Supporting Information

Synthesis, Structures, and Temperature-Dependent Photoluminescence of 1,4-Diphenyl-1-telluro-1,3-butadiene Incorporated in a Dibenzobarrelene Skeleton and Derivatives

Tatsuro Annaka, Norio Nakata, and Akihiko Ishii*

Department of Chemistry, Graduate School of Science and Engineering, Saitama University
255 Shimo-okubo, Sakura-ku, Saitama 338-8570, Japan
ishiiaki@chem.saitama-u.ac.jp

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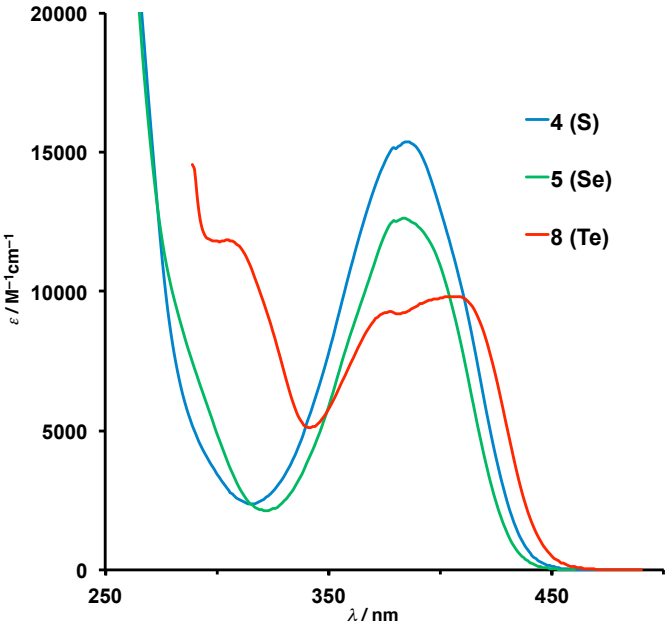


Figure S1. Optical absorption spectra of **4**, **5**, and **8** in 2-methyltetrahydrofuran at room temperature

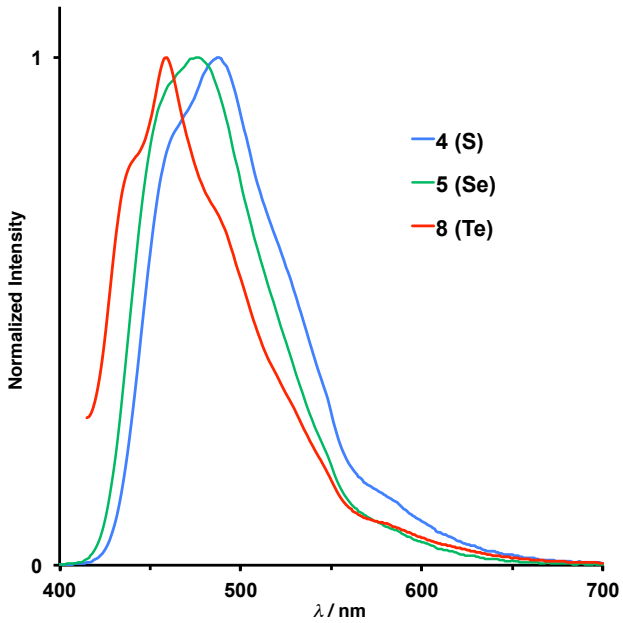


Figure S2. Emission spectra of **4**, **5**, and **8** in 2-methyltetrahydrofuran at room temperature

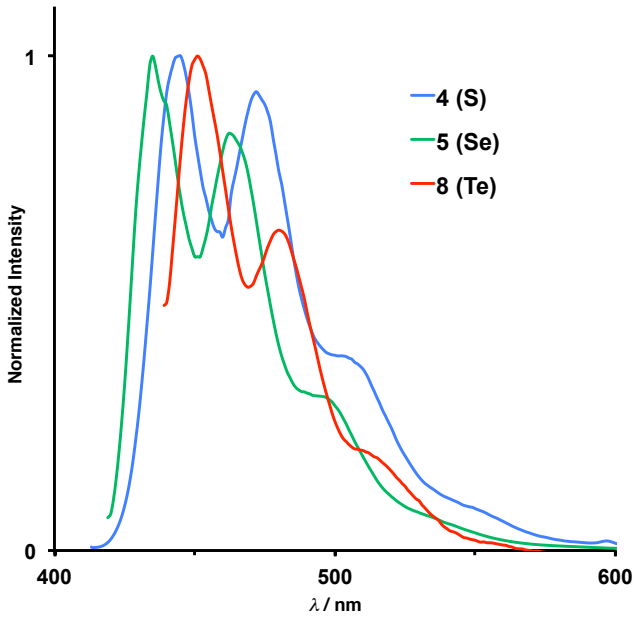
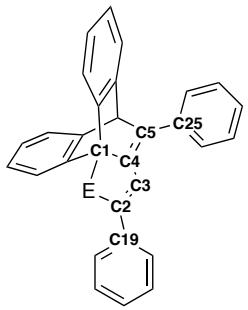


Figure S3. Emission spectra of **4**, **5**, and **8** in 2-methyltetrahydrofuran at 77 K

Table S1. Selected geometrical parameters of **4**, **5**, and **8** obtained by X-ray crystallography



	4 (E = S) [1]	**5** (E = Se)[1]	**8** (E = Te)
C1–E	1.814(2)	1.961(2)	2.153(2)
E–C2	1.780(2)	1.923(2)	2.109(2)
C2–C3	1.352(3)	1.342(3)	1.344(3)
C3–C4	1.428(3)	1.435(3)	1.438(3)
C4–C1	1.550(3)	1.544(3)	1.549(3)
C4–C5	1.342(3)	1.352(3)	1.354(3)
C2–C19	1.462(3)	1.476(2)	1.469(3)
C5–C25	1.470(3)	1.468(3)	1.465(3)
C1–E–C2	92.42(11)	87.79(8)	82.63(8)
E–C2–C3	113.30(19)	113.44(14)	113.31(15)
C2–C3–C4	116.0(2)	117.68(18)	120.42(19)
C3–C4–C1	111.3(2)	113.71(16)	116.17(17)
C4–C1–E	106.83(16)	106.47(12)	106.56(13)
C3–C4–C5	134.7(2)	131.5(2)	129.65(19)
C1–C4–C5	114.0(2)	114.2(2)	113.60(18)
E–C2–C19	118.16(18)	119.74(14)	120.35(15)
C2–C3–C4–C5	–177.4(2)	174.4(2)	176.2(2)
C2–E–C1–C4	3.0(2)	–8.9(1)	8.07(13)
C1–E–C2–C3	2.6(2)	–7.6(2)	–6.08(15)
E–C2–C3–C4	–1.3(3)	3.7(2)	2.1(2)
C2–C3–C4–C1	–1.1(3)	4.1(3)	5.5(3)
E–C1–C4–C5	–180.0(2)	178.6(1)	178.21(14)
E–C1–C4–C3	2.9(2)	–9.3(2)	–9.6(2)

(1) Ishii, A.; Annaka, T.; Nakata, N. *Chem.—Eur. J.* **2012**, *18*, 6428–6432.

