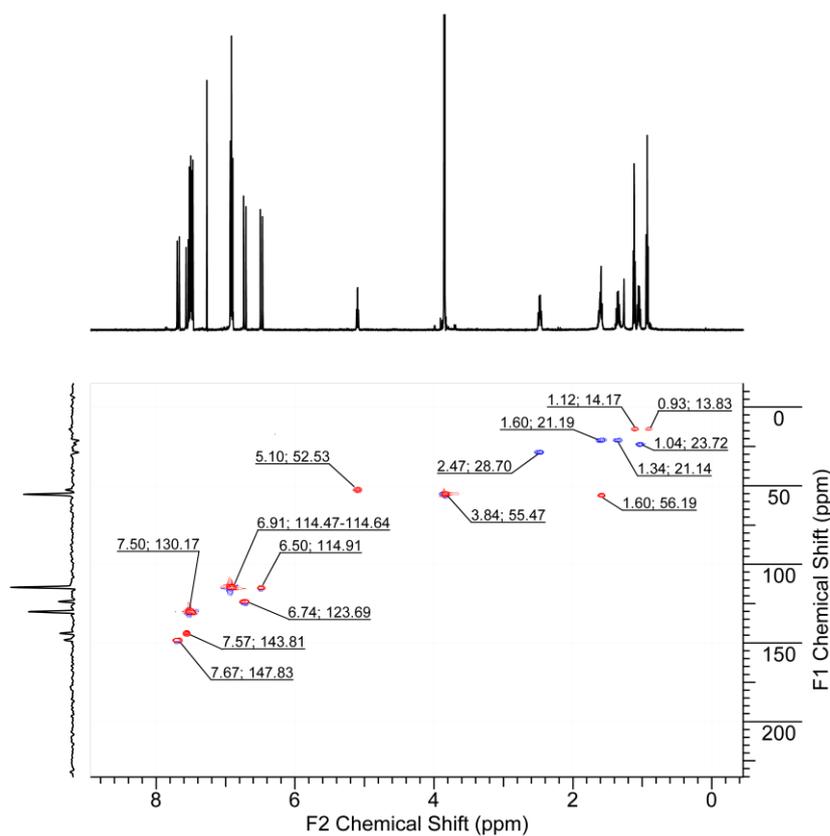
Fig. S20 ^{1}H-^{13}C HSQC NMR spectrum of **6d** (CDCl$_3$, 293 K).
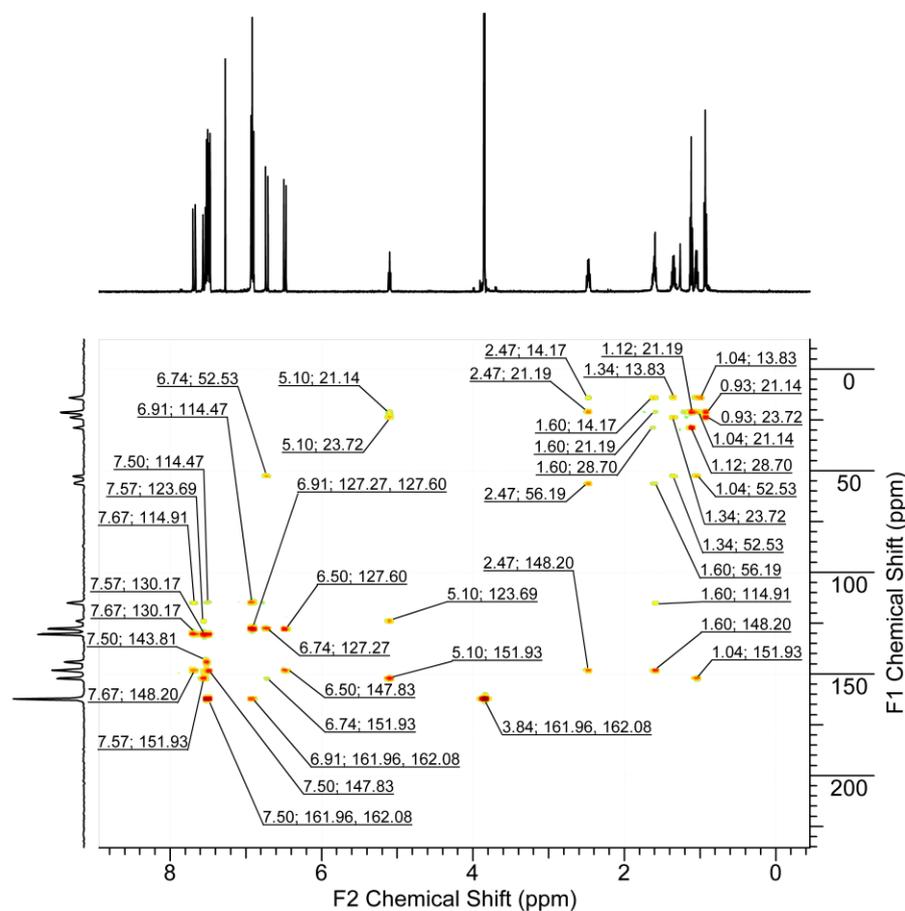
Fig. S21 ^{1}H-^{13}C HMBC NMR spectrum of **6d** (CDCl$_3$, 293 K).

Table S1 Proton-carbon connectivities from ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC spectra for **6d**[§]

Proton (ppm)		^3J (Hz)	carbon atom attached	α-carbon atom	β-carbon atom
^{Pr}CH$_3$* 0.94-0.92		t, 7.4	13.84	21.14	23.72
^{α}CH$_2$* 1.07-1.03		q, 7.7	23.72	21.14; 52.53	13.84; 151.93
^{Pr}CH$_3$** 1.13-1.10		t, 7.3	14.17	21.19	28.70
^{β}CH$_2$* 1.39-1.31		-	21.14	13.83; 23.72	52.53
^{β}CH$_2$**	1.65-1.57	-	21.19	14.17; 28.70	56.19
6-H**		-	56.19	28.70; 148.20	21.19; 114.91
^{α}CH$_2$** 2.50-2.45		q, 7.7	28.70	21.19; 56.19	14.17; 148.20
OCH$_3$*,** 3.85-3,84		s	55.47	-	161.96, 162.08
6-H* 5.12-5.09		t, 7.5	52.53	23.72; 151.93	21.14; 123.69
1'-H** 6.50-6.47		d, 15.3	114.91	147.83	127.60
1'-H* 6.74-6.71		d, 15.9	123.69	151.93	52.53; 127.27
m-Ar*,** 6.93-6.90		-	114.47, 114.64	161.96,162.08	127.27, 127.60
o-Ar*,** 7.52-7.47		-	130.17	114.47, 114.64	143.81, 147.83; 161.96, 162.08
2'-H* 7.57-7.54		d, 15.9	143.81	123.69	151.93; 130.17
2'-H** 7.70-7.67		d, 15.3	147.83	114.91	148.20; 130.17

[§]Proton signals of conformers with either axial or equatorial position of the 6-propyl group are designated as * and **, respectively.
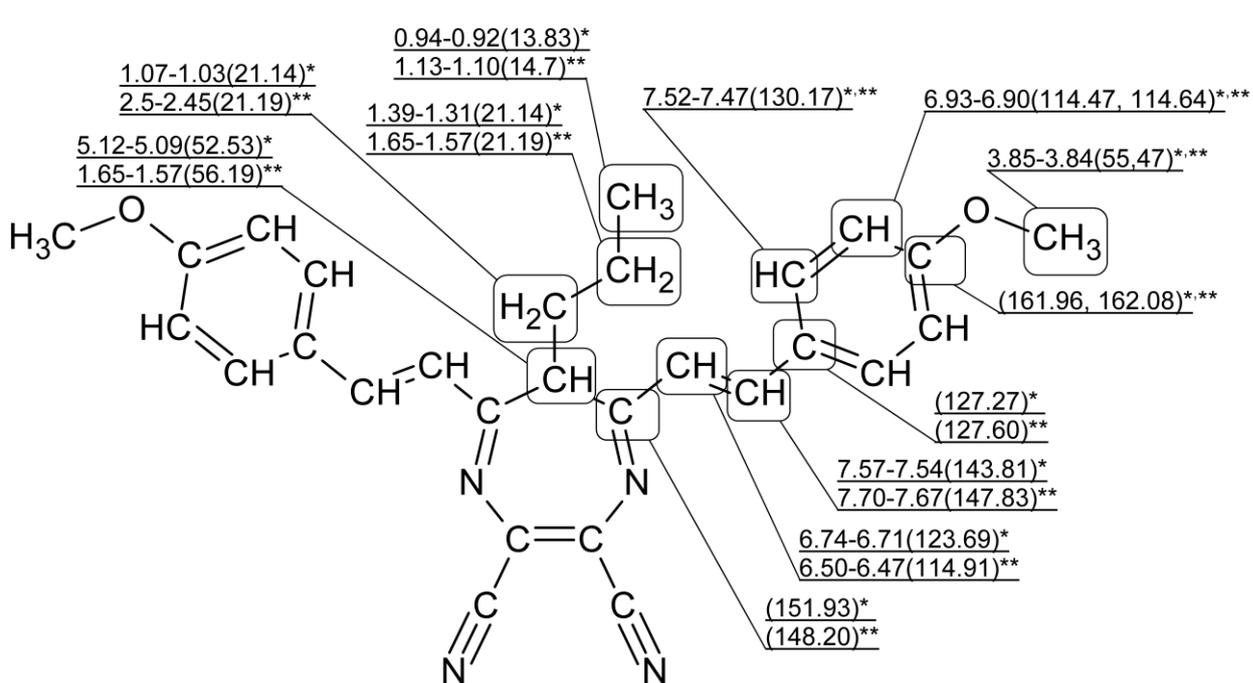
Fig. S22 NMR data analysis for **6d**.
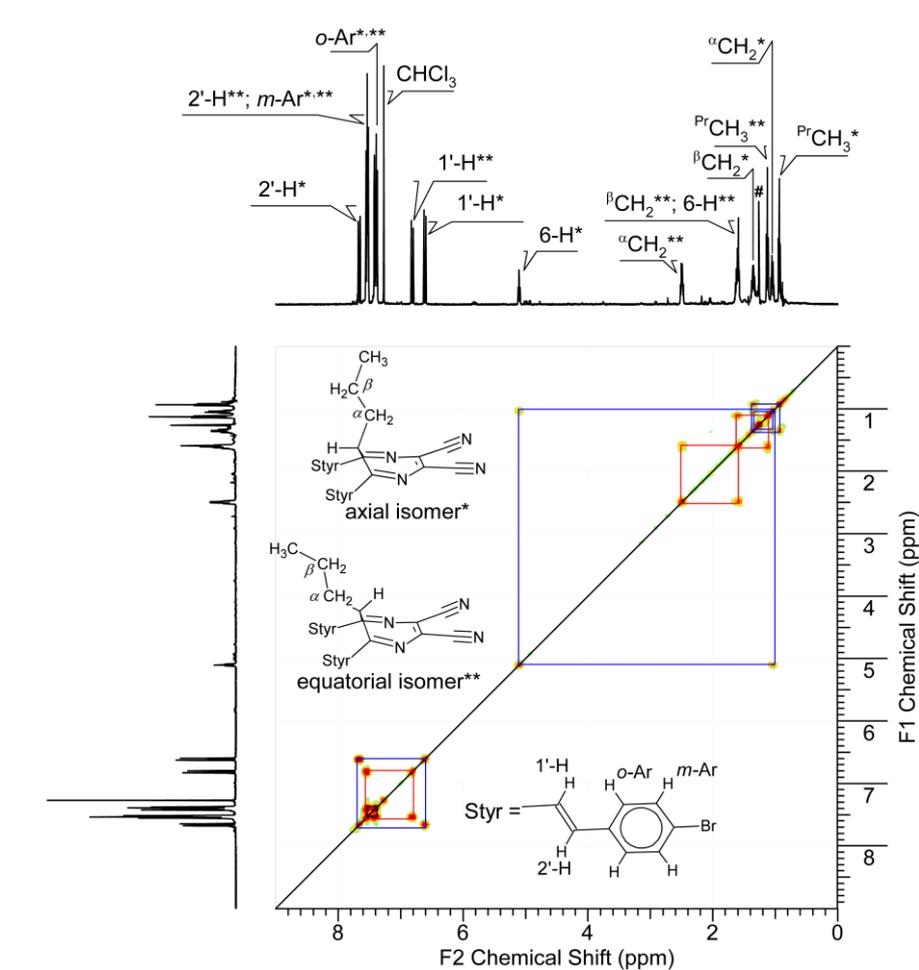
Fig. S23 ^{1}H-^{1}H COSY NMR spectrum of **6b** (CDCl$_3$, 293 K).
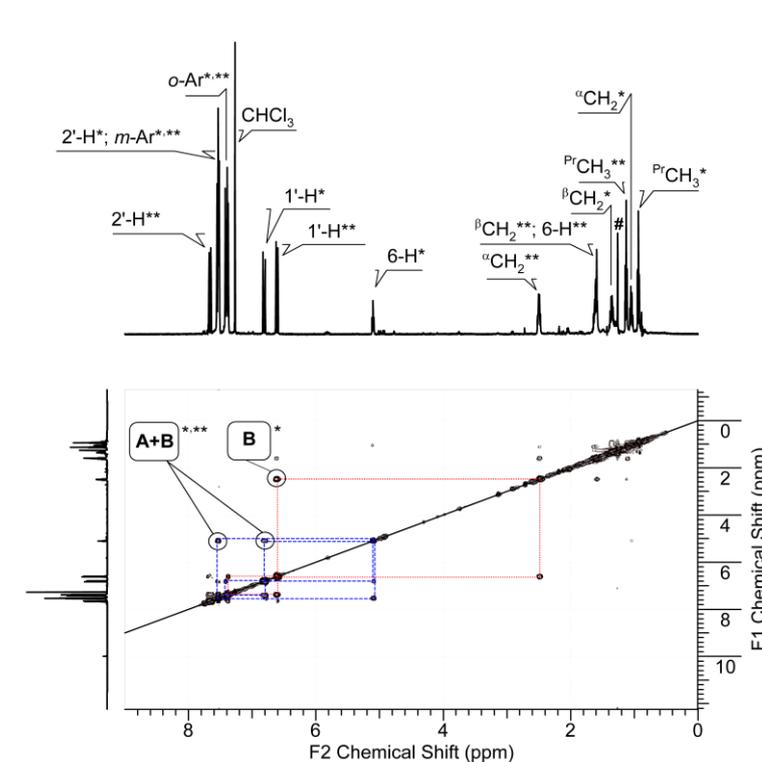
Fig. S24 ^{1}H-^{1}H NOESY NMR spectrum of **6b** (CDCl$_3$, 293 K).
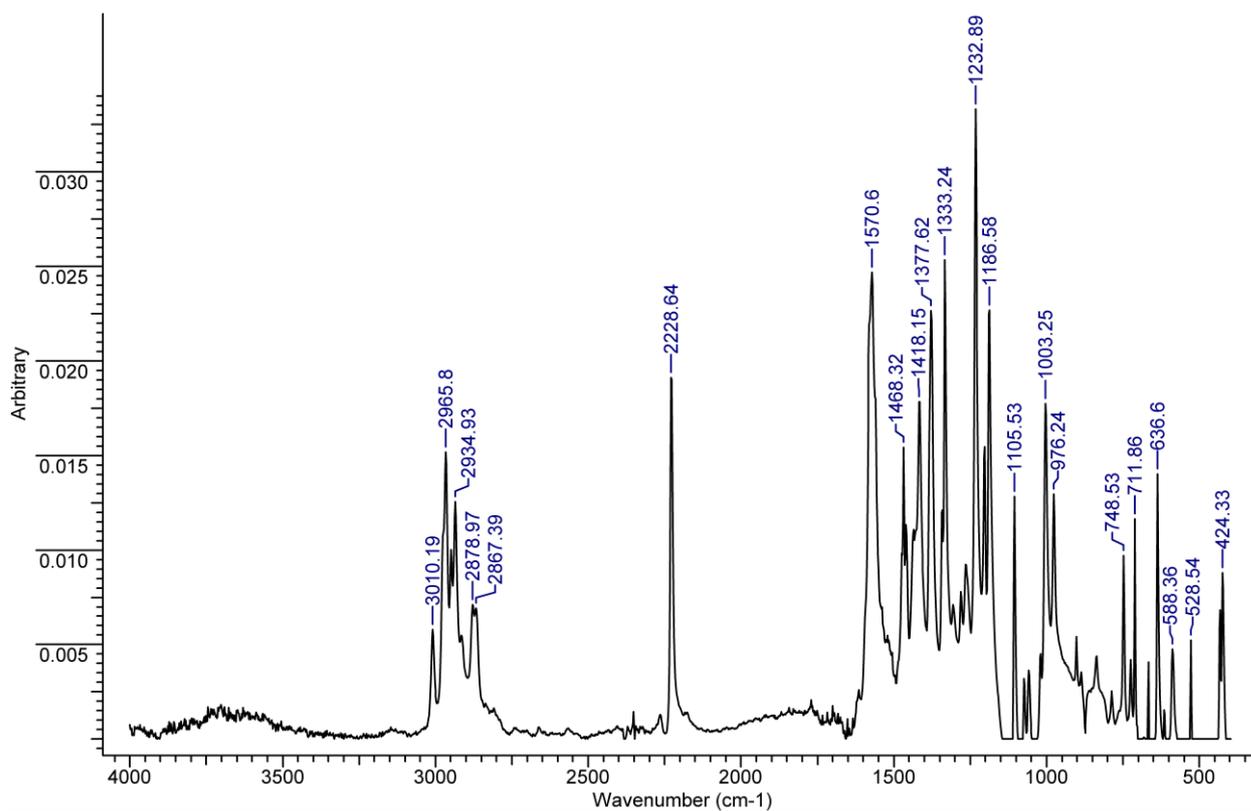
Fig. S25 IR spectrum of **4**.
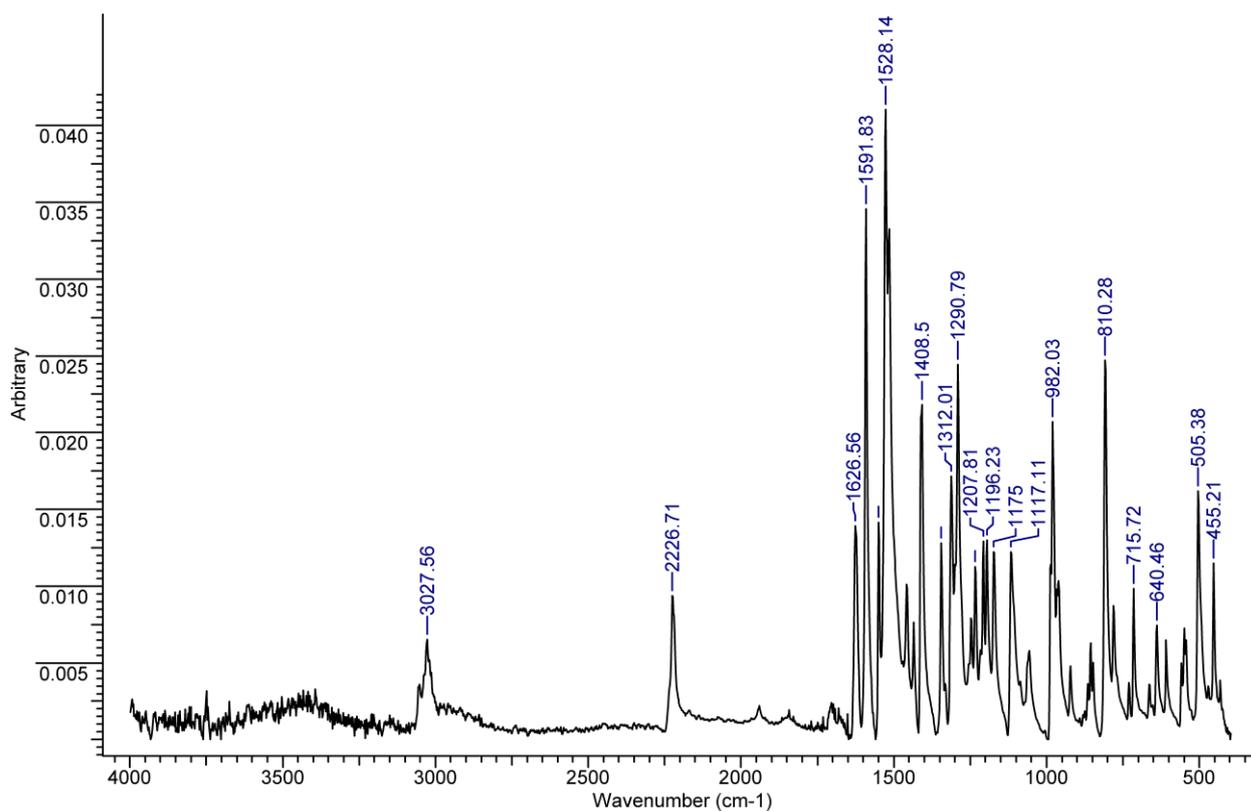
Fig. S26 IR spectrum of **5a**.
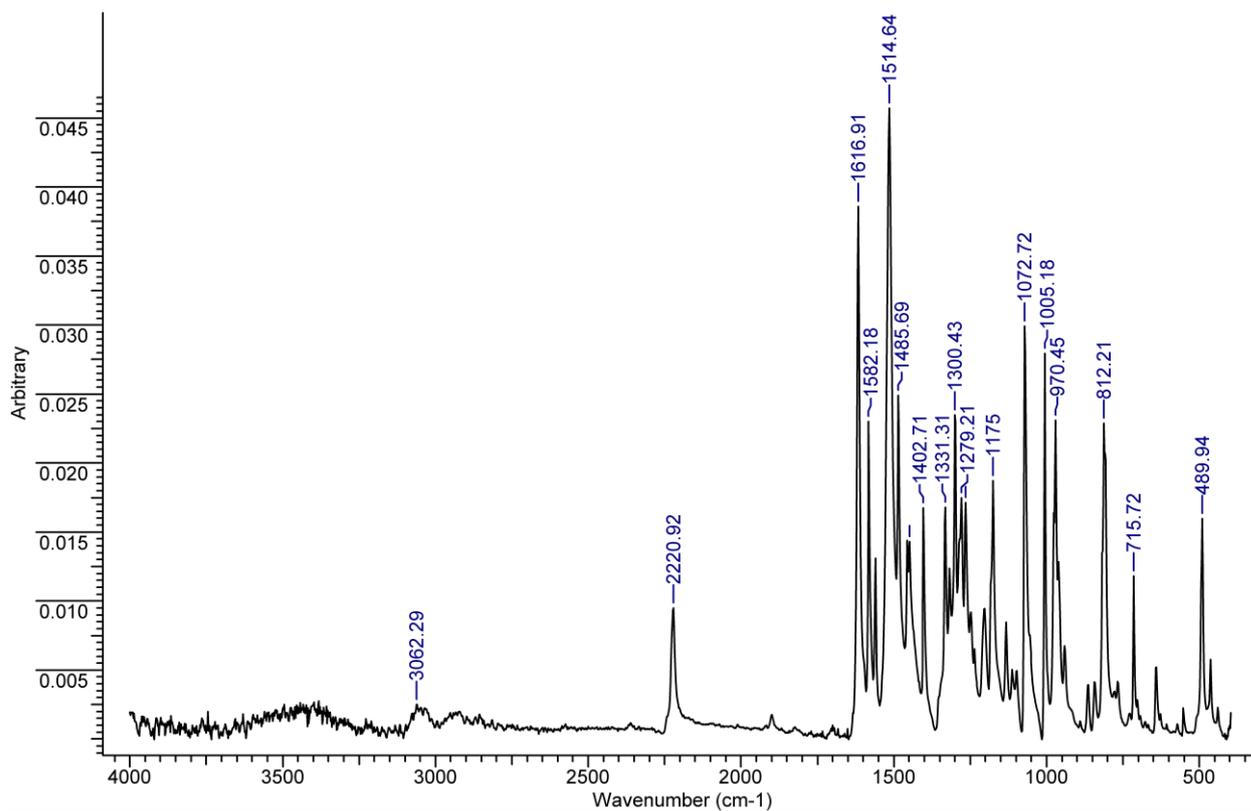
Fig. S27 IR spectrum of **5b**.
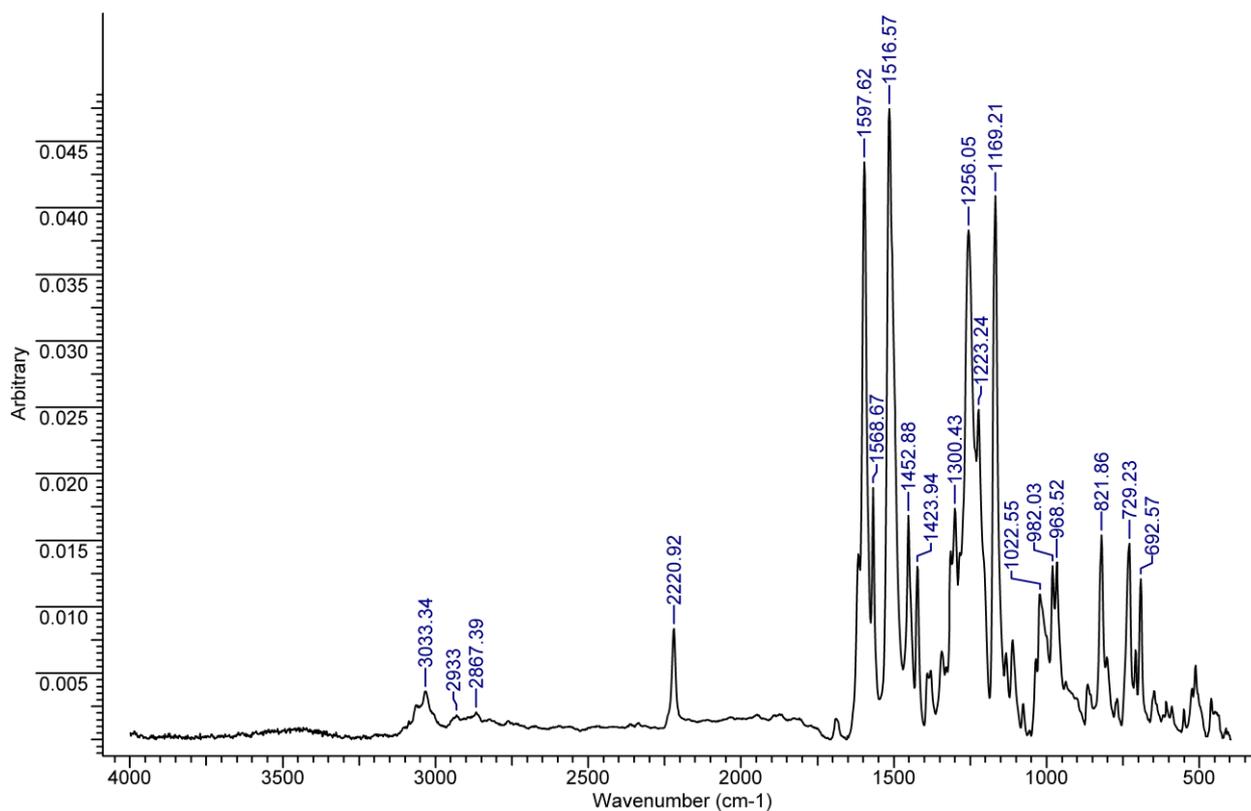
Fig. S28 IR spectrum of **5c**.
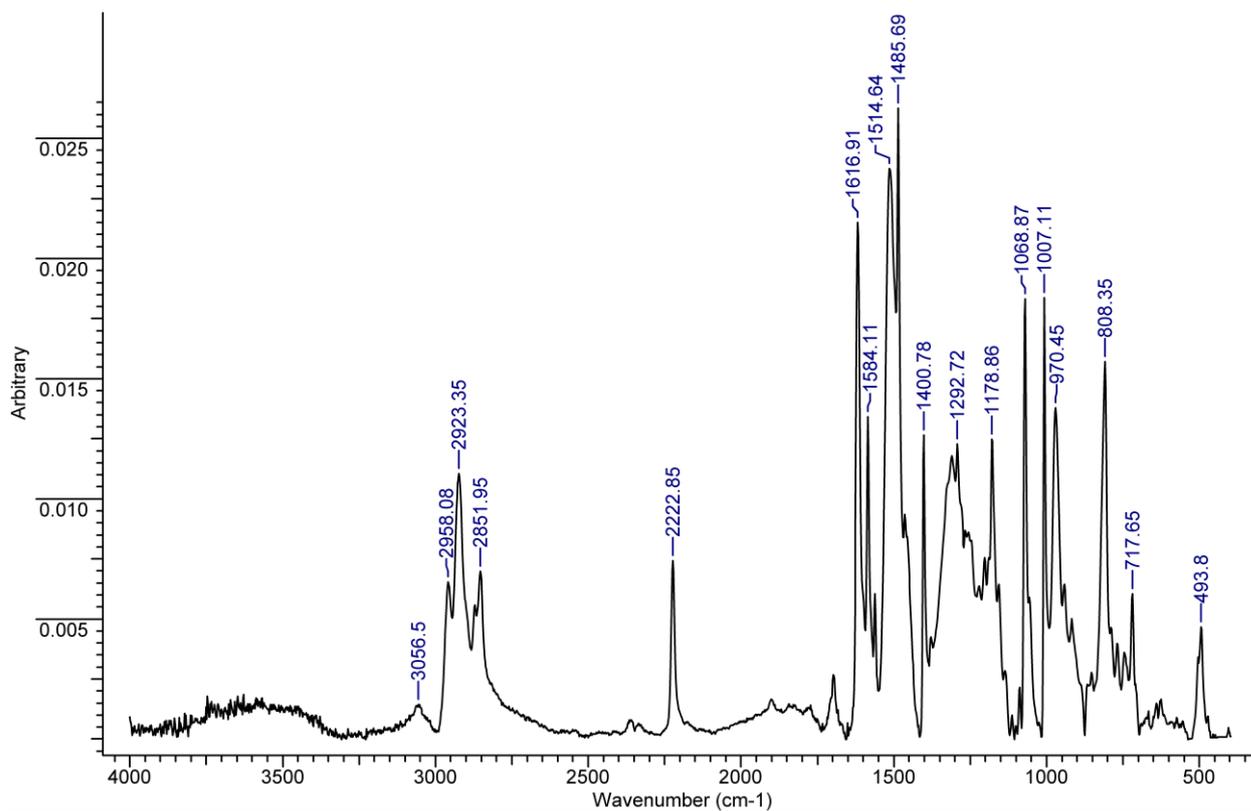
Fig. S29 IR spectrum of **6b**.
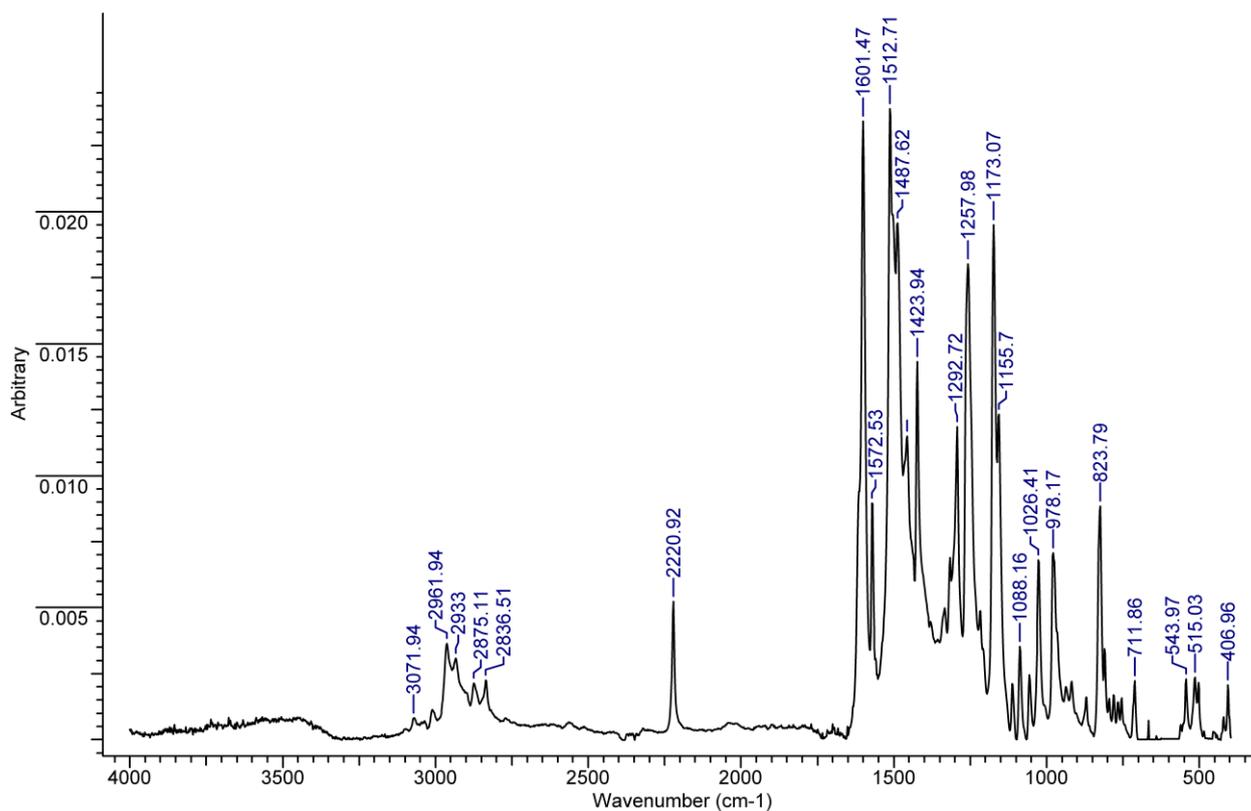
Fig. S30 IR spectrum of **6d**.
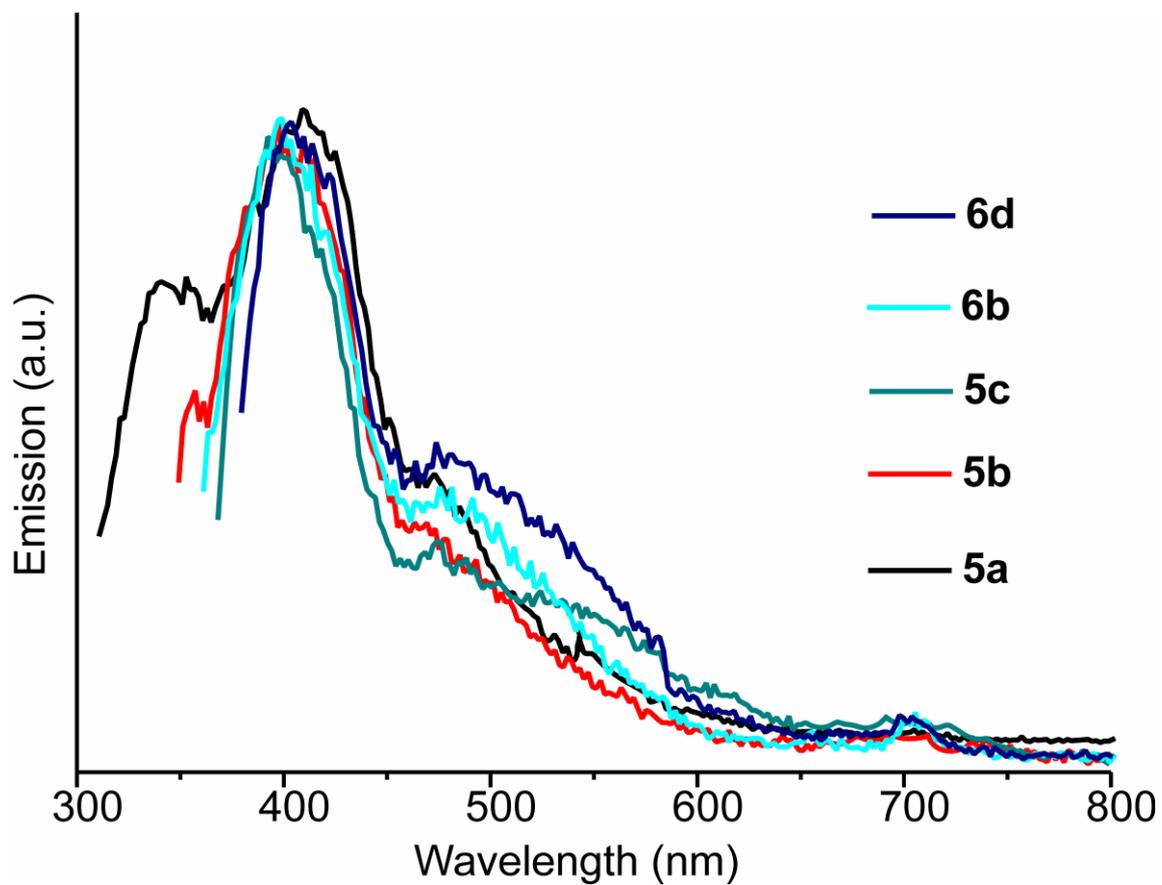
Fig. S31 Fluorescence of 5,7-bis(2'-arylethenyl)-6*H*-1,4-diazepine-2,3-dicarbonitriles in MeOH solution.
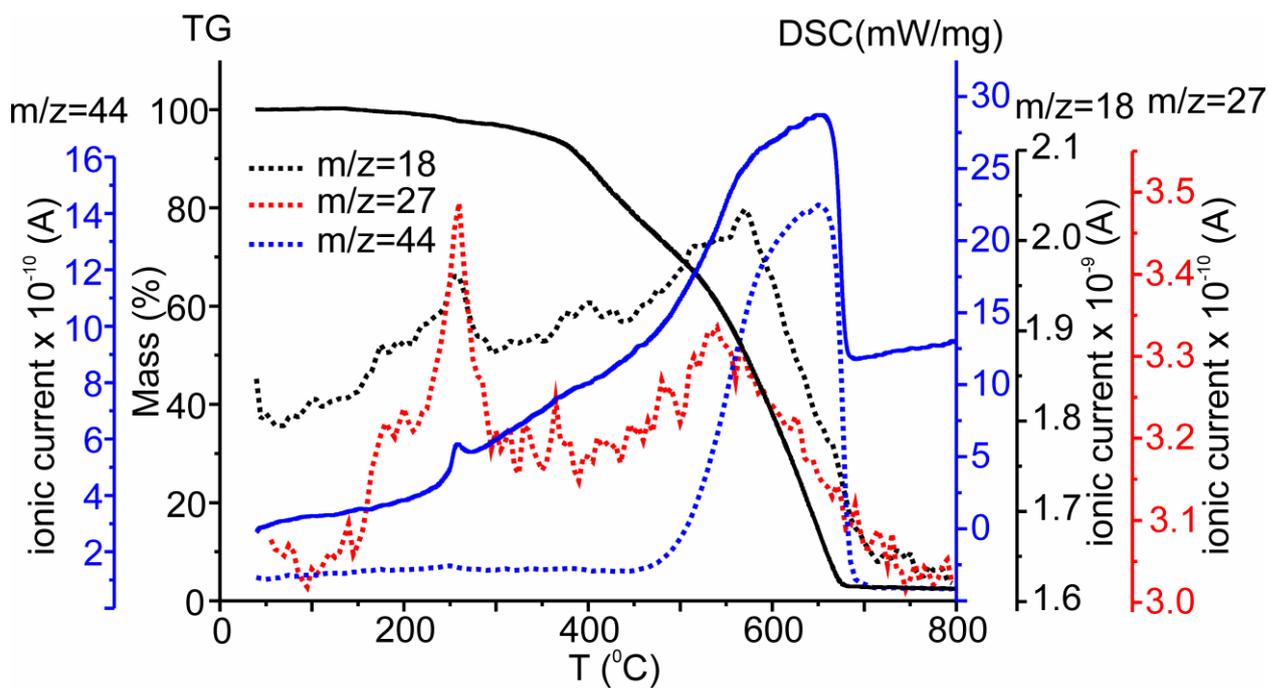
Fig. S32 Thermogravimetric analysis of **5b**.
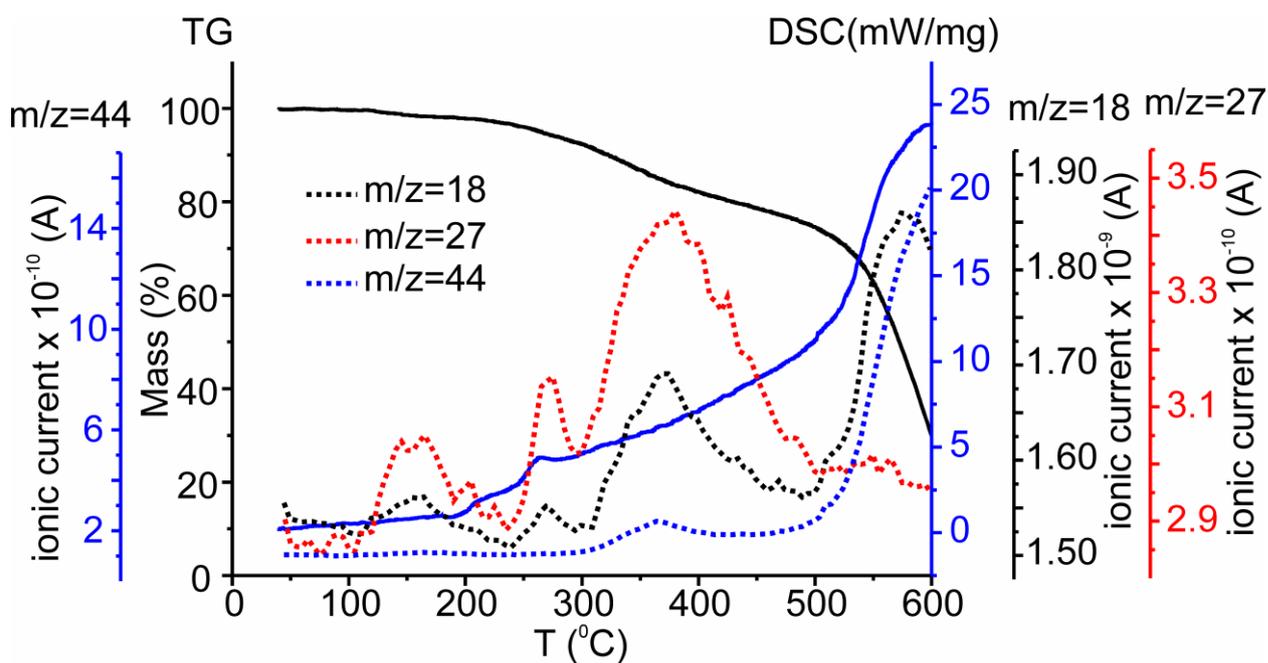
Fig. S33 Thermogravimetric analysis of **5c**.
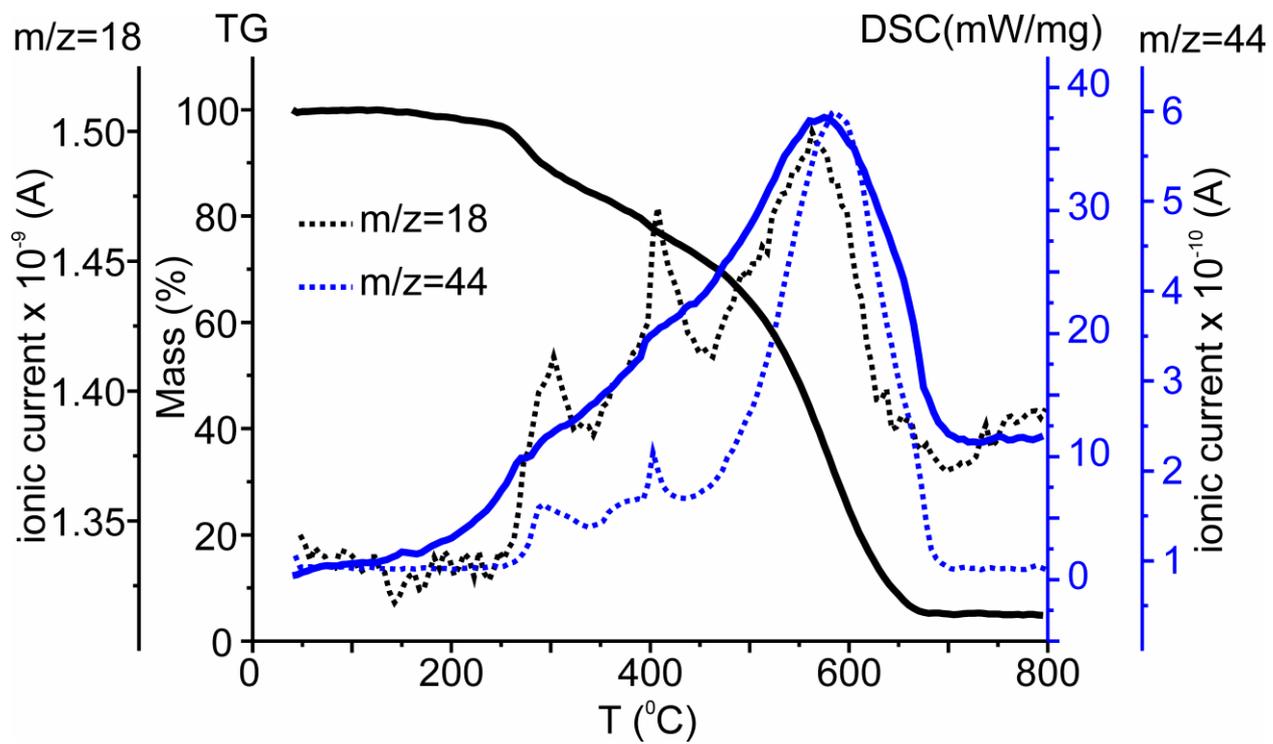
Fig. S34 Thermogravimetric analysis of **6d**.

