Supporting Information

Planarity of Thioamides. Nonplanar Structures of Thioamides Bearing 7-Azabicyclo[2.2.1]heptane

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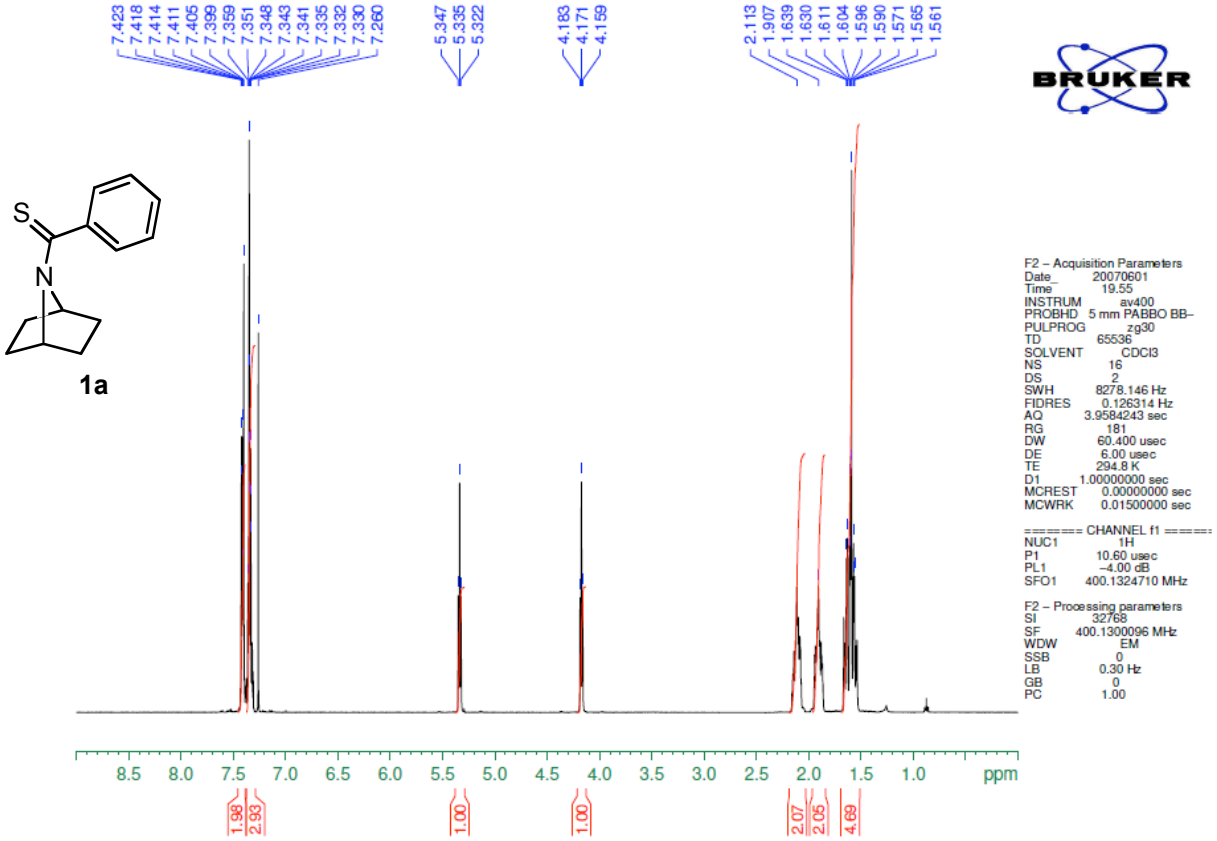
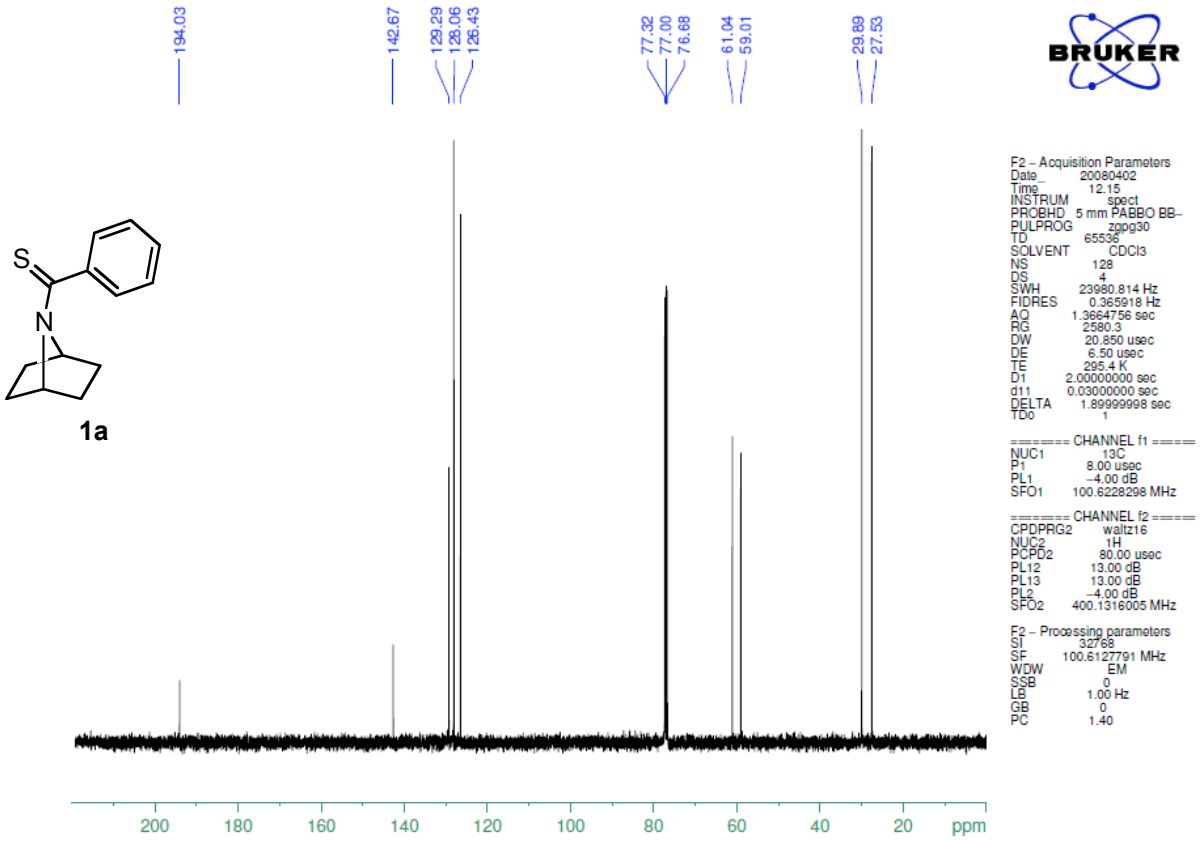
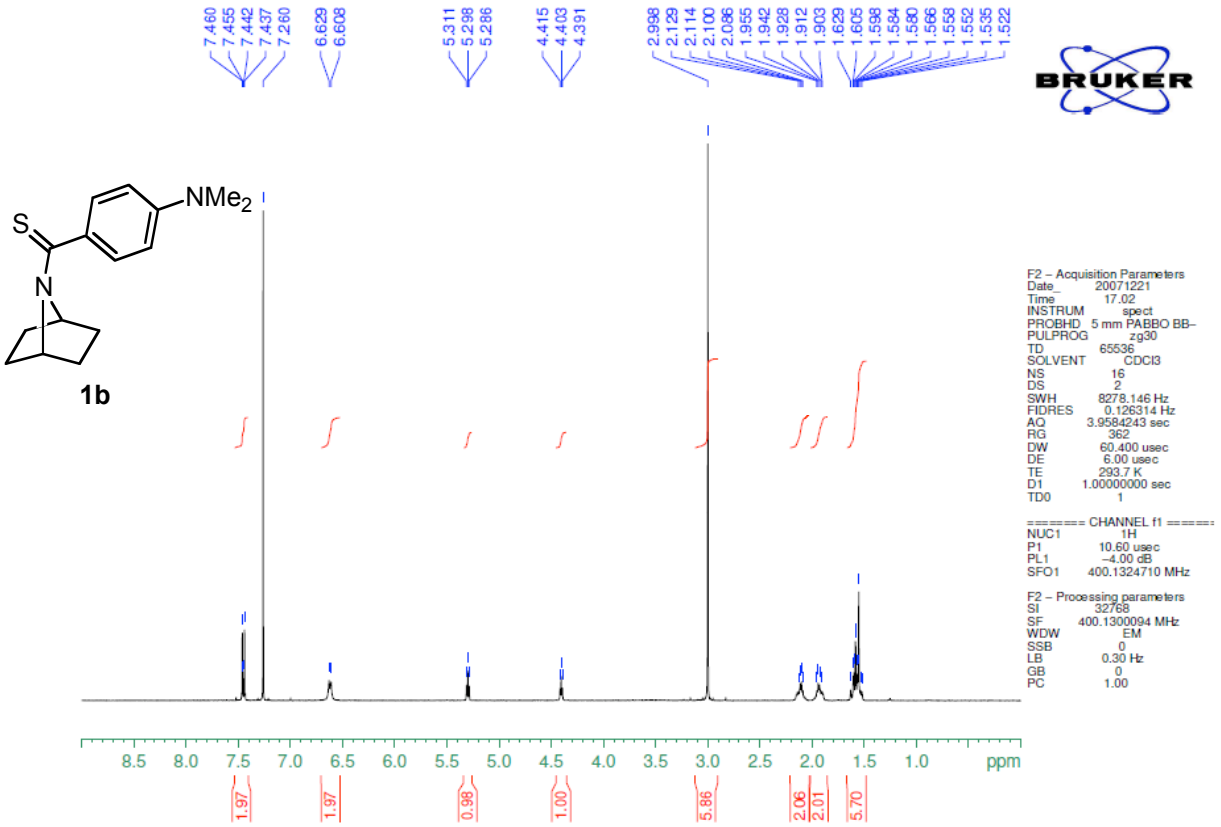
1. General Methods

All the reagents were commercial products, and were used without further purification. Proton (400 MHz) NMR spectra and carbon (100 MHz) NMR spectra were measured and chemical shifts (δ) are shown in ppm and were referenced to internal tetramethylsilane (δ = 0 ppm). Coupling constants are given in hertz. Electron spray ionization time-of-flight mass spectra (ESI-TOF MS) were also recorded. Flash column chromatography was carried out on silica gel (silica gel (40-63 μm)). All the melting points were measured with a micro melting point apparatus and are uncorrected. The combustion analyses were carried out in the microanalytical laboratory of this faculty.