Table S2. Cartesian coordinate of **8**

#p opt freq rb3lyp/gen geom=connectivity pseudo=read
(C H 0 6-31G(d)/Te 0 LANL2DZ/Te 0 LANL2DZ)
SCF energy = -1163.23712118 hartree

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	0.505900	-1.051200	-0.003900
C	-2.078900	0.196900	-0.001600
C	-1.001800	1.019800	-0.001300
H	-1.138900	2.097700	0.017200
C	0.338500	0.494100	-0.030200
C	1.520800	1.167700	-0.028500
C	1.408400	-1.409000	-1.196800
C	1.163900	-2.305200	-2.230400
H	0.222500	-2.844900	-2.275100
C	2.130600	-2.494500	-3.228100
H	1.934200	-3.193100	-4.037000
C	3.332700	-1.791100	-3.189900
H	4.077100	-1.940200	-3.967500
C	3.582900	-0.887100	-2.149100
H	4.518900	-0.334600	-2.113200
C	2.623700	-0.702200	-1.161200
C	1.334400	-1.368200	1.255600
C	1.027700	-2.228700	2.303000
H	0.083600	-2.765300	2.311100
C	1.935800	-2.388000	3.359200
H	1.690600	-3.059200	4.177900
C	3.142500	-1.691800	3.365200
H	3.842400	-1.819300	4.186700
C	3.454900	-0.823400	2.310700
H	4.397100	-0.279700	2.307600
C	2.552400	-0.664400	1.266300
C	2.738200	0.228000	0.043600
H	3.683900	0.772800	0.055900
C	-3.483800	0.614400	0.056100
C	-4.511000	-0.181600	-0.483800
H	-4.260600	-1.123200	-0.967100
C	-5.841500	0.230800	-0.441300
H	-6.613000	-0.401200	-0.872800
C	-6.181400	1.449100	0.149200
C	-5.176000	2.248000	0.700900
H	-5.429700	3.191600	1.176800
C	-3.846900	1.835900	0.660700
H	-3.080400	2.450700	1.122400
C	1.711800	2.626500	-0.094900

C	0.979800	3.424600	-0.995300
H	0.279600	2.950000	-1.675900
C	1.174300	4.804300	-1.051400
H	0.603600	5.397800	-1.760900
C	2.850500	4.640600	0.676000
H	3.579200	5.109000	1.332400
C	2.659900	3.261400	0.731100
H	3.231400	2.669000	1.440500
C	2.107400	5.419600	-0.214600
H	-7.218900	1.769500	0.187400
H	2.259900	6.494500	-0.260500
Te	-1.530700	-1.869100	-0.050700

Table S3. TD-DFT of **8**
#p td=(50-50,nstates=10) rb3lyp/gen geom=connectivity pseudo=read
(C H 0 6-31G(d)/Te 0 LANL2DZ/Te 0 LANL2DZ)
103 = HOMO, 104 = LUMO; transitions from S_0 to a triplet state are omitted.

Excited State 3: Singlet-A 2.9766 eV 416.53 nm f=0.1521 <S**2>=0.000
103 ->104 0.56842
103 ->105 0.39963
Excited State 4: Singlet-A 3.0702 eV 403.84 nm f=0.1020 <S**2>=0.000
103 ->104 -0.39842
103 ->105 0.57007
Excited State 10: Singlet-A 3.8038 eV 325.94 nm f=0.0988 <S**2>=0.000
102 ->104 0.69163
Excited State 13: Singlet-A 3.9851 eV 311.12 nm f=0.0115 <S**2>=0.000
103 ->106 0.65984
103 ->107 -0.22325
Excited State 15: Singlet-A 4.0369 eV 307.13 nm f=0.0022 <S**2>=0.000
101 ->105 0.13605
102 ->105 0.66643
103 ->105 -0.10988
Excited State 16: Singlet-A 4.1110 eV 301.59 nm f=0.0231 <S**2>=0.000
103 ->106 0.19955
103 ->107 0.65507
Excited State 17: Singlet-A 4.1630 eV 297.82 nm f=0.0223 <S**2>=0.000
101 ->104 0.21983
103 ->108 0.64893
Excited State 18: Singlet-A 4.1847 eV 296.28 nm f=0.2218 <S**2>=0.000
101 ->104 0.64247
103 ->108 -0.22481
103 ->110 -0.13425
Excited State 19: Singlet-A 4.2474 eV 291.91 nm f=0.0020 <S**2>=0.000
97 ->104 0.12212
103 ->109 0.67411
Excited State 20: Singlet-A 4.3250 eV 286.67 nm f=0.0195 <S**2>=0.000
95 ->104 0.14695
100 ->104 0.15968
103 ->110 0.63768

Table S4. Cartesian coordinate of **10**
#p opt freq rb3lyp/gen geom=connectivity pseudo=read
(C H O 0 6-31G(d)/Te 0 LANL2DZ/Te 0 LANL2DZ)
SCF energy = -1238.38977661 hartree

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	0.515700	-0.994900	0.007900
C	-1.998000	0.393900	-0.093700
C	-0.869300	1.145500	-0.092800
H	-0.934800	2.228300	-0.186000
C	0.440000	0.546700	-0.020400
C	1.656300	1.153100	-0.019300
C	-3.371900	0.904100	-0.123500
C	-4.413900	0.178200	-0.731100
H	-4.203800	-0.783500	-1.193000
C	-5.712700	0.680100	-0.775100
H	-6.496000	0.100200	-1.255400
C	-6.006100	1.920300	-0.205100
H	-7.019900	2.309700	-0.232900
C	-4.987600	2.650100	0.413600
H	-5.207800	3.609400	0.874400
C	-3.689900	2.148000	0.459100
H	-2.913600	2.708800	0.970900
C	1.929900	2.600700	-0.024000
C	1.245400	3.480000	0.836100
H	0.524000	3.077900	1.540900
C	1.517900	4.847700	0.824100
H	0.984800	5.507300	1.503700
C	2.481200	5.366400	-0.043400
H	2.694000	6.431800	-0.050800
C	3.177500	4.504400	-0.894500
H	3.929600	4.898600	-1.572700
C	2.910800	3.137000	-0.880000
H	3.447300	2.477500	-1.556900
C	1.336300	-1.352800	1.255900
C	0.967600	-2.156800	2.330700
H	-0.024800	-2.596100	2.368000
C	1.884500	-2.348900	3.374700
H	1.604100	-2.973800	4.218400
C	3.140500	-1.745600	3.344500
H	3.841200	-1.903500	4.160200
C	3.502300	-0.925500	2.267200
H	4.477500	-0.444700	2.242800
C	2.597500	-0.730500	1.231500
C	1.363000	-1.411900	-1.202600