<h1 style="text-align: center;">Full Computational Details</h1>

Quantum-chemical calculations were performed at the DFT level using hybrid functional B3LYP with 6-31G(d,p) basis sets as provided by the GAMESS package.

equatorial isomer of **4:**

Table S2.

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 C                -0.95257000    0.25194500   -0.14019000
 C                 1.84692300    0.58300500   -0.16802100
 N                 1.04445700    1.63036100    0.19992200
 C                -0.23885100    1.51242300    0.33139600
 C                -1.50320100   -1.06647700    2.07303000
 C                -1.00135200    2.62541700    0.98639300
 C                 2.69629000   -1.70900700   -0.06365700
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 C                 3.07317000    0.96553100   -0.81841400
 N                 4.04300400    1.29020400   -1.37213000
 C                -2.45170500    0.38299900   -0.44165600
 C                -3.02301400   -0.84195100   -1.17171800
 C                -4.51645900   -0.69990000   -1.47784500
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 H                -1.51678900    2.26551800    1.88448400
 H                -0.43281900   -0.07899900   -1.05007900
 H                -3.02026600    0.57062300    0.47633100
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 H                -2.46723100   -0.98935400   -2.10660700
 H                -2.85653000   -1.74813900   -0.57573100
 H                -4.89495000   -1.57851600   -2.00876400
 H                -5.10150200   -0.58786500   -0.55825000
 H                -4.71034200    0.17791100   -2.10407600
 H                -2.41362700   -1.53017300    1.68146700
 H                -1.77272200    3.01951700    0.31694600
 H                -0.31940100    3.42746900    1.26807100
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Table S3.

TD–DFT output

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      56      58  -0.303260     0.000000
      56      61  -0.120730     0.000000
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STATE #   3  ENERGY =    5.103700 EV
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      57      58  -0.249200     0.000000
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         57      60   0.257820        0.000000
         57      61   0.479180        0.000000
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         55      59   0.306210        0.000000
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         57      60   0.154910        0.000000


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       50      58   0.148110      0.000000
       51      58   0.520620      0.000000
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       49      58   0.386970      0.000000
       54      58   0.270840      0.000000
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       56      61   0.100260      0.000000
       57      59   0.198480      0.000000


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        I       A    X(I->A)        Y(A->I)
       ---     ---   --------       --------
       47      60   0.184410      0.000000
       51      62  -0.135140      0.000000
       55      61   0.130200      0.000000
       56      59   0.116580      0.000000
       56      60  -0.230810      0.000000
       57      62   0.474760      0.000000


STATE #  14   ENERGY =    7.408300 EV
OSCILLATOR STRENGTH =    0.004400
                    EXCITATION  DE-EXCITATION
       OCC     VIR   AMPLITUDE      AMPLITUDE
        I       A    X(I->A)        Y(A->I)
       ---     ---   --------       --------
       46      58  -0.276600      0.000000
       47      58  -0.146300      0.000000
       48      58  -0.186010      0.000000
       50      58  -0.312310      0.000000
       52      58   0.150650      0.000000
       53      58   0.364830      0.000000


STATE #  15   ENERGY =    7.482000 EV
OSCILLATOR STRENGTH =    0.079800
                    EXCITATION  DE-EXCITATION
```

```
        OCC      VIR   AMPLITUDE      AMPLITUDE
         I        A     X(I->A)        Y(A->I)
        ---      ---   --------       --------
         46       58   -0.236270      0.000000
         47       58    0.399930      0.000000
         48       60    0.116020      0.000000
         52       58    0.285630      0.000000
         53       58   -0.132700      0.000000
         55       59    0.200990      0.000000
         56       61    0.148270      0.000000


STATE #  16   ENERGY =    7.595800 EV
OSCILLATOR STRENGTH =     0.018700
                  EXCITATION  DE-EXCITATION
        OCC      VIR   AMPLITUDE      AMPLITUDE
         I        A     X(I->A)        Y(A->I)
        ---      ---   --------       --------
         45       58    0.140830      0.000000
         47       58    0.132250      0.000000
         48       58    0.104550      0.000000
         50       58    0.140790      0.000000
         51       58   -0.111190      0.000000
         52       58   -0.261800      0.000000
         53       58    0.458350      0.000000
         54       58   -0.107700      0.000000
         56       61    0.161990      0.000000


STATE #  17   ENERGY =    7.717300 EV
OSCILLATOR STRENGTH =     0.036500
                  EXCITATION  DE-EXCITATION
        OCC      VIR   AMPLITUDE      AMPLITUDE
         I        A     X(I->A)        Y(A->I)
        ---      ---   --------       --------
         45       58    0.148840      0.000000
         47       58    0.248460      0.000000
         51       58    0.167600      0.000000
         52       58   -0.217770      0.000000
         55       60    0.318510      0.000000
         55       61    0.132570      0.000000
         56       59    0.144670      0.000000
         56       60   -0.201870      0.000000
         56       61   -0.246400      0.000000


STATE #  18   ENERGY =    7.726200 EV
OSCILLATOR STRENGTH =     0.021400
                  EXCITATION  DE-EXCITATION
        OCC      VIR   AMPLITUDE      AMPLITUDE
         I        A     X(I->A)        Y(A->I)
        ---      ---   --------       --------
         47       62    0.104780      0.000000
         50       60   -0.113090      0.000000
         51       58    0.163390      0.000000
         51       60   -0.100910      0.000000
```

```
52     58   -0.157330        0.000000
55     59    0.127030        0.000000
55     60   -0.125450        0.000000
55     61    0.438910        0.000000
56     60    0.252450        0.000000
57     60   -0.120630        0.000000


STATE #  19  ENERGY =    7.859900 EV
OSCILLATOR STRENGTH =    0.004500
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------      --------
    44     58   -0.101070        0.000000
    45     58   -0.103420        0.000000
    46     58    0.125120        0.000000
    50     58    0.210810        0.000000
    51     58   -0.167500        0.000000
    52     58    0.231860        0.000000
    53     58    0.144470        0.000000
    54     59    0.163970        0.000000
    55     61    0.328740        0.000000
    56     60   -0.233400        0.000000
    57     62   -0.260380        0.000000


STATE #  20  ENERGY =    7.879100 EV
OSCILLATOR STRENGTH =    0.108300
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------      --------
    45     58   -0.228950        0.000000
    47     58   -0.130220        0.000000
    55     59    0.102730        0.000000
    55     60    0.384790        0.000000
    56     60    0.144830        0.000000
    56     61    0.327990        0.000000
    56     62    0.137540        0.000000


STATE #  21  ENERGY =    7.910800 EV
OSCILLATOR STRENGTH =    0.027300
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------      --------
    48     58   -0.140840        0.000000
    50     58   -0.211320        0.000000
    51     58    0.179180        0.000000
    52     58   -0.143740        0.000000
    53     58   -0.106130        0.000000
    54     59    0.193670        0.000000
    56     59   -0.146220        0.000000
    56     60   -0.278430        0.000000
```

```
        56       61   0.308070         0.000000
        57       62  -0.244100         0.000000


STATE #  22   ENERGY =      8.001700 EV
OSCILLATOR STRENGTH =     0.038600
                     EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE     AMPLITUDE
        I        A    X(I->A)       Y(A->I)
       ---      ---   --------     --------
        43       58   0.164260         0.000000
        48       58  -0.132140         0.000000
        54       59   0.492030         0.000000
        55       60   0.124350         0.000000
        55       62   0.121600         0.000000
        56       60   0.181180         0.000000
        56       61  -0.123550         0.000000
        57       62   0.195560         0.000000


STATE #  23   ENERGY =      8.082700 EV
OSCILLATOR STRENGTH =     0.026700
                     EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE     AMPLITUDE
        I        A    X(I->A)       Y(A->I)
       ---      ---   --------     --------
        42       58   0.208310         0.000000
        44       58   0.124920         0.000000
        45       58   0.130890         0.000000
        46       59  -0.156870         0.000000
        51       59   0.310620         0.000000
        52       59   0.271780         0.000000
        53       59   0.229300         0.000000
        57       63  -0.235780         0.000000


STATE #  24   ENERGY =      8.126400 EV
OSCILLATOR STRENGTH =     0.061200
                     EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE     AMPLITUDE
        I        A    X(I->A)       Y(A->I)
       ---      ---   --------     --------
        43       58   0.120060         0.000000
        44       58   0.232240         0.000000
        45       58   0.467790         0.000000
        51       59  -0.118770         0.000000
        52       58   0.136450         0.000000
        52       59  -0.123200         0.000000
        53       59  -0.106040         0.000000
        55       60   0.142890         0.000000
        56       61   0.175640         0.000000


STATE #  25   ENERGY =      8.170700 EV
OSCILLATOR STRENGTH =     0.013600
                     EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE     AMPLITUDE
```

```
           I        A     X(I->A)        Y(A->I)
          ---      ---    --------       --------
          43       58     0.396480       0.000000
          44       58    -0.240900       0.000000
          46       58     0.256000       0.000000
          47       58     0.133220       0.000000
          50       58    -0.170700       0.000000
          54       59    -0.207250       0.000000
          55       60    -0.145920       0.000000
          55       61    -0.156670       0.000000


STATE #  26   ENERGY =     8.194800 EV
OSCILLATOR STRENGTH =      0.004500
                    EXCITATION   DE-EXCITATION
         OCC      VIR   AMPLITUDE      AMPLITUDE
          I        A     X(I->A)        Y(A->I)
          ---      ---    --------       --------
          46       59    -0.102080       0.000000
          47       58    -0.126520       0.000000
          50       59    -0.174950       0.000000
          51       59     0.109980       0.000000
          52       59     0.152840       0.000000
          53       59     0.121330       0.000000
          57       63     0.548800       0.000000


STATE #  27   ENERGY =     8.296300 EV
OSCILLATOR STRENGTH =      0.046800
                    EXCITATION   DE-EXCITATION
         OCC      VIR   AMPLITUDE      AMPLITUDE
          I        A     X(I->A)        Y(A->I)
          ---      ---    --------       --------
          41       58     0.225280       0.000000
          43       58     0.411610       0.000000
          46       58    -0.217010       0.000000
          47       59     0.135570       0.000000
          48       58     0.105400       0.000000
          50       58     0.216240       0.000000


STATE #  28   ENERGY =     8.412000 EV
OSCILLATOR STRENGTH =      0.082400
                    EXCITATION   DE-EXCITATION
         OCC      VIR   AMPLITUDE      AMPLITUDE
          I        A     X(I->A)        Y(A->I)
          ---      ---    --------       --------
          42       58     0.442090       0.000000
          46       59     0.107850       0.000000
          47       58     0.104830       0.000000
          50       59     0.245050       0.000000
          52       59    -0.135070       0.000000
          54       61     0.119650       0.000000
          55       60    -0.129980       0.000000
          57       63     0.170820       0.000000
```

```
          STATE #  29   ENERGY =     8.520500 EV
          OSCILLATOR STRENGTH =     0.004900
                         EXCITATION  DE-EXCITATION
            OCC      VIR   AMPLITUDE     AMPLITUDE
             I        A     X(I->A)       Y(A->I)
            ---      ---   --------      --------
             42       58   0.276860      0.000000
             45       58  -0.110450      0.000000
             47       60  -0.100600      0.000000
             47       62   0.145630      0.000000
             50       60  -0.112790      0.000000
             51       60  -0.261060      0.000000
             51       61   0.122170      0.000000
             54       60  -0.108140      0.000000
             54       61  -0.112510      0.000000
             54       62   0.122490      0.000000
             55       60   0.230090      0.000000
             55       61  -0.141190      0.000000
             56       60  -0.139810      0.000000
             56       62  -0.109000      0.000000

          STATE #  30   ENERGY =     8.575400 EV
          OSCILLATOR STRENGTH =     0.009100
                         EXCITATION  DE-EXCITATION
            OCC      VIR   AMPLITUDE     AMPLITUDE
             I        A     X(I->A)       Y(A->I)
            ---      ---   --------      --------
             40       58   0.191650      0.000000
             43       58  -0.156540      0.000000
             46       58   0.255160      0.000000
             47       58   0.112050      0.000000
             47       59   0.161670      0.000000
             47       60   0.102140      0.000000
             48       58  -0.145250      0.000000
             49       59  -0.177780      0.000000
             51       61   0.131460      0.000000
             52       59   0.110450      0.000000
             53       59  -0.168330      0.000000
             54       60   0.169740      0.000000
             54       61  -0.133130      0.000000
             55       61  -0.132140      0.000000
             57       62  -0.104890      0.000000
```

Inversion Ts for **4**:

Table S4.