^{1}H and ^{13}C NMR Charts of Synthesized Compounds



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2.998
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2.100
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1.942
1.928
1.912
1.903
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S
N
1b
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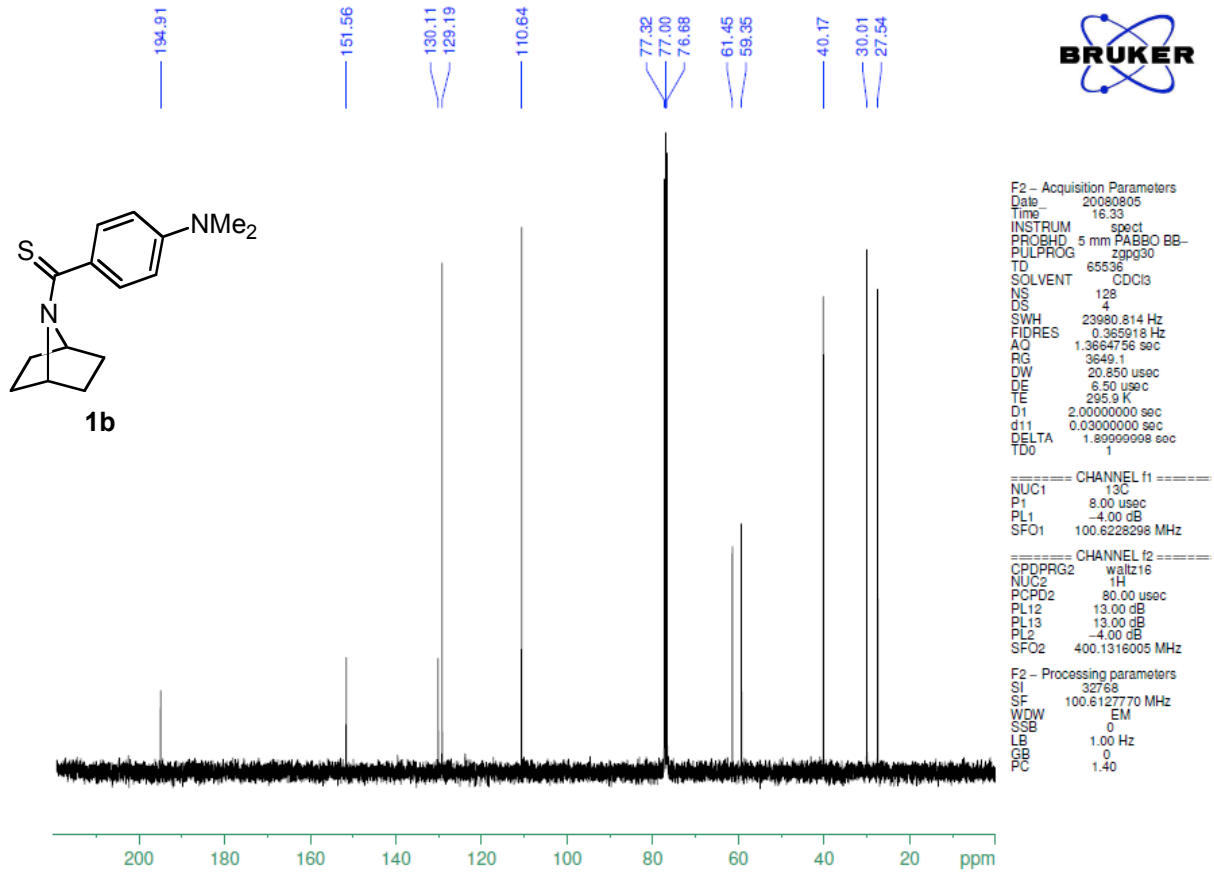
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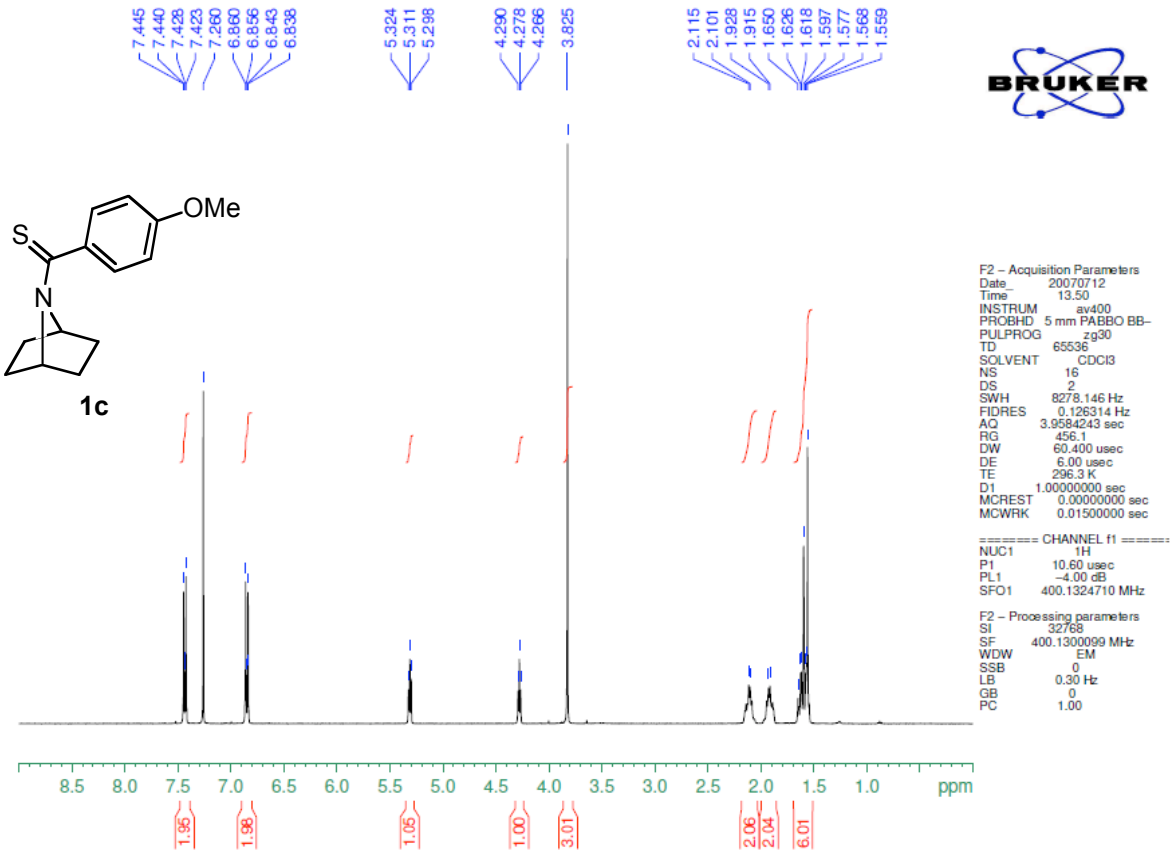
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4.278
4.266
3.825
2.115
2.101
1.928
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1.618
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OMe
S
N