C	1.043200	-2.311500	-2.214200
H	0.082600	-2.818400	-2.222100
C	1.969200	-2.569600	-3.234800
H	1.713500	-3.270500	-4.024500
C	3.209900	-1.936700	-3.236300
H	3.924900	-2.141700	-4.028300
C	3.541800	-1.038900	-2.212200
H	4.514700	-0.552600	-2.202700
C	2.621100	-0.781400	-1.204600
C	2.818200	0.139600	-0.005800
H	3.793900	0.628800	-0.001400
Te	-1.568500	-1.728900	-0.117100
O	-2.011800	-2.441800	1.493300

Table S5. TD-DFT of **10**
#p td=(50-50,nstates=10) rb3lyp/gen geom=connectivity pseudo=read
(C H O 0 6-31G(d)/Te 0 LANL2DZ/Te 0 LANL2DZ)
107 = HOMO, 108 = LUMO; transitions from S_0 to a triplet state are omitted.

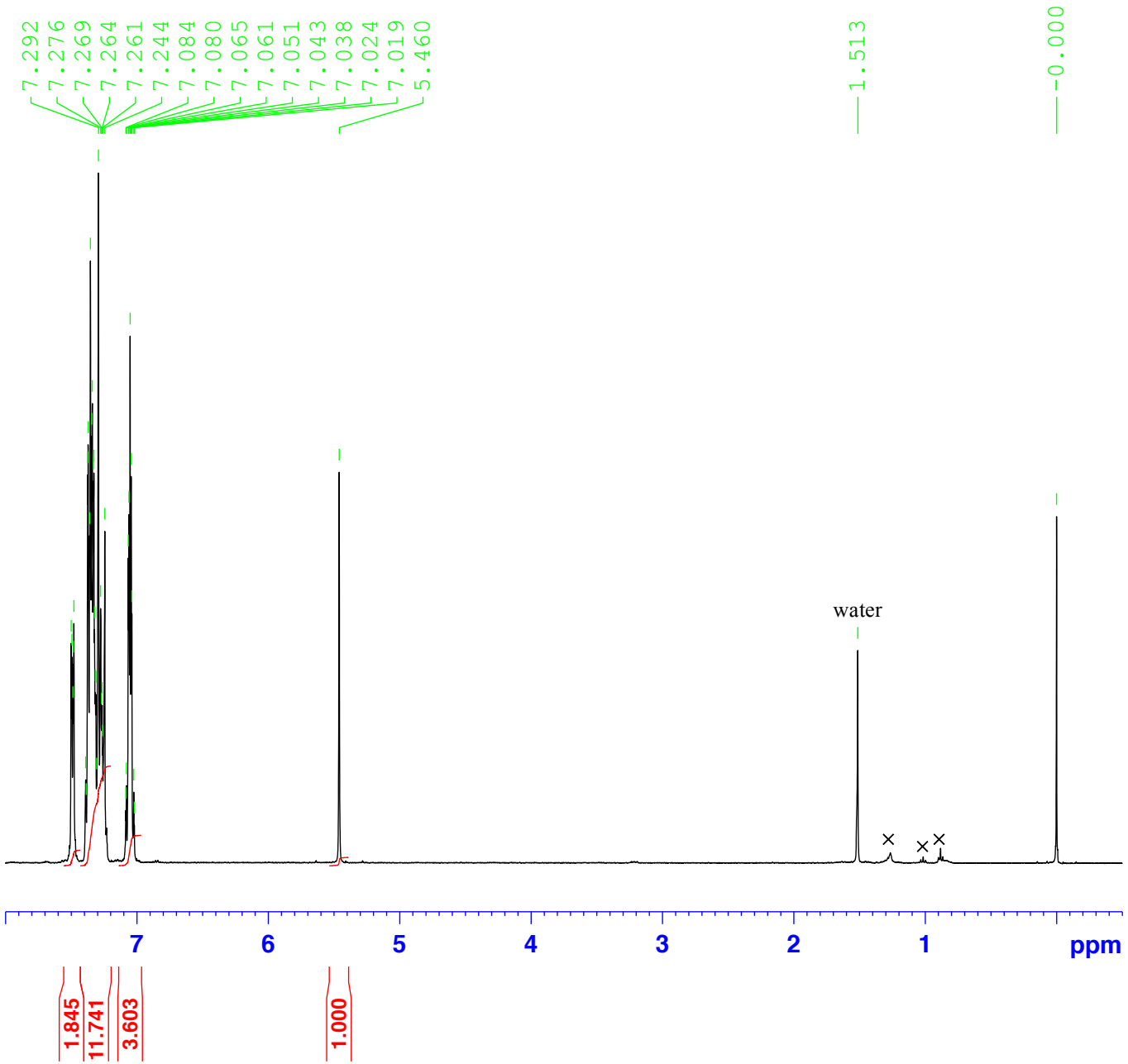
Excited State 3: Singlet-A 3.2141 eV 385.75 nm f=0.1553 <S**2>=0.000
106 ->108 -0.42608
107 ->108 0.54326
Excited State 5: Singlet-A 3.2887 eV 377.00 nm f=0.1659 <S**2>=0.000
106 ->108 0.54988
107 ->108 0.41848
Excited State 12: Singlet-A 3.7361 eV 331.86 nm f=0.0159 <S**2>=0.000
104 ->108 0.38239
105 ->108 0.57315
Excited State 14: Singlet-A 3.8819 eV 319.39 nm f=0.0056 <S**2>=0.000
104 ->108 0.23548
105 ->108 -0.23257
107 ->109 0.61102
Excited State 15: Singlet-A 3.9305 eV 315.44 nm f=0.0394 <S**2>=0.000
104 ->108 -0.36201
105 ->108 0.22350
106 ->109 0.51389
107 ->109 0.16997
Excited State 16: Singlet-A 4.0334 eV 307.40 nm f=0.1839 <S**2>=0.000
103 ->108 0.28935
104 ->108 0.36109
105 ->108 -0.18562
106 ->109 0.39521
107 ->108 0.12640
107 ->109 -0.23649
Excited State 17: Singlet-A 4.0651 eV 305.00 nm f=0.0528 <S**2>=0.000
103 ->108 0.63668
104 ->108 -0.11120
105 ->108 0.12369
106 ->109 -0.16948
107 ->109 0.14522
Excited State 18: Singlet-A 4.2282 eV 293.23 nm f=0.0081 <S**2>=0.000
102 ->108 0.47113
107 ->110 0.50503
Excited State 19: Singlet-A 4.2892 eV 289.06 nm f=0.0203 <S**2>=0.000
99 ->108 -0.12988
100 ->108 0.10829
101 ->108 -0.17263
102 ->108 0.47757
107 ->110 -0.42179
Excited State 20: Singlet-A 4.3875 eV 282.58 nm f=0.0037 <S**2>=0.000
100 ->108 -0.10113