```
TOTAL FREE ENERGY IN SOLVENT = -684.453041 A.U.
 N                 -0.87701600    1.57330800   -0.05700100
 C                  0.38039400    1.32656700    0.05246300
 C                 -1.93595100    0.68582400   -0.03303900
 C                  1.12906400    0.00000600    0.29182400
 C                 -1.93594700   -0.68582900   -0.03304000
 N                 -0.87700900   -1.57330700   -0.05700000
```

```
C               0.38040000      -1.32656000       0.05246400
C               1.24554500       2.56868900       0.01751800
C               1.24555800      -2.56867600       0.01752100
C              -3.20823800       1.36834000      -0.02061000
N              -4.21690600       1.94761600      -0.00625500
C              -3.20823100      -1.36835100      -0.02061200
N              -4.21689600      -1.94763200      -0.00625700
C               2.52002900       0.00000700      -0.44368700
C               3.73145700       0.00000300       0.49951500
C               5.06443700      -0.00001100      -0.25293400
H               2.10250200       2.49132600       0.69209800
H               1.63768300      -2.74875600      -0.98966400
H               1.35066200       0.00000600       1.37337300
H               2.58613500      -0.86278700      -1.10878900
H               2.58613500       0.86280300      -1.10878700
H               3.68233100       0.87565300       1.15985300
H               3.68231800      -0.87563800       1.15986300
H               5.15851000      -0.88435000      -0.89283300
H               5.15852400       0.88432100      -0.89284100
H               5.90959900      -0.00001500       0.44202200
H               2.10251800      -2.49130400       0.69209800
H               0.63455800      -3.42815600       0.29228300
H               1.63767200       2.74876600      -0.98966700
H               0.63453800       3.42816600       0.29227400
```

Axial isomer of **4:**

Table S5.

```
TOTAL FREE ENERGY IN SOLVENT = -684.488174 A.U.
N               0.22560900      -0.19426900       1.63495400
C              -0.91195000       0.34946500       1.35141800
C               1.24527400      -0.36407700       0.73393300
C              -1.37115300       0.66745600      -0.06807600
C               1.53510100       0.47175700      -0.33736100
N               0.84858600       1.60740800      -0.68354400
C              -0.41795000       1.77876500      -0.49255400
C              -1.83232900       0.71186600       2.48049700
C              -0.99338500       3.15090200      -0.69030600
C               2.17333600      -1.40944100       1.08081900
N               2.89417400      -2.27834400       1.36033800
C               2.75685100       0.27237800      -1.07333000
N               3.72353400       0.11201800      -1.69993200
C              -1.44712100      -0.53617100      -1.03765600
C              -2.47686200      -1.58601300      -0.59797000
C              -2.59905800      -2.73840100      -1.59929100
H              -2.05467300       1.78530500       2.45941900
H              -1.76706900       3.12698100      -1.46683200
H              -2.37593300       1.09589400      -0.00426600
H              -1.72397600      -0.14132100      -2.02265800
H              -0.47145900      -1.01213500      -1.15945400
H              -2.19638900      -1.98675000       0.38433400
H              -3.45554800      -1.10504800      -0.46934500
H              -2.90958400      -2.37544400      -2.58525900
```

```
H                     -1.64326100    -3.25922600    -1.72217600
H                     -3.33841100    -3.47279600    -1.26553600
H                     -1.48247100     3.49698100     0.22806700
H                     -0.21461700     3.85971700    -0.97124100
H                     -2.79046800     0.19104500     2.37055200
H                     -1.38398200     0.45819500     3.44094600
```

Table S6.

TD–DFT output

HOMO: 57, LUMO: 58
```
STATE #   1   ENERGY =     4.201300 EV
 OSCILLATOR STRENGTH =     0.252200
                   EXCITATION   DE-EXCITATION
      OCC      VIR  AMPLITUDE      AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---  --------      --------
       55       58   0.228580      0.000000
       56       58   0.171110      0.000000
       56       59  -0.119570      0.000000
       57       58   0.602510      0.000000

STATE #   2   ENERGY =     4.847000 EV
 OSCILLATOR STRENGTH =     0.081600
                   EXCITATION   DE-EXCITATION
      OCC      VIR  AMPLITUDE      AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---  --------      --------
       55       58  -0.210530      0.000000
       55       59  -0.175510      0.000000
       56       58   0.480050      0.000000
       56       59  -0.140560      0.000000
       56       61  -0.127170      0.000000
       57       59  -0.342630      0.000000

STATE #   3   ENERGY =     4.950300 EV
 OSCILLATOR STRENGTH =     0.119600
                   EXCITATION   DE-EXCITATION
      OCC      VIR  AMPLITUDE      AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---  --------      --------
       55       58   0.490970      0.000000
       56       58   0.353910      0.000000
       57       58  -0.281320      0.000000
       57       59   0.168870      0.000000

STATE #   4   ENERGY =     5.034000 EV
 OSCILLATOR STRENGTH =     0.018300
                   EXCITATION   DE-EXCITATION
      OCC      VIR  AMPLITUDE      AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---  --------      --------
```

```
           55      58  -0.362340      0.000000
           56      58   0.273490      0.000000
           57      59   0.513940      0.000000


STATE #   5  ENERGY =    5.863200 EV
OSCILLATOR STRENGTH =    0.040900
                    EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
           54      59  -0.134050      0.000000
           55      59  -0.286470      0.000000
           55      61   0.153390      0.000000
           56      59   0.414490      0.000000
           56      61   0.137510      0.000000
           57      58   0.130850      0.000000
           57      61   0.343940      0.000000


STATE #   6  ENERGY =    5.973800 EV
OSCILLATOR STRENGTH =    0.007000
                    EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
           52      58  -0.105860      0.000000
           53      58   0.144970      0.000000
           54      58   0.526390      0.000000
           55      59  -0.287230      0.000000
           56      59  -0.199040      0.000000
           57      60  -0.149280      0.000000


STATE #   7  ENERGY =    6.034900 EV
OSCILLATOR STRENGTH =    0.006500
                    EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
           54      58   0.146730      0.000000
           57      60   0.642360      0.000000


STATE #   8  ENERGY =    6.462600 EV
OSCILLATOR STRENGTH =    0.007800
                    EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
           55      59   0.149120      0.000000
           56      59  -0.316740      0.000000
           57      61   0.542600      0.000000


STATE #   9  ENERGY =    6.476700 EV
OSCILLATOR STRENGTH =    0.081000
                    EXCITATION  DE-EXCITATION
```

```
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A     X(I->A)          Y(A->I)
          ---      ---   --------         --------
          49       58    0.267860         0.000000
          50       58    0.423330         0.000000
          52       58    0.113510         0.000000
          55       59   -0.310290         0.000000
          56       59   -0.128700         0.000000
          57       59    0.113030         0.000000
          57       60    0.155670         0.000000
          57       61   -0.100590         0.000000


STATE #  10   ENERGY =    6.671300 EV
OSCILLATOR STRENGTH =    0.000500
                        EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A     X(I->A)          Y(A->I)
          ---      ---   --------         --------
          46       58   -0.110770         0.000000
          48       58    0.563930         0.000000
          48       61    0.124390         0.000000
          49       58    0.220360         0.000000
          50       58   -0.141210         0.000000
          50       63   -0.105070         0.000000
          52       58    0.100730         0.000000


STATE #  11   ENERGY =    6.744600 EV
OSCILLATOR STRENGTH =    0.048700
                        EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A     X(I->A)          Y(A->I)
          ---      ---   --------         --------
          48       58    0.169510         0.000000
          49       58   -0.174920         0.000000
          50       58    0.105570         0.000000
          50       60   -0.128500         0.000000
          51       58    0.434310         0.000000
          52       58   -0.336970         0.000000
          53       58    0.128010         0.000000
          54       58   -0.143230         0.000000


STATE #  12   ENERGY =    6.808500 EV
OSCILLATOR STRENGTH =    0.707800
                        EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A     X(I->A)          Y(A->I)
          ---      ---   --------         --------
          48       60   -0.114920         0.000000
          49       58    0.134400         0.000000
          50       58    0.353100         0.000000
          51       58    0.122480         0.000000
          53       58    0.109610         0.000000
          54       58    0.296790         0.000000
```

```
    55       59    0.262780          0.000000
    56       59    0.188210          0.000000
    57       59   -0.188850          0.000000


STATE #  13   ENERGY =     7.101700 EV
OSCILLATOR STRENGTH =      0.009000
                    EXCITATION  DE-EXCITATION
     OCC      VIR   AMPLITUDE      AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---   --------      --------
     46       58   -0.201830          0.000000
     47       58   -0.155020          0.000000
     51       58   -0.212770          0.000000
     53       58    0.571410          0.000000
     54       58   -0.152740          0.000000


STATE #  14   ENERGY =     7.216200 EV
OSCILLATOR STRENGTH =      0.015700
                    EXCITATION  DE-EXCITATION
     OCC      VIR   AMPLITUDE      AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---   --------      --------
     45       58    0.164600          0.000000
     46       58    0.130630          0.000000
     47       58   -0.169180          0.000000
     50       58   -0.109770          0.000000
     51       58    0.328070          0.000000
     52       58    0.464110          0.000000
     53       58    0.137420          0.000000
     57       62    0.106910          0.000000


STATE #  15   ENERGY =     7.310800 EV
OSCILLATOR STRENGTH =      0.008700
                    EXCITATION  DE-EXCITATION
     OCC      VIR   AMPLITUDE      AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---   --------      --------
     47       60    0.166020          0.000000
     48       58   -0.131360          0.000000
     51       58   -0.127460          0.000000
     54       60   -0.127450          0.000000
     55       60    0.102180          0.000000
     55       61    0.111690          0.000000
     56       60   -0.162870          0.000000
     57       61    0.104360          0.000000
     57       62    0.482030          0.000000


STATE #  16   ENERGY =     7.390000 EV
OSCILLATOR STRENGTH =      0.048900
                    EXCITATION  DE-EXCITATION
     OCC      VIR   AMPLITUDE      AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---   --------      --------
```

```
42      58    0.102500          0.000000
47      58    0.127760          0.000000
48      58   -0.143670          0.000000
49      58    0.452260          0.000000
50      58   -0.231230          0.000000
51      58    0.181850          0.000000
52      58   -0.135260          0.000000
53      58    0.181100          0.000000
56      59    0.100680          0.000000


STATE #  17  ENERGY =     7.522000 EV
OSCILLATOR STRENGTH =     0.067400
                    EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A     X(I->A)       Y(A->I)
      ---      ---   --------      --------
       45      58    0.190730          0.000000
       46      58   -0.224080          0.000000
       47      58    0.402340          0.000000
       48      60    0.150810          0.000000
       49      58   -0.146320          0.000000
       52      58    0.196790          0.000000
       55      59    0.150160          0.000000
       56      59    0.118770          0.000000
       56      61   -0.176990          0.000000


STATE #  18  ENERGY =     7.656400 EV
OSCILLATOR STRENGTH =     0.004200
                    EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A     X(I->A)       Y(A->I)
      ---      ---   --------      --------
       47      58   -0.114110          0.000000
       47      62   -0.109040          0.000000
       51      60   -0.145480          0.000000
       52      60    0.118210          0.000000
       55      60    0.393540          0.000000
       55      61    0.118030          0.000000
       56      60    0.334310          0.000000
       56      61   -0.242520          0.000000
       56      62    0.105830          0.000000
       57      60    0.120280          0.000000


STATE #  19  ENERGY =     7.728300 EV
OSCILLATOR STRENGTH =     0.034100
                    EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A     X(I->A)       Y(A->I)
      ---      ---   --------      --------
       43      58   -0.139690          0.000000
       55      59    0.128990          0.000000
       55      61    0.455000          0.000000
       56      59   -0.156580          0.000000
```

```
             56      61    0.342580           0.000000
             57      62   -0.169240           0.000000


STATE #  20   ENERGY =     7.850600 EV
OSCILLATOR STRENGTH =      0.066100
                      EXCITATION  DE-EXCITATION
          OCC      VIR  AMPLITUDE     AMPLITUDE
           I        A    X(I->A)       Y(A->I)
          ---      ---  --------      --------
           44      58    0.195520           0.000000
           45      58    0.271160           0.000000
           46      58   -0.124950           0.000000
           55      60    0.130140           0.000000
           55      61   -0.300650           0.000000
           56      60    0.184290           0.000000
           56      61    0.342140           0.000000
           56      62    0.106730           0.000000


STATE #  21   ENERGY =     7.853900 EV
OSCILLATOR STRENGTH =      0.005800
                      EXCITATION  DE-EXCITATION
          OCC      VIR  AMPLITUDE     AMPLITUDE
           I        A    X(I->A)       Y(A->I)
          ---      ---  --------      --------
           47      60   -0.108420           0.000000
           54      59   -0.136450           0.000000
           55      60   -0.350420           0.000000
           55      62    0.109640           0.000000
           56      60    0.387450           0.000000
           57      62    0.327510           0.000000


STATE #  22   ENERGY =     8.019700 EV
OSCILLATOR STRENGTH =      0.031500
                      EXCITATION  DE-EXCITATION
          OCC      VIR  AMPLITUDE     AMPLITUDE
           I        A    X(I->A)       Y(A->I)
          ---      ---  --------      --------
           44      58   -0.307850           0.000000
           47      58   -0.167690           0.000000
           48      60    0.153560           0.000000
           51      59    0.196330           0.000000
           54      59   -0.145770           0.000000
           57      63    0.410360           0.000000


STATE #  23   ENERGY =     8.038600 EV
OSCILLATOR STRENGTH =      0.037200
                      EXCITATION  DE-EXCITATION
          OCC      VIR  AMPLITUDE     AMPLITUDE
           I        A    X(I->A)       Y(A->I)
          ---      ---  --------      --------
           43      58   -0.205920           0.000000
           44      58   -0.265740           0.000000
           45      58   -0.252120           0.000000
```

```
        47      58    0.159360          0.000000
        54      59    0.367130          0.000000
        56      61    0.192210          0.000000


STATE #  24   ENERGY =      8.069800 EV
OSCILLATOR STRENGTH =      0.066700
                   EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
        43      58   -0.130130          0.000000
        44      58    0.263700          0.000000
        45      58    0.174660          0.000000
        47      58   -0.211710          0.000000
        52      59   -0.160380          0.000000
        53      59    0.116850          0.000000
        54      59    0.347720          0.000000
        55      60   -0.145790          0.000000
        55      61    0.175380          0.000000
        57      63    0.125320          0.000000


STATE #  25   ENERGY =      8.115700 EV
OSCILLATOR STRENGTH =      0.034600
                   EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
        42      58    0.105150          0.000000
        44      58    0.322880          0.000000
        45      58   -0.108220          0.000000
        46      58    0.221840          0.000000
        47      58    0.113630          0.000000
        51      59   -0.113350          0.000000
        53      58    0.109820          0.000000
        57      63    0.425000          0.000000


STATE #  26   ENERGY =      8.164100 EV
OSCILLATOR STRENGTH =      0.005100
                   EXCITATION  DE-EXCITATION
       OCC      VIR   AMPLITUDE      AMPLITUDE
        I        A     X(I->A)        Y(A->I)
       ---      ---   --------      --------
        43      58    0.578560          0.000000
        43      61    0.100230          0.000000
        51      59   -0.125830          0.000000
        54      59    0.186600          0.000000
        55      61    0.143530          0.000000
        56      61    0.110090          0.000000
        57      63    0.126790          0.000000


STATE #  27   ENERGY =      8.238500 EV
OSCILLATOR STRENGTH =      0.013500
                   EXCITATION  DE-EXCITATION
```

```
           OCC      VIR   AMPLITUDE        AMPLITUDE
            I        A     X(I->A)          Y(A->I)
           ---      ---   --------         --------
            43       58    0.116620         0.000000
            45       58    0.148140         0.000000
            46       58    0.409030         0.000000
            47       58    0.110680         0.000000
            48       58    0.136710         0.000000
            49       59    0.115280         0.000000
            51       58   -0.156630         0.000000
            51       59    0.221430         0.000000
            52       59   -0.207610         0.000000
            53       58    0.112310         0.000000


 STATE #  28  ENERGY =    8.316800 EV
 OSCILLATOR STRENGTH =    0.082700
                   EXCITATION  DE-EXCITATION
           OCC      VIR   AMPLITUDE        AMPLITUDE
            I        A     X(I->A)          Y(A->I)
           ---      ---   --------         --------
            44       58    0.184830         0.000000
            45       58   -0.219640         0.000000
            45       59    0.101550         0.000000
            46       59    0.165470         0.000000
            48       59    0.115230         0.000000
            49       59    0.158330         0.000000
            50       59   -0.131830         0.000000
            51       59    0.455480         0.000000
            53       59   -0.192940         0.000000


 STATE #  29  ENERGY =    8.379200 EV
 OSCILLATOR STRENGTH =    0.003500
                   EXCITATION  DE-EXCITATION
           OCC      VIR   AMPLITUDE        AMPLITUDE
            I        A     X(I->A)          Y(A->I)
           ---      ---   --------         --------
            45       58   -0.202420         0.000000
            46       59   -0.129280         0.000000
            51       59    0.103170         0.000000
            53       59    0.571800         0.000000
            54       59   -0.113180         0.000000


 STATE #  30  ENERGY =    8.447400 EV
 OSCILLATOR STRENGTH =    0.042600
                   EXCITATION  DE-EXCITATION
           OCC      VIR   AMPLITUDE        AMPLITUDE
            I        A     X(I->A)          Y(A->I)
           ---      ---   --------         --------
            45       58    0.163290         0.000000
            46       58    0.104630         0.000000
            47       59   -0.107520         0.000000
            47       62    0.118260         0.000000
            49       60   -0.157030         0.000000
```

```
50        60   0.163700         0.000000
51        60   0.174320         0.000000
52        59   0.252760         0.000000
54        59   0.115310         0.000000
54        60  -0.113440         0.000000
54        61   0.123670         0.000000
54        62  -0.114450         0.000000
55        60   0.189000         0.000000
56        60   0.182950         0.000000
```

A conformer of **5a:**

Table S7.

```
TOTAL FREE ENERGY IN SOLVENT = -1136.860193 A.U.
N              2.71027600    -1.51093800    -0.14176900
 C             1.55064400    -1.20206600     0.37437100
 C             3.80219700    -0.69973600    -0.05400500
 C             1.41502600    -0.00000700     1.28692900
 C             3.80220500     0.69970900    -0.05399500
 N             2.71029500     1.51092400    -0.14175000
 C             1.55065800     1.20205800     0.37438200
 C             5.06128600     1.39155600    -0.17048600
 N             6.06663500     1.97250000    -0.23579100
 C             5.06126900    -1.39159700    -0.17050800
 N             6.06661100    -1.97255200    -0.23582300
 C             0.43522100    -2.05829300     0.01057300
 C            -0.82179500    -1.98214700     0.50141200
 C             0.43524500     2.05830000     0.01058800
 C            -0.82178100     1.98214500     0.50140100
 C            -3.01135300     4.58408900    -1.15664100
 C            -1.88819800     3.80603300    -0.89662200
 C            -1.94133600     2.85064800     0.13414500
 C            -4.21938800     3.57196800     0.49693200
 C            -3.15282000     2.74247000     0.83678500
 C            -4.21939700    -3.57198200     0.49697800
 C            -3.15282100    -2.74249600     0.83683500
 C            -1.94135900    -2.85063700     0.13415100
 C            -3.01141200    -4.58401800    -1.15668400
 C            -1.88825200    -3.80597100    -0.89666400
 H             0.69912000    -2.82367100    -0.71284700
 H            -1.05996800    -1.23434300     1.25275300
 H             0.69916000     2.82369400    -0.71280900
 H            -1.05997200     1.23431600     1.25271200
 H             0.48637700    -0.00000400     1.85251600
 H             2.25029100    -0.00001500     1.99650700
 H            -2.98213200     5.32557500    -1.95201900
 H            -0.99586300     3.94210900    -1.49713700
 H            -5.16016800     3.49636300     1.03805500
 H            -3.26105200     2.02276400     1.64247400
 H            -5.16016000    -3.49640700     1.03813500
 H            -3.26103000    -2.02282900     1.64256200
 H            -2.98221500    -5.32546500    -1.95210000
 H            -0.99593700    -3.94201300    -1.49721600
```

```
N                     -4.16831800     -4.48524100     -0.48178100
N                     -4.16828000      4.48527400     -0.48178000
```

B conformer of **5a:**

Table S8.

```
TOTAL FREE ENERGY IN SOLVENT = -1136.862906 A.U.
N                     -2.15964300      0.15456900      1.51209700
 C                    -1.13700600      0.89856000      1.19148500
 C                    -3.24040600     -0.00442500      0.70152400
 C                    -1.21181200      1.82992900      0.00000000
 C                    -3.24040600     -0.00442500     -0.70152400
 N                    -2.15964300      0.15456900     -1.51209700
 C                    -1.13700600      0.89856000     -1.19148500
 C                     0.09787400      0.82910800      1.96119600
 C                     0.28264700     -0.03127600      2.98749900
 C                     0.09787400      0.82910800     -1.96119600
 C                     0.28264700     -0.03127600     -2.98749900
 C                     2.62394400     -1.21690400     -5.66287300
 C                     1.49080100     -1.09686000     -4.86083100
 C                     1.47400300     -0.14712300     -3.82561300
 C                     3.70886100      0.43771200     -4.52008400
 C                     2.63072200      0.63778600     -3.66517400
 C                     2.62394400     -1.21690400      5.66287300
 C                     1.49080100     -1.09686000      4.86083100
 C                     1.47400300     -0.14712300      3.82561300
 C                     3.70886100      0.43771200      4.52008400
 C                     2.63072200      0.63778600      3.66517400
 C                    -4.44497400     -0.39488000      1.39054600
 N                    -5.41140600     -0.68234700      1.97025800
 C                    -4.44497400     -0.39488000     -1.39054600
 N                    -5.41140600     -0.68234700     -1.97025800
 H                     0.87760400      1.52647300      1.67132600
 H                    -0.53534700     -0.70659700      3.22799400
 H                     0.87760400      1.52647300     -1.67132600
 H                    -0.53534700     -0.70659700     -3.22799400
 H                    -2.17678500      2.34903000      0.00000000
 H                     2.64522100     -1.94944400     -6.46691700
 H                     0.62917700     -1.73322400     -5.03707100
 H                     4.60861100      1.03847400     -4.40574700
 H                     2.69884000      1.39432600     -2.89118000
 H                     2.64522100     -1.94944400      6.46691700
 H                     0.62917700     -1.73322400      5.03707100
 H                     4.60861100      1.03847400      4.40574700
 H                     2.69884000      1.39432600      2.89118000
 H                    -0.40389900      2.56191200      0.00000000
 N                     3.72574400     -0.47014400     -5.51002000
 N                     3.72574400     -0.47014400      5.51002000
```

Table S9.

TD–DFT output

HOMO: 91, LUMO: 92

```
STATE #  1  ENERGY =   3.297400 EV
 OSCILLATOR STRENGTH =    1.058500
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE    AMPLITUDE
      I        A    X(I->A)      Y(A->I)
     ---      ---  --------    --------
      90       93   0.128280    0.000000
      91       92   0.676920    0.000000


 STATE #  2  ENERGY =   3.926600 EV
 OSCILLATOR STRENGTH =    0.267500
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE    AMPLITUDE
      I        A    X(I->A)      Y(A->I)
     ---      ---  --------    --------
      85       93   0.190010    0.000000
      90       92  -0.152890    0.000000
      91       93   0.618670    0.000000


 STATE #  3  ENERGY =   4.230800 EV
 OSCILLATOR STRENGTH =    0.020900
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE    AMPLITUDE
      I        A    X(I->A)      Y(A->I)
     ---      ---  --------    --------
      83       93  -0.185290    0.000000
      84       92   0.366870    0.000000
      85       92   0.524720    0.000000
      87       92   0.112750    0.000000


 STATE #  4  ENERGY =   4.399400 EV
 OSCILLATOR STRENGTH =    1.161400
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE    AMPLITUDE
      I        A    X(I->A)      Y(A->I)
     ---      ---  --------    --------
      90       92   0.657330    0.000000
      91       93   0.179230    0.000000


 STATE #  5  ENERGY =   4.568200 EV
 OSCILLATOR STRENGTH =    0.002000
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE    AMPLITUDE
      I        A    X(I->A)      Y(A->I)
     ---      ---  --------    --------
      83       92  -0.138830    0.000000
      85       93   0.131060    0.000000
      86       92   0.455530    0.000000
      86       94  -0.227420    0.000000
      86       98   0.143050    0.000000
      87       93  -0.358920    0.000000
      87       95  -0.175130    0.000000
```

```
STATE #   6  ENERGY =    4.573300 EV
OSCILLATOR STRENGTH =    0.001100
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE    AMPLITUDE
    I       A    X(I->A)      Y(A->I)
   ---     ---  --------    --------
    86      93  -0.392610    0.000000
    86      95  -0.183510    0.000000
    87      92   0.456570    0.000000
    87      94  -0.230880    0.000000
    87      98   0.145910    0.000000

STATE #   7  ENERGY =    4.658000 EV
OSCILLATOR STRENGTH =    0.032500
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE    AMPLITUDE
    I       A    X(I->A)      Y(A->I)
   ---     ---  --------    --------
    83      92   0.536180    0.000000
    83      98  -0.106640    0.000000
    84      93  -0.237630    0.000000
    85      93  -0.204640    0.000000
    87      93  -0.150220    0.000000
    91      93   0.175810    0.000000

STATE #   8  ENERGY =    4.740900 EV
OSCILLATOR STRENGTH =    0.029500
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE    AMPLITUDE
    I       A    X(I->A)      Y(A->I)
   ---     ---  --------    --------
    88      93  -0.357990    0.000000
    89      92   0.523340    0.000000
    89      94  -0.167430    0.000000
    90      97   0.125880    0.000000
    91      96  -0.123780    0.000000

STATE #   9  ENERGY =    4.744300 EV
OSCILLATOR STRENGTH =    0.056900
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE    AMPLITUDE
    I       A    X(I->A)      Y(A->I)
   ---     ---  --------    --------
    88      92   0.523610    0.000000
    88      94  -0.166810    0.000000
    89      93  -0.356980    0.000000
    90      96   0.139750    0.000000
    91      97  -0.113830    0.000000

STATE #  10  ENERGY =    4.916100 EV
OSCILLATOR STRENGTH =    0.228300
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
```

```
        I       A     X(I->A)        Y(A->I)
       ---     ---    --------       --------
        83      93    0.186070       0.000000
        84      92    0.182720       0.000000
        85      94    0.198020       0.000000
        90      93    0.582400       0.000000


 STATE #  11   ENERGY =     5.070100 EV
 OSCILLATOR STRENGTH =      0.245300
                   EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I       A     X(I->A)        Y(A->I)
         ---     ---    --------       --------
          83      92    0.359890       0.000000
          83      94    0.138080       0.000000
          84      93    0.178700       0.000000
          85      93    0.479520       0.000000
          90      94    0.143110       0.000000
          91      93   -0.135270       0.000000


 STATE #  12   ENERGY =     5.179700 EV
 OSCILLATOR STRENGTH =      0.001400
                   EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I       A     X(I->A)        Y(A->I)
         ---     ---    --------       --------
          83      93   -0.124910       0.000000
          91      94    0.648660       0.000000


 STATE #  13   ENERGY =     5.379300 EV
 OSCILLATOR STRENGTH =      0.000600
                   EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I       A     X(I->A)        Y(A->I)
         ---     ---    --------       --------
          81      92    0.111870       0.000000
          82      93    0.116890       0.000000
          83      93   -0.141500       0.000000
          84      92    0.482860       0.000000
          85      92   -0.392440       0.000000


 STATE #  14   ENERGY =     5.640300 EV
 OSCILLATOR STRENGTH =      0.003400
                   EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I       A     X(I->A)        Y(A->I)
         ---     ---    --------       --------
          83      93    0.447970       0.000000
          83      95   -0.106720       0.000000
          84      92    0.173080       0.000000
          84      94    0.231590       0.000000
          85      94    0.199740       0.000000
          90      93   -0.321230       0.000000
```

```
      91       92    0.104380        0.000000


STATE #  15  ENERGY =    5.756200 EV
OSCILLATOR STRENGTH =    0.000000
                 EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---   --------      --------
      86       96    0.496420        0.000000
      87       95    0.204610        0.000000
      87       97    0.439890        0.000000


STATE #  16  ENERGY =    5.756200 EV
OSCILLATOR STRENGTH =    0.000000
                 EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---   --------      --------
      85       96   -0.107060        0.000000
      86       95    0.209350        0.000000
      86       97    0.450760        0.000000
      87       96    0.484600        0.000000


STATE #  17  ENERGY =    5.824400 EV
OSCILLATOR STRENGTH =    0.002300
                 EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---   --------      --------
      88       92    0.468550        0.000000
      88       94    0.154840        0.000000
      89       93    0.429000        0.000000
      90       96   -0.130000        0.000000
      91       97    0.127800        0.000000


STATE #  18  ENERGY =    5.825400 EV
OSCILLATOR STRENGTH =    0.000200
                 EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---   --------      --------
      88       93    0.430250        0.000000
      89       92    0.468570        0.000000
      89       94    0.154460        0.000000
      90       97   -0.116570        0.000000
      91       96    0.145980        0.000000


STATE #  19  ENERGY =    5.928100 EV
OSCILLATOR STRENGTH =    0.001700
                 EXCITATION  DE-EXCITATION
      OCC      VIR   AMPLITUDE     AMPLITUDE
       I        A    X(I->A)        Y(A->I)
      ---      ---   --------      --------
```

```
        82       92    -0.138320          0.000000
        84       99    -0.101330          0.000000
        85       99     0.219210          0.000000
        91       95     0.326810          0.000000
        91       97    -0.127280          0.000000
        91       99     0.502910          0.000000