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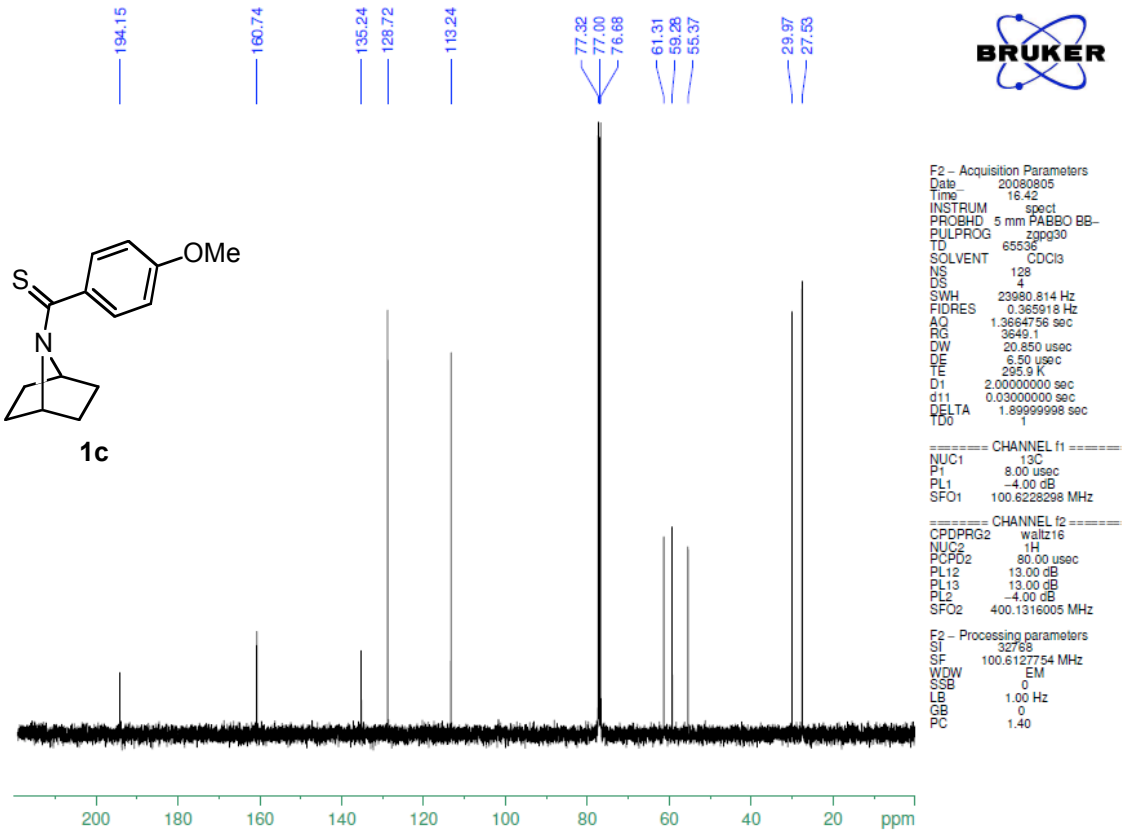
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OMe
S
N
1c
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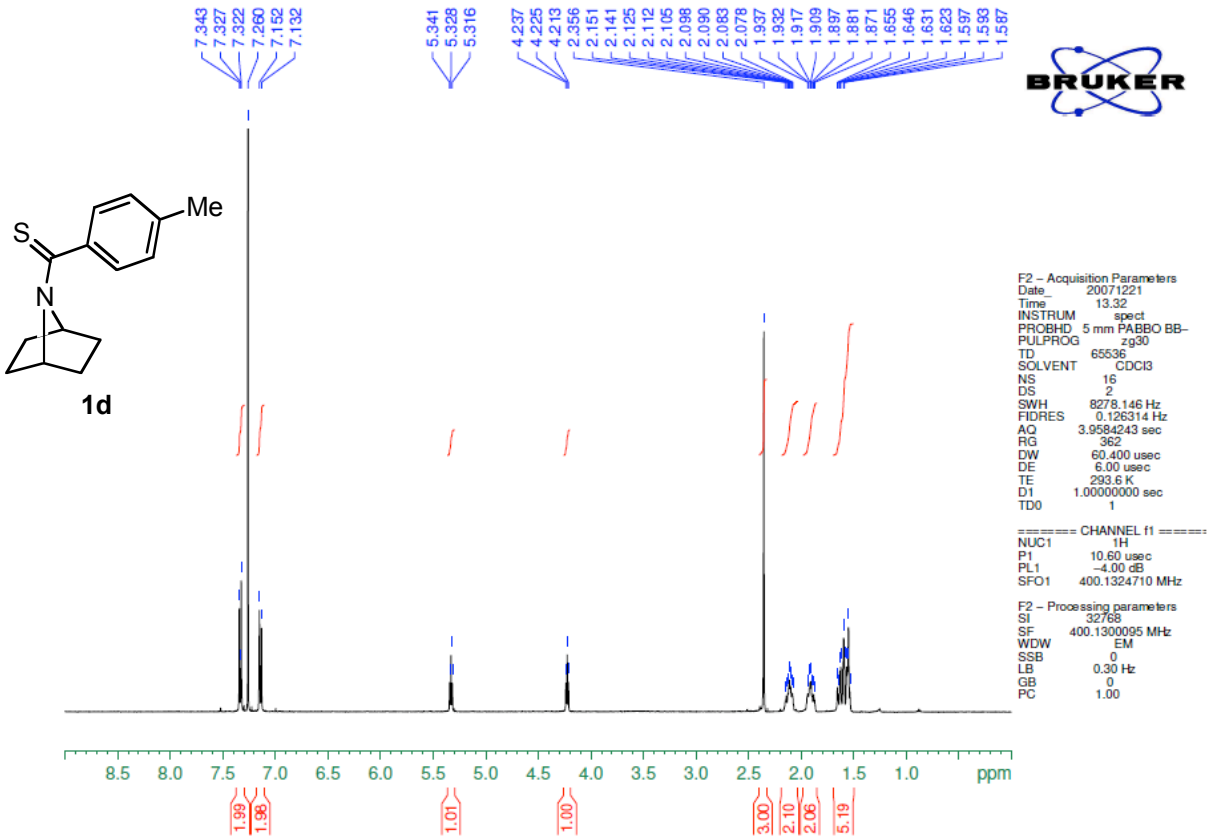
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2.098
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N
Me
1d
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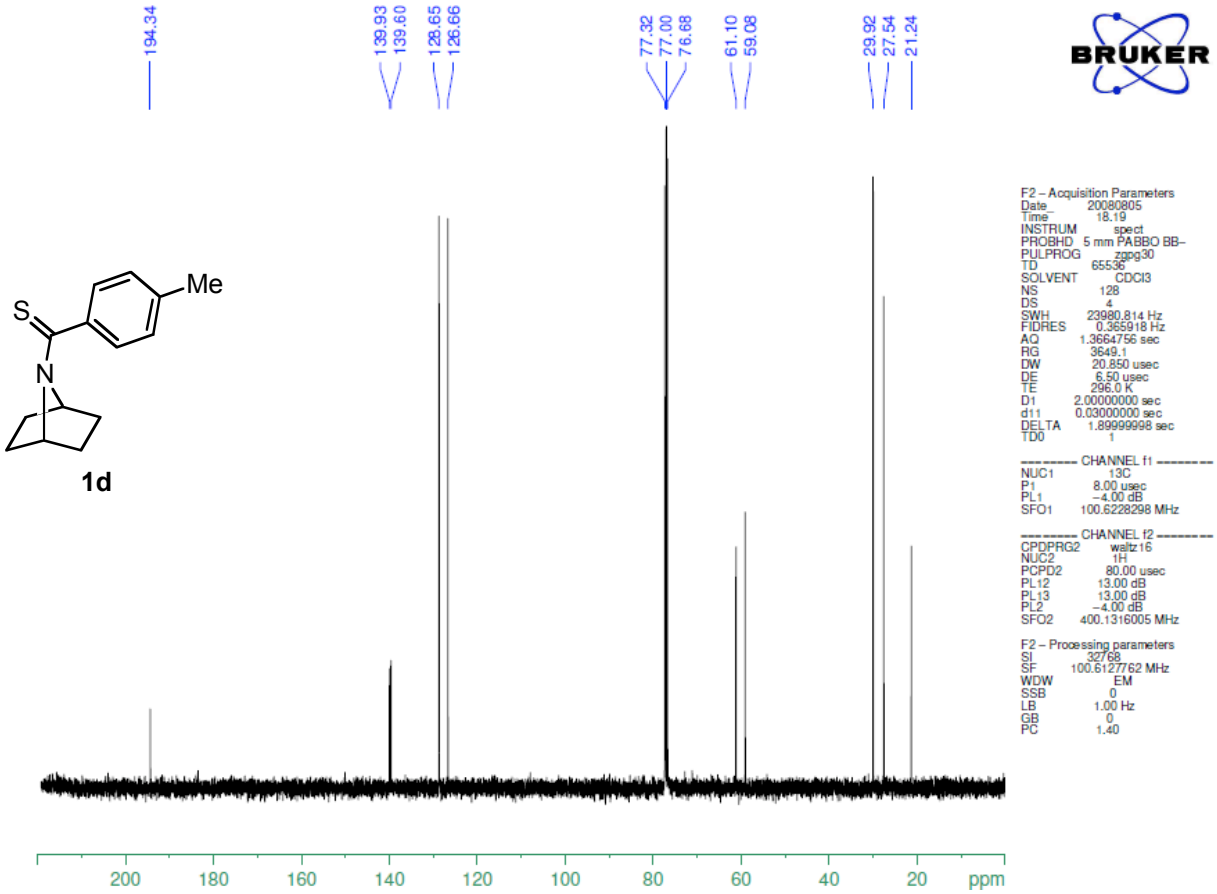
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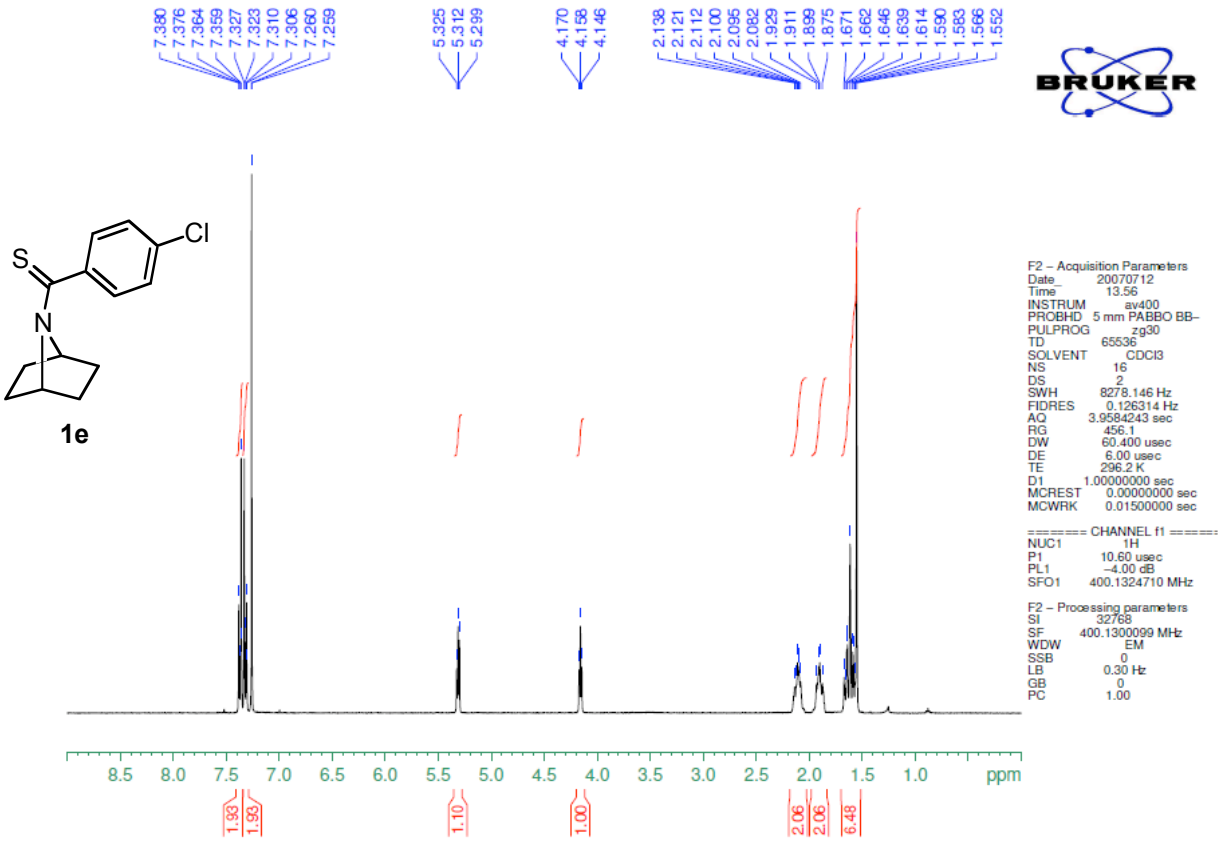
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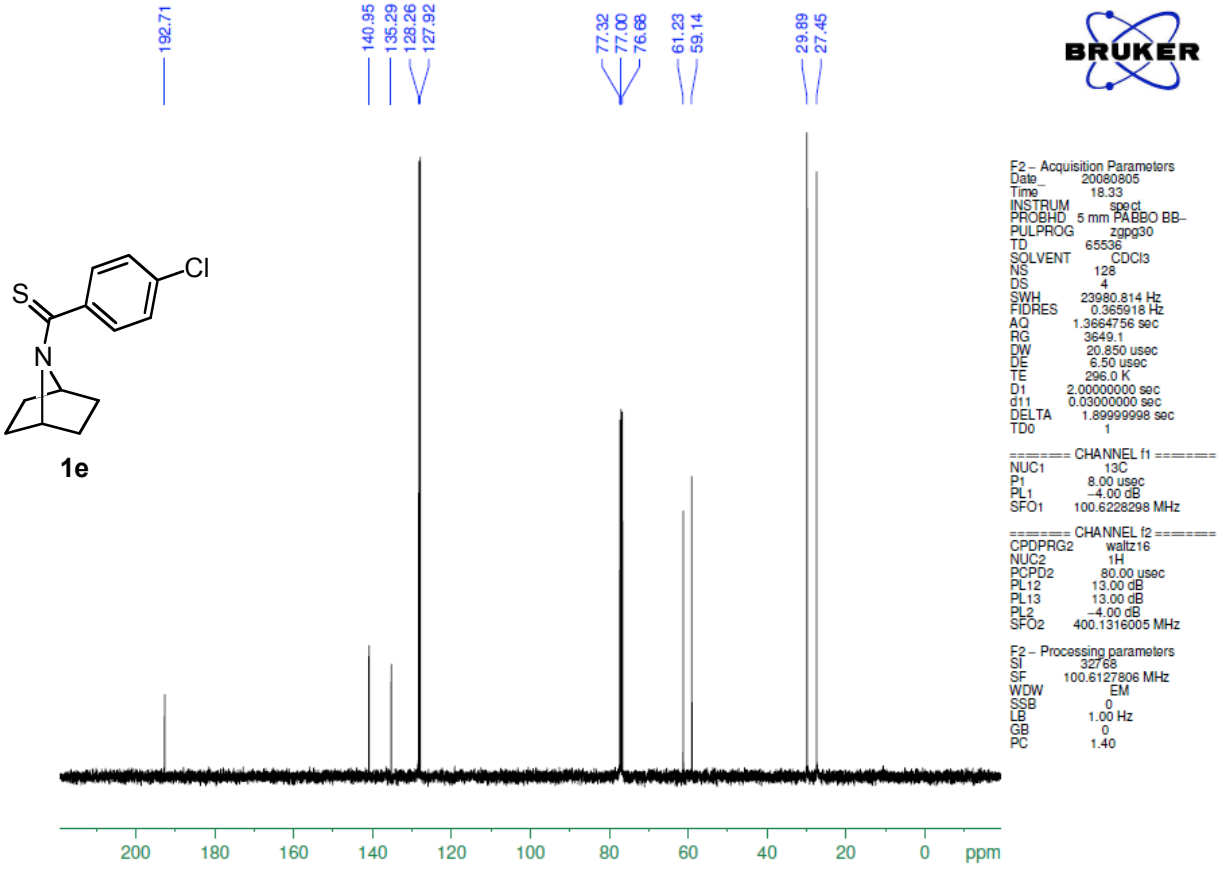
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DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======= CHANNEL f1 ======