101 ->108	0.16961
106 ->108	0.10100
106 ->109	-0.11999
106 ->110	0.48994
106 ->111	-0.24167
106 ->114	-0.15065
106 ->115	-0.26070

Table S6. TD-DFT of **11**
#p td=(50-50,nstates=10) rb3lyp/gen geom=connectivity pseudo=read
(C H 0 6-31G(d)/Te 0 LANL2DZ/Te Br 0 LANL2DZ)
110 = HOMO, 111 = LUMO; transitions from S_0 to a triplet state are omitted.

Excited State 3: Singlet-A	2.7360 eV	453.15 nm	f=0.0859	<S**2>=0.000
110 ->111	0.67640			
110 ->113	0.18620			
Excited State 6: Singlet-A	3.0233 eV	410.10 nm	f=0.0012	<S**2>=0.000
110 ->112	0.63046			
110 ->113	0.30641			
Excited State 10: Singlet-A	3.3569 eV	369.34 nm	f=0.0338	<S**2>=0.000
107 ->111	0.26554			
109 ->111	0.52052			
110 ->112	-0.18040			
110 ->113	0.32136			
Excited State 13: Singlet-A	3.4041 eV	364.23 nm	f=0.1254	<S**2>=0.000
107 ->111	0.46543			
110 ->111	0.12876			
110 ->112	0.20579			
110 ->113	-0.42373			
Excited State 14: Singlet-A	3.4404 eV	360.38 nm	f=0.0088	<S**2>=0.000
105 ->111	0.32661			
108 ->111	0.58222			
Excited State 16: Singlet-A	3.5324 eV	350.99 nm	f=0.1571	<S**2>=0.000
105 ->111	0.10053			
106 ->111	-0.21378			
107 ->111	-0.36035			
109 ->111	0.43638			
110 ->111	0.10070			
110 ->112	0.13501			
110 ->113	-0.25967			
Excited State 17: Singlet-A	3.6191 eV	342.58 nm	f=0.0189	<S**2>=0.000
98 ->111	0.10517			
105 ->111	-0.10779			
106 ->111	0.61710			
107 ->111	-0.21038			
109 ->111	0.11156			
Excited State 18: Singlet-A	3.7545 eV	330.23 nm	f=0.0060	<S**2>=0.000
102 ->111	-0.16718			
105 ->111	0.43038			
106 ->111	0.11053			
107 ->112	0.19525			
108 ->111	-0.19257			
108 ->112	-0.37327			
109 ->112	0.15337			
Excited State 19: Singlet-A	3.8151 eV	324.98 nm	f=0.0085	<S**2>=0.000

107 ->112 0.10997
108 ->112 0.27233
109 ->112 0.57795
109 ->113 0.25054
Excited State 20: Singlet-A 3.8588 eV 321.30 nm f=0.0244 <S**2>=0.000
101 ->111 -0.14743
102 ->111 0.42961
105 ->111 -0.19342
108 ->112 -0.38440
108 ->113 -0.18057
109 ->112 0.14107

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PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       2
SWH               8305.647 Hz
FIDRES             0.126734 Hz
AQ                3.9453173 sec
RG                     5.1
DW                  60.200 usec
DE                  10.00 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
SI                   32768
SF            400.1300152 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
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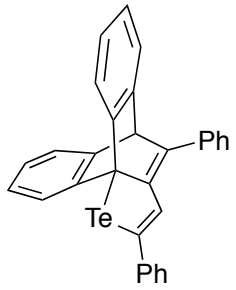
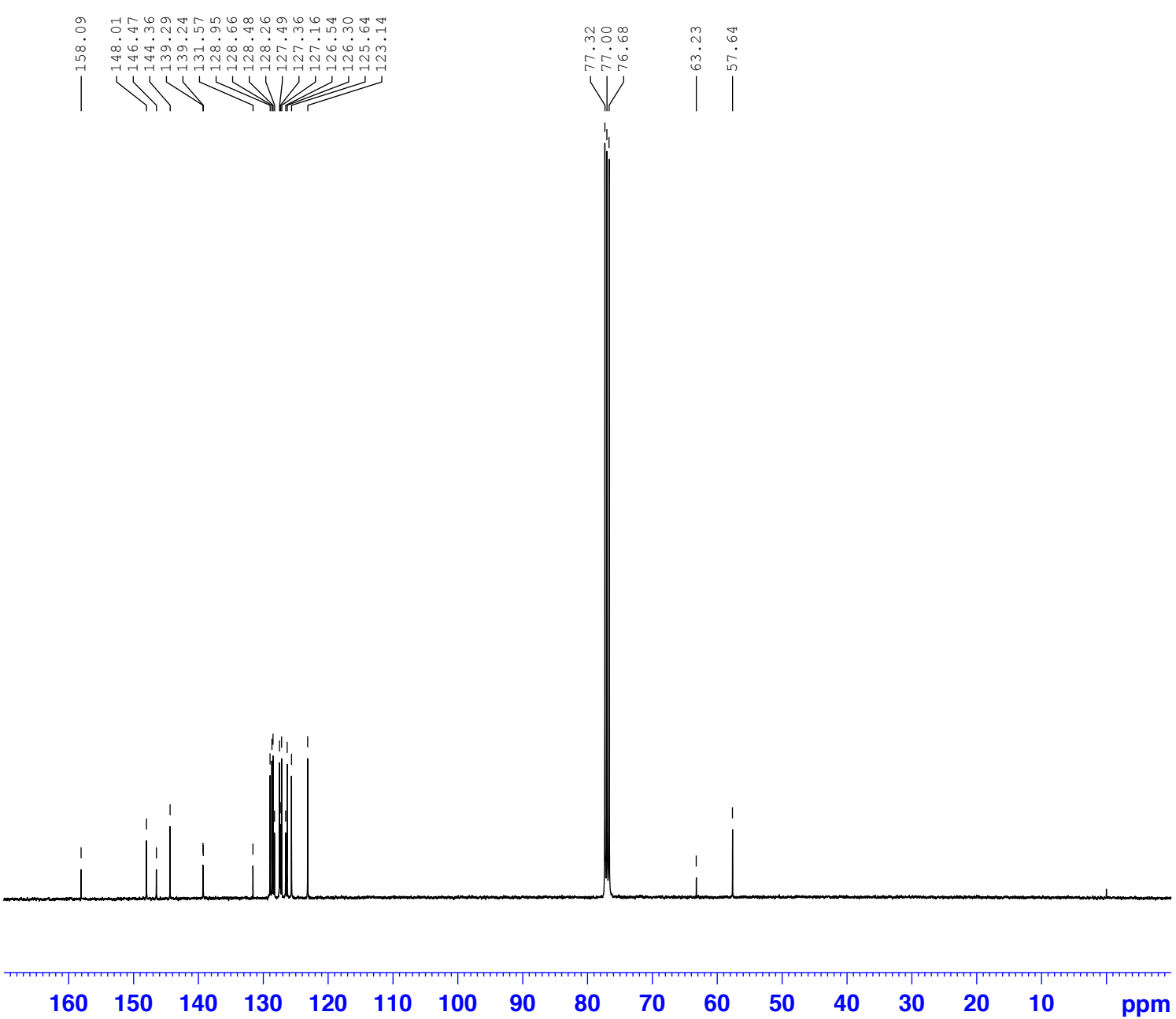
Figure S4. ^{1}H NMR spectrum of **8**