   STATE #  20   ENERGY =    6.028200 EV
   OSCILLATOR STRENGTH =     0.004400
                    EXCITATION  DE-EXCITATION
         OCC      VIR  AMPLITUDE    AMPLITUDE
          I        A    X(I->A)      Y(A->I)
         ---      ---   --------     --------
         80       92    -0.275620          0.000000
         80       94    -0.167370          0.000000
         82       92     0.386140          0.000000
         82       94     0.101080          0.000000
         90       94    -0.175390          0.000000
         91       95    -0.196410          0.000000
         91       99     0.257380          0.000000


   STATE #  21   ENERGY =    6.102700 EV
   OSCILLATOR STRENGTH =     0.003300
                    EXCITATION  DE-EXCITATION
         OCC      VIR  AMPLITUDE    AMPLITUDE
          I        A    X(I->A)      Y(A->I)
         ---      ---   --------     --------
         85       92    -0.130650          0.000000
         86       93     0.398210          0.000000
         86       95     0.101820          0.000000
         87       92     0.507160          0.000000
         87       94     0.154410          0.000000
         87       98    -0.119110          0.000000


   STATE #  22   ENERGY =    6.102900 EV
   OSCILLATOR STRENGTH =     0.001900
                    EXCITATION  DE-EXCITATION
         OCC      VIR  AMPLITUDE    AMPLITUDE
          I        A    X(I->A)      Y(A->I)
         ---      ---   --------     --------
         86       92     0.506170          0.000000
         86       94     0.149170          0.000000
         86       98    -0.115640          0.000000
         87       93     0.395520          0.000000


   STATE #  23   ENERGY =    6.153700 EV
   OSCILLATOR STRENGTH =     0.048300
                    EXCITATION  DE-EXCITATION
         OCC      VIR  AMPLITUDE    AMPLITUDE
          I        A    X(I->A)      Y(A->I)
         ---      ---   --------     --------
         80       92     0.107120          0.000000
         84       93     0.428060          0.000000
```

```
    85      93    -0.317150        0.000000
    90      94     0.150120        0.000000
    91      95    -0.256450        0.000000
    91      97     0.108730        0.000000
    91      99     0.145810        0.000000


STATE #  24   ENERGY =      6.254500 EV
OSCILLATOR STRENGTH =     0.035300
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I       A     X(I->A)      Y(A->I)
    ---     ---   --------     --------
    84      93    -0.290550        0.000000
    88      96     0.120520        0.000000
    89      93     0.193920        0.000000
    89      97     0.139810        0.000000
    90      94     0.404750        0.000000
    90      96     0.123070        0.000000
    91      95    -0.278310        0.000000
    91      99     0.134680        0.000000


STATE #  25   ENERGY =      6.319400 EV
OSCILLATOR STRENGTH =     0.005800
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I       A     X(I->A)      Y(A->I)
    ---     ---   --------     --------
    83      93    -0.228760        0.000000
    85      94     0.327990        0.000000
    88      93     0.217930        0.000000
    88      97     0.109580        0.000000
    90      95     0.192630        0.000000
    91      94    -0.113600        0.000000
    91      96    -0.233890        0.000000
    91      98     0.288050        0.000000


STATE #  26   ENERGY =      6.400100 EV
OSCILLATOR STRENGTH =     0.038600
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I       A     X(I->A)      Y(A->I)
    ---     ---   --------     --------
    83      93    -0.171480        0.000000
    84      94     0.100700        0.000000
    85      94     0.194890        0.000000
    85      96    -0.107710        0.000000
    88      93    -0.325010        0.000000
    88      95     0.144230        0.000000
    89      94     0.122580        0.000000
    89      98    -0.117190        0.000000
    90      97    -0.225040        0.000000
    91      96     0.331670        0.000000
    91      98     0.159290        0.000000
```

```
STATE #  27   ENERGY =    6.402400 EV
OSCILLATOR STRENGTH =    0.007900
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------    --------
     75       92   0.130240    0.000000
     80       92  -0.359590    0.000000
     80       94  -0.203540    0.000000
     89       93  -0.138260    0.000000
     90       94   0.393290    0.000000
     91       95   0.186060    0.000000
     91       99  -0.118930    0.000000

STATE #  28   ENERGY =    6.416700 EV
OSCILLATOR STRENGTH =    0.074500
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------    --------
     80       92   0.193840    0.000000
     80       94   0.124030    0.000000
     84       93  -0.179370    0.000000
     88       94   0.117510    0.000000
     88       98  -0.114560    0.000000
     89       93  -0.314860    0.000000
     89       95   0.152340    0.000000
     90       96  -0.206260    0.000000
     91       97   0.355430    0.000000
     91       99   0.109500    0.000000

STATE #  29   ENERGY =    6.525000 EV
OSCILLATOR STRENGTH =    0.006000
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------    --------
     76       92   0.140490    0.000000
     77       92  -0.131260    0.000000
     79       92   0.115890    0.000000
     81       92   0.512150    0.000000
     82       93  -0.211170    0.000000
     85       94  -0.163070    0.000000
     91       98   0.120710    0.000000

STATE #  30   ENERGY =    6.549200 EV
OSCILLATOR STRENGTH =    0.011100
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------    --------
     76       92  -0.112300    0.000000
```

77	92	-0.281700	0.000000
77	94	-0.185990	0.000000
78	93	0.192260	0.000000
79	92	-0.299350	0.000000
84	94	-0.138630	0.000000
85	94	-0.109830	0.000000
91	98	0.306320	0.000000

B conformer of **5b:**

Table S10.

TOTAL FREE ENERGY IN SOLVENT = -6247.006420 A.U.

N	3.58616800	-0.11518500	1.51684200
C	2.61359800	-0.92606900	1.19561100
C	4.64944900	0.12051500	0.70171500
C	2.75082000	-1.84595400	0.00000000
C	4.64944900	0.12051500	-0.70171500
N	3.58616800	-0.11518500	-1.51684200
C	2.61359800	-0.92606900	-1.19561100
C	1.38104300	-0.94732400	1.96525700
C	1.13451200	-0.09694000	2.99050100
C	1.38104300	-0.94732400	-1.96525700
C	1.13451200	-0.09694000	-2.99050100
C	-2.25448100	-0.83390200	-4.52217100
C	-1.14819400	-0.92351800	-3.68730100
C	-2.27418500	0.13647000	-5.52727800
C	-0.04936800	-0.05223400	-3.83823400
C	-1.20677900	1.01382100	-5.70689300
C	-0.10496100	0.91311500	-4.86259900
C	-1.20677900	1.01382100	5.70689300
C	-0.10496100	0.91311500	4.86259900
C	-2.27418500	0.13647000	5.52727800
C	-0.04936800	-0.05223400	3.83823400
C	-2.25448100	-0.83390200	4.52217100
C	-1.14819400	-0.92351800	3.68730100
C	5.82567600	0.59336000	1.38842500
N	6.77026200	0.94817700	1.96728800
C	5.82567600	0.59336000	-1.38842500
N	6.77026200	0.94817700	-1.96728800
H	0.65542800	-1.70175400	1.67794300
H	1.90680300	0.63461900	3.21839600
H	0.65542800	-1.70175400	-1.67794300
H	1.90680300	0.63461900	-3.21839600
H	1.99493600	-2.63180900	0.00000000
H	-3.09391400	-1.50805300	-4.39815000
H	-1.14424900	-1.68171500	-2.91144500
H	-1.23537600	1.76124700	-6.49102100
H	0.73002900	1.59428500	-4.99782200
H	-1.23537600	1.76124700	6.49102100
H	0.73002900	1.59428500	4.99782200
H	-3.09391400	-1.50805300	4.39815000
H	-1.14424900	-1.68171500	2.91144500
Br	-3.79530900	0.25971500	6.67579400

```
Br                     -3.79530900    0.25971500   -6.67579400
H                       3.74856700   -2.29917000    0.00000000
```

Table S11.

TD–DFT output
HOMO: 125, LUMO: 126

```
STATE #   1  ENERGY =     3.138800 EV
 OSCILLATOR STRENGTH =     1.242400
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---      ---  --------      --------
    124      127   0.155110     0.000000
    125      126   0.669870     0.000000


STATE #   2  ENERGY =     3.880000 EV
 OSCILLATOR STRENGTH =     0.336000
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---      ---  --------      --------
    123      127   0.197820     0.000000
    124      126  -0.164440     0.000000
    125      127   0.613400     0.000000


STATE #   3  ENERGY =     4.073500 EV
 OSCILLATOR STRENGTH =     1.422300
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---      ---  --------      --------
    119      126   0.132780     0.000000
    124      126   0.640490     0.000000
    125      127   0.207710     0.000000


STATE #   4  ENERGY =     4.216100 EV
 OSCILLATOR STRENGTH =     0.006000
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---      ---  --------      --------
    115      126   0.155290     0.000000
    116      127   0.181480     0.000000
    120      126   0.464770     0.000000
    123      126   0.425390     0.000000


STATE #   5  ENERGY =     4.654800 EV
 OSCILLATOR STRENGTH =     0.220300
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
```

```
          I      A     X(I->A)      Y(A->I)
         ---    ---   --------     --------
         116    127  -0.126520     0.000000
         119    127   0.100560     0.000000
         120    126   0.166490     0.000000
         123    128   0.129970     0.000000
         124    127   0.601730     0.000000
         125    126  -0.135550     0.000000


STATE #   6  ENERGY =    4.677400 EV
OSCILLATOR STRENGTH =    0.027700
                  EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I      A     X(I->A)      Y(A->I)
         ---    ---   --------     --------
         115    127   0.140980     0.000000
         116    126   0.501300     0.000000
         116    133  -0.108270     0.000000
         120    127   0.310740     0.000000
         123    127   0.212910     0.000000
         125    127  -0.169130     0.000000


STATE #   7  ENERGY =    4.809100 EV
OSCILLATOR STRENGTH =    0.000900
                  EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I      A     X(I->A)      Y(A->I)
         ---    ---   --------     --------
         121    126   0.451600     0.000000
         121    128  -0.173740     0.000000
         122    127  -0.332860     0.000000
         122    131   0.110730     0.000000
         123    130   0.121940     0.000000
         124    129  -0.225250     0.000000
         125    130  -0.229390     0.000000


STATE #   8  ENERGY =    4.809600 EV
OSCILLATOR STRENGTH =    0.014800
                  EXCITATION  DE-EXCITATION
         OCC     VIR  AMPLITUDE    AMPLITUDE
          I      A     X(I->A)      Y(A->I)
         ---    ---   --------     --------
         121    127  -0.333370     0.000000
         121    131   0.110910     0.000000
         122    126   0.452780     0.000000
         122    128  -0.174230     0.000000
         123    129  -0.117500     0.000000
         124    130   0.231020     0.000000
         125    129   0.229300     0.000000


STATE #   9  ENERGY =    4.994900 EV
OSCILLATOR STRENGTH =    0.168700
                  EXCITATION  DE-EXCITATION
```

```
          OCC     VIR  AMPLITUDE      AMPLITUDE
           I       A    X(I->A)        Y(A->I)
          ---     ---  --------       --------
          116     126   0.415810       0.000000
          116     128   0.130560       0.000000
          120     127  -0.250540       0.000000
          123     127  -0.411730       0.000000
          124     128  -0.149240       0.000000
          125     127   0.111140       0.000000


  STATE #  10  ENERGY =     5.079300 EV
  OSCILLATOR STRENGTH =     0.000700
                    EXCITATION  DE-EXCITATION
          OCC     VIR  AMPLITUDE      AMPLITUDE
           I       A    X(I->A)        Y(A->I)
          ---     ---  --------       --------
          115     126   0.133040       0.000000
          120     126   0.122290       0.000000
          123     126  -0.104600       0.000000
          123     128   0.156840       0.000000
          125     128   0.619850       0.000000


  STATE #  11  ENERGY =     5.108700 EV
  OSCILLATOR STRENGTH =     0.007300
                    EXCITATION  DE-EXCITATION
          OCC     VIR  AMPLITUDE      AMPLITUDE
           I       A    X(I->A)        Y(A->I)
          ---     ---  --------       --------
          115     126  -0.255980       0.000000
          119     127   0.131810       0.000000
          120     126  -0.288360       0.000000
          123     126   0.490840       0.000000
          124     127   0.137800       0.000000
          125     128   0.178000       0.000000


  STATE #  12  ENERGY =     5.575600 EV
  OSCILLATOR STRENGTH =     0.019100
                    EXCITATION  DE-EXCITATION
          OCC     VIR  AMPLITUDE      AMPLITUDE
           I       A    X(I->A)        Y(A->I)
          ---     ---  --------       --------
          115     128  -0.108240       0.000000
          116     127   0.473580       0.000000
          116     131   0.118800       0.000000
          120     126  -0.100650       0.000000
          120     128  -0.296960       0.000000
          123     128  -0.156260       0.000000
          124     127   0.226880       0.000000


  STATE #  13  ENERGY =     5.688700 EV
  OSCILLATOR STRENGTH =     0.050900
                    EXCITATION  DE-EXCITATION
          OCC     VIR  AMPLITUDE      AMPLITUDE
```

I	A	X(I->A)	Y(A->I)
114	126	-0.219660	0.000000
119	126	0.535500	0.000000
120	127	-0.105760	0.000000
124	126	-0.147840	0.000000
124	128	0.175710	0.000000
125	127	0.110920	0.000000
125	131	-0.169970	0.000000

STATE # 14 ENERGY =   5.796500 EV
OSCILLATOR STRENGTH =   0.026800

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
121	131	-0.105880	0.000000
122	126	0.456940	0.000000
122	133	-0.106110	0.000000
124	128	-0.141510	0.000000
124	130	-0.239460	0.000000
125	129	-0.347470	0.000000
125	132	0.113640	0.000000

STATE # 15 ENERGY =   5.810400 EV
OSCILLATOR STRENGTH =   0.041800

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
121	126	0.495580	0.000000
121	133	-0.113780	0.000000
122	131	-0.109040	0.000000
123	130	-0.109880	0.000000
124	129	0.258170	0.000000
125	130	0.339830	0.000000

STATE # 16 ENERGY =   5.855100 EV
OSCILLATOR STRENGTH =   0.018100

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
115	132	-0.117390	0.000000
119	126	-0.107610	0.000000
122	126	-0.159210	0.000000
123	132	0.275550	0.000000
125	131	-0.248650	0.000000
125	132	0.486590	0.000000

STATE # 17 ENERGY =   5.880300 EV
OSCILLATOR STRENGTH =   0.090400

EXCITATION DE-EXCITATION

```
          OCC     VIR   AMPLITUDE      AMPLITUDE
           I       A     X(I->A)        Y(A->I)
          ---     ---   --------       --------
          115     127   -0.201320      0.000000
          116     126    0.102840      0.000000
          119     128   -0.143240      0.000000
          120     127   -0.356620      0.000000
          123     127    0.422440      0.000000
          124     128   -0.187470      0.000000
          125     131   -0.110260      0.000000


STATE #  18   ENERGY =    5.917100 EV
OSCILLATOR STRENGTH =    0.000900
                  EXCITATION  DE-EXCITATION
          OCC     VIR   AMPLITUDE      AMPLITUDE
           I       A     X(I->A)        Y(A->I)
          ---     ---   --------       --------
          119     135   -0.194310      0.000000
          120     134   -0.135990      0.000000
          123     134    0.283730      0.000000
          124     132    0.101620      0.000000
          124     135    0.419120      0.000000
          125     134   -0.388270      0.000000


STATE #  19   ENERGY =    5.917600 EV
OSCILLATOR STRENGTH =    0.001600
                  EXCITATION  DE-EXCITATION
          OCC     VIR   AMPLITUDE      AMPLITUDE
           I       A     X(I->A)        Y(A->I)
          ---     ---   --------       --------
          119     134   -0.195490      0.000000
          120     135   -0.135190      0.000000
          123     135    0.273620      0.000000
          124     134    0.422050      0.000000
          125     135   -0.394090      0.000000


STATE #  20   ENERGY =    6.014100 EV
OSCILLATOR STRENGTH =    0.022300
                  EXCITATION  DE-EXCITATION
          OCC     VIR   AMPLITUDE      AMPLITUDE
           I       A     X(I->A)        Y(A->I)
          ---     ---   --------       --------
          114     126    0.112270      0.000000
          120     127   -0.195760      0.000000
          121     127    0.116510      0.000000
          122     126    0.140080      0.000000
          124     128    0.484590      0.000000
          125     131    0.234180      0.000000
          125     132    0.182950      0.000000


STATE #  21   ENERGY =    6.057700 EV
OSCILLATOR STRENGTH =    0.000000
                  EXCITATION  DE-EXCITATION
```

```
           OCC       VIR   AMPLITUDE        AMPLITUDE
            I         A      X(I->A)          Y(A->I)
           ---       ---    --------         --------
           113       126    0.173410         0.000000
           115       126    0.503550         0.000000
           119       127    0.270440         0.000000
           120       126   -0.255750         0.000000
           123       128   -0.130850         0.000000


STATE #  22   ENERGY =    6.163200 EV
OSCILLATOR STRENGTH =    0.003700
                     EXCITATION  DE-EXCITATION
           OCC       VIR   AMPLITUDE        AMPLITUDE
            I         A      X(I->A)          Y(A->I)
           ---       ---    --------         --------
           115       127    0.146640         0.000000
           119       126    0.251550         0.000000
           119       128   -0.102040         0.000000
           124       128   -0.291610         0.000000
           124       133   -0.143000         0.000000
           125       129    0.174920         0.000000
           125       131    0.382790         0.000000
           125       132    0.179250         0.000000


STATE #  23   ENERGY =    6.190700 EV
OSCILLATOR STRENGTH =    0.000000
                     EXCITATION  DE-EXCITATION
           OCC       VIR   AMPLITUDE        AMPLITUDE
            I         A      X(I->A)          Y(A->I)
           ---       ---    --------         --------
           117       126    0.529850         0.000000
           117       128   -0.189570         0.000000
           117       133    0.113110         0.000000
           118       127    0.349030         0.000000
           118       131   -0.145820         0.000000


STATE #  24   ENERGY =    6.190900 EV
OSCILLATOR STRENGTH =    0.000000
                     EXCITATION  DE-EXCITATION
           OCC       VIR   AMPLITUDE        AMPLITUDE
            I         A      X(I->A)          Y(A->I)
           ---       ---    --------         --------
           117       127    0.350910         0.000000
           117       131   -0.148590         0.000000
           118       126    0.530040         0.000000
           118       128   -0.189220         0.000000
           118       133    0.113590         0.000000


STATE #  25   ENERGY =    6.201900 EV
OSCILLATOR STRENGTH =    0.000700
                     EXCITATION  DE-EXCITATION
           OCC       VIR   AMPLITUDE        AMPLITUDE
            I         A      X(I->A)          Y(A->I)
```

```
---     ---   --------      --------
116     127   0.216540      0.000000
120     126  -0.104640      0.000000
120     128   0.128310      0.000000
121     126   0.121620      0.000000
122     127   0.256200      0.000000
123     128   0.291630      0.000000
124     131  -0.188120      0.000000
125     128  -0.119380      0.000000
125     130  -0.109830      0.000000
125     133   0.336690      0.000000


STATE #  26   ENERGY =    6.284300 EV
OSCILLATOR STRENGTH =     0.088400
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---     ---   --------      --------
    121     127   0.551370      0.000000
    122     126   0.179130      0.000000
    124     130   0.154470      0.000000
    125     129   0.259540      0.000000
    125     131  -0.169300      0.000000


STATE #  27   ENERGY =    6.287500 EV
OSCILLATOR STRENGTH =     0.102200
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---     ---   --------      --------
    116     127  -0.116170      0.000000
    121     126   0.162910      0.000000
    122     127   0.512730      0.000000
    123     128  -0.154280      0.000000
    124     129  -0.121810      0.000000
    124     131   0.125030      0.000000
    125     130  -0.276960      0.000000
    125     133  -0.153140      0.000000


STATE #  28   ENERGY =    6.370500 EV
OSCILLATOR STRENGTH =     0.011800
                  EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)       Y(A->I)
    ---     ---   --------      --------
    106     126  -0.129970      0.000000
    112     126   0.463020      0.000000
    112     128   0.257250      0.000000
    114     126  -0.213490      0.000000
    114     128  -0.112940      0.000000
    124     128  -0.100050      0.000000
    125     131   0.152020      0.000000
    125     132   0.124210      0.000000
```

```
STATE #  29   ENERGY =    6.487900 EV
OSCILLATOR STRENGTH =     0.004500
               EXCITATION  DE-EXCITATION
    OCC    VIR  AMPLITUDE    AMPLITUDE
     I      A    X(I->A)      Y(A->I)
    ---    ---  --------     --------
    113    126   0.102310    0.000000
    116    127  -0.240570    0.000000
    119    127  -0.140610    0.000000
    120    128  -0.237290    0.000000
    123    128  -0.239260    0.000000
    124    131  -0.230100    0.000000
    125    133   0.350140    0.000000


STATE #  30   ENERGY =    6.535600 EV
OSCILLATOR STRENGTH =     0.008200
               EXCITATION  DE-EXCITATION
    OCC    VIR  AMPLITUDE    AMPLITUDE
     I      A    X(I->A)      Y(A->I)
    ---    ---  --------     --------
    107    126  -0.170030    0.000000
    107    128  -0.120490    0.000000
    113    126  -0.144730    0.000000
    114    127  -0.129750    0.000000
    115    126  -0.148930    0.000000
    115    128  -0.126840    0.000000
    119    127   0.448220    0.000000
    120    126   0.149510    0.000000
    123    126  -0.101210    0.000000
    123    128  -0.170590    0.000000
    125    133   0.165300    0.000000
```

B conformer of **5c:**

Table S12.

```
TOTAL FREE ENERGY IN SOLVENT = -1795.746848 A.U.
 N          4.76035500   -0.02941000    1.52333500
 C          3.82929600   -0.89098200    1.20113500
 C          5.80328700    0.26815600    0.70209900
 C          4.01464200   -1.79626200    0.00000000
 C          5.80328700    0.26815600   -0.70209900
 N          4.76035500   -0.02941000   -1.52333500
 C          3.82929600   -0.89098200   -1.20113500
 C          2.60668800   -0.98838000    1.97196500
 C          2.30779200   -0.15204200    2.99974400
 C          2.60668800   -0.98838000   -1.97196500
 C          2.30779200   -0.15204200   -2.99974400
 C         -0.07907200    0.82750700   -5.72769200
 C          1.01703800    0.78774900   -4.87069300
 C         -1.10230700   -0.12007200   -5.57953200
 C          1.13550300   -0.17709200   -3.85281500
 C         -1.00498100   -1.09549500   -4.56636400
```

C	0.08944800	-1.12197800	-3.72418000
O	-2.21622700	-0.18759600	-6.34938900
C	-2.38414800	0.77617900	-7.41115200
C	-0.07907200	0.82750700	5.72769200
C	1.01703800	0.78774900	4.87069300
C	-1.10230700	-0.12007200	5.57953200
C	1.13550300	-0.17709200	3.85281500
C	-1.00498100	-1.09549500	4.56636400
C	0.08944800	-1.12197800	3.72418000
O	-2.21622700	-0.18759600	6.34938900
C	-2.38414800	0.77617900	7.41115200
C	6.95347200	0.80583800	1.38561700
N	7.87745100	1.21398100	1.96327000
C	6.95347200	0.80583800	-1.38561700
N	7.87745100	1.21398100	-1.96327000
H	1.92756300	-1.78624400	1.68803800
H	3.03511600	0.62721400	3.21971700
H	1.92756300	-1.78624400	-1.68803800
H	3.03511600	0.62721400	-3.21971700
H	5.03497400	-2.19668900	0.00000000
H	-0.12612000	1.58837600	-6.49655700
H	1.80576100	1.52499400	-4.99243800
H	-1.80679900	-1.81969800	-4.46910700
H	0.13769700	-1.88634600	-2.95534000
H	-1.53910300	0.69959600	-8.10535300
H	-2.39296900	1.78586200	-6.98394000
H	-0.12612000	1.58837600	6.49655700
H	1.80576100	1.52499400	4.99243800
H	-1.80679900	-1.81969800	4.46910700
H	0.13769700	-1.88634600	2.95534000
H	-2.39296900	1.78586200	6.98394000
H	-1.53910300	0.69959600	8.10535300
H	3.30184200	-2.62160200	0.00000000
C	-3.68300200	0.47631400	-8.11024900
C	-4.87797600	1.05505800	-7.66548800
C	-3.71606900	-0.40485000	-9.19794500
C	-6.08624000	0.75979600	-8.29765900
H	-4.86013000	1.74087500	-6.82250900
C	-4.92278600	-0.70205600	-9.83227300
H	-2.79248900	-0.85711000	-9.54975400
C	-6.10988500	-0.11973600	-9.38242700
H	-7.00651100	1.21718400	-7.94680700
H	-4.93633200	-1.38392400	-10.67729300
H	-7.04920000	-0.34755200	-9.87756900
C	-3.68300200	0.47631400	8.11024900
C	-3.71606900	-0.40485000	9.19794500
C	-4.87797600	1.05505800	7.66548800
C	-4.92278600	-0.70205600	9.83227300
H	-2.79248900	-0.85711000	9.54975400
C	-6.08624000	0.75979600	8.29765900
H	-4.86013000	1.74087500	6.82250900
C	-6.10988500	-0.11973600	9.38242700
H	-4.93633200	-1.38392400	10.67729300