NUC1 13C
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PL1 –4.00 dB
SFO1 100.6228298 MHz
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NUC2 1H
PCPD2 80.00 usec
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PL13 13.00 dB
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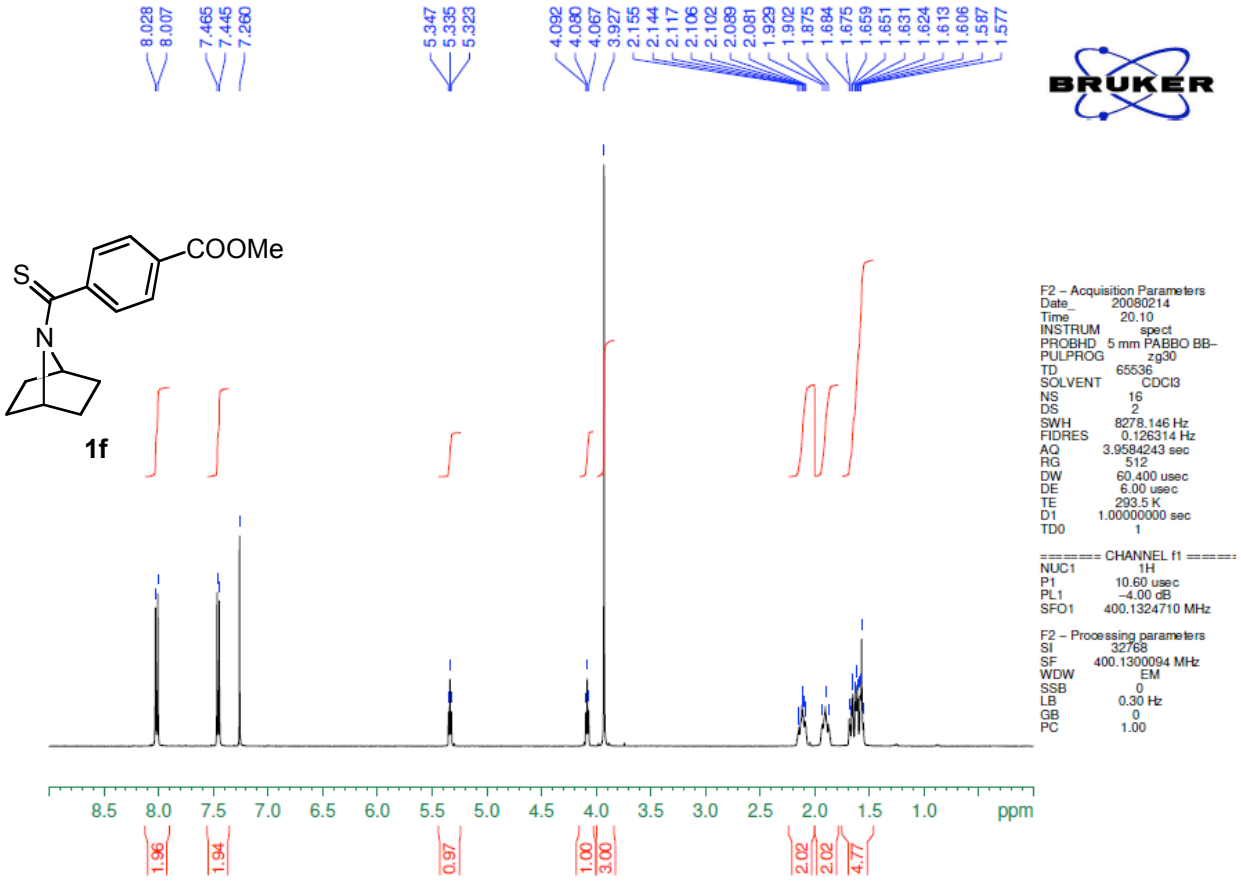
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COOMe
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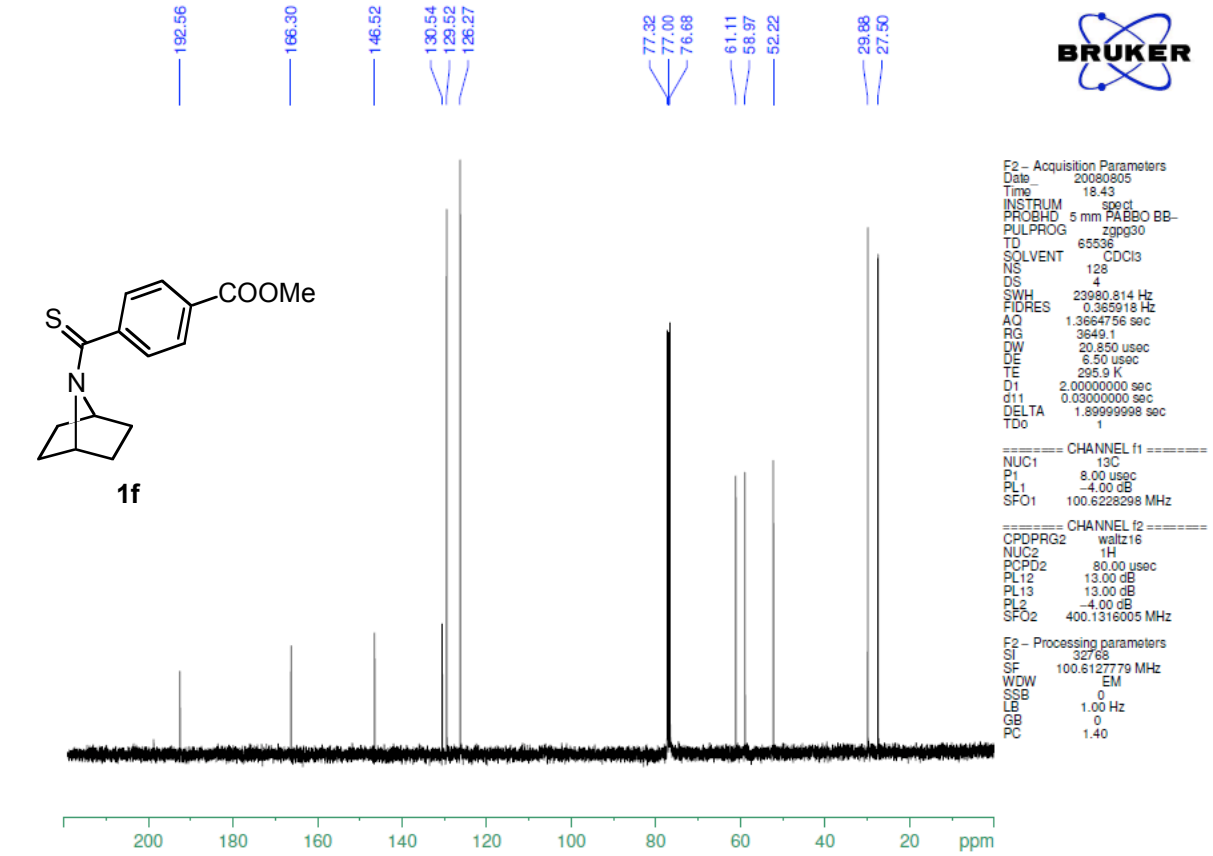
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COOMe
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RG 3649.1
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DE 6.50 usec
TE 295.9 K