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PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         158
DS                           2
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010548 sec
RG                       126.99
DW                       16.800 usec
DE                       18.00 usec
TE                       300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                       12.00 usec
SI                        32768
SF                100.6127711 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40
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Figure S5. ^{13}C NMR spectrum of **8**

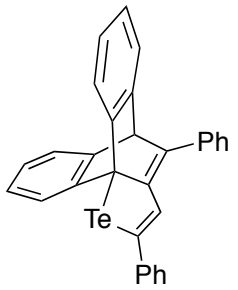
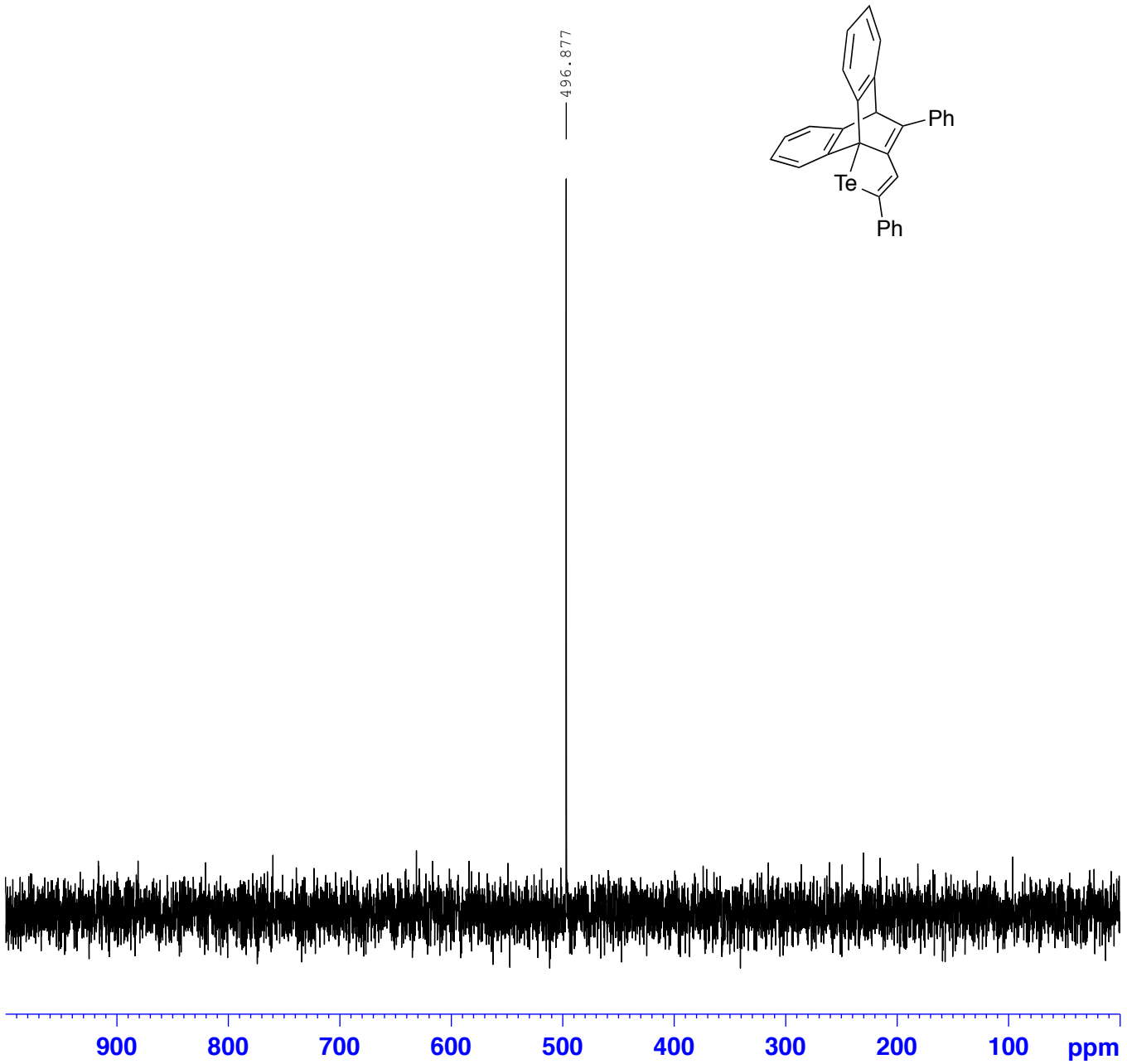