```
H                          -7.00651100    1.21718400    7.94680700
H                          -7.04920000   -0.34755200    9.87756900
```

Table S13.

TD–DFT output
HOMO: 147, LUMO: 148
STATE #   1   ENERGY =   2.999600 EV
 OSCILLATOR STRENGTH =   1.329100
                  EXCITATION DE-EXCITATION
     OCC   VIR AMPLITUDE   AMPLITUDE
      I   A   X(I->A)   Y(A->I)
     ---   --- --------   --------
     146   149 -0.165200   0.000000
     147   148   0.666040   0.000000

 STATE #   2   ENERGY =   3.811800 EV
 OSCILLATOR STRENGTH =   0.004400
                  EXCITATION DE-EXCITATION
     OCC   VIR AMPLITUDE   AMPLITUDE
      I   A   X(I->A)   Y(A->I)
     ---   --- --------   --------
     137   148 -0.138370   0.000000
     143   149 -0.120990   0.000000
     145   149 -0.164160   0.000000
     146   148   0.450100   0.000000
     147   149   0.458670   0.000000

 STATE #   3   ENERGY =   3.869300 EV
 OSCILLATOR STRENGTH =   1.849700
                  EXCITATION DE-EXCITATION
     OCC   VIR AMPLITUDE   AMPLITUDE
      I   A   X(I->A)   Y(A->I)
     ---   --- --------   --------
     146   148   0.494980   0.000000
     147   149 -0.466660   0.000000

 STATE #   4   ENERGY =   4.225200 EV
 OSCILLATOR STRENGTH =   0.000000
                  EXCITATION DE-EXCITATION
     OCC   VIR AMPLITUDE   AMPLITUDE
      I   A   X(I->A)   Y(A->I)
     ---   --- --------   --------
     135   148   0.120000   0.000000
     136   149   0.175950   0.000000
     138   148   0.466090   0.000000
     143   148   0.277250   0.000000
     145   148   0.336560   0.000000
     147   150   0.103370   0.000000

 STATE #   5   ENERGY =   4.470300 EV
 OSCILLATOR STRENGTH =   0.232000
                  EXCITATION DE-EXCITATION
```

```
       OCC     VIR   AMPLITUDE      AMPLITUDE
        I       A    X(I->A)        Y(A->I)
       ---     ---   --------      --------
       136     149   -0.109070     0.000000
       138     148    0.131050     0.000000
       146     149    0.624350     0.000000
       147     148    0.158060     0.000000


STATE #   6  ENERGY =    4.710700 EV
OSCILLATOR STRENGTH =    0.034800
                  EXCITATION  DE-EXCITATION
       OCC     VIR   AMPLITUDE      AMPLITUDE
        I       A    X(I->A)        Y(A->I)
       ---     ---   --------      --------
       135     149    0.117800     0.000000
       136     148    0.444650     0.000000
       138     149    0.353620     0.000000
       143     149    0.177710     0.000000
       145     149    0.216680     0.000000
       147     149    0.160600     0.000000


STATE #   7  ENERGY =    4.808600 EV
OSCILLATOR STRENGTH =    0.001600
                  EXCITATION  DE-EXCITATION
       OCC     VIR   AMPLITUDE      AMPLITUDE
        I       A    X(I->A)        Y(A->I)
       ---     ---   --------      --------
       139     148    0.417130     0.000000
       139     150   -0.166020     0.000000
       140     149   -0.304880     0.000000
       145     148   -0.102200     0.000000
       146     151   -0.195730     0.000000
       146     153    0.168800     0.000000
       147     152   -0.210870     0.000000
       147     154    0.178350     0.000000


STATE #   8  ENERGY =    4.810600 EV
OSCILLATOR STRENGTH =    0.001400
                  EXCITATION  DE-EXCITATION
       OCC     VIR   AMPLITUDE      AMPLITUDE
        I       A    X(I->A)        Y(A->I)
       ---     ---   --------      --------
       139     149   -0.304720     0.000000
       140     148    0.421540     0.000000
       140     150   -0.165920     0.000000
       146     152   -0.197220     0.000000
       146     154    0.168960     0.000000
       147     151   -0.212700     0.000000
       147     153    0.179890     0.000000


STATE #   9  ENERGY =    4.974200 EV
OSCILLATOR STRENGTH =    0.124500
                  EXCITATION  DE-EXCITATION
```

```
       OCC      VIR    AMPLITUDE        AMPLITUDE
        I        A      X(I->A)          Y(A->I)
       ---      ---    --------         --------
       136      148    0.477920         0.000000
       136      150    0.111440         0.000000
       138      149   -0.183670         0.000000
       143      149   -0.248700         0.000000
       145      149   -0.307480         0.000000
       146      150   -0.154970         0.000000


 STATE #  10   ENERGY =     4.981800 EV
 OSCILLATOR STRENGTH =     0.003800
                     EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE        AMPLITUDE
        I        A      X(I->A)          Y(A->I)
       ---      ---    --------         --------
       135      148   -0.233970         0.000000
       138      148   -0.385790         0.000000
       143      148    0.266410         0.000000
       145      148    0.406050         0.000000


 STATE #  11   ENERGY =     5.004100 EV
 OSCILLATOR STRENGTH =     0.001600
                     EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE        AMPLITUDE
        I        A      X(I->A)          Y(A->I)
       ---      ---    --------         --------
       143      150   -0.104930         0.000000
       145      150   -0.149070         0.000000
       147      150    0.634780         0.000000


 STATE #  12   ENERGY =     5.569700 EV
 OSCILLATOR STRENGTH =     0.059700
                     EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE        AMPLITUDE
        I        A      X(I->A)          Y(A->I)
       ---      ---    --------         --------
       132      148   -0.122810         0.000000
       135      149   -0.104230         0.000000
       137      148    0.429180         0.000000
       140      148   -0.174440         0.000000
       144      148   -0.335740         0.000000
       146      148    0.132010         0.000000
       146      150   -0.147660         0.000000
       147      151   -0.116300         0.000000
       147      153    0.118010         0.000000


 STATE #  13   ENERGY =     5.576800 EV
 OSCILLATOR STRENGTH =     0.030600
                     EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE        AMPLITUDE
        I        A      X(I->A)          Y(A->I)
       ---      ---    --------         --------
```

```
       136      149   0.477950       0.000000
       138      150  -0.326270       0.000000
       143      150  -0.118240       0.000000
       145      150  -0.132540       0.000000
       146      149   0.183090       0.000000


STATE #  14   ENERGY =     5.593800 EV
OSCILLATOR STRENGTH =    0.000000
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)       Y(A->I)
       ---      ---   --------      --------
       141      152   0.248260       0.000000
       141      154   0.241450       0.000000
       142      151   0.248270       0.000000
       142      153   0.240990       0.000000
       143      156   0.258140       0.000000
       144      155   0.335240       0.000000
       145      156  -0.213260       0.000000


STATE #  15   ENERGY =     5.594000 EV
OSCILLATOR STRENGTH =    0.000700
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)       Y(A->I)
       ---      ---   --------      --------
       141      151   0.246990       0.000000
       141      153   0.239100       0.000000
       142      152   0.248470       0.000000
       142      154   0.243200       0.000000
       143      155   0.258330       0.000000
       144      156   0.334100       0.000000
       145      155  -0.212670       0.000000


STATE #  16   ENERGY =     5.642900 EV
OSCILLATOR STRENGTH =    0.047200
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)       Y(A->I)
       ---      ---   --------      --------
       139      148   0.355310       0.000000
       143      148   0.318530       0.000000
       145      148  -0.257840       0.000000
       146      151   0.189780       0.000000
       146      153  -0.149540       0.000000
       147      152   0.240300       0.000000
       147      154  -0.189890       0.000000


STATE #  17   ENERGY =     5.660800 EV
OSCILLATOR STRENGTH =    0.046400
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)       Y(A->I)
```

```
    ---       ---    --------     --------
    137       148    0.197770     0.000000
    140       148    0.350780     0.000000
    144       148    0.129170     0.000000
    145       149    0.125360     0.000000
    146       150   -0.323070     0.000000
    146       152    0.173460     0.000000
    146       154   -0.133340     0.000000
    147       149    0.101400     0.000000
    147       151    0.218320     0.000000
    147       153   -0.173550     0.000000


STATE #  18   ENERGY =     5.712200 EV
OSCILLATOR STRENGTH =     0.025100
                  EXCITATION  DE-EXCITATION
    OCC       VIR  AMPLITUDE     AMPLITUDE
     I         A    X(I->A)       Y(A->I)
    ---       ---    --------     --------
    139       148   -0.331720     0.000000
    143       148    0.437310     0.000000
    144       149   -0.138940     0.000000
    145       148   -0.298850     0.000000
    146       151   -0.122310     0.000000
    147       152   -0.158900     0.000000
    147       154    0.122600     0.000000


STATE #  19   ENERGY =     5.713400 EV
OSCILLATOR STRENGTH =     0.003900
                  EXCITATION  DE-EXCITATION
    OCC       VIR  AMPLITUDE     AMPLITUDE
     I         A    X(I->A)       Y(A->I)
    ---       ---    --------     --------
    140       148   -0.226640     0.000000
    144       148    0.508870     0.000000
    145       149    0.141200     0.000000
    145       158   -0.102270     0.000000
    147       153    0.103320     0.000000
    147       157    0.207320     0.000000
    147       158    0.148750     0.000000


STATE #  20   ENERGY =     5.743400 EV
OSCILLATOR STRENGTH =     0.016900
                  EXCITATION  DE-EXCITATION
    OCC       VIR  AMPLITUDE     AMPLITUDE
     I         A    X(I->A)       Y(A->I)
    ---       ---    --------     --------
    140       148    0.158210     0.000000
    143       157   -0.103780     0.000000
    143       158   -0.156610     0.000000
    144       148   -0.194780     0.000000
    145       157   -0.157820     0.000000
    145       158   -0.190470     0.000000
    146       150    0.129060     0.000000
```

```
  147     157   0.376630        0.000000
  147     158   0.339760        0.000000


STATE #  21  ENERGY =    5.817500 EV
OSCILLATOR STRENGTH =    0.152800
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------       --------
  137     148   0.353450        0.000000
  137     150  -0.111260        0.000000
  138     149   0.247590        0.000000
  143     149  -0.193420        0.000000
  144     148   0.167470        0.000000
  145     149  -0.241330        0.000000
  146     150   0.313710        0.000000
  147     158  -0.134510        0.000000


STATE #  22  ENERGY =    5.862200 EV
OSCILLATOR STRENGTH =    0.000100
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------       --------
  141     148   0.685400        0.000000
  142     149  -0.143410        0.000000


STATE #  23  ENERGY =    5.862600 EV
OSCILLATOR STRENGTH =    0.003800
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------       --------
  141     149  -0.143460        0.000000
  142     148   0.679540        0.000000


STATE #  24  ENERGY =    5.882300 EV
OSCILLATOR STRENGTH =    0.073100
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
   ---     ---  --------       --------
  135     149  -0.119440        0.000000
  136     148   0.154930        0.000000
  138     149  -0.382320        0.000000
  145     149   0.197910        0.000000
  146     150   0.407420        0.000000


STATE #  25  ENERGY =    6.119500 EV
OSCILLATOR STRENGTH =    0.003900
                EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
    I       A    X(I->A)        Y(A->I)
```

```
---     ---    --------       --------
131     148   -0.106710       0.000000
135     148    0.524540       0.000000
137     149   -0.238700       0.000000
138     148   -0.192030       0.000000
143     150   -0.103300       0.000000
145     150   -0.139610       0.000000


STATE #  26  ENERGY =    6.168100 EV
OSCILLATOR STRENGTH =    0.002100
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I       A    X(I->A)       Y(A->I)
   ---     ---    --------       --------
   137     148    0.151690       0.000000
   139     149   -0.147370       0.000000
   146     150    0.102910       0.000000
   146     159    0.180900       0.000000
   147     153   -0.187850       0.000000
   147     157   -0.355090       0.000000
   147     158    0.372080       0.000000


STATE #  27  ENERGY =    6.197200 EV
OSCILLATOR STRENGTH =    0.014400
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I       A    X(I->A)       Y(A->I)
   ---     ---    --------       --------
   136     149   -0.239980       0.000000
   138     148    0.131230       0.000000
   138     150   -0.103990       0.000000
   139     148   -0.123740       0.000000
   140     149   -0.232470       0.000000
   143     150   -0.212870       0.000000
   145     150   -0.255820       0.000000
   146     157   -0.139770       0.000000
   146     158    0.120260       0.000000
   147     150   -0.129140       0.000000
   147     159    0.293910       0.000000


STATE #  28  ENERGY =    6.230400 EV
OSCILLATOR STRENGTH =    0.085200
              EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I       A    X(I->A)       Y(A->I)
   ---     ---    --------       --------
   135     148   -0.133910       0.000000
   139     148    0.217180       0.000000
   140     149    0.488540       0.000000
   144     149    0.207860       0.000000
   145     150   -0.147040       0.000000
   146     151   -0.121910       0.000000
   147     152   -0.206530       0.000000
```

```
         147       159    0.107690          0.000000


 STATE #  29  ENERGY =     6.242900 EV
 OSCILLATOR STRENGTH =      0.059700
                    EXCITATION  DE-EXCITATION
        OCC      VIR  AMPLITUDE     AMPLITUDE
         I        A    X(I->A)       Y(A->I)
        ---      ---   --------      --------
        139      149    0.533050      0.000000
        140      148    0.238550      0.000000
        143      149    0.155280      0.000000
        145      149   -0.121540      0.000000
        146      152   -0.124410      0.000000
        147      151   -0.210780      0.000000
        147      157   -0.106300      0.000000


 STATE #  30  ENERGY =     6.368400 EV
 OSCILLATOR STRENGTH =      0.010500
                    EXCITATION  DE-EXCITATION
        OCC      VIR  AMPLITUDE     AMPLITUDE
         I        A    X(I->A)       Y(A->I)
        ---      ---   --------      --------
        141      156    0.104950      0.000000
        142      155    0.104930      0.000000
        144      151   -0.123290      0.000000
        144      153   -0.108030      0.000000
        145      152    0.157670      0.000000
        145      154    0.165860      0.000000
        146      151    0.216740      0.000000
        146      153    0.280730      0.000000
        147      152    0.276930      0.000000
        147      154    0.360340      0.000000
```

B+B conformer of equatorial isomer of **6b:**
Table S14.
```
TOTAL FREE ENERGY IN SOLVENT = -6364.871323 A.U.
 N              -1.51060600     3.36462900    -0.55743800
 C              -1.17793800     2.50403300     0.37066500
 C              -0.72793600     4.41456000    -0.91240400
 C              -0.01526300     2.82244500     1.30813800
 C               0.67702300     4.44411800    -0.89813000
 N               1.49782100     3.43071400    -0.52216500
 C               1.18244900     2.55835500     0.40117800
 C              -1.90239100     1.24679200     0.47581900
 C              -2.88236100     0.88724900    -0.38764800
 C               1.96829200     1.34292800     0.54403100
 C               2.97231800     1.01168500    -0.30305600
 C               5.65241000    -1.44420400    -1.24374300
 C               4.80362900    -0.34111400    -1.24059600
 C               5.53061900    -2.38935600    -0.22738200
 C               3.83053200    -0.16438700    -0.23760000
 C               4.57894200    -2.24659900     0.78550200
```

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```
C                         3.73852000    -1.14082400     0.77598800
C                        -5.44995700    -1.66038000    -1.39514100
C                        -4.65412100    -0.51906600    -1.35966600
C                        -5.27377400    -2.63387800    -0.41412500
C                        -3.68138400    -0.33119700    -0.35835800
C                        -4.31962800    -2.48200200     0.59511800
C                        -3.53284500    -1.33765700     0.61846700
C                        -1.43533900     5.50112100    -1.54242000
N                        -2.02901800     6.37850600    -2.02301700
C                         1.35024900     5.55963900    -1.51466000
N                         1.91581800     6.46136300    -1.98406300
C                        -0.00679400     2.14676000     2.68708700
C                        -1.13906600     2.64076500     3.59963300
C                        -1.09742400     1.99716200     4.98825500
H                        -1.62642200     0.59301700     1.29428800
H                        -3.11078400     1.58219900    -1.19265000
H                         1.71688100     0.69746900     1.37701000
H                         3.17072900     1.69548500    -1.12542600
H                        -0.04170700     3.90898100     1.46677500
H                         6.39579500    -1.56693500    -2.02261900
H                         4.89380000     0.39876500    -2.03047100
H                         4.50065400    -2.99086100     1.56939400
H                         3.00675000    -1.03943700     1.57046000
H                        -6.19434800    -1.79071100    -2.17182200
H                        -4.78691100     0.24308900    -2.12185000
H                        -4.19767700    -3.24943700     1.35057800
H                        -2.79763200    -1.23074900     1.40902400
H                        -0.05708800     1.05544300     2.60190500
H                         0.95710700     2.36765300     3.16134300
H                        -1.06975100     3.73175500     3.69661300
H                        -2.10945300     2.43770300     3.12951900
H                        -1.90870100     2.37090500     5.62011200
H                        -1.19927600     0.90789600     4.92502700
H                        -0.15128200     2.21306400     5.49672900
Br                       -6.35666800    -4.20724100    -0.44557700
Br                        6.68691500    -3.91000100    -0.21404900
```

Table S15.

TD–DFT output

HOMO: 137, LUMO: 138

```
STATE #   1   ENERGY =     3.177800 EV
 OSCILLATOR STRENGTH =     1.209600
               EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A     X(I->A)        Y(A->I)
    ---      ---  --------       --------
    136      139  -0.160640       0.000000
    137      138   0.668230       0.000000


 STATE #   2   ENERGY =     3.814000 EV
 OSCILLATOR STRENGTH =     0.441200
               EXCITATION  DE-EXCITATION
```

```
       OCC      VIR    AMPLITUDE       AMPLITUDE
        I        A      X(I->A)         Y(A->I)
       ---      ---    --------        --------
       135      139    0.201260        0.000000
       136      138    0.102260        0.000000
       137      139    0.628020        0.000000


STATE #   3   ENERGY =    4.099900 EV
OSCILLATOR STRENGTH =     1.280300
                      EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE       AMPLITUDE
        I        A      X(I->A)         Y(A->I)
       ---      ---    --------        --------
       131      138    0.140930        0.000000
       135      139    0.109740        0.000000
       136      138    0.651510        0.000000
       137      139   -0.150130        0.000000


STATE #   4   ENERGY =    4.233500 EV
OSCILLATOR STRENGTH =     0.009800
                      EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE       AMPLITUDE
        I        A      X(I->A)         Y(A->I)
       ---      ---    --------        --------
       127      138    0.126690        0.000000
       130      139   -0.195830        0.000000
       132      138    0.442520        0.000000
       135      138    0.443460        0.000000


STATE #   5   ENERGY =    4.614400 EV
OSCILLATOR STRENGTH =     0.166900
                      EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE       AMPLITUDE
        I        A      X(I->A)         Y(A->I)
       ---      ---    --------        --------
       130      138   -0.241950        0.000000
       130      139   -0.123720        0.000000
       132      138   -0.161370        0.000000
       132      139    0.146180        0.000000
       135      139    0.117260        0.000000
       135      140    0.114620        0.000000
       136      139    0.522660        0.000000
       137      138    0.123910        0.000000


STATE #   6   ENERGY =    4.625200 EV
OSCILLATOR STRENGTH =     0.071600
                      EXCITATION  DE-EXCITATION
       OCC      VIR    AMPLITUDE       AMPLITUDE
        I        A      X(I->A)         Y(A->I)
       ---      ---    --------        --------
       127      139   -0.100280        0.000000
       130      138    0.423980        0.000000
       132      139   -0.265110        0.000000
```

```
       135      139   -0.196310         0.000000
       136      139    0.303470         0.000000
       137      139    0.144980         0.000000


STATE #   7  ENERGY =     4.821000 EV
OSCILLATOR STRENGTH =      0.004500
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE     AMPLITUDE
      I        A    X(I->A)       Y(A->I)
     ---      ---  --------     --------
       133      138   -0.211470         0.000000
       134      138    0.385650         0.000000
       134      139   -0.336610         0.000000
       134      140    0.154650         0.000000
       134      143   -0.114870         0.000000
       135      142    0.109520         0.000000
       136      141   -0.192240         0.000000
       136      142   -0.125550         0.000000
       137      141   -0.112980         0.000000
       137      142   -0.206390         0.000000


STATE #   8  ENERGY =     4.821400 EV
OSCILLATOR STRENGTH =      0.010000
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE     AMPLITUDE
      I        A    X(I->A)       Y(A->I)
     ---      ---  --------     --------
       133      138    0.383250         0.000000
       133      139    0.339780         0.000000
       133      140    0.151850         0.000000
       133      143    0.116100         0.000000
       134      138    0.209630         0.000000
       135      141    0.101830         0.000000
       136      141    0.123940         0.000000
       136      142   -0.198350         0.000000
       137      141   -0.203920         0.000000
       137      142    0.112650         0.000000


STATE #   9  ENERGY =     4.914900 EV
OSCILLATOR STRENGTH =      0.185200
                  EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE     AMPLITUDE
      I        A    X(I->A)       Y(A->I)
     ---      ---  --------     --------
       130      138    0.410990         0.000000
       130      140   -0.123940         0.000000
       132      139    0.243490         0.000000
       135      139    0.410060         0.000000
       136      140    0.135100         0.000000
       137      139   -0.129120         0.000000


STATE #  10  ENERGY =     5.063700 EV
OSCILLATOR STRENGTH =      0.000300
```

```
                    EXCITATION   DE-EXCITATION
       OCC      VIR  AMPLITUDE      AMPLITUDE
        I        A    X(I->A)        Y(A->I)
       ---      ---  --------      --------
       135      140  0.160920      0.000000
       137      140  0.644300      0.000000


STATE #  11  ENERGY =    5.170400 EV
OSCILLATOR STRENGTH =    0.006600
                    EXCITATION   DE-EXCITATION
       OCC      VIR  AMPLITUDE      AMPLITUDE
        I        A    X(I->A)        Y(A->I)
       ---      ---  --------      --------
       127      138 -0.272160      0.000000
       130      139  0.123150      0.000000
       131      139 -0.109810      0.000000
       132      138 -0.341450      0.000000
       135      138  0.488400      0.000000


STATE #  12  ENERGY =    5.464100 EV
OSCILLATOR STRENGTH =    0.014400
                    EXCITATION   DE-EXCITATION
       OCC      VIR  AMPLITUDE      AMPLITUDE
        I        A    X(I->A)        Y(A->I)
       ---      ---  --------      --------
       130      139  0.490010      0.000000
       130      143 -0.114810      0.000000
       132      138  0.139520      0.000000
       132      140 -0.255180      0.000000
       135      140 -0.146620      0.000000
       136      139  0.233700      0.000000


STATE #  13  ENERGY =    5.703300 EV
OSCILLATOR STRENGTH =    0.042300
                    EXCITATION   DE-EXCITATION
       OCC      VIR  AMPLITUDE      AMPLITUDE
        I        A    X(I->A)        Y(A->I)
       ---      ---  --------      --------
       126      138 -0.217080      0.000000
       131      138  0.515780      0.000000
       132      139  0.113380      0.000000
       136      138 -0.142640      0.000000
       136      140 -0.196820      0.000000
       137      139 -0.111370      0.000000
       137      143 -0.182350      0.000000


STATE #  14  ENERGY =    5.814900 EV
OSCILLATOR STRENGTH =    0.017000
                    EXCITATION   DE-EXCITATION
       OCC      VIR  AMPLITUDE      AMPLITUDE
        I        A    X(I->A)        Y(A->I)
       ---      ---  --------      --------
       133      138  0.220590      0.000000
```

```
134     138    0.358380         0.000000
135     144    0.106250         0.000000
136     140   -0.174110         0.000000
136     142    0.217410         0.000000
137     141    0.349430         0.000000
137     143    0.116460         0.000000
137     144    0.176220         0.000000


STATE #  15  ENERGY =    5.836400 EV
OSCILLATOR STRENGTH =    0.044500
                EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I        A     X(I->A)       Y(A->I)
   ---      ---   --------      --------
   133     138    0.427780         0.000000
   134     138   -0.255270         0.000000
   135     142    0.106280         0.000000
   136     141   -0.254280         0.000000
   137     142   -0.345470         0.000000


STATE #  16  ENERGY =    5.856400 EV
OSCILLATOR STRENGTH =    0.106700
                EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I        A     X(I->A)       Y(A->I)
   ---      ---   --------      --------
   127     139   -0.190020         0.000000
   131     140   -0.118460         0.000000
   132     139   -0.382160         0.000000
   135     139    0.392450         0.000000
   136     140   -0.150340         0.000000
   137     144   -0.168150         0.000000


STATE #  17  ENERGY =    5.863700 EV
OSCILLATOR STRENGTH =    0.016700
                EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I        A     X(I->A)       Y(A->I)
   ---      ---   --------      --------
   127     144   -0.111890         0.000000
   133     138   -0.109970         0.000000
   134     138   -0.186470         0.000000
   135     139    0.125760         0.000000
   135     144    0.244620         0.000000
   136     142   -0.108630         0.000000
   137     143    0.228970         0.000000
   137     144    0.447720         0.000000


STATE #  18  ENERGY =    5.909400 EV
OSCILLATOR STRENGTH =    0.001200
                EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I        A     X(I->A)       Y(A->I)
```

```
---     ---     --------        --------
131     146     -0.172680       0.000000
135     145      0.190390       0.000000
135     146     -0.150250       0.000000
135     147      0.143980       0.000000
136     144      0.107930       0.000000
136     145     -0.153370       0.000000
136     146      0.372210       0.000000
136     147     -0.100680       0.000000
137     145     -0.266010       0.000000
137     146      0.221170       0.000000
137     147     -0.192710       0.000000


STATE #  19  ENERGY =     5.910700 EV
OSCILLATOR STRENGTH =     0.001800
                EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE      AMPLITUDE
     I       A   X(I->A)         Y(A->I)
    ---     ---  --------        --------
    131     145   0.133880       0.000000
    131     147   0.113820       0.000000
    132     146   0.114770       0.000000
    135     145  -0.118010       0.000000
    135     146  -0.216420       0.000000
    135     147  -0.105610       0.000000
    136     145  -0.296100       0.000000
    136     146  -0.176430       0.000000
    136     147  -0.250060       0.000000
    137     145   0.162020       0.000000
    137     146   0.324090       0.000000
    137     147   0.151030       0.000000


STATE #  20  ENERGY =     6.003500 EV
OSCILLATOR STRENGTH =     0.044100
                EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE      AMPLITUDE
     I       A   X(I->A)         Y(A->I)
    ---     ---  --------        --------
    126     138  -0.108920       0.000000
    132     139  -0.179870       0.000000
    133     139  -0.110300       0.000000
    134     138   0.153780       0.000000
    136     140   0.445440       0.000000
    137     143  -0.284110       0.000000
    137     144   0.190010       0.000000


STATE #  21  ENERGY =     6.084900 EV
OSCILLATOR STRENGTH =     0.000400
                EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE      AMPLITUDE
     I       A   X(I->A)         Y(A->I)
    ---     ---  --------        --------
    123     138   0.137330       0.000000
```

```
        127     138     0.497980        0.000000
        131     139    -0.284340        0.000000
        132     138    -0.214310        0.000000
        135     140     0.156010        0.000000


STATE #  22   ENERGY =     6.139500 EV
OSCILLATOR STRENGTH =      0.006300
                   EXCITATION  DE-EXCITATION
        OCC     VIR  AMPLITUDE      AMPLITUDE
         I       A    X(I->A)        Y(A->I)
        ---     ---  --------      --------
        127     139    -0.139930        0.000000
        131     138     0.263100        0.000000
        131     140     0.108940        0.000000
        136     140     0.333910        0.000000
        137     141     0.177160        0.000000
        137     143     0.350120        0.000000
        137     144    -0.147190        0.000000


STATE #  23   ENERGY =     6.159900 EV
OSCILLATOR STRENGTH =      0.005700
                   EXCITATION  DE-EXCITATION
        OCC     VIR  AMPLITUDE      AMPLITUDE
         I       A    X(I->A)        Y(A->I)
        ---     ---  --------      --------
        130     139     0.210630        0.000000
        131     139     0.137860        0.000000
        132     138     0.121540        0.000000
        132     140     0.187810        0.000000
        134     139    -0.177680        0.000000
        135     140     0.316980        0.000000
        136     143     0.160890        0.000000
        137     140    -0.139420        0.000000
        137     145    -0.184020        0.000000
        137     147     0.232950        0.000000


STATE #  24   ENERGY =     6.216200 EV
OSCILLATOR STRENGTH =      0.000100
                   EXCITATION  DE-EXCITATION
        OCC     VIR  AMPLITUDE      AMPLITUDE
         I       A    X(I->A)        Y(A->I)
        ---     ---  --------      --------
        128     138    -0.315790        0.000000
        128     139     0.257300        0.000000
        128     140    -0.117240        0.000000
        128     143     0.108180        0.000000
        129     138     0.413850        0.000000
        129     139    -0.248440        0.000000
        129     140     0.153650        0.000000
        129     143    -0.105080        0.000000


STATE #  25   ENERGY =     6.216500 EV
OSCILLATOR STRENGTH =      0.000100
```

```
                    EXCITATION  DE-EXCITATION
      OCC     VIR   AMPLITUDE    AMPLITUDE
       I       A     X(I->A)      Y(A->I)
      ---     ---   --------     --------
      128     138   0.408370     0.000000
      128     139   0.249650     0.000000
      128     140   0.150000     0.000000
      128     143   0.105320     0.000000
      129     138   0.317210     0.000000
      129     139   0.263440     0.000000
      129     140   0.116510     0.000000
      129     143   0.111830     0.000000


STATE #  26  ENERGY =    6.251700 EV
OSCILLATOR STRENGTH =    0.089800
                    EXCITATION  DE-EXCITATION
      OCC     VIR   AMPLITUDE    AMPLITUDE
       I       A     X(I->A)      Y(A->I)
      ---     ---   --------     --------
      133     138  -0.184690     0.000000
      133     139   0.423400     0.000000
      134     139   0.336090     0.000000
      135     140   0.122660     0.000000
      136     141  -0.124360     0.000000
      137     142  -0.256680     0.000000


STATE #  27  ENERGY =    6.257300 EV
OSCILLATOR STRENGTH =    0.087200
                    EXCITATION  DE-EXCITATION
      OCC     VIR   AMPLITUDE    AMPLITUDE
       I       A     X(I->A)      Y(A->I)
      ---     ---   --------     --------
      133     139  -0.354160     0.000000
      134     138   0.188390     0.000000
      134     139   0.429740     0.000000
      136     142  -0.142990     0.000000
      137     141  -0.221470     0.000000
      137     142  -0.103770     0.000000
      137     143   0.178820     0.000000


STATE #  28  ENERGY =    6.394900 EV
OSCILLATOR STRENGTH =    0.004800
                    EXCITATION  DE-EXCITATION
      OCC     VIR   AMPLITUDE    AMPLITUDE
       I       A     X(I->A)      Y(A->I)
      ---     ---   --------     --------
      121     138   0.161060     0.000000
      122     138   0.302850     0.000000
      122     140  -0.151920     0.000000
      124     138  -0.159890     0.000000
      125     138   0.253220     0.000000
      131     139   0.149760     0.000000
      132     140   0.104270     0.000000
```

```
          136     143   -0.170010       0.000000
          137     145    0.138390       0.000000
          137     147   -0.169170       0.000000


STATE #  29  ENERGY =     6.400800 EV
OSCILLATOR STRENGTH =     0.007900
                  EXCITATION  DE-EXCITATION
        OCC     VIR  AMPLITUDE     AMPLITUDE
         I       A     X(I->A)       Y(A->I)
        ---     ---  --------      --------
          116     138    0.100200       0.000000
          121     138   -0.136760       0.000000
          122     138    0.328790       0.000000
          122     140   -0.201220       0.000000
          124     138    0.242820       0.000000
          126     138   -0.209320       0.000000
          131     139   -0.111550       0.000000
          136     143    0.122960       0.000000
          137     145   -0.100860       0.000000
          137     147    0.127520       0.000000


STATE #  30  ENERGY =     6.474700 EV
OSCILLATOR STRENGTH =     0.022600
                  EXCITATION  DE-EXCITATION
        OCC     VIR  AMPLITUDE     AMPLITUDE
         I       A     X(I->A)       Y(A->I)
        ---     ---  --------      --------
          118     138    0.126600       0.000000
          121     138    0.113570       0.000000
          124     138   -0.185790       0.000000
          125     138    0.228110       0.000000
          130     139   -0.148230       0.000000
          132     140   -0.216020       0.000000
          135     140   -0.255490       0.000000
          136     143    0.150730       0.000000
          137     145   -0.211900       0.000000
          137     147    0.264860       0.000000
```

B+B conformer of axial isomer of **6b:**
Table S16.
```
TOTAL FREE ENERGY IN SOLVENT = -6364.871324 A.U.
 N                 -1.54460800    3.02459100   -0.62374000
 C                 -1.20929600    2.16850900    0.30536400
 C                 -0.76189200    4.04428200   -1.05766400
 C                 -0.02788500    2.39186300    1.24451300
 C                  0.63886800    4.09051400   -1.04537400
 N                  1.47979900    3.12663800   -0.59310800
 C                  1.18492800    2.25101000    0.33123900
 C                 -1.98291900    0.94449900    0.46037500
 C                 -3.00832100    0.60489300   -0.35752300
 C                  2.04169700    1.08767100    0.51261300
 C                  3.10618200    0.81727100   -0.28068300
```