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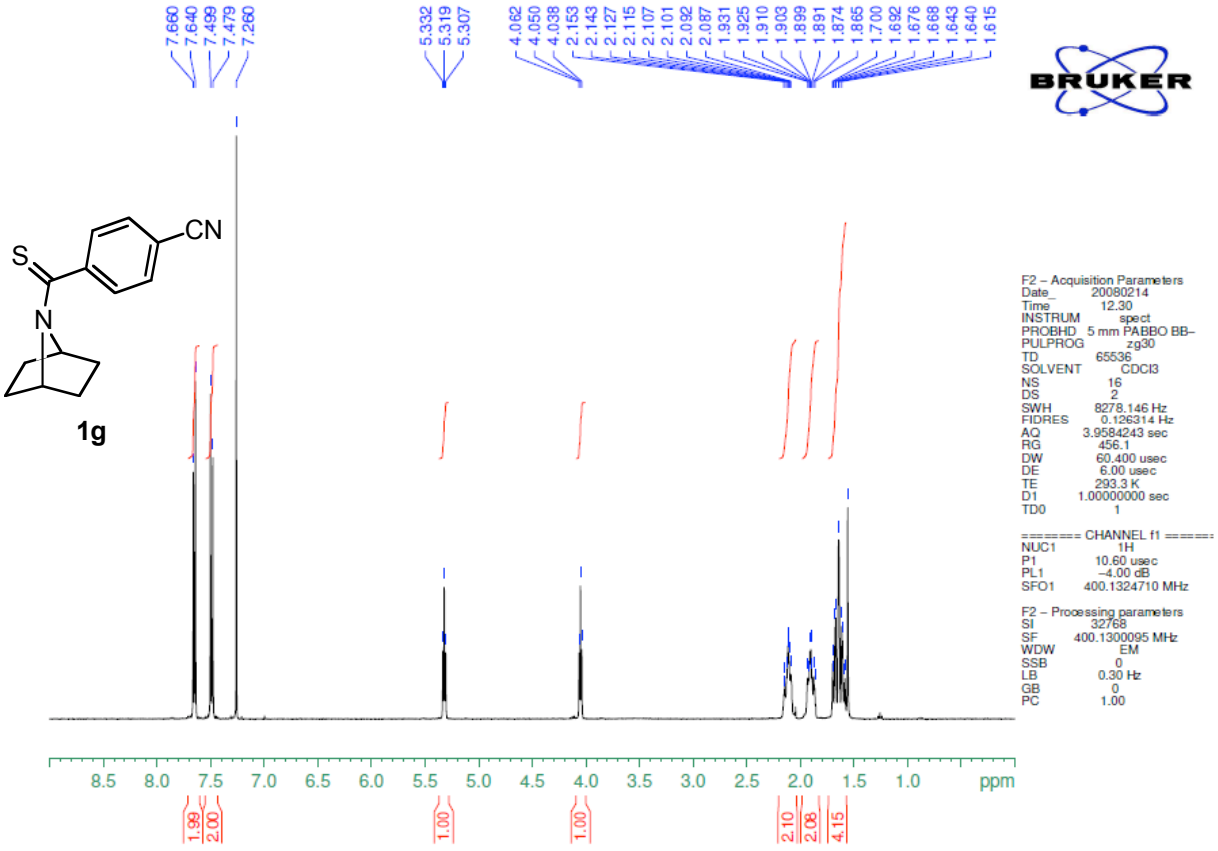
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BRUKER
S
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P1 10.60 usec
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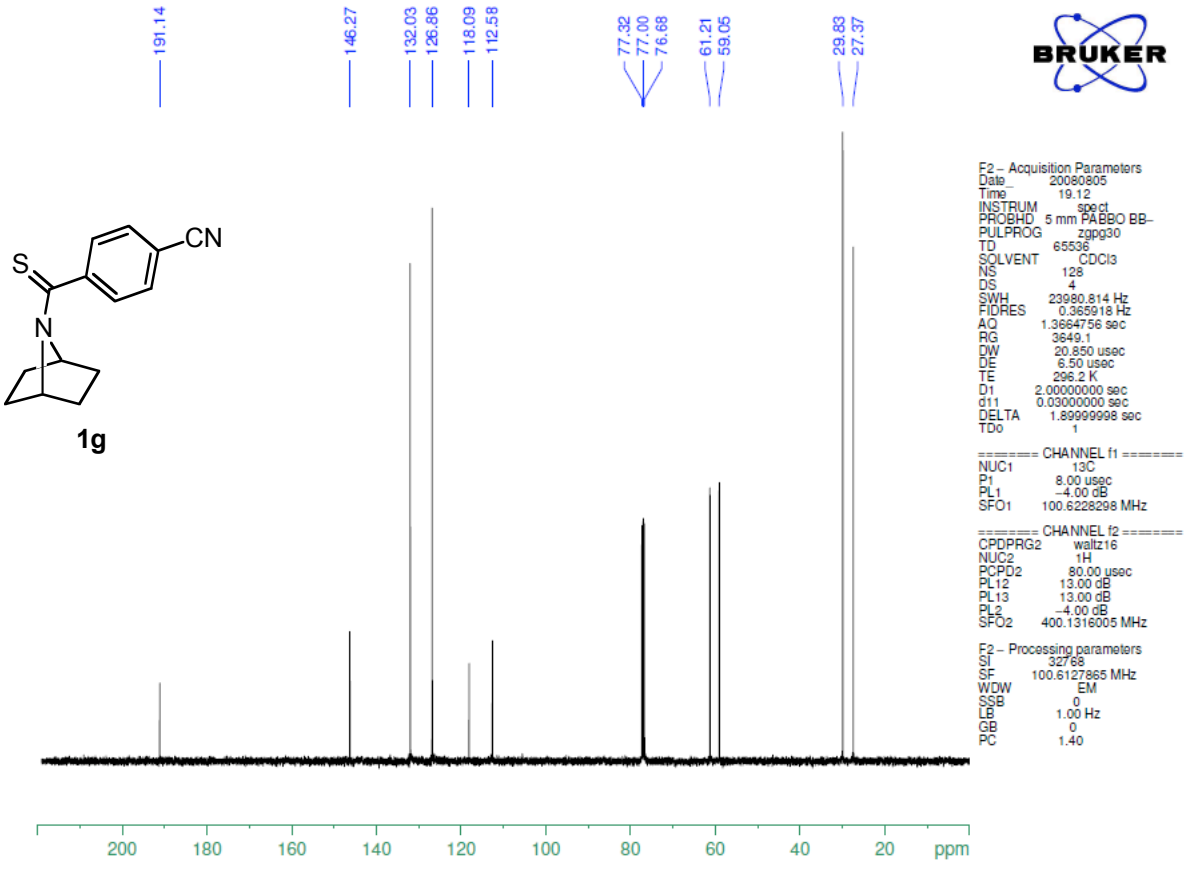
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S
CN
N
1g
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FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3649.1
DW 20.850 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 =======
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P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 =======
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NUC2 1H
PCPD2 80.00 usec