Figure S6. ^{125}Te NMR spectrum of **8**

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PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   157
DS                     2
SWH           312500.000 Hz
FIDRES          9.536743 Hz
AQ             0.0524788 sec
RG                   203
DW                 1.600 usec
DE                30.00 usec
TE                300.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1               125Te
P1                 10.00 usec
PL1                 0.00 dB
PL1W         75.35659027 W
SFO1        157.8246575 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                 2.40 dB
PL12               19.02 dB
PL13               22.02 dB
PL2W         15.17711735 W
PL12W         0.33051354 W
PL13W         0.16564916 W
SFO2        500.0320005 MHz
SI                 16384
SF          157.7583748 MHz
WDW                   EM
SSB                    0
LB                 10.00 Hz
GB                     0
PC                  1.40
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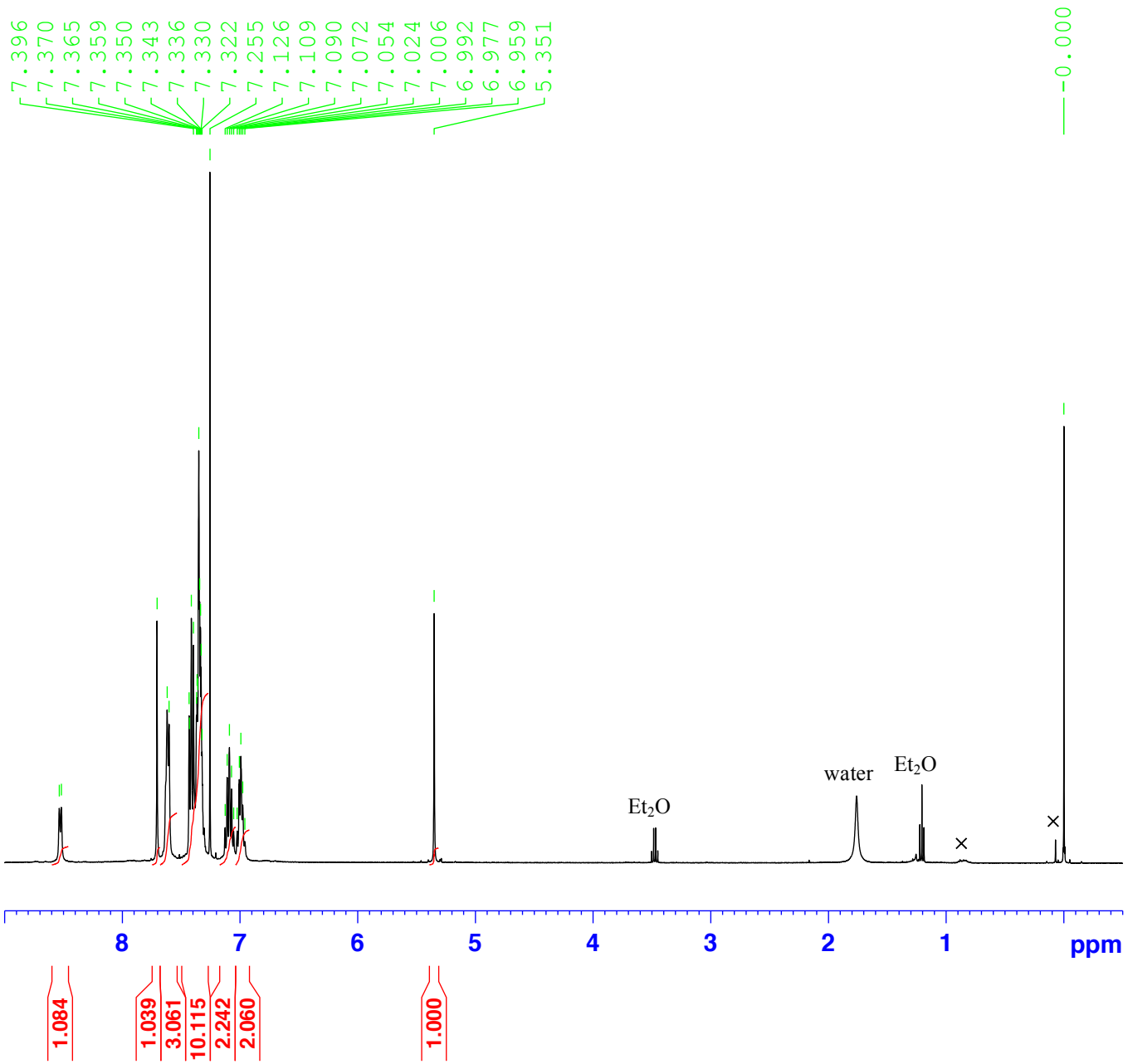