```
C          4.84447900    -2.34256000     0.89049900
C          3.93702700    -1.29276100     0.83254100
C          5.86816700    -2.41306100    -0.05777800
C          4.03237500    -0.30145600    -0.16639500
C          5.99523100    -1.45125800    -1.05782900
C          5.07853400    -0.40505400    -1.10413600
C         -5.71880700    -1.85154200    -1.20299200
C         -4.87529900    -0.74477300    -1.22612500
C         -5.54366100    -2.80991300    -0.20691600
C         -3.85562000    -0.57678400    -0.26876300
C         -4.54375800    -2.67695300     0.75989900
C         -3.70957500    -1.56707900     0.72503500
C         -1.47925000     5.08561100    -1.75069300
N         -2.08149500     5.92677500    -2.28286400
C          1.29819900     5.17697500    -1.72629200
N          1.85309700     6.05606200    -2.24862900
C         -0.07032300     3.69960300     2.06895500
C         -1.25255500     3.74694900     3.04657200
C         -1.24955300     5.01596700     3.90395300
H         -1.69871700     0.30358100     1.28886500
H         -3.23702400     1.29149800    -1.16983900
H          1.78561300     0.43299700     1.33957100
H          3.30234500     1.51320700    -1.09354300
H         -0.00767200     1.56362300     1.95832600
H          4.76244900    -3.09924700     1.66200700
H          3.14826200    -1.24784500     1.57591600
H          6.79463700    -1.51790100    -1.78641400
H          5.17250800     0.34745900    -1.88149900
H         -6.49897900    -1.96708800    -1.94615900
H         -5.00708300     0.00553900    -2.00011900
H         -4.42338000    -3.43218700     1.52779600
H         -2.93853400    -1.47387100     1.48247300
H          0.87078900     3.75993900     2.62884200
H         -0.09967200     4.57922100     1.42165000
H         -2.19464600     3.68665700     2.48773800
H         -1.22230400     2.86322900     3.69790000
H         -0.33328100     5.08964000     4.50021700
H         -1.31368300     5.91478200     3.28100900
H         -2.09886800     5.02749600     4.59395500
Br        -6.69182800    -4.33581100    -0.15841000
Br         7.11662400    -3.85658100     0.02227600
```

Table S17.

TD–DFT output
```
HOMO: 137, LUMO: 138
STATE #   1   ENERGY =      2.920900 EV
 OSCILLATOR STRENGTH =      1.294000
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I       A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
```

```
118      121   -0.156290         0.000000
119      120    0.668650         0.000000


STATE #   2   ENERGY =      3.705400 EV
OSCILLATOR STRENGTH =     0.150600
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    113      120    0.114730         0.000000
    117      121   -0.221690         0.000000
    118      120    0.260950         0.000000
    119      121    0.577100         0.000000


STATE #   3   ENERGY =      3.823600 EV
OSCILLATOR STRENGTH =     1.410000
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    113      120    0.104570         0.000000
    118      120    0.615350         0.000000
    119      121   -0.292150         0.000000


STATE #   4   ENERGY =      4.068500 EV
OSCILLATOR STRENGTH =     0.008000
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    112      121   -0.174460         0.000000
    114      120    0.446380         0.000000
    117      120    0.463210         0.000000


STATE #   5   ENERGY =      4.450300 EV
OSCILLATOR STRENGTH =     0.221100
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    112      121    0.106040         0.000000
    113      121    0.117110         0.000000
    114      120    0.155830         0.000000
    117      122    0.112940         0.000000
    118      121    0.618650         0.000000
    119      120    0.148370         0.000000


STATE #   6   ENERGY =      4.568900 EV
OSCILLATOR STRENGTH =     0.022800
                EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
```

```
111     121    -0.101560          0.000000
112     120     0.505250          0.000000
114     121    -0.311440          0.000000
117     121    -0.228620          0.000000
119     121    -0.174190          0.000000


STATE #   7  ENERGY =     4.788900 EV
OSCILLATOR STRENGTH =     0.029000
                    EXCITATION  DE-EXCITATION
      OCC      VIR  AMPLITUDE     AMPLITUDE
       I        A    X(I->A)       Y(A->I)
      ---      ---  --------      --------
      112      120   0.223630      0.000000
      114      121   0.119460      0.000000
      115      121   0.213850      0.000000
      116      120   0.358880      0.000000
      116      121  -0.100400      0.000000
      116      122  -0.133760      0.000000
      117      121   0.242010      0.000000
      118      124   0.220010      0.000000
      119      123   0.236530      0.000000


STATE #   8  ENERGY =     4.794000 EV
OSCILLATOR STRENGTH =     0.001300
                    EXCITATION  DE-EXCITATION
      OCC      VIR  AMPLITUDE     AMPLITUDE
       I        A    X(I->A)       Y(A->I)
      ---      ---  --------      --------
      115      120   0.421580      0.000000
      115      121   0.134650      0.000000
      115      122  -0.159810      0.000000
      116      121   0.268040      0.000000
      117      120   0.104130      0.000000
      117      124  -0.108910      0.000000
      118      123  -0.253200      0.000000
      119      124  -0.258930      0.000000


STATE #   9  ENERGY =     4.821800 EV
OSCILLATOR STRENGTH =     0.117100
                    EXCITATION  DE-EXCITATION
      OCC      VIR  AMPLITUDE     AMPLITUDE
       I        A    X(I->A)       Y(A->I)
      ---      ---  --------      --------
      112      120   0.332250      0.000000
      114      121   0.188870      0.000000
      115      121  -0.172780      0.000000
      116      120  -0.240740      0.000000
      117      121   0.354950      0.000000
      118      122   0.111300      0.000000
      118      124  -0.134470      0.000000
      119      121   0.107940      0.000000
      119      123  -0.123050      0.000000
```

```
STATE #  10   ENERGY =     4.889800 EV
OSCILLATOR STRENGTH =     0.007200
                  EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------     --------
     111     120  -0.249170     0.000000
     112     120   0.100020     0.000000
     114     120  -0.392380     0.000000
     117     120   0.443640     0.000000
     119     122   0.117130     0.000000

STATE #  11   ENERGY =     4.953500 EV
OSCILLATOR STRENGTH =     0.003100
                  EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------     --------
     117     120  -0.114550     0.000000
     117     122  -0.183960     0.000000
     119     122   0.629000     0.000000

STATE #  12   ENERGY =     5.447200 EV
OSCILLATOR STRENGTH =     0.018800
                  EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------     --------
     112     121   0.498420     0.000000
     112     125  -0.101340     0.000000
     113     121   0.135760     0.000000
     114     120   0.108510     0.000000
     114     122   0.279910     0.000000
     117     122   0.147330     0.000000
     118     121  -0.202100     0.000000

STATE #  13   ENERGY =     5.564000 EV
OSCILLATOR STRENGTH =     0.057500
                  EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------     --------
     107     120   0.138040     0.000000
     111     121   0.137240     0.000000
     113     120   0.473950     0.000000
     116     120   0.225140     0.000000
     118     120  -0.141520     0.000000
     118     122   0.109220     0.000000
     118     124  -0.125160     0.000000
     119     123  -0.180300     0.000000
     119     125  -0.154600     0.000000

STATE #  14   ENERGY =     5.633200 EV
```

```
OSCILLATOR STRENGTH =    0.060700
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------     --------
    115      120   0.454400    0.000000
    116      120  -0.145130    0.000000
    117      124   0.105380    0.000000
    118      123   0.284240    0.000000
    119      124   0.366500    0.000000

STATE #  15  ENERGY =     5.639100 EV
OSCILLATOR STRENGTH =    0.062900
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------     --------
    113      120  -0.194410    0.000000
    115      120   0.116130    0.000000
    116      120   0.380340    0.000000
    117      121   0.122780    0.000000
    118      122  -0.244040    0.000000
    118      124  -0.236540    0.000000
    119      123  -0.308770    0.000000

STATE #  16  ENERGY =     5.657400 EV
OSCILLATOR STRENGTH =    0.003500
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------     --------
    111      126   0.101450    0.000000
    113      120   0.131320    0.000000
    117      125  -0.163870    0.000000
    117      126  -0.297710    0.000000
    119      125   0.313600    0.000000
    119      126   0.470260    0.000000

STATE #  17  ENERGY =     5.761600 EV
OSCILLATOR STRENGTH =    0.166000
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE    AMPLITUDE
     I        A    X(I->A)      Y(A->I)
    ---      ---  --------     --------
    111      121   0.122970    0.000000
    112      120   0.150610    0.000000
    113      120  -0.253350    0.000000
    113      122   0.115830    0.000000
    114      121   0.406720    0.000000
    117      121  -0.371480    0.000000
    118      122   0.134910    0.000000
    119      125   0.105970    0.000000
```

```
STATE #  18  ENERGY =    5.856800 EV
OSCILLATOR STRENGTH =    0.074000
              EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE    AMPLITUDE
    I        A    X(I->A)      Y(A->I)
   ---      ---  --------    --------
   113      120  -0.149980    0.000000
   114      121  -0.242430    0.000000
   116      120   0.101660    0.000000
   118      122   0.560300    0.000000

STATE #  19  ENERGY =    6.026900 EV
OSCILLATOR STRENGTH =    0.009100
              EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE    AMPLITUDE
    I        A    X(I->A)      Y(A->I)
   ---      ---  --------    --------
   104      120   0.123160    0.000000
   111      120   0.565440    0.000000
   113      121   0.229310    0.000000
   114      120  -0.218650    0.000000

STATE #  20  ENERGY =    6.108200 EV
OSCILLATOR STRENGTH =    0.005400
              EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE    AMPLITUDE
    I        A    X(I->A)      Y(A->I)
   ---      ---  --------    --------
   113      120   0.157200    0.000000
   115      121  -0.113600    0.000000
   115      123  -0.112580    0.000000
   116      124   0.107510    0.000000
   118      122  -0.129610    0.000000
   118      127   0.166580    0.000000
   119      123   0.112090    0.000000
   119      125   0.460030    0.000000
   119      126  -0.300890    0.000000

STATE #  21  ENERGY =    6.134500 EV
OSCILLATOR STRENGTH =    0.032000
              EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE    AMPLITUDE
    I        A    X(I->A)      Y(A->I)
   ---      ---  --------    --------
   112      121  -0.247970    0.000000
   114      120  -0.107120    0.000000
   114      122   0.154510    0.000000
   116      121   0.110390    0.000000
   117      122   0.435910    0.000000
   118      125   0.153260    0.000000
   119      122   0.151320    0.000000
   119      127   0.260980    0.000000
```

```
STATE #  22   ENERGY =    6.227900 EV
OSCILLATOR STRENGTH =    0.065700
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    115      120  -0.228130      0.000000
    115      121   0.129340      0.000000
    116      120   0.101320      0.000000
    116      121   0.566590      0.000000
    117      122  -0.113810      0.000000
    119      124   0.215590      0.000000


STATE #  23   ENERGY =    6.240500 EV
OSCILLATOR STRENGTH =    0.067700
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    115      120  -0.101700      0.000000
    115      121   0.568020      0.000000
    116      120  -0.225500      0.000000
    116      121  -0.126280      0.000000
    119      123  -0.196650      0.000000
    119      125   0.125670      0.000000


STATE #  24   ENERGY =    6.390000 EV
OSCILLATOR STRENGTH =    0.006900
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    103      120   0.404920      0.000000
    103      122   0.209460      0.000000
    106      120   0.277560      0.000000
    106      122   0.121800      0.000000
    107      120  -0.219410      0.000000
    107      122  -0.110120      0.000000
    110      120   0.109330      0.000000
    119      126   0.102520      0.000000


STATE #  25   ENERGY =    6.428400 EV
OSCILLATOR STRENGTH =    0.009400
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---  --------      --------
    112      121   0.183620      0.000000
    114      122  -0.187320      0.000000
    115      124  -0.115450      0.000000
    116      123   0.116900      0.000000
    117      122  -0.205080      0.000000
    118      125   0.275380      0.000000
```

```
118     126   -0.125430        0.000000
119     127    0.428110        0.000000


STATE #  26  ENERGY =     6.511200 EV
OSCILLATOR STRENGTH =     0.028200
                 EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------      --------
     105     120   -0.149950        0.000000
     106     120    0.115940        0.000000
     111     120   -0.158450        0.000000
     111     122   -0.116470        0.000000
     112     121   -0.134200        0.000000
     113     121    0.473560        0.000000
     114     120    0.102910        0.000000
     117     122   -0.141010        0.000000
     119     127    0.192980        0.000000


STATE #  27  ENERGY =     6.612800 EV
OSCILLATOR STRENGTH =     0.048200
                 EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------      --------
      96     120    0.113910        0.000000
     101     121    0.106960        0.000000
     102     120    0.101860        0.000000
     105     120    0.371200        0.000000
     106     120   -0.234030        0.000000
     107     120   -0.151230        0.000000
     108     120    0.125200        0.000000
     108     121    0.134990        0.000000
     109     120    0.225540        0.000000
     110     120    0.115470        0.000000
     113     121    0.158740        0.000000


STATE #  28  ENERGY =     6.637600 EV
OSCILLATOR STRENGTH =     0.003300
                 EXCITATION  DE-EXCITATION
     OCC     VIR  AMPLITUDE     AMPLITUDE
      I       A    X(I->A)       Y(A->I)
     ---     ---  --------      --------
      99     120   -0.110930        0.000000
     101     120    0.162340        0.000000
     101     121    0.147440        0.000000
     102     120    0.268380        0.000000
     102     121    0.105440        0.000000
     105     120   -0.141150        0.000000
     106     120    0.119290        0.000000
     108     120    0.232730        0.000000
     108     121    0.212740        0.000000
     108     122   -0.107370        0.000000
```

```
     109     120    0.138990          0.000000
     110     120   -0.245170          0.000000


  STATE #  29  ENERGY =     6.645900 EV
  OSCILLATOR STRENGTH =      0.001100
                   EXCITATION  DE-EXCITATION
       OCC     VIR  AMPLITUDE     AMPLITUDE
        I       A    X(I->A)       Y(A->I)
       ---     ---  --------      --------
       101     120    0.242500          0.000000
       102     120   -0.188210          0.000000
       102     121    0.188510          0.000000
       108     120    0.266040          0.000000
       109     120   -0.260770          0.000000
       109     121    0.269750          0.000000
       109     122    0.106100          0.000000


  STATE #  30  ENERGY =     6.706400 EV
  OSCILLATOR STRENGTH =      0.006500
                   EXCITATION  DE-EXCITATION
       OCC     VIR  AMPLITUDE     AMPLITUDE
        I       A    X(I->A)       Y(A->I)
       ---     ---  --------      --------
        99     120   -0.165240          0.000000
       100     120    0.322530          0.000000
       100     122    0.145980          0.000000
       102     122    0.131080          0.000000
       106     120   -0.113960          0.000000
       109     120   -0.129500          0.000000
       110     120    0.192010          0.000000
       113     121    0.161240          0.000000
       114     122    0.113300          0.000000
       117     122   -0.127980          0.000000
       118     125    0.137740          0.000000
       119     128    0.158830          0.000000
```

A+A conformer of equatorial isomer of **6d:**

Table S18.

```
TOTAL FREE ENERGY IN SOLVENT = -1451.625086 A.U.
N              3.62050400     1.14178500    -0.56996700
 C             2.50801700     0.91986500     0.08935000
 C             4.56393100     0.18420800    -0.76184500
 C             2.41409000    -0.33186400     0.96638800
 C             4.32388200    -1.19388800    -0.89699300
 N             3.12159800    -1.82365200    -0.82721000
 C             2.12940800    -1.43114500    -0.05636300
 C             1.47080600     1.91700300    -0.10165000
 C             0.13825200     1.77912700     0.10898600
 C             0.86674200    -2.09497400    -0.31025500
 C            -0.29917300    -1.99671300     0.37861800
 C            -3.85588200    -3.15963000     0.73253500
 C            -2.63478800    -2.52720400     0.95004500
 C            -4.01246500    -3.98090900    -0.39267800
```

```
C                        -1.54356700      -2.68690000       0.07612100
C                        -2.93491500      -4.15148400      -1.28414600
C                        -1.72898200      -3.51773100      -1.05384200
O                        -5.14891600      -4.64688500      -0.71246200
C                        -6.28096300      -4.52059100       0.14801500
C                        -3.28009900       3.30683400      -0.24411900
C                        -2.24131300       2.41062100      -0.00495000
C                        -2.97957600       4.61404100      -0.65020000
C                        -0.89143400       2.77238700      -0.16200600
C                        -1.63444500       4.99956900      -0.81002700
C                        -0.61486500       4.09733600      -0.57175800
O                        -3.90086000       5.57539300      -0.91018900
C                        -5.28346000       5.25081700      -0.77056700
C                         5.88096900       0.69052500      -1.05461600
N                         6.94320700       1.11890500      -1.25865700
C                         5.40379800      -2.03796500      -1.34419100
N                         6.26676800      -2.74333600      -1.67795300
C                         1.63075100      -0.23137700       2.28874900
C                         2.35455400       0.66453400       3.30620300
C                         1.61271200       0.75416500       4.64238000
H                         1.85340600       2.82433600      -0.56072300
H                        -0.24274800       0.83036800       0.47101300
H                         0.92399000      -2.76163400      -1.16578200
H                        -0.34634500      -1.36539800       1.25816700
H                         3.45255800      -0.52255800       1.27014200
H                        -4.66736200      -3.01059600       1.43390400
H                        -2.52104600      -1.89578400       1.82737000
H                        -3.07752500      -4.78725100      -2.15149800
H                        -0.92034500      -3.66362700      -1.76212300
H                        -6.62177200      -3.48095700       0.20755200
H                        -7.06367700      -5.13332900      -0.29874100
H                        -6.05885800      -4.89069000       1.15502800
H                        -4.30525400       2.98313000      -0.11402800
H                        -2.48443200       1.39791000       0.30568200
H                        -1.42158000       6.01678500      -1.12136300
H                         0.41148800       4.42589700      -0.69779600
H                        -5.52293800       4.96113000       0.25880800
H                        -5.82969600       6.15824500      -1.02761700
H                        -5.57447100       4.44491300      -1.45357600
H                         0.61908100       0.15411900       2.15432100
H                         1.53409300      -1.24110000       2.70460600
H                         3.36801700       0.27706900       3.47262500
H                         2.47415500       1.67040600       2.88452800
H                         2.15231600       1.39060500       5.35024800
H                         0.61002100       1.17676700       4.51286800
H                         1.50069200      -0.23468500       5.10099200
```

Rotational transition state **Ts₂** of equatorial isomer of **6d:**
Table S19.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.617293 A.U.
  N                        3.80651600       0.12378400      -0.45582400
  C                        2.65626800       0.28772300       0.16190500
  C                        4.37672200      -1.08994300      -0.65527700
```

```
C        2.11586100    -0.88514500     0.98014400
C        3.69933700    -2.30034200    -0.86180200
N        2.33714100    -2.44916900    -0.89439400
C        1.54662900    -1.75447400    -0.13653000
C        2.02352300     1.57507200    -0.05025500
C        0.74290500     1.93175800     0.22263400
C        0.09020200    -1.74936800    -0.43199300
C       -0.77719700    -2.60999600     0.12592300
C       -4.35347000    -3.75913000     0.45602300
C       -2.97581900    -3.62211400     0.62757000
C       -5.01008700    -2.96578000    -0.49212700
C       -2.21949000    -2.70736000    -0.12036100
C       -4.26919400    -2.04707200    -1.25790600
C       -2.90262000    -1.92399900    -1.07477200
O       -6.34509700    -3.00751100    -0.75006800
C       -7.14897900    -3.92493500    -0.01193000
C       -1.90384300     4.59227000     0.01381300
C       -1.23852700     3.39365200     0.25619000
C       -1.20595500     5.65947500    -0.56830300
C        0.11939200     3.21428300    -0.06511200
C        0.15486000     5.50273700    -0.89781600
C        0.80085200     4.30639300    -0.65189300
O       -1.74234200     6.87134600    -0.85274500
C       -3.11895200     7.09812800    -0.54970300
C        5.80319300    -1.05126900    -0.87354500
N        6.95642400    -1.00404100    -1.01451600
C        4.44079900    -3.45620900    -1.28649600
N        5.02647400    -4.41124700    -1.60125900
C        1.22002400    -0.65118800     2.20557900
C        1.88026300     0.21861100     3.28426900
C        1.01380000     0.34788300     4.54032600
H        2.68103100     2.27383200    -0.55931700
H        0.07792900     1.20518900     0.67682400
H       -0.23699000    -1.00298700    -1.15486400
H       -0.38893000    -3.33284800     0.84248300
H        3.01259600    -1.40707500     1.34037500
H       -4.89618500    -4.47826300     1.05701500
H       -2.47638200    -4.24354600     1.36626800
H       -4.79207800    -1.44603500    -1.99459600
H       -2.35726400    -1.21405400    -1.68885100
H       -7.11834500    -3.70931500     1.06236900
H       -8.16714800    -3.79194100    -0.37804600
H       -6.83399900    -4.96067700    -0.18309700
H       -2.94990600     4.68502900     0.27752700
H       -1.78840300     2.57232200     0.70793200
H        0.67759800     6.34026100    -1.34741700
H        1.84901400     4.21692400    -0.91721300
H       -3.31204200     6.99846700     0.52419900
H       -3.32712400     8.12135100    -0.86178400
H       -3.76691200     6.40940500    -1.10308900
H        0.24471200    -0.24275300     1.93251200
H        1.00983900    -1.64149400     2.62911500
H        2.85270900    -0.21506200     3.55173600
```

```
H                    2.08922100      1.21503900      2.87835900
H                    1.50545000      0.96730400      5.29664700
H                    0.04693500      0.80905700      4.30947000
H                    0.81531800     -0.63206400      4.98856500
```

A+B conformer of equatorial isomer of **6d:**
Table S20.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.631566 A.U.
 N                  -2.37905600      2.65611700     -0.86661100
 C                  -1.98396700      1.72970500     -0.02522900
 C                  -1.78463100      3.87420300     -0.95855500
 C                  -1.06160800      2.13981700      1.12427500
 C                  -0.42417100      4.15154200     -0.73478300
 N                   0.53507800      3.27346000     -0.34406500
 C                   0.28913500      2.23998200      0.42670600
 C                  -2.47898700      0.39340200     -0.30635200
 C                  -1.97339700     -0.79129400      0.11623500
 C                   1.28885500      1.20644700      0.59873400
 C                   2.44650400      1.17219500     -0.11269000
 C                   5.71349300     -0.53929500     -0.81234600
 C                   4.64253500      0.34845500     -0.85177000
 C                   5.68536500     -1.60967500      0.09289500
 C                   3.52398300      0.20787800     -0.00855400
 C                   4.57636400     -1.77004500      0.94786900
 C                   3.52132200     -0.88016300      0.89680000
 O                   6.66443300     -2.53683000      0.22470000
 C                   7.82043400     -2.43461300     -0.60773700
 C                  -2.16494100     -4.54395700     -0.06587600
 C                  -1.75992400     -3.24469900      0.23037100
 C                  -3.30510500     -4.74467000     -0.85532300
 C                  -2.45815900     -2.11817100     -0.23941800
 C                  -4.02188100     -3.63122200     -1.33475800
 C                  -3.60605400     -2.34808600     -1.03285700
 O                  -3.79797600     -5.95800800     -1.21026800
 C                  -3.11704100     -7.12861000     -0.76040400
 C                  -2.61205200      4.89980000     -1.54173300
 N                  -3.30635600      5.72038700     -1.98712400
 C                   0.08286900      5.44563100     -1.11909800
 N                   0.51175700      6.49054000     -1.39837700
 C                  -1.12874300      1.37833000      2.45847400
 C                  -2.49665100      1.50604500      3.14460500
 C                  -2.53472900      0.81492700      4.51037600
 H                  -3.29798900      0.40432700     -1.02013100
 H                  -1.09543600     -0.79470700      0.75407000
 H                   1.07914600      0.44676800      1.34279600
 H                   2.59115600      1.96301800     -0.84610200
 H                  -1.35078500      3.17517200      1.35107700
 H                   6.55360800     -0.39290200     -1.47963200
 H                   4.67093300      1.17558100     -1.55560800
 H                   4.57597400     -2.60367700      1.64211500
 H                   2.68200500     -1.02703400      1.56870800
 H                   8.35408800     -1.49397200     -0.43304000
```

```
H            8.46067100     -3.27187800     -0.33073000
H            7.55530300     -2.51340800     -1.66775200
H           -1.59494000     -5.38114100      0.31732700
H           -0.87432300     -3.10022000      0.84345200
H           -4.90330800     -3.80620700     -1.94259100
H           -4.18175400     -1.51137000     -1.41453000
H           -3.10312600     -7.18605100      0.33379700
H           -3.67955000     -7.97230900     -1.15998400
H           -2.08989900     -7.16314200     -1.14060600
H           -0.87938300      0.32004400      2.35367800
H           -0.35923400      1.80738100      3.11240700
H           -2.74187200      2.56944600      3.26323900
H           -3.27183200      1.08083000      2.49606400
H           -3.51647600      0.92562000      4.98085500
H           -2.32909700     -0.25750700      4.41854000
H           -1.78841900      1.23935200      5.19121800
```

Rotational transition state **Ts₁** of equatorial isomer of **6d**:
Table S21.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.624081 A.U.
 N            3.53785300      0.41981800     -0.87186800
 C            2.67991000      0.58671200      0.08362500
 C            4.16496000     -0.77730900     -1.09588900
 C            2.50950900     -0.47004500      1.17376600
 C            3.58202300     -2.03828800     -0.91149600
 N            2.33362800     -2.29545800     -0.45074000
 C            1.71443800     -1.52945400      0.41731800
 C            1.85875300      1.82817300      0.08292400
 C            0.61745300      1.89611400     -0.42572300
 C            0.29247200     -1.69030500      0.64515800
 C           -0.47678400     -2.54810700     -0.07645600
 C           -3.86581000     -4.03438000     -0.70340300
 C           -2.50939100     -3.73545300     -0.78661800
 C           -4.65081700     -3.39846300      0.26904400
 C           -1.89413200     -2.80970400      0.07747100
 C           -4.05623100     -2.46913300      1.14637000
 C           -2.70840600     -2.18317900      1.05139100
 O           -5.97749100     -3.60543800      0.44741400
 C           -6.64563400     -4.53790900     -0.40358500
 C           -2.39876400      4.02832500     -1.18853900
 C           -1.51382200      2.95334600     -1.09857900
 C           -2.03544200      5.26495600     -0.64269400
 C           -0.26171300      3.06923900     -0.47666600
 C           -0.78522300      5.40225000     -0.01251800
 C            0.08083000      4.32532600      0.06734700
 O           -2.81014200      6.38331800     -0.66614400
 C           -4.08656900      6.30920100     -1.29631200
 C            5.42936800     -0.67856200     -1.77261300
 N            6.46573600     -0.57850500     -2.29247300
 C            4.27450200     -3.19751800     -1.42371700
 N            4.82450000     -4.14898500     -1.80383700
 C            1.93425900      0.01779300      2.50906400
 C            2.94073600      0.84782300      3.31925200
```

```
C                    2.37143500      1.31592900      4.66129600
H                    2.34034300      2.70203400      0.51884500
H                    0.19408800      0.99187400     -0.86120400
H                   -0.14299800     -1.09301600      1.43700900
H                    0.02429100     -3.11289100     -0.86019900
H                    3.50487100     -0.90064800      1.35103100
H                   -4.29789100     -4.75282900     -1.38862500
H                   -1.90691800     -4.23187100     -1.54220400
H                   -4.68130500     -1.99049700      1.89270900
H                   -2.27748500     -1.46585300      1.74218000
H                   -6.22848900     -5.54497100     -0.29473800
H                   -7.68687200     -4.53978600     -0.08202000
H                   -6.58858700     -4.22958500     -1.45326000
H                   -3.35422900      3.89180000     -1.67998100
H                   -1.80610700      1.99836400     -1.52743100
H                   -0.51944200      6.36716900      0.40659800
H                    1.03745900      4.46303200      0.56169100
H                   -4.73586700      5.57778100     -0.80124200
H                   -4.52482800      7.30293200     -1.20209100
H                   -3.99447200      6.05219100     -2.35784700
H                    1.02789800      0.60913100      2.34016600
H                    1.63861200     -0.85851600      3.09849700
H                    3.84503800      0.24971400      3.49079000
H                    3.25888000      1.71985700      2.73374800
H                    3.10942500      1.89783200      5.22183700
H                    1.48712300      1.94693400      4.51876000
H                    2.07503300      0.46443000      5.28392000
```

B+B conformer of equatorial isomer of **6d:**
Table S22.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.637789 A.U.
 N                  -1.49395600      2.70542600     -0.57608600
 C                  -1.16631600      1.85143100      0.36317700
 C                  -0.70433700      3.74781200     -0.93850200
 C                  -0.00770800      2.18255600      1.30264800
 C                   0.70104300      3.77969700     -0.91272900
 N                   1.52507900      2.77670600     -0.51616800
 C                   1.20210000      1.90989600      0.41304400
 C                  -1.88684000      0.59832100      0.48056000
 C                  -2.85052800      0.21532300     -0.39673300
 C                   1.98535400      0.70129000      0.58021400
 C                   2.99873900      0.35664500     -0.25608800
 C                   5.70966500     -2.08433600     -1.14667900
 C                   4.85064700     -0.98917300     -1.15599700
 C                   5.58990600     -3.04258000     -0.13052600
 C                   3.85861800     -0.80900600     -0.17391400
 C                   4.60492800     -2.88274400      0.86444000
 C                   3.76009600     -1.78987700      0.84158100
 O                   6.36555600     -4.14840400     -0.01518100
 C                   7.38569300     -4.37155600     -0.98896000
 C                  -5.40169300     -2.34487700     -1.41530900
 C                  -4.60115700     -1.20682800     -1.37818200
```