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PL13 13.00 dB
PL2 –4.00 dB
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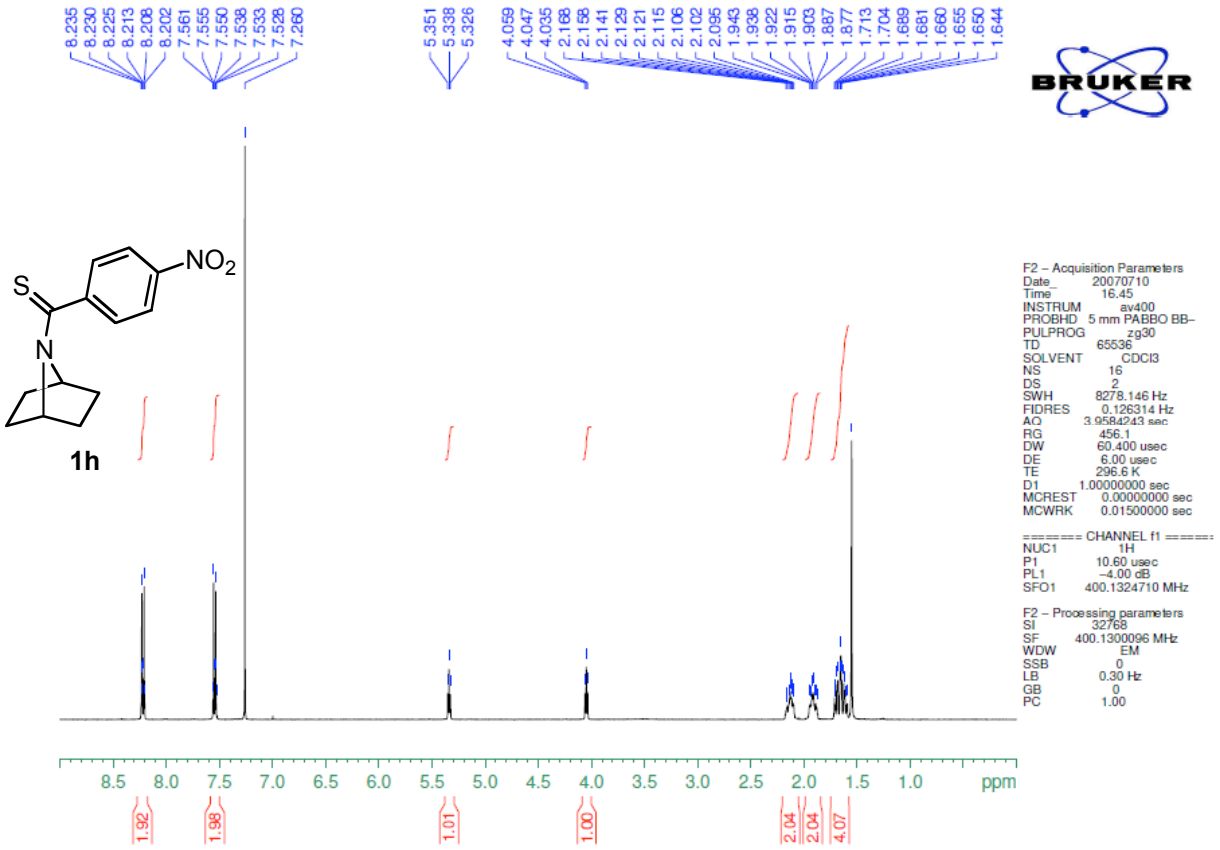
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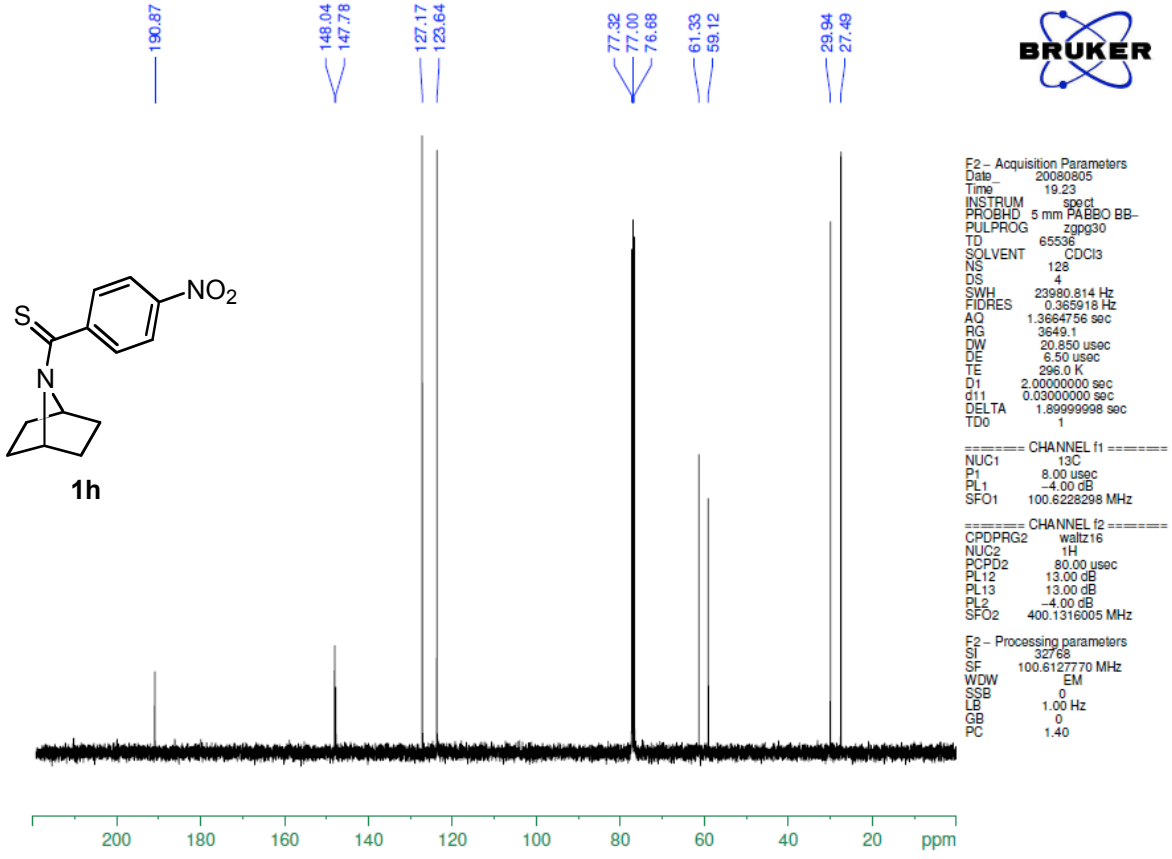
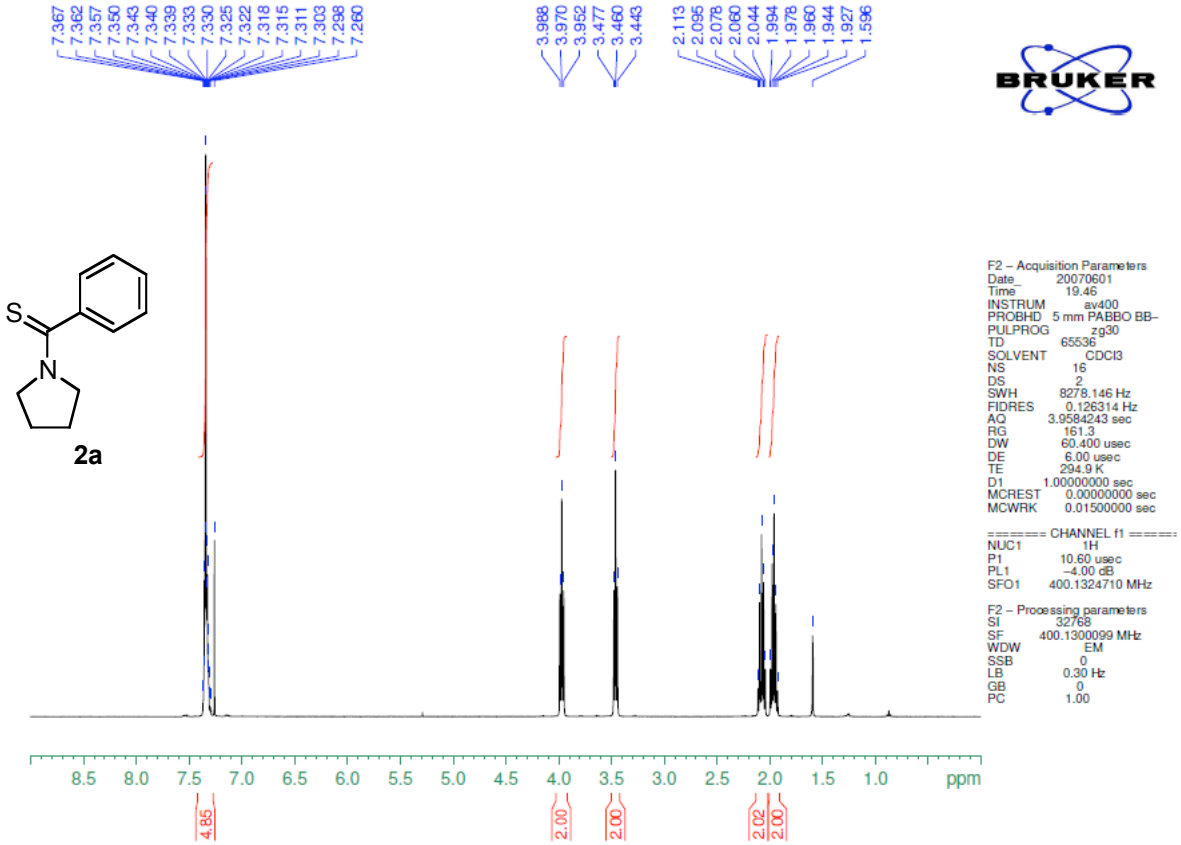
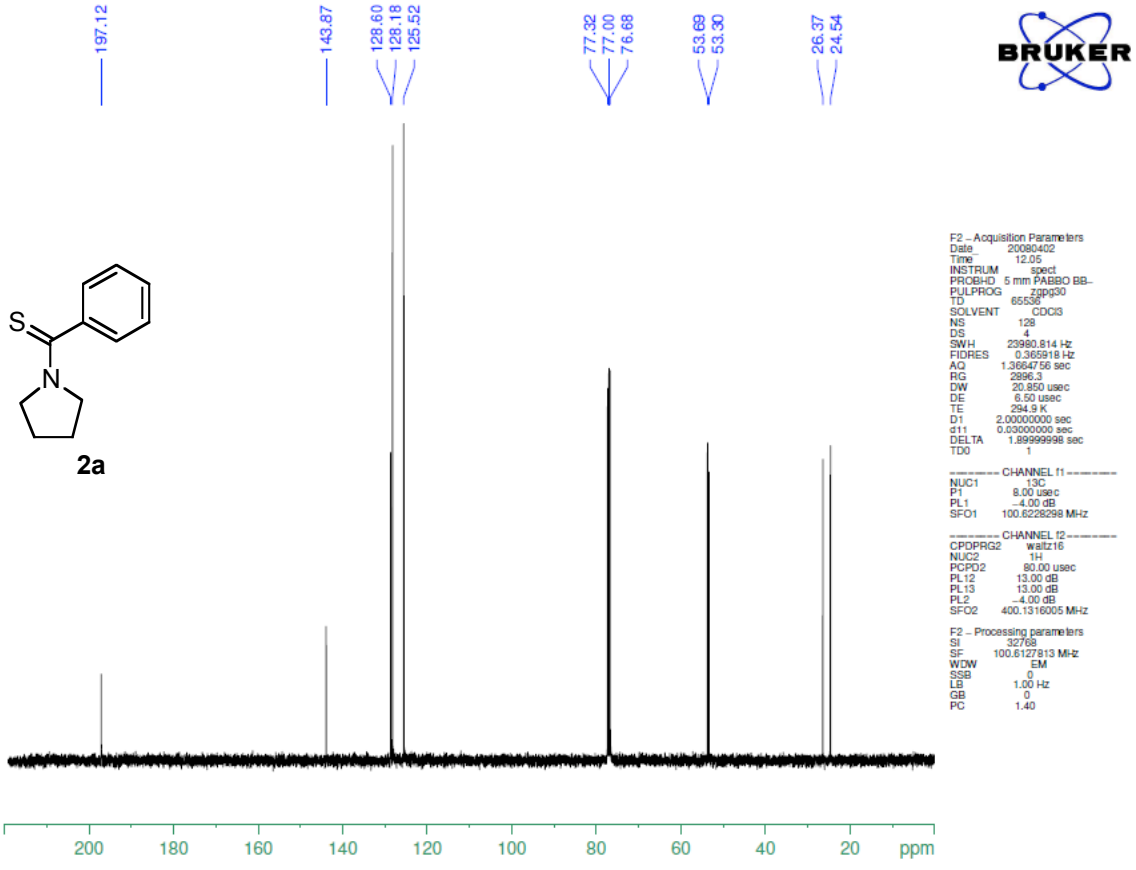
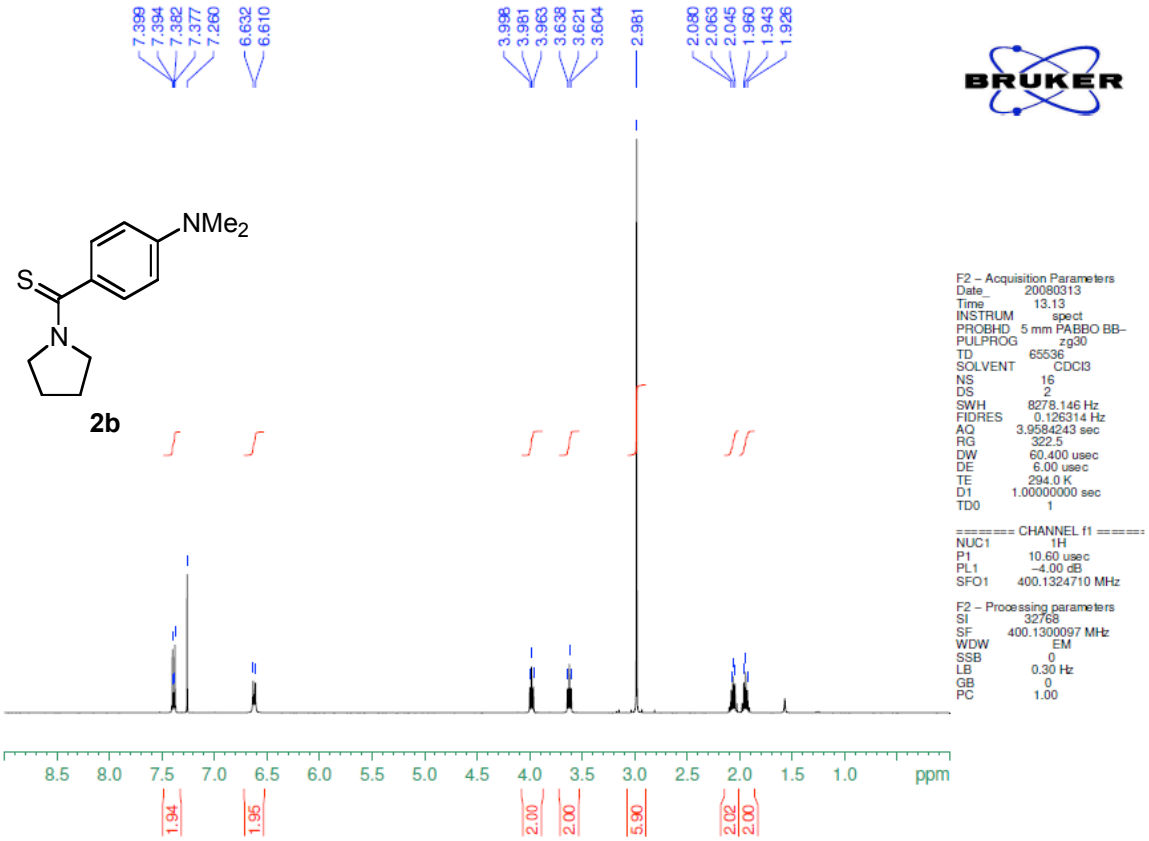
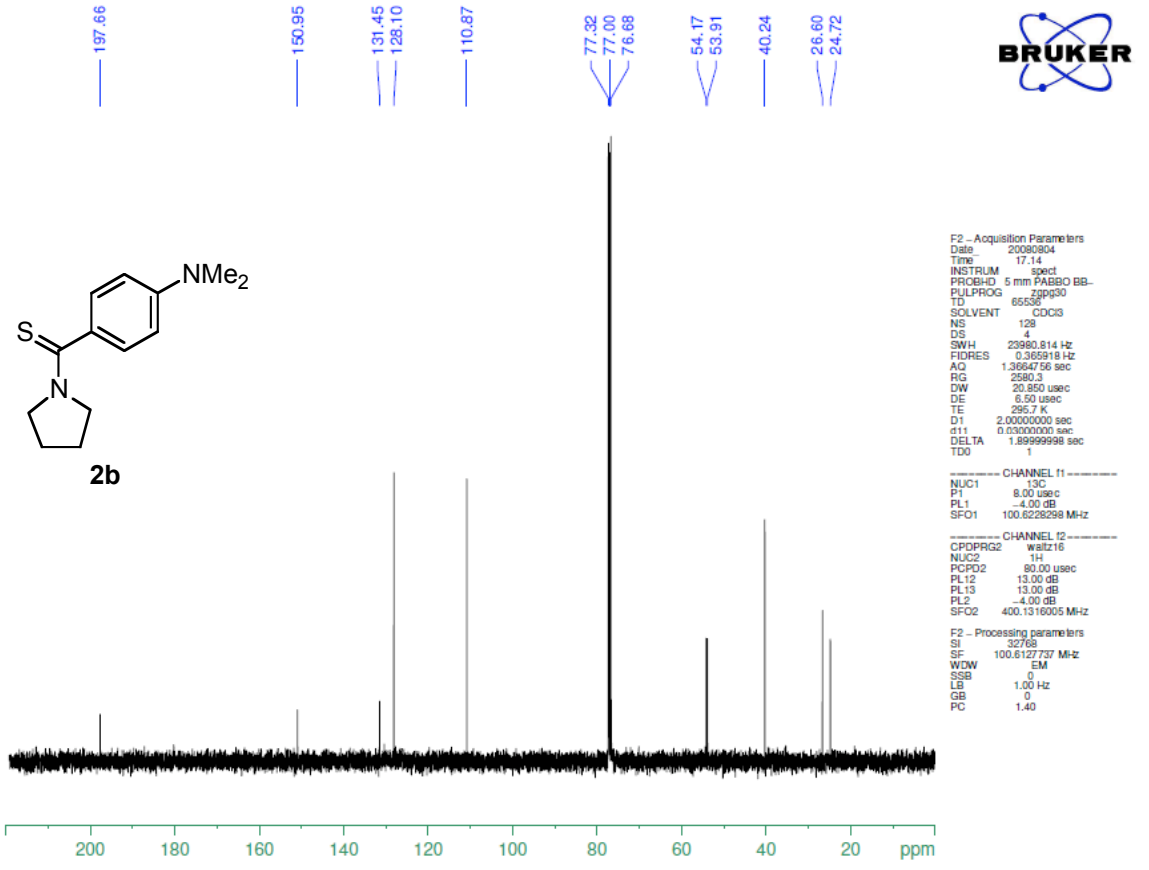
NO2
S
N
1h
F2 – Acquisition Parameters
Date_ 20070710
Time 16.45
INSTRUM av400
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.92
1.98
1.01
1.00
2.04
2.04
4.07

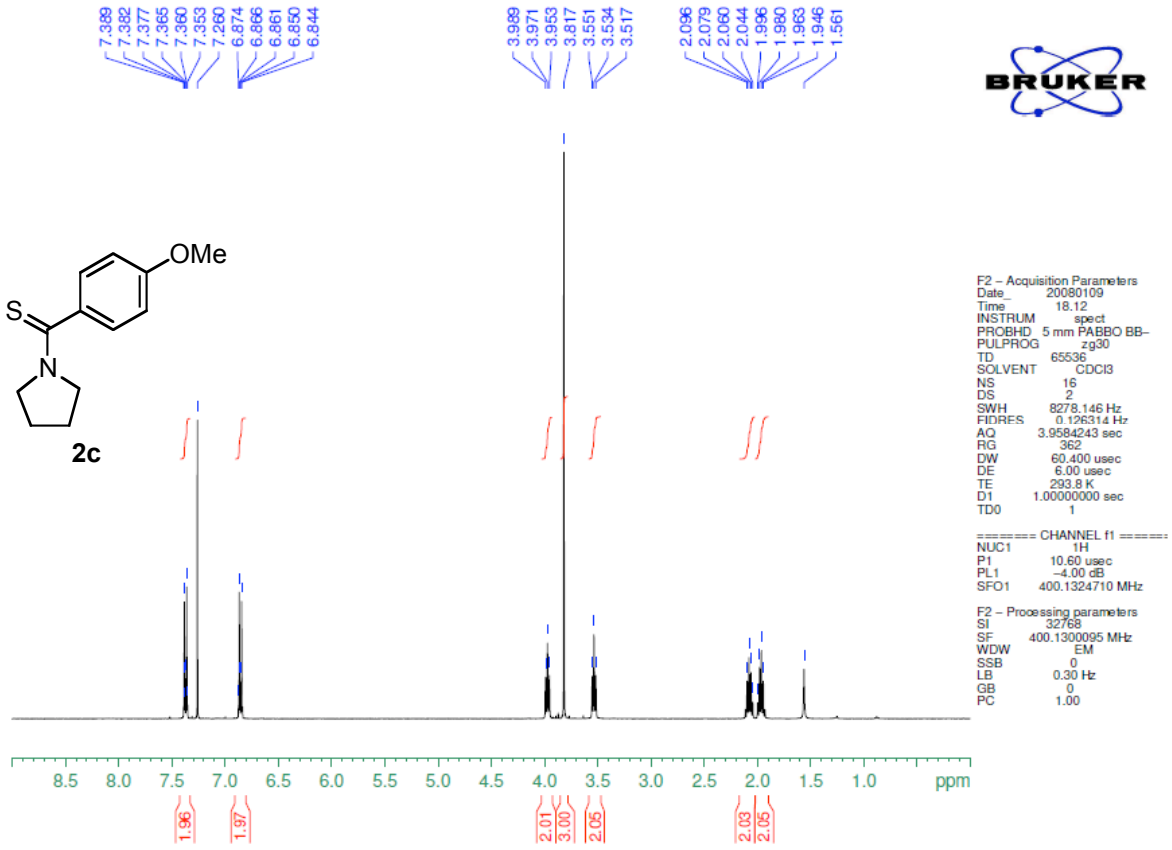

190.87
148.04
147.78
127.17
123.64
77.32
77.00
76.68
61.33
59.12
29.94
27.49
BRUKER
NO2
S
N
1h