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Date_               20140203
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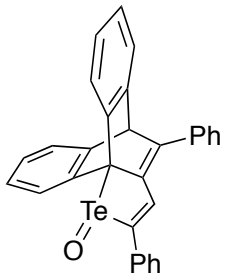
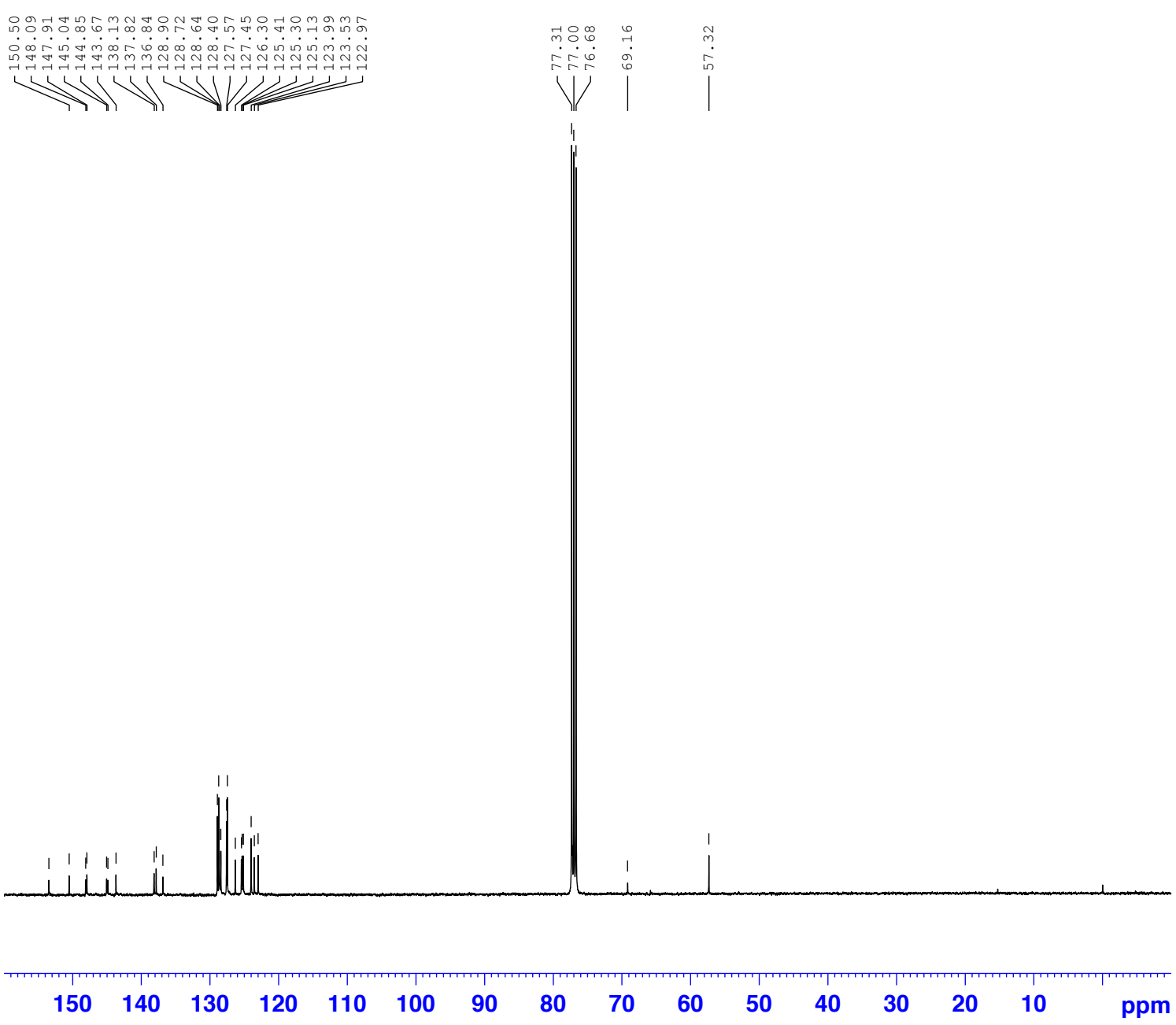
SOLVENT                CDCl3
NS                         4
DS                         2
SWH                 8305.647 Hz
FIDRES              0.126734 Hz
AQ                  3.9453173 sec
RG                      12.9
DW                     60.200 usec
DE                     10.00 usec
TE                     300.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
SI                     32768
SF               400.1300114 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

Figure S7. ^{1}H NMR spectrum of **10**

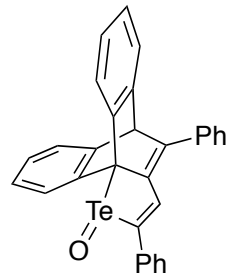


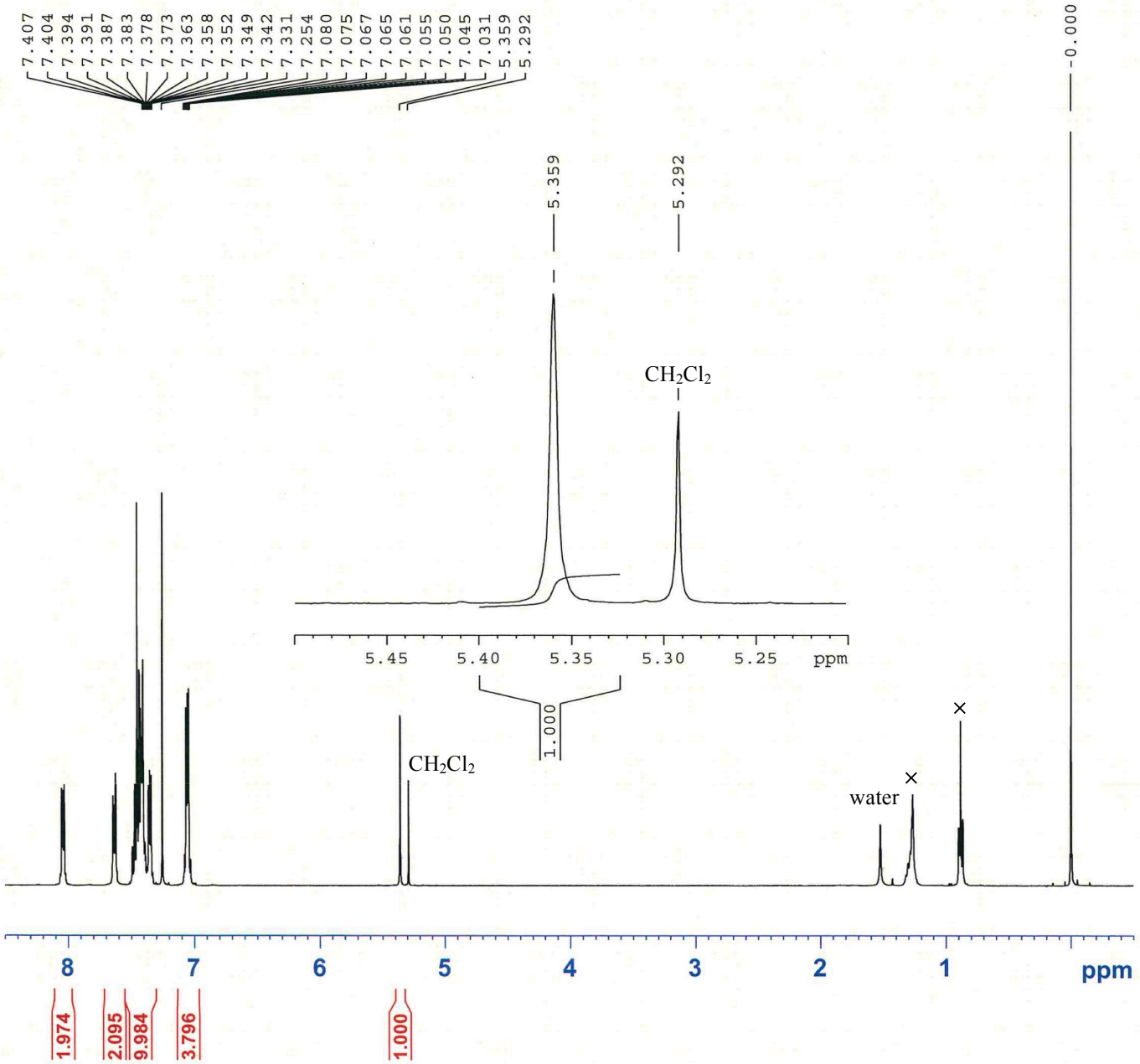



```
NAME                A12ds001aa
EXPNO                    20303
PROCNO                       1
Date_                 20140203
Time                     18.19
INSTRUM                  spect
PROBHD    5 mm CPQNP 1H/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         210
DS                           2
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010548 sec
RG                       126.99
DW                       16.800 usec
DE                       18.00 usec
TE                       300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                       12.00 usec
SI                        32768
SF                100.6127716 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40
```