```
C              -5.26054300    -3.31686700    -0.41507900
C              -3.64792000    -0.99629500    -0.36424300
C              -4.31250500    -3.12804300     0.61022600
C              -3.52577000    -1.99267700     0.63340400
O              -5.98117800    -4.46282300    -0.34320400
C              -6.96421700    -4.71534400    -1.34749600
C              -1.40525900     4.82817300    -1.58637900
N              -1.99495300     5.69986400    -2.08279500
C               1.37509100     4.89120700    -1.53579600
N               1.94223900     5.78912900    -2.01135900
C              -0.00923200     1.52596900     2.69097900
C              -1.14594900     2.03390600     3.59006600
C              -1.11439100     1.40951700     4.98776500
H              -1.62577600    -0.03904300     1.31671800
H              -3.06041100     0.89555400    -1.21977200
H               1.72947600     0.06711000     1.42051000
H               3.19923500     1.03234800    -1.08522800
H              -0.03693600     3.27094900     1.44816500
H               6.45865000    -2.18254300    -1.92249000
H               4.94927900    -0.25073400    -1.94681600
H               4.53030100    -3.63470000     1.64287600
H               3.01299400    -1.69191600     1.62257200
H               8.12113300    -3.55949800    -0.98794000
H               7.87321700    -5.30267600    -0.70070700
H               6.96080900    -4.47822500    -1.99318200
H              -6.12249200    -2.46520300    -2.21436500
H              -4.71640600    -0.45770400    -2.15660100
H              -4.21990500    -3.89178100     1.37514100
H              -2.80620400    -1.87340700     1.43694900
H              -6.50924500    -4.78166900    -2.34195800
H              -7.41317700    -5.67432000    -1.08951600
H              -7.73789100    -3.93959600    -1.35064500
H              -0.06123900     0.43378100     2.61990000
H               0.95222100     1.75107900     3.16846200
H              -1.07561600     3.12612400     3.67276100
H              -2.11340400     1.82573300     3.11637500
H              -1.92878800     1.79314300     5.60983200
H              -1.21792200     0.31963800     4.93870100
H              -0.17088000     1.63025400     5.49924300
```

Table S23.

TD–DFT output

HOMO: 119, LUMO: 120
STATE #   1   ENERGY =   3.041200 EV
 OSCILLATOR STRENGTH =   1.230000
                 EXCITATION DE-EXCITATION
     OCC   VIR AMPLITUDE   AMPLITUDE
      I   A   X(I->A)   Y(A->I)
     ---   --- --------   --------
     118   121 -0.170800   0.000000
     119   120   0.664640   0.000000

```
STATE #   2   ENERGY =    3.764500 EV
OSCILLATOR STRENGTH =    0.342100
              EXCITATION  DE-EXCITATION
   OCC    VIR  AMPLITUDE    AMPLITUDE
    I      A    X(I->A)      Y(A->I)
   ---    ---  --------    --------
   117    121  -0.206500     0.000000
   118    120   0.178710     0.000000
   119    121   0.617200     0.000000


STATE #   3   ENERGY =    3.879200 EV
OSCILLATOR STRENGTH =    1.328500
              EXCITATION  DE-EXCITATION
   OCC    VIR  AMPLITUDE    AMPLITUDE
    I      A    X(I->A)      Y(A->I)
   ---    ---  --------    --------
   113    120  -0.120980     0.000000
   118    120   0.644350     0.000000
   119    121  -0.211440     0.000000


STATE #   4   ENERGY =    4.243200 EV
OSCILLATOR STRENGTH =    0.000200
              EXCITATION  DE-EXCITATION
   OCC    VIR  AMPLITUDE    AMPLITUDE
    I      A    X(I->A)      Y(A->I)
   ---    ---  --------    --------
   111    120   0.101970     0.000000
   112    121  -0.191420     0.000000
   114    120   0.445590     0.000000
   117    120   0.447660     0.000000
   119    122  -0.100690     0.000000


STATE #   5   ENERGY =    4.421300 EV
OSCILLATOR STRENGTH =    0.192900
              EXCITATION  DE-EXCITATION
   OCC    VIR  AMPLITUDE    AMPLITUDE
    I      A    X(I->A)      Y(A->I)
   ---    ---  --------    --------
   112    121   0.118100     0.000000
   114    120   0.137990     0.000000
   117    122  -0.101380     0.000000
   118    121   0.625360     0.000000
   119    120   0.167100     0.000000


STATE #   6   ENERGY =    4.656300 EV
OSCILLATOR STRENGTH =    0.042500
              EXCITATION  DE-EXCITATION
   OCC    VIR  AMPLITUDE    AMPLITUDE
    I      A    X(I->A)      Y(A->I)
   ---    ---  --------    --------
   111    121  -0.104040     0.000000
   112    120   0.417240     0.000000
```

```
114    121  -0.353070        0.000000
117    121  -0.307210        0.000000
119    121  -0.168660        0.000000


STATE #   7  ENERGY =    4.820000 EV
OSCILLATOR STRENGTH =    0.001000
                 EXCITATION  DE-EXCITATION
   OCC      VIR   AMPLITUDE      AMPLITUDE
    I        A     X(I->A)        Y(A->I)
   ---      ---   --------      --------
   115      120   0.350220        0.000000
   115      121  -0.120710        0.000000
   115      122   0.146140        0.000000
   116      120  -0.205530        0.000000
   116      121   0.283540        0.000000
   117      124  -0.102610        0.000000
   118      123  -0.227900        0.000000
   118      124  -0.136250        0.000000
   119      123  -0.113630        0.000000
   119      124  -0.261700        0.000000


STATE #   8  ENERGY =    4.821300 EV
OSCILLATOR STRENGTH =    0.000400
                 EXCITATION  DE-EXCITATION
   OCC      VIR   AMPLITUDE      AMPLITUDE
    I        A     X(I->A)        Y(A->I)
   ---      ---   --------      --------
   115      120   0.205650        0.000000
   115      121   0.279030        0.000000
   116      120   0.349590        0.000000
   116      121   0.131110        0.000000
   116      122   0.142790        0.000000
   117      123   0.100650        0.000000
   118      123  -0.140330        0.000000
   118      124   0.226670        0.000000
   119      123   0.262140        0.000000
   119      124  -0.112640        0.000000


STATE #   9  ENERGY =    4.894300 EV
OSCILLATOR STRENGTH =    0.116700
                 EXCITATION  DE-EXCITATION
   OCC      VIR   AMPLITUDE      AMPLITUDE
    I        A     X(I->A)        Y(A->I)
   ---      ---   --------      --------
   112      120   0.484310        0.000000
   112      122  -0.101830        0.000000
   114      121   0.167330        0.000000
   117      121   0.372230        0.000000
   118      122  -0.132150        0.000000


STATE #  10  ENERGY =    4.988300 EV
OSCILLATOR STRENGTH =    0.001200
                 EXCITATION  DE-EXCITATION
```

```
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A      X(I->A)          Y(A->I)
          ---      ---    --------         --------
          117      122   -0.183400        0.000000
          119      122    0.634150        0.000000


STATE #  11  ENERGY =     5.052000 EV
OSCILLATOR STRENGTH =     0.006400
                    EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A      X(I->A)          Y(A->I)
          ---      ---    --------         --------
          111      120   -0.227570        0.000000
          114      120   -0.405420        0.000000
          117      120    0.473250        0.000000


STATE #  12  ENERGY =     5.470900 EV
OSCILLATOR STRENGTH =     0.027100
                    EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A      X(I->A)          Y(A->I)
          ---      ---    --------         --------
          112      121    0.510550        0.000000
          114      120    0.107740        0.000000
          114      122   -0.287050        0.000000
          117      122   -0.164680        0.000000
          118      121   -0.182460        0.000000


STATE #  13  ENERGY =     5.605900 EV
OSCILLATOR STRENGTH =     0.035000
                    EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A      X(I->A)          Y(A->I)
          ---      ---    --------         --------
          107      120    0.179480        0.000000
          111      121   -0.125520        0.000000
          113      120    0.470040        0.000000
          116      120   -0.163330        0.000000
          118      120    0.139410        0.000000
          118      122    0.261430        0.000000
          119      121    0.114750        0.000000
          119      123    0.121850        0.000000
          119      125    0.132220        0.000000


STATE #  14  ENERGY =     5.671200 EV
OSCILLATOR STRENGTH =     0.075000
                    EXCITATION  DE-EXCITATION
          OCC      VIR   AMPLITUDE        AMPLITUDE
           I        A      X(I->A)          Y(A->I)
          ---      ---    --------         --------
          116      120    0.411770        0.000000
          117      121    0.125590        0.000000
          118      122    0.310570        0.000000
```

```
118     124  -0.237370       0.000000
119     123  -0.319070       0.000000


STATE #  15   ENERGY =     5.686200 EV
OSCILLATOR STRENGTH =      0.069100
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)       Y(A->I)
    ---     ---  --------      --------
    115     120   0.482750      0.000000
    118     123   0.284610      0.000000
    119     124   0.366810      0.000000


STATE #  16   ENERGY =     5.739500 EV
OSCILLATOR STRENGTH =      0.017000
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)       Y(A->I)
    ---     ---  --------      --------
    111     126   0.107720      0.000000
    116     120   0.103160      0.000000
    117     125  -0.191620      0.000000
    117     126  -0.287630      0.000000
    119     125   0.376760      0.000000
    119     126   0.419270      0.000000


STATE #  17   ENERGY =     5.799400 EV
OSCILLATOR STRENGTH =      0.179700
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)       Y(A->I)
    ---     ---  --------      --------
    113     120   0.326680      0.000000
    113     122   0.100820      0.000000
    114     121   0.359390      0.000000
    116     120   0.139780      0.000000
    117     121  -0.347240      0.000000
    118     122  -0.195210      0.000000


STATE #  18   ENERGY =     5.863800 EV
OSCILLATOR STRENGTH =      0.096800
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)       Y(A->I)
    ---     ---  --------      --------
    107     120  -0.109150      0.000000
    111     121   0.108460      0.000000
    112     120   0.148730      0.000000
    113     120  -0.172320      0.000000
    114     121   0.315110      0.000000
    116     120  -0.113940      0.000000
    117     121  -0.146550      0.000000
    118     122   0.460650      0.000000
```

```
 119     123    0.110630         0.000000

STATE #  19  ENERGY =     6.130000 EV
OSCILLATOR STRENGTH =     0.007400
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)        Y(A->I)
    ---     ---  --------      --------
    111     120    0.425290         0.000000
    112     121    0.157990         0.000000
    113     121   -0.167450         0.000000
    115     124    0.113600         0.000000
    116     123   -0.116020         0.000000
    117     122    0.295040         0.000000
    119     125    0.137830         0.000000
    119     126   -0.113380         0.000000
    119     127   -0.146030         0.000000

STATE #  20  ENERGY =     6.141800 EV
OSCILLATOR STRENGTH =     0.003700
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)        Y(A->I)
    ---     ---  --------      --------
    111     120   -0.185180         0.000000
    113     120   -0.137850         0.000000
    115     121   -0.176260         0.000000
    115     123   -0.106230         0.000000
    116     120    0.111520         0.000000
    116     124    0.114500         0.000000
    118     127    0.159770         0.000000
    119     123    0.120350         0.000000
    119     125    0.380250         0.000000
    119     126   -0.318340         0.000000

STATE #  21  ENERGY =     6.160200 EV
OSCILLATOR STRENGTH =     0.005500
               EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A   X(I->A)        Y(A->I)
    ---     ---  --------      --------
    111     120   -0.246770         0.000000
    112     121    0.197760         0.000000
    113     121    0.235050         0.000000
    114     120    0.186110         0.000000
    114     122    0.166470         0.000000
    115     120    0.137050         0.000000
    116     121   -0.232840         0.000000
    117     122    0.266470         0.000000
    119     122    0.136530         0.000000
    119     127   -0.200630         0.000000

STATE #  22  ENERGY =     6.218300 EV
```

```
OSCILLATOR STRENGTH =    0.065000
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------     --------
       111      120  -0.121960    0.000000
       115      120  -0.244780    0.000000
       115      121   0.173540    0.000000
       116      121   0.513720    0.000000
       117      122   0.161030    0.000000
       119      124   0.180560    0.000000


STATE #  23  ENERGY =    6.230400 EV
OSCILLATOR STRENGTH =    0.068500
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------     --------
       115      121   0.535010    0.000000
       116      120  -0.253180    0.000000
       116      121  -0.170670    0.000000
       118      124  -0.102800    0.000000
       119      123  -0.152380    0.000000
       119      125   0.161560    0.000000
       119      126  -0.110260    0.000000


STATE #  24  ENERGY =    6.408200 EV
OSCILLATOR STRENGTH =    0.003700
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------     --------
       106      120  -0.125340    0.000000
       110      120   0.122500    0.000000
       111      120   0.182120    0.000000
       112      121   0.132940    0.000000
       113      121   0.250400    0.000000
       114      122   0.146990    0.000000
       115      124  -0.129600    0.000000
       116      123   0.130620    0.000000
       118      125   0.278670    0.000000
       118      126  -0.125940    0.000000
       119      127   0.339420    0.000000


STATE #  25  ENERGY =    6.448000 EV
OSCILLATOR STRENGTH =    0.008000
                  EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------     --------
       104      120   0.404050    0.000000
       104      122  -0.219680    0.000000
       107      120   0.338570    0.000000
```

```
107    122  -0.169950        0.000000
112    122   0.101190        0.000000
113    120  -0.108170        0.000000
119    126   0.108640        0.000000


STATE #  26  ENERGY =    6.490700 EV
OSCILLATOR STRENGTH =    0.021500
                EXCITATION  DE-EXCITATION
     OCC    VIR  AMPLITUDE      AMPLITUDE
      I      A    X(I->A)        Y(A->I)
     ---    ---  --------      --------
     102    120   0.112960        0.000000
     106    120  -0.148870        0.000000
     110    120   0.160340        0.000000
     111    120   0.141570        0.000000
     113    121   0.366230        0.000000
     114    120  -0.115950        0.000000
     114    122  -0.106120        0.000000
     117    122  -0.258940        0.000000
     119    127  -0.306110        0.000000


STATE #  27  ENERGY =    6.544800 EV
OSCILLATOR STRENGTH =    0.002500
                EXCITATION  DE-EXCITATION
     OCC    VIR  AMPLITUDE      AMPLITUDE
      I      A    X(I->A)        Y(A->I)
     ---    ---  --------      --------
     100    121  -0.109340        0.000000
     101    120  -0.124680        0.000000
     102    120   0.136610        0.000000
     103    120   0.251650        0.000000
     106    120  -0.230240        0.000000
     109    121  -0.105730        0.000000
     110    120   0.329400        0.000000
     113    121  -0.259620        0.000000
     118    125  -0.107920        0.000000


STATE #  28  ENERGY =    6.671600 EV
OSCILLATOR STRENGTH =    0.001500
                EXCITATION  DE-EXCITATION
     OCC    VIR  AMPLITUDE      AMPLITUDE
      I      A    X(I->A)        Y(A->I)
     ---    ---  --------      --------
      97    120  -0.148240        0.000000
     100    120   0.258840        0.000000
     101    121   0.185910        0.000000
     108    121   0.141670        0.000000
     109    120   0.364770        0.000000
     109    122   0.155680        0.000000
     110    121  -0.284320        0.000000


STATE #  29  ENERGY =    6.730400 EV
OSCILLATOR STRENGTH =    0.023200
```

```
                    EXCITATION  DE-EXCITATION
      OCC      VIR  AMPLITUDE     AMPLITUDE
       I        A    X(I->A)       Y(A->I)
      ---      ---  --------     --------
       98      120  -0.163190    0.000000
       99      120   0.142820    0.000000
      102      120   0.146600    0.000000
      106      120  -0.114820    0.000000
      110      120   0.105140    0.000000
      111      120  -0.124200    0.000000
      111      122  -0.114810    0.000000
      113      121  -0.189850    0.000000
      114      122  -0.156620    0.000000
      117      122   0.100870    0.000000
      117      127   0.121270    0.000000
      117      128  -0.110800    0.000000
      118      123   0.150310    0.000000
      118      125   0.212300    0.000000
      119      124  -0.149900    0.000000
      119      128   0.194460    0.000000


  STATE #  30  ENERGY =    6.746600 EV
  OSCILLATOR STRENGTH =    0.020900
                    EXCITATION  DE-EXCITATION
      OCC      VIR  AMPLITUDE     AMPLITUDE
       I        A    X(I->A)       Y(A->I)
      ---      ---  --------     --------
       96      120   0.101120    0.000000
       98      120   0.110610    0.000000
       99      120  -0.108140    0.000000
      100      121   0.164480    0.000000
      101      120   0.184600    0.000000
      103      120   0.105630    0.000000
      105      120   0.113950    0.000000
      106      120  -0.183390    0.000000
      108      120   0.310080    0.000000
      108      122   0.102680    0.000000
      109      121   0.293040    0.000000
      110      120  -0.156180    0.000000
      110      122  -0.120530    0.000000
```

A+A conformer of axial isomer of **6d:**

Table S24.

```
TOTAL FREE ENERGY IN SOLVENT = -1451.635479 A.U.
  N              3.30748300    1.14579000   -0.80081200
  C              2.17851300    0.94958100   -0.16260500
  C              4.31144000    0.23559200   -0.90066400
  C              1.96681100   -0.22357900    0.78931300
  C              4.18889300   -1.15823000   -0.87226700
  N              3.04316800   -1.87531400   -0.73243600
  C              1.96975500   -1.45867800   -0.10451800
  C              1.14038400    1.92509200   -0.42435700
```

C	−0.07804100	2.00158700	0.17026800
C	0.78050600	−2.25974100	−0.30911400
C	−0.42655100	−2.09813400	0.29137200
C	−2.86360700	−4.68770600	−1.01126200
C	−1.70213900	−3.95511400	−0.85893400
C	−3.99908200	−4.39558100	−0.23015000
C	−1.62080500	−2.89958300	0.07989700
C	−3.94547200	−3.35261200	0.70501800
C	−2.76810300	−2.62348700	0.84604900
O	−5.08496800	−5.17378600	−0.45971300
C	−6.27211300	−4.93079900	0.29488900
C	−3.34337100	3.84086000	0.46035700
C	−2.30416000	2.93639300	0.65950500
C	−3.21710500	4.82437700	−0.53056100
C	−1.12188400	2.97589600	−0.10230500
C	−2.04377400	4.88089600	−1.30826300
C	−1.02100300	3.97615500	−1.09811000
O	−4.15753100	5.75708300	−0.81863700
C	−5.37312200	5.75575600	−0.07016800
C	5.58868100	0.80738200	−1.24844100
N	6.61580400	1.29256300	−1.50042800
C	5.34459400	−1.95754700	−1.19527700
N	6.26945900	−2.62429600	−1.42773600
C	2.96556800	−0.29420200	1.97066900
C	2.85190500	0.90611100	2.92009600
C	3.80475700	0.79753200	4.11425300
H	1.42157700	2.65233100	−1.18018200
H	−0.33373300	1.28220100	0.94426900
H	0.92875600	−3.06654100	−1.02067300
H	−0.55099000	−1.30256600	1.02192400
H	0.97742800	−0.12699900	1.23349500
H	−2.92625100	−5.49589100	−1.73220600
H	−0.84634600	−4.20021200	−1.47893300
H	−4.80333000	−3.10570300	1.31791600
H	−2.73545900	−1.81754300	1.57438600
H	−6.65770400	−3.92091300	0.11600100
H	−7.00032600	−5.66342800	−0.05247700
H	−6.09777300	−5.07087600	1.36748300
H	−4.23479000	3.77393800	1.07146200
H	−2.41090900	2.17822200	1.43081600
H	−1.96662000	5.64678900	−2.07265100
H	−0.13209600	4.04173200	−1.71646300
H	−5.96748800	6.57850100	−0.46703800
H	−5.91982300	4.81519200	−0.20074100
H	−5.18431100	5.92381200	0.99591600
H	2.75078600	−1.21814300	2.52122400
H	3.99569200	−0.37960500	1.61692600
H	3.06100900	1.83161500	2.36968000
H	1.81807800	0.98946700	3.28137400
H	3.60067700	−0.10278800	4.70451900
H	4.84824200	0.74861100	3.78442200
H	3.70544600	1.66192700	4.77808300

Rotational transition state **Ts$_2$** of axial isomer of **6d**:
Table S25.

```
TOTAL FREE ENERGY IN SOLVENT = -1451.620397 A.U.
 N              3.12200300     1.02540800    -1.09674000
 C              2.12904600     0.93519800    -0.24245400
 C              4.17478300     0.17022600    -1.16310900
 C              2.18620900     0.00926400     0.96793300
 C              4.19040300    -1.17918300    -0.80788400
 N              3.11568300    -1.89488700    -0.34685200
 C              2.14896500    -1.38433900     0.34177800
 C              0.97935700     1.76993000    -0.52561800
 C             -0.13548100     1.90004100     0.23936500
 C              0.93028200    -2.21300100     0.56039600
 C             -0.18562300    -2.10006600    -0.17729100
 C             -2.84795000    -4.50406100     1.07615600
 C             -1.64699400    -3.82222700     0.97789000
 C             -3.89176900    -4.24146800     0.17054300
 C             -1.43627400    -2.85208800    -0.02478000
 C             -3.70691000    -3.28338500    -0.83274800
 C             -2.49028300    -2.60532900    -0.91688900
 O             -5.02977400    -4.96510700     0.35505300
 C             -6.12054500    -4.74887700    -0.53660700
 C             -3.48826100     3.53066500     0.69700500
 C             -2.35134300     2.75151600     0.88920400
 C             -3.58845300     4.32706200    -0.45261200
 C             -1.29096500     2.73579200    -0.03609300
 C             -2.53963400     4.32581600    -1.39386600
 C             -1.41738700     3.54707200    -1.18886100
 O             -4.64170500     5.12525800    -0.75023000
 C             -5.74031100     5.17700500     0.16065300
 C              5.32965600     0.71720900    -1.83618900
 N              6.25857600     1.18770100    -2.35399500
 C              5.35040300    -1.97329800    -1.10908300
 N              6.28954900    -2.62826600    -1.31749000
 C              3.36412500     0.26621100     1.93842000
 C              3.26734500     1.63066200     2.63500400
 C              4.40293600     1.85417700     3.63804400
 H              1.07631900     2.33097000    -1.45012600
 H             -0.20762700     1.33321300     1.16440700
 H              0.99944400    -2.92199300     1.38465800
 H             -0.18870200    -1.37515800    -0.99057000
 H              1.26881000     0.11969800     1.54649800
 H             -3.00689300    -5.25009400     1.84791100
 H             -0.86111700    -4.04837000     1.69189800
 H             -4.49130700    -3.05981400    -1.54527400
 H             -2.35809500    -1.86420100    -1.70077900
 H             -5.84474200    -4.98352000    -1.57120500
 H             -6.91137000    -5.42525900    -0.21160800
 H             -6.48255500    -3.71545600    -0.48377700
 H             -4.27971800     3.51256800     1.43571600
 H             -2.28191200     2.13726400     1.78290600
 H             -2.63727100     4.94798300    -2.27712100
 H             -0.62706300     3.56594600    -1.93180700
```

```
H                 -6.45576400        5.87321700       -0.27637000
H                 -6.21032300        4.19377300        0.27311200
H                 -5.42532800        5.54632500        1.14279400
H                  3.34456800       -0.53069400        2.69167400
H                  4.32775600        0.18571900        1.43055100
H                  3.28189100        2.42914700        1.88294900
H                  2.30077900        1.70940600        3.15010800
H                  4.39572000        1.08926300        4.42252100
H                  5.38029700        1.81500700        3.14482500
H                  4.31339900        2.83101500        4.12320200
```

A+B conformer of axial isomer of **6d**:

Table S26.

```
TOTAL FREE ENERGY IN SOLVENT = -1451.636151 A.U.
 N                 -1.37586100        2.89644600       -1.03277400
 C                 -1.33617500        1.87341000       -0.21295600
 C                 -0.44342700        3.88411700       -1.09091700
 C                 -0.38261900        1.81765300        0.97540400
 C                  0.91453300        3.78280100       -0.76198200
 N                  1.56680600        2.68111300       -0.31253400
 C                  1.00250300        1.70082900        0.34678900
 C                 -2.25727600        0.79557500       -0.51421100
 C                 -2.43708900       -0.34583000        0.19792000
 C                  1.71014900        0.44455600        0.50643600
 C                  2.91287700        0.18823600       -0.07217600
 C                  4.13403900       -3.26900600        0.86228400
 C                  3.33073400       -2.14728100        0.79800300
 C                  5.35951700       -3.30845700        0.16717800
 C                  3.71244600       -1.01571300        0.03782800
 C                  5.76117700       -2.20066500       -0.59267900
 C                  4.94066000       -1.07809500       -0.64759000
 O                  6.07009700       -4.45472800        0.29820200
 C                  7.32329200       -4.56387600       -0.37789800
 C                 -4.27928200       -3.60487700        0.54018400
 C                 -3.42452800       -2.52970300        0.76749000
 C                 -5.09550500       -3.60412100       -0.59934700
 C                 -3.35141200       -1.43346600       -0.11136700
 C                 -5.03797500       -2.51792200       -1.49451400
 C                 -4.18442100       -1.45811300       -1.25478900
 O                 -5.96476300       -4.59108900       -0.92927300
 C                 -6.07010200       -5.72450500       -0.06798800
 C                 -0.90746700        5.09109200       -1.72814800
 N                 -1.31079500        6.06523800       -2.22073000
 C                  1.78189600        4.89157600       -1.07550900
 N                  2.49909600        5.78078100       -1.29674500
 C                 -0.53845900        2.97759800        1.98810200
 C                 -1.89305800        2.95908400        2.70952100
 C                 -2.01921400        4.08282800        3.74243700
 H                 -2.83565900        0.97075000       -1.41648200
 H                 -1.85439000       -0.50005300        1.10304300
 H                  1.22700300       -0.30164800        1.12901200
 H                  3.33496000        0.98164500       -0.68613000
```

H	-0.56501400	0.89542000	1.52940000
H	3.84277100	-4.13658600	1.44487500
H	2.39342100	-2.14452600	1.34480100
H	6.69771100	-2.20486700	-1.13610100
H	5.25804800	-0.22334300	-1.23835200
H	8.02954300	-3.80113600	-0.03198000
H	7.70843800	-5.55314600	-0.13154700
H	7.19809600	-4.48120300	-1.46308900
H	-4.30309500	-4.42656700	1.24505100
H	-2.79615500	-2.53914500	1.65416800
H	-5.67578100	-2.53676500	-2.37185900
H	-4.16003800	-0.63793400	-1.96448600
H	-6.81602200	-6.37570900	-0.52329200
H	-5.11629200	-6.25875900	0.00543700
H	-6.40379800	-5.43346600	0.93421600
H	0.26892900	2.87837900	2.72378500
H	-0.39851000	3.94826800	1.50675400
H	-2.70254100	3.04649600	1.97436100
H	-2.02964200	1.98829600	3.20450000
H	-1.24127400	4.00530600	4.51021000
H	-1.92277400	5.06674400	3.27051700
H	-2.99020800	4.04869000	4.24620600

Rotational transition state **Ts₁** of axial isomer of **6d**:
Table S27.
TOTAL FREE ENERGY IN SOLVENT = -1451.621427 A.U.

N	-1.21346700	2.49330300	-1.08210500
C	-1.09683900	1.53681800	-0.21954300
C	-0.38219600	3.58135400	-1.14012100
C	-0.17905400	1.59967200	1.00271200
C	0.97301700	3.58704300	-0.79792600
N	1.70013000	2.55030600	-0.31622100
C	1.20892200	1.54965700	0.37439800
C	-1.83970000	0.26880600	-0.46736800
C	-3.07577700	0.03301800	-0.00046300
C	1.99231000	0.34359100	0.55515000
C	3.19733100	0.14459600	-0.04230300
C	4.65169400	-3.19778900	0.96762400
C	3.77997900	-2.12953800	0.89118600
C	5.85870700	-3.18596900	0.23932000
C	4.07203200	-1.00303800	0.08470000
C	6.17249600	-2.08116300	-0.56543900
C	5.28389300	-1.01281800	-0.63229700
O	6.64031700	-4.28209200	0.38516100
C	7.87969000	-4.33927300	-0.32279600
C	-5.98093800	-2.35864100	0.26172100
C	-5.15502700	-1.24285900	0.40249600
C	-5.54397000	-3.44450900	-0.50561800
C	-3.89102000	-1.17026600	-0.20139300
C	-4.28109900	-3.39109700	-1.12284800
C	-3.47473100	-2.27572700	-0.97311600
O	-6.25651800	-4.58482200	-0.71663400
C	-7.54831100	-4.69422900	-0.12425100