F2 – Acquisition Parameters
Date_ 20080805
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3649.1
DW 20.850 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 =======
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127770 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

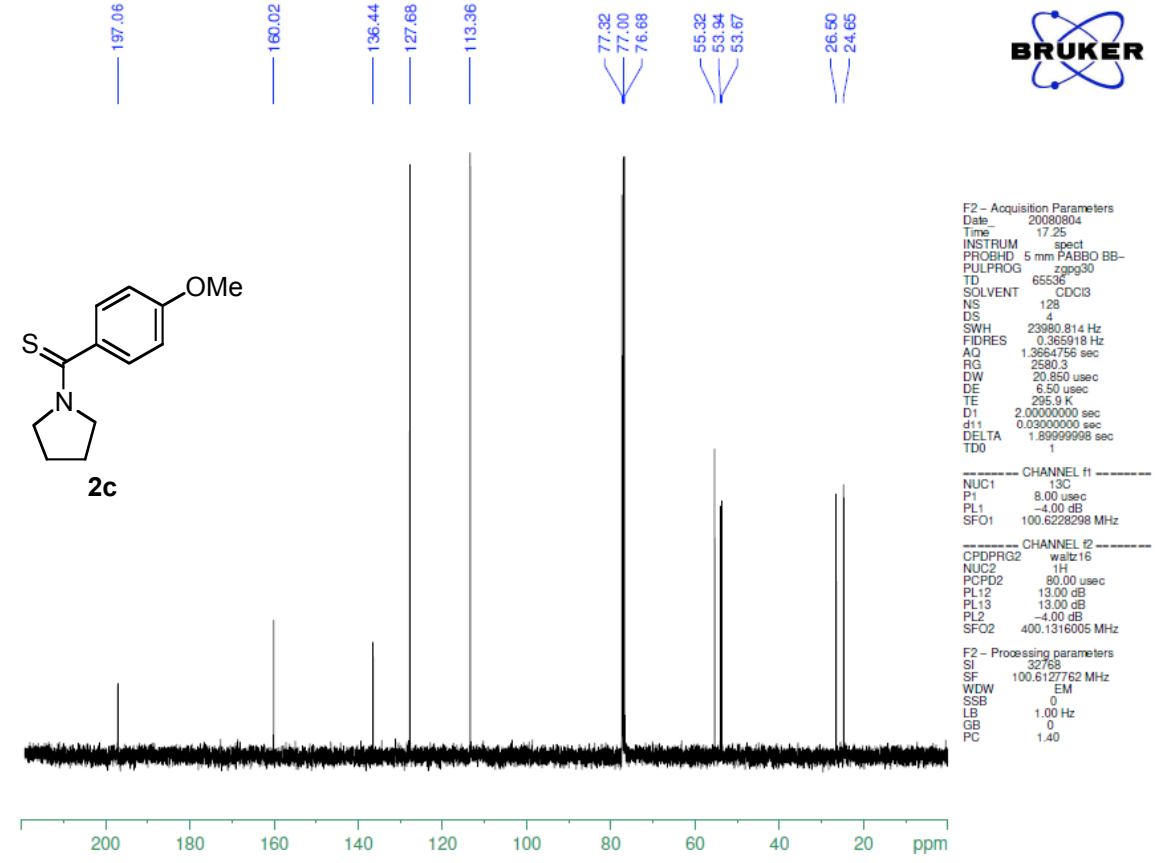

7.367
7.362
7.357
7.350
7.343
7.340
7.339
7.333
7.330
7.325
7.322
7.318
7.315
7.311
7.303
7.298
7.260
3.988
3.970
3.952
3.477
3.460
3.443
2.113
2.095
2.078
2.060
2.044
1.994
1.978
1.960
1.944
1.927
1.596
BRUKER
S
N
2a
F2 – Acquisition Parameters
Date_ 20070601
Time 19.46
INSTRUM av400
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 161.3
DW 60.400 usec
DE 6.00 usec
TE 294.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.85