Figure S8. ^{13}C NMR spectrum of **10**





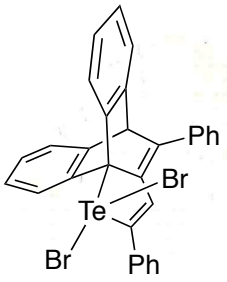

```
Current Data Parameters
NAME          A12ds001aa
EXPNO              40405
PROCNO                 1

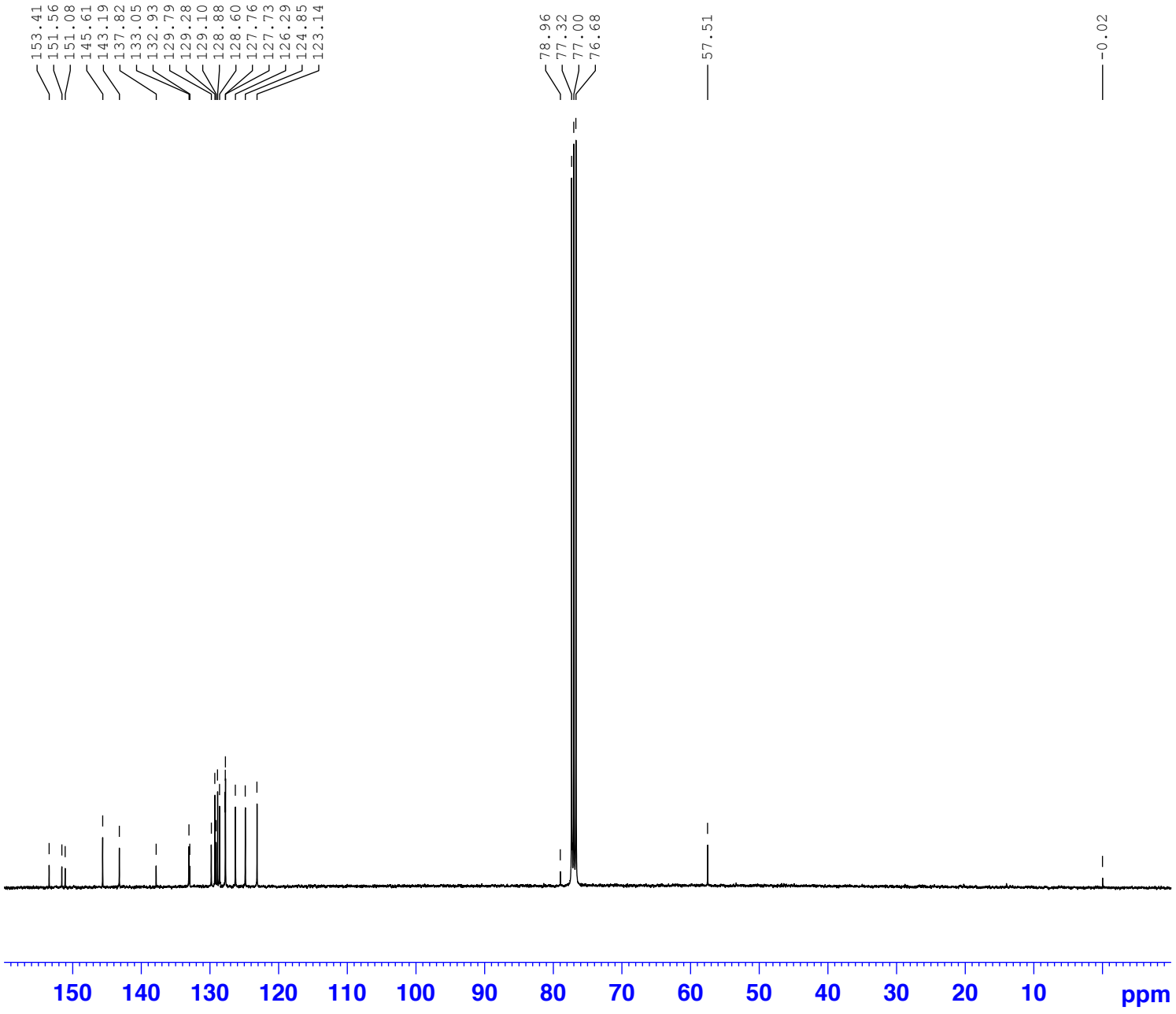
F2 - Acquisition Parameters
Date_           20130404
Time               16.55
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             8305.647 Hz
FIDRES          0.126734 Hz
AQ             3.9453173 sec
RG                  6.55
DW                60.200 usec
DE                10.00 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1          5.19999981 W
SFO1        400.1324708 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300128 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Figure S9. ^{1}H NMR spectrum of **11**





BRUKER

NAME	A12ds001a
EXPNO	1492503
PROCNO	1
Date_	20140925
Time	11.13
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	171
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	126.99
DW	16.800 usec
DE	18.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	12.00 usec
SI	32768
SF	100.6127707 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

Figure S10. ^{13}C NMR spectrum of **11**

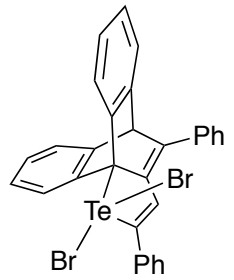
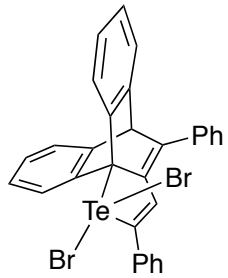


Figure S11. ^{125}Te NMR spectrum of **11**




```
NAME          A12ds001aa
EXPNO              40408
PROCNO                 1
Date_           20130404
Time               17.43
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   529
DS                     2
SWH           312500.000 Hz
FIDRES          9.536743 Hz
AQ             0.0524788 sec
RG                   203
DW                 1.600 usec
DE                30.00 usec
TE                300.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1               125Te
P1                 10.00 usec
PL1                 0.00 dB
PL1W         75.35659027 W
SFO1        157.8246575 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                 2.40 dB
PL12               19.02 dB
PL13               22.02 dB
PL2W         15.17711735 W
PL12W         0.33051354 W
PL13W         0.16564916 W
SFO2        500.0320005 MHz
SI                 16384
SF          157.7583748 MHz
WDW                   EM
SSB                    0
LB                 10.00 Hz
GB                     0
PC                  1.40
```