```
C              -0.94545800      4.72823400     -1.79871100
N              -1.42872400      5.65739800     -2.30644100
C               1.75976200      4.75197500     -1.13059300
N               2.40907200      5.68797500     -1.36459900
C              -0.41441400      2.78120500      1.97236400
C              -1.80883000      2.76376100      2.61292500
C              -1.98759600      3.87690700      3.64971300
H              -1.30865200     -0.47103000     -1.06510200
H              -3.55379000      0.81049700      0.59442200
H               1.56638600     -0.40966900      1.21002000
H               3.55628600      0.94283100     -0.68927300
H              -0.33000800      0.67750900      1.56906300
H               4.42982200     -4.06160800      1.58519800
H               2.85940100     -2.16490200      1.46457900
H               7.09330900     -2.04672100     -1.13398300
H               5.53272800     -0.16016600     -1.25787900
H               8.54814400     -3.52600500     -0.01986100
H               8.32888100     -5.29606100     -0.05761400
H               7.72072700     -4.29854100     -1.40589100
H              -6.94912800     -2.36906900      0.74698800
H              -5.50532300     -0.40517700      0.99991400
H              -3.95917400     -4.23918500     -1.71829300
H              -2.50843500     -2.26255200     -1.46770000
H              -7.93253100     -5.67001400     -0.42217000
H              -7.49305000     -4.64459200      0.96944400
H              -8.22366700     -3.91155200     -0.48875500
H               0.34842400      2.70449700      2.75665600
H              -0.25472200      3.74331400      1.48066600
H              -2.57224800      2.87052300      1.83185600
H              -1.98223000      1.78825200      3.08611200
H              -1.26127300      3.77959400      4.46422100
H              -1.84953200      4.86507800      3.19751500
H              -2.98904400      3.84887600      4.09008700
```

B+B conformer of axial isomer of **6d**:
Table S28.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.637357 A.U.
N              -1.53935600      2.33732300     -0.64906500
C              -1.20077400      1.51152700      0.30934400
C              -0.75662700      3.34290300     -1.11515700
C              -0.02304100      1.77600100      1.24322600
C               0.64432800      3.40257300     -1.09518300
N               1.49637100      2.46894000     -0.60188100
C               1.20193400      1.61760300      0.34840000
C              -1.96164000      0.29131900      0.50617200
C              -2.97050200     -0.09966400     -0.31549000
C               2.06495000      0.47375900      0.57970000
C               3.13597000      0.17742200     -0.20175700
C               4.90738500     -2.91316000      1.07654600
C               3.98957700     -1.88480300      0.98477700
C               5.95179500     -3.02184000      0.13666300
C               4.07095700     -0.92037300     -0.04808700
```

C	6.05583900	-2.07863800	-0.89531200
C	5.12298900	-1.04885800	-0.97455500
O	6.79675200	-4.06611400	0.31775100
C	7.87929000	-4.23607100	-0.59779900
C	-5.64021800	-2.61462600	-1.11813000
C	-4.80238500	-1.50429200	-1.16449100
C	-5.49433900	-3.54214200	-0.07703100
C	-3.80630900	-1.27861700	-0.19570500
C	-4.50466300	-3.33681600	0.90498700
C	-3.68105700	-2.22941200	0.84540200
O	-6.24796400	-4.65844800	0.07513200
C	-7.27132500	-4.92785400	-0.88357100
C	-1.47539400	4.35486500	-1.84932100
N	-2.08009800	5.17186800	-2.41597200
C	1.29519600	4.47245100	-1.80991900
N	1.84412000	5.33832300	-2.36062500
C	-0.08342200	3.10951000	2.02412500
C	-1.26983100	3.17624500	2.99539000
C	-1.28626400	4.47343100	3.80943900
H	-1.68467400	-0.31049100	1.36594200
H	-3.18754900	0.54949600	-1.16167500
H	1.81273700	-0.14962500	1.43176300
H	3.32407900	0.84435000	-1.04102400
H	-0.00000800	0.97222900	1.98459300
H	4.84563600	-3.65276300	1.86783100
H	3.19697700	-1.82546100	1.72357600
H	6.84896100	-2.13871600	-1.62999100
H	5.20975300	-0.32174800	-1.77713800
H	8.55469400	-3.37363000	-0.57980800
H	8.41549600	-5.12360400	-0.26238600
H	7.51552500	-4.39413700	-1.61906800
H	-6.39328800	-2.74828400	-1.88460200
H	-4.92116600	-0.78966100	-1.97415000
H	-4.40967300	-4.06576400	1.70284600
H	-2.92960300	-2.09574700	1.61679500
H	-7.73818800	-5.85998600	-0.56593400
H	-8.02246800	-4.13044900	-0.89833300
H	-6.85229500	-5.05367100	-1.88800600
H	0.85456300	3.20024600	2.58545100
H	-0.12054800	3.96646200	1.34728400
H	-2.20869600	3.08515900	2.43535500
H	-1.23188600	2.31543700	3.67648300
H	-0.37325800	4.57897000	4.40607800
H	-1.35880700	5.34979700	3.15606100
H	-2.13838400	4.49823900	4.49581500

Table S29.
TD–DFT output
HOMO: 119, LUMO: 120
STATE # 1 ENERGY =   2.920900 EV
 OSCILLATOR STRENGTH =   1.294000
                EXCITATION DE-EXCITATION
    OCC   VIR AMPLITUDE   AMPLITUDE

```
    I      A     X(I->A)       Y(A->I)
   ---    ---   --------      --------
   118    121   -0.156290     0.000000
   119    120    0.668650     0.000000


STATE #   2  ENERGY =    3.705400 EV
OSCILLATOR STRENGTH =    0.150600
                 EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I      A     X(I->A)       Y(A->I)
   ---    ---   --------      --------
   113    120    0.114730     0.000000
   117    121   -0.221690     0.000000
   118    120    0.260950     0.000000
   119    121    0.577100     0.000000


STATE #   3  ENERGY =    3.823600 EV
OSCILLATOR STRENGTH =    1.410000
                 EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I      A     X(I->A)       Y(A->I)
   ---    ---   --------      --------
   113    120    0.104570     0.000000
   118    120    0.615350     0.000000
   119    121   -0.292150     0.000000


STATE #   4  ENERGY =    4.068500 EV
OSCILLATOR STRENGTH =    0.008000
                 EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I      A     X(I->A)       Y(A->I)
   ---    ---   --------      --------
   112    121   -0.174460     0.000000
   114    120    0.446380     0.000000
   117    120    0.463210     0.000000


STATE #   5  ENERGY =    4.450300 EV
OSCILLATOR STRENGTH =    0.221100
                 EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE     AMPLITUDE
    I      A     X(I->A)       Y(A->I)
   ---    ---   --------      --------
   112    121    0.106040     0.000000
   113    121    0.117110     0.000000
   114    120    0.155830     0.000000
   117    122    0.112940     0.000000
   118    121    0.618650     0.000000
   119    120    0.148370     0.000000


STATE #   6  ENERGY =    4.568900 EV
OSCILLATOR STRENGTH =    0.022800
                 EXCITATION  DE-EXCITATION
   OCC     VIR  AMPLITUDE      AMPLITUDE
```

```
   I       A     X(I->A)        Y(A->I)
  ---     ---    --------       --------
  111     121   -0.101560      0.000000
  112     120    0.505250      0.000000
  114     121   -0.311440      0.000000
  117     121   -0.228620      0.000000
  119     121   -0.174190      0.000000


STATE #   7  ENERGY =     4.788900 EV
OSCILLATOR STRENGTH =     0.029000
                 EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I       A     X(I->A)        Y(A->I)
   ---     ---    --------       --------
   112     120    0.223630      0.000000
   114     121    0.119460      0.000000
   115     121    0.213850      0.000000
   116     120    0.358880      0.000000
   116     121   -0.100400      0.000000
   116     122   -0.133760      0.000000
   117     121    0.242010      0.000000
   118     124    0.220010      0.000000
   119     123    0.236530      0.000000


STATE #   8  ENERGY =     4.794000 EV
OSCILLATOR STRENGTH =     0.001300
                 EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I       A     X(I->A)        Y(A->I)
   ---     ---    --------       --------
   115     120    0.421580      0.000000
   115     121    0.134650      0.000000
   115     122   -0.159810      0.000000
   116     121    0.268040      0.000000
   117     120    0.104130      0.000000
   117     124   -0.108910      0.000000
   118     123   -0.253200      0.000000
   119     124   -0.258930      0.000000


STATE #   9  ENERGY =     4.821800 EV
OSCILLATOR STRENGTH =     0.117100
                 EXCITATION  DE-EXCITATION
   OCC      VIR  AMPLITUDE     AMPLITUDE
    I       A     X(I->A)        Y(A->I)
   ---     ---    --------       --------
   112     120    0.332250      0.000000
   114     121    0.188870      0.000000
   115     121   -0.172780      0.000000
   116     120   -0.240740      0.000000
   117     121    0.354950      0.000000
   118     122    0.111300      0.000000
   118     124   -0.134470      0.000000
   119     121    0.107940      0.000000
```

```
119      123   -0.123050        0.000000


STATE #  10   ENERGY =     4.889800 EV
OSCILLATOR STRENGTH =      0.007200
                 EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE       AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---  --------       --------
     111      120   -0.249170        0.000000
     112      120    0.100020        0.000000
     114      120   -0.392380        0.000000
     117      120    0.443640        0.000000
     119      122    0.117130        0.000000


STATE #  11   ENERGY =     4.953500 EV
OSCILLATOR STRENGTH =      0.003100
                 EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE       AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---  --------       --------
     117      120   -0.114550        0.000000
     117      122   -0.183960        0.000000
     119      122    0.629000        0.000000


STATE #  12   ENERGY =     5.447200 EV
OSCILLATOR STRENGTH =      0.018800
                 EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE       AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---  --------       --------
     112      121    0.498420        0.000000
     112      125   -0.101340        0.000000
     113      121    0.135760        0.000000
     114      120    0.108510        0.000000
     114      122    0.279910        0.000000
     117      122    0.147330        0.000000
     118      121   -0.202100        0.000000


STATE #  13   ENERGY =     5.564000 EV
OSCILLATOR STRENGTH =      0.057500
                 EXCITATION  DE-EXCITATION
     OCC      VIR  AMPLITUDE       AMPLITUDE
      I        A    X(I->A)        Y(A->I)
     ---      ---  --------       --------
     107      120    0.138040        0.000000
     111      121    0.137240        0.000000
     113      120    0.473950        0.000000
     116      120    0.225140        0.000000
     118      120   -0.141520        0.000000
     118      122    0.109220        0.000000
     118      124   -0.125160        0.000000
     119      123   -0.180300        0.000000
     119      125   -0.154600        0.000000
```

```
STATE #  14  ENERGY =    5.633200 EV
OSCILLATOR STRENGTH =    0.060700
                 EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE    AMPLITUDE
     I       A    X(I->A)      Y(A->I)
    ---     ---  --------    --------
    115     120   0.454400    0.000000
    116     120  -0.145130    0.000000
    117     124   0.105380    0.000000
    118     123   0.284240    0.000000
    119     124   0.366500    0.000000

STATE #  15  ENERGY =    5.639100 EV
OSCILLATOR STRENGTH =    0.062900
                 EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE    AMPLITUDE
     I       A    X(I->A)      Y(A->I)
    ---     ---  --------    --------
    113     120  -0.194410    0.000000
    115     120   0.116130    0.000000
    116     120   0.380340    0.000000
    117     121   0.122780    0.000000
    118     122  -0.244040    0.000000
    118     124  -0.236540    0.000000
    119     123  -0.308770    0.000000

STATE #  16  ENERGY =    5.657400 EV
OSCILLATOR STRENGTH =    0.003500
                 EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE    AMPLITUDE
     I       A    X(I->A)      Y(A->I)
    ---     ---  --------    --------
    111     126   0.101450    0.000000
    113     120   0.131320    0.000000
    117     125  -0.163870    0.000000
    117     126  -0.297710    0.000000
    119     125   0.313600    0.000000
    119     126   0.470260    0.000000

STATE #  17  ENERGY =    5.761600 EV
OSCILLATOR STRENGTH =    0.166000
                 EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE    AMPLITUDE
     I       A    X(I->A)      Y(A->I)
    ---     ---  --------    --------
    111     121   0.122970    0.000000
    112     120   0.150610    0.000000
    113     120  -0.253350    0.000000
    113     122   0.115830    0.000000
    114     121   0.406720    0.000000
    117     121  -0.371480    0.000000
    118     122   0.134910    0.000000
```

```
119     125   0.105970        0.000000


STATE #  18  ENERGY =     5.856800 EV
OSCILLATOR STRENGTH =    0.074000
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A   X(I->A)        Y(A->I)
    ---      ---  --------      --------
    113      120  -0.149980       0.000000
    114      121  -0.242430       0.000000
    116      120   0.101660       0.000000
    118      122   0.560300       0.000000


STATE #  19  ENERGY =     6.026900 EV
OSCILLATOR STRENGTH =    0.009100
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A   X(I->A)        Y(A->I)
    ---      ---  --------      --------
    104      120   0.123160       0.000000
    111      120   0.565440       0.000000
    113      121   0.229310       0.000000
    114      120  -0.218650       0.000000


STATE #  20  ENERGY =     6.108200 EV
OSCILLATOR STRENGTH =    0.005400
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A   X(I->A)        Y(A->I)
    ---      ---  --------      --------
    113      120   0.157200       0.000000
    115      121  -0.113600       0.000000
    115      123  -0.112580       0.000000
    116      124   0.107510       0.000000
    118      122  -0.129610       0.000000
    118      127   0.166580       0.000000
    119      123   0.112090       0.000000
    119      125   0.460030       0.000000
    119      126  -0.300890       0.000000


STATE #  21  ENERGY =     6.134500 EV
OSCILLATOR STRENGTH =    0.032000
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE     AMPLITUDE
     I        A   X(I->A)        Y(A->I)
    ---      ---  --------      --------
    112      121  -0.247970       0.000000
    114      120  -0.107120       0.000000
    114      122   0.154510       0.000000
    116      121   0.110390       0.000000
    117      122   0.435910       0.000000
    118      125   0.153260       0.000000
    119      122   0.151320       0.000000
```

```
       119     127    0.260980        0.000000


STATE #  22  ENERGY =     6.227900 EV
OSCILLATOR STRENGTH =     0.065700
                 EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------    --------
       115      120  -0.228130       0.000000
       115      121   0.129340       0.000000
       116      120   0.101320       0.000000
       116      121   0.566590       0.000000
       117      122  -0.113810       0.000000
       119      124   0.215590       0.000000


STATE #  23  ENERGY =     6.240500 EV
OSCILLATOR STRENGTH =     0.067700
                 EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------    --------
       115      120  -0.101700       0.000000
       115      121   0.568020       0.000000
       116      120  -0.225500       0.000000
       116      121  -0.126280       0.000000
       119      123  -0.196650       0.000000
       119      125   0.125670       0.000000


STATE #  24  ENERGY =     6.390000 EV
OSCILLATOR STRENGTH =     0.006900
                 EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------    --------
       103      120   0.404920       0.000000
       103      122   0.209460       0.000000
       106      120   0.277560       0.000000
       106      122   0.121800       0.000000
       107      120  -0.219410       0.000000
       107      122  -0.110120       0.000000
       110      120   0.109330       0.000000
       119      126   0.102520       0.000000


STATE #  25  ENERGY =     6.428400 EV
OSCILLATOR STRENGTH =     0.009400
                 EXCITATION  DE-EXCITATION
       OCC      VIR  AMPLITUDE    AMPLITUDE
        I        A    X(I->A)      Y(A->I)
       ---      ---  --------    --------
       112      121   0.183620       0.000000
       114      122  -0.187320       0.000000
       115      124  -0.115450       0.000000
       116      123   0.116900       0.000000
```

```
117     122    -0.205080        0.000000
118     125     0.275380        0.000000
118     126    -0.125430        0.000000
119     127     0.428110        0.000000


STATE #  26   ENERGY =     6.511200 EV
OSCILLATOR STRENGTH =     0.028200
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---   --------      --------
    105     120    -0.149950       0.000000
    106     120     0.115940       0.000000
    111     120    -0.158450       0.000000
    111     122    -0.116470       0.000000
    112     121    -0.134200       0.000000
    113     121     0.473560       0.000000
    114     120     0.102910       0.000000
    117     122    -0.141010       0.000000
    119     127     0.192980       0.000000


STATE #  27   ENERGY =     6.612800 EV
OSCILLATOR STRENGTH =     0.048200
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---   --------      --------
     96     120     0.113910       0.000000
    101     121     0.106960       0.000000
    102     120     0.101860       0.000000
    105     120     0.371200       0.000000
    106     120    -0.234030       0.000000
    107     120    -0.151230       0.000000
    108     120     0.125200       0.000000
    108     121     0.134990       0.000000
    109     120     0.225540       0.000000
    110     120     0.115470       0.000000
    113     121     0.158740       0.000000


STATE #  28   ENERGY =     6.637600 EV
OSCILLATOR STRENGTH =     0.003300
                 EXCITATION  DE-EXCITATION
    OCC      VIR  AMPLITUDE      AMPLITUDE
     I        A    X(I->A)        Y(A->I)
    ---      ---   --------      --------
     99     120    -0.110930       0.000000
    101     120     0.162340       0.000000
    101     121     0.147440       0.000000
    102     120     0.268380       0.000000
    102     121     0.105440       0.000000
    105     120    -0.141150       0.000000
    106     120     0.119290       0.000000
    108     120     0.232730       0.000000
```

```
108     121    0.212740          0.000000
108     122   -0.107370          0.000000
109     120    0.138990          0.000000
110     120   -0.245170          0.000000


STATE #  29  ENERGY =    6.645900 EV
OSCILLATOR STRENGTH =    0.001100
                EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A    X(I->A)       Y(A->I)
    ---     ---  --------      --------
    101     120    0.242500          0.000000
    102     120   -0.188210          0.000000
    102     121    0.188510          0.000000
    108     120    0.266040          0.000000
    109     120   -0.260770          0.000000
    109     121    0.269750          0.000000
    109     122    0.106100          0.000000


STATE #  30  ENERGY =    6.706400 EV
OSCILLATOR STRENGTH =    0.006500
                EXCITATION  DE-EXCITATION
    OCC     VIR  AMPLITUDE     AMPLITUDE
     I       A    X(I->A)       Y(A->I)
    ---     ---  --------      --------
     99     120   -0.165240          0.000000
    100     120    0.322530          0.000000
    100     122    0.145980          0.000000
    102     122    0.131080          0.000000
    106     120   -0.113960          0.000000
    109     120   -0.129500          0.000000
    110     120    0.192010          0.000000
    113     121    0.161240          0.000000
    114     122    0.113300          0.000000
    117     122   -0.127980          0.000000
    118     125    0.137740          0.000000
    119     128    0.158830          0.000000
```

Inversion transition state **Ts** of B+B conformer of **6d:**
Table S30.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.602670 A.U.
 N                 1.53343600    2.11427400    0.26884300
 C                 1.30594700    0.84573900    0.45092100
 C                 0.67446500    3.16479500    0.27071800
 C                -0.02497800    0.16628800    0.89291300
 C                -0.70760800    3.15709700    0.18161300
 N                -1.56060600    2.09895300    0.14893300
 C                -1.34172500    0.84228800    0.41114600
 C                 2.48559900   -0.00946400    0.33747000
 C                 3.68389800    0.43530600   -0.12829400
 C                -2.53721000   -0.00032600    0.37105300
 C                -3.69724000    0.37987000   -0.22586000
```

```
C           -6.38148800     -2.23800700      0.30415200
C           -5.16041300     -1.59571200      0.37236400
C           -7.45319500     -1.65792000     -0.40354500
C           -4.95199500     -0.34700100     -0.26142400
C           -7.27390600     -0.42181300     -1.04027800
C           -6.03760700      0.21252100     -0.96219500
O           -8.60640800     -2.37047200     -0.40767500
C           -9.73535400     -1.84003200     -1.10248500
C            7.28722600     -0.30871100     -0.86945100
C            6.06376100      0.34025000     -0.73533900
C            7.39258700     -1.65827700     -0.50370800
C            4.91916500     -0.31443000     -0.24009000
C            6.26062200     -2.33569200     -0.00735800
C            5.05333400     -1.67729500      0.12049900
O            8.52575800     -2.39624700     -0.58901000
C            9.71166200     -1.77387900     -1.08465900
C            1.35088600      4.44094300      0.29932400
N            1.92474000      5.45303800      0.33264000
C           -1.39059100      4.42557700      0.07957900
N           -1.96969900      5.43229700      0.00056300
C           -0.00797500     -1.36592200      0.56668700
C            0.24292400     -2.26056600      1.78855400
C            0.29233500     -3.74940300      1.43546200
H            2.40359200     -1.03421000      0.66991900
H            3.72868000      1.47255100     -0.45176000
H           -2.49681800     -0.95324100      0.88329600
H           -3.69135200      1.33881000     -0.73885300
H           -0.04412900      0.26817200      1.99069400
H           -6.54139700     -3.19441800      0.79066300
H           -4.35478300     -2.06637000      0.92644200
H           -8.08066600      0.04650500     -1.59015400
H           -5.90646900      1.17079900     -1.45698400
H           -9.52505600     -1.72069300     -2.17110400
H          -10.53509300     -2.56841700     -0.96961000
H          -10.04545600     -0.87736100     -0.68125200
H            8.14130300      0.23492500     -1.25356400
H            5.98931800      1.38602400     -1.02006000
H            6.36351400     -3.37987000      0.26839300
H            4.19911000     -2.22569200      0.50375800
H           10.48219400     -2.54429800     -1.06401600
H            9.57564600     -1.42146400     -2.11302800
H           10.01654800     -0.93591600     -0.44827500
H           -0.94746700     -1.66622400      0.10437400
H            0.73632400     -1.56893200     -0.20710000
H            1.17871100     -1.96759900      2.28301700
H           -0.54932700     -2.08203500      2.52823400
H           -0.64503100     -4.07852300      0.97316900
H            1.10113200     -3.96307700      0.72752700
H            0.45832200     -4.36295700      2.32627600
```

Inversion transition state **Ts** of B+A conformer of **6d:**
Table S31.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.596353 A.U.
```

```
N        1.32359600    2.60993600   -0.53452800
C        1.34510200    1.32950100   -0.28287400
C        0.39830900    3.54924400   -0.18570400
C        0.24309600    0.42841400    0.33624900
C       -0.87870000    3.36178300    0.31770100
N       -1.59461400    2.21454000    0.35420700
C       -1.21445700    0.97567800    0.23364100
C        2.68088900    0.78769400   -0.55324700
C        3.31779400   -0.20714300    0.11468900
C       -2.30258300    0.01227500    0.10705300
C       -3.61447200    0.37855300    0.07776300
C       -5.83036800   -2.66765600   -0.28459500
C       -4.69020200   -1.89557600   -0.18429400
C       -7.10472100   -2.06596300   -0.24103800
C       -4.76776000   -0.48895100   -0.03485300
C       -7.21022400   -0.67482600   -0.09655600
C       -6.05230500    0.08924600    0.00295900
O       -8.15522200   -2.91337600   -0.34785200
C       -9.47760600   -2.37387400   -0.31481500
C        6.54772300   -2.03796300    0.72054900
C        5.22538600   -1.60892500    0.80312800
C        7.40277300   -1.45116100   -0.22197800
C        4.71310200   -0.59832600   -0.03065600
C        6.91163300   -0.43839100   -1.06852000
C        5.59709500   -0.02222600   -0.97290000
O        8.70629600   -1.78428700   -0.39886900
C        9.26817800   -2.80198700    0.42863500
C        0.86744300    4.89855100   -0.38167600
N        1.26981600    5.97872700   -0.54593800
C       -1.62910300    4.51773200    0.75016400
N       -2.25109100    5.42889100    1.12045400
C        0.33222400   -1.04024800   -0.19964300
C        0.17322000   -2.11751900    0.88409800
C        0.20214200   -3.53770500    0.31210300
H        3.24355300    1.41238100   -1.24006200
H        2.77426200   -0.77082700    0.86901900
H       -2.05762700   -1.03636800    0.05077600
H       -3.82752900    1.44192300    0.15728100
H        0.45605700    0.39934300    1.41773200
H       -5.77193700   -3.74473200   -0.40002300
H       -3.72354400   -2.38663600   -0.22548200
H       -8.17667200   -0.18781500   -0.06178300
H       -6.14091500    1.16619600    0.11478600
H       -9.64425300   -1.68005100   -1.14596800
H      -10.14840000   -3.22695300   -0.41391100
H       -9.67452400   -1.86302600    0.63397600
H        6.89803300   -2.81860200    1.38431500
H        4.57055700   -2.07085300    1.53723600
H        7.58797300    0.00338300   -1.79269200
H        5.24848300    0.75876000   -1.64041500
H       10.30760100   -2.90004000    0.11570800
H        9.23169400   -2.52052400    1.48701400
H        8.75389900   -3.75939200    0.28801200
```

```
H                        -0.41038300    -1.18287600    -0.99013500
H                         1.28569300    -1.19464800    -0.69791500
H                         0.98042700    -2.00303000     1.62056900
H                        -0.75585700    -1.96554600     1.44736800
H                        -0.62085200    -3.69925200    -0.39341800
H                         1.13768500    -3.72914100    -0.22505500
H                         0.11240000    -4.28641900     1.10516100
```

Inversion transition state **Ts** of A+A conformer of **6d:**
Table S32.
```
TOTAL FREE ENERGY IN SOLVENT = -1451.589332 A.U.
N                        -1.52741000     2.80846600     0.17773300
C                        -1.30591800     1.53686800     0.03551500
C                        -0.68905300     3.85960200    -0.05919100
C                         0.00000000     0.83497900    -0.44828600
C                         0.68905300     3.85960200    -0.05919200
N                         1.52741000     2.80846600     0.17773300
C                         1.30591800     1.53686800     0.03551500
C                        -2.53084300     0.76807500     0.33042200
C                        -3.07680800    -0.21536000    -0.42210400
C                         2.53084300     0.76807500     0.33042200
C                         3.07680800    -0.21536000    -0.42210400
C                         6.44263200    -1.20310600     1.01980900
C                         5.21767600    -0.57680600     0.88297200
C                         6.88554400    -2.12266600     0.04981000
C                         4.38100600    -0.84018900    -0.22545700
C                         6.07392000    -2.40236900    -1.05742700
C                         4.84154200    -1.76401200    -1.17944800
O                         8.10157500    -2.68021200     0.28047100
C                         8.61063900    -3.61948600    -0.66514600
C                        -6.07392000    -2.40236900    -1.05742700
C                        -4.84154100    -1.76401200    -1.17944800
C                        -6.88554400    -2.12266600     0.04981000
C                        -4.38100600    -0.84018900    -0.22545700
C                        -6.44263200    -1.20310600     1.01980900
C                        -5.21767600    -0.57680600     0.88297200
O                        -8.10157500    -2.68021200     0.28047100
C                        -8.61063900    -3.61948600    -0.66514600
C                        -1.38571400     5.11122100    -0.23247100
N                        -1.97017500     6.10537700    -0.38712200
C                         1.38571400     5.11122100    -0.23247100
N                         1.97017500     6.10537700    -0.38712200
C                         0.00000000    -0.67241700    -0.04992700
C                         0.00000000    -0.95677200     1.45879900
C                         0.00000000    -2.45882100     1.75826100
H                        -3.12249700     1.21579400     1.12386300
H                        -2.54448200    -0.56674900    -1.30249100
H                         3.12249700     1.21579400     1.12386300
H                         2.54448200    -0.56674900    -1.30249100
H                         0.00000000     0.89983100    -1.54788900
H                         7.08300800    -1.00151600     1.87206100
H                         4.90223700     0.12290100     1.64997000
H                         6.38781600    -3.10608600    -1.81834900
```

```
H                      4.21939800   -1.98826400   -2.04190900
H                      8.73605500   -3.16270200   -1.65327300
H                      9.58353600   -3.92898200   -0.28343100
H                      7.95731600   -4.49534200   -0.74879000
H                     -6.38781600   -3.10608600   -1.81834900
H                     -4.21939800   -1.98826400   -2.04190900
H                     -7.08300800   -1.00151600    1.87206100
H                     -4.90223700    0.12290100    1.64997000
H                     -9.58353600   -3.92898200   -0.28343200
H                     -8.73605500   -3.16270200   -1.65327300
H                     -7.95731600   -4.49534200   -0.74879000
H                     -0.86250300   -1.16059900   -0.49940200
H                      0.86250300   -1.16059900   -0.49940200
H                      0.87748100   -0.49381100    1.92440200
H                     -0.87748100   -0.49381100    1.92440200
H                     -0.88470500   -2.94774700    1.33481100
H                      0.88470500   -2.94774700    1.33481100
H                      0.00000000   -2.64710500    2.83636900
```


Table S33. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis.

	Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
5a	2. BD (2) N1 - C2	435. BD*(2) C8 - C9	7.18	0.36	0.046
	18. BD (2) C8 - C9	419. BD*(2) N1 - C2	20.18	0.28	0.069
5b	2. BD (2) N1 - C2	493. BD*(2) C8 - C9	7.19	0.36	0.046
	18. BD (2) C8 - C9	477. BD*(2) N1 - C2	20.82	0.28	0.070
5c	2. BD (2) N1 - C2	707. BD*(2) C8 - C9	7.16	0.36	0.046
	18. BD (2) C8 - C9	691. BD*(2) N1 - C2	21.72	0.28	0.072
6b	2. BD (2) N1 - C2	559. BD*(2) C8 - C9	7.16	0.36	0.046
	18. BD (2) C8 - C9	543. BD*(2) N1 - C2	20.34	0.28	0.070
6d	2. BD (2) N1 - C2	581. BD*(2) C8 - C9	7.12	0.36	0.046
	18. BD (2) C8 - C9	565. BD*(2) N1 - C2	21.26	0.28	0.071

Threshold for printing: 0.50 kcal/mol