2.00
2.00
2.02
2.00

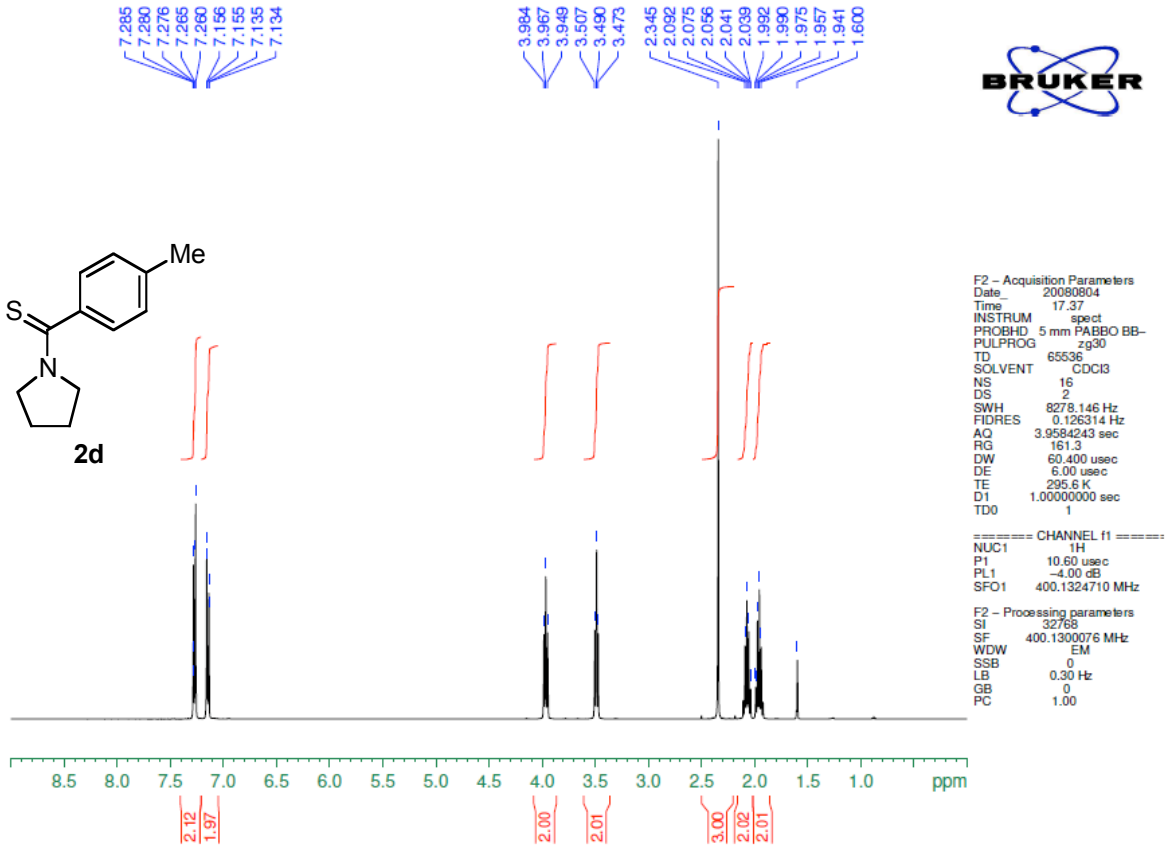

197.12
143.87
128.60
128.18
125.52
77.32
77.00
76.68
53.69
53.30
26.37
24.54
BRUKER
S
N
2a
F2 – Acquisition Parameters
Date_ 20080402
Time 12.05
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2896.3
DW 20.850 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127813 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

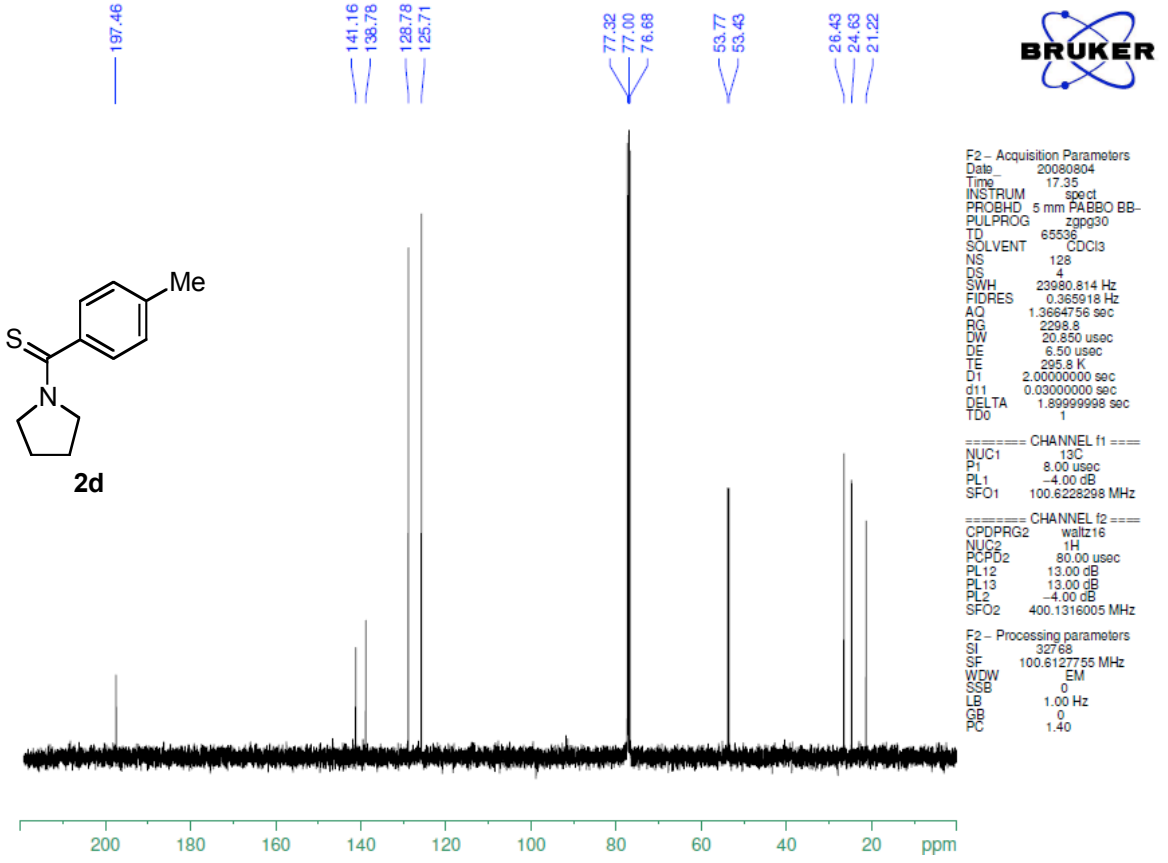

7.399
7.394
7.382
7.377
7.260
6.632
6.610
3.998
3.981
3.963
3.638
3.621
3.604
2.981
2.080
2.063
2.045
1.960
1.943
1.926
NMe2
S
N
2b
F2 – Acquisition Parameters
Date_ 20080313
Time 13.13
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.94
1.95
2.00
2.00
5.90
2.02
2.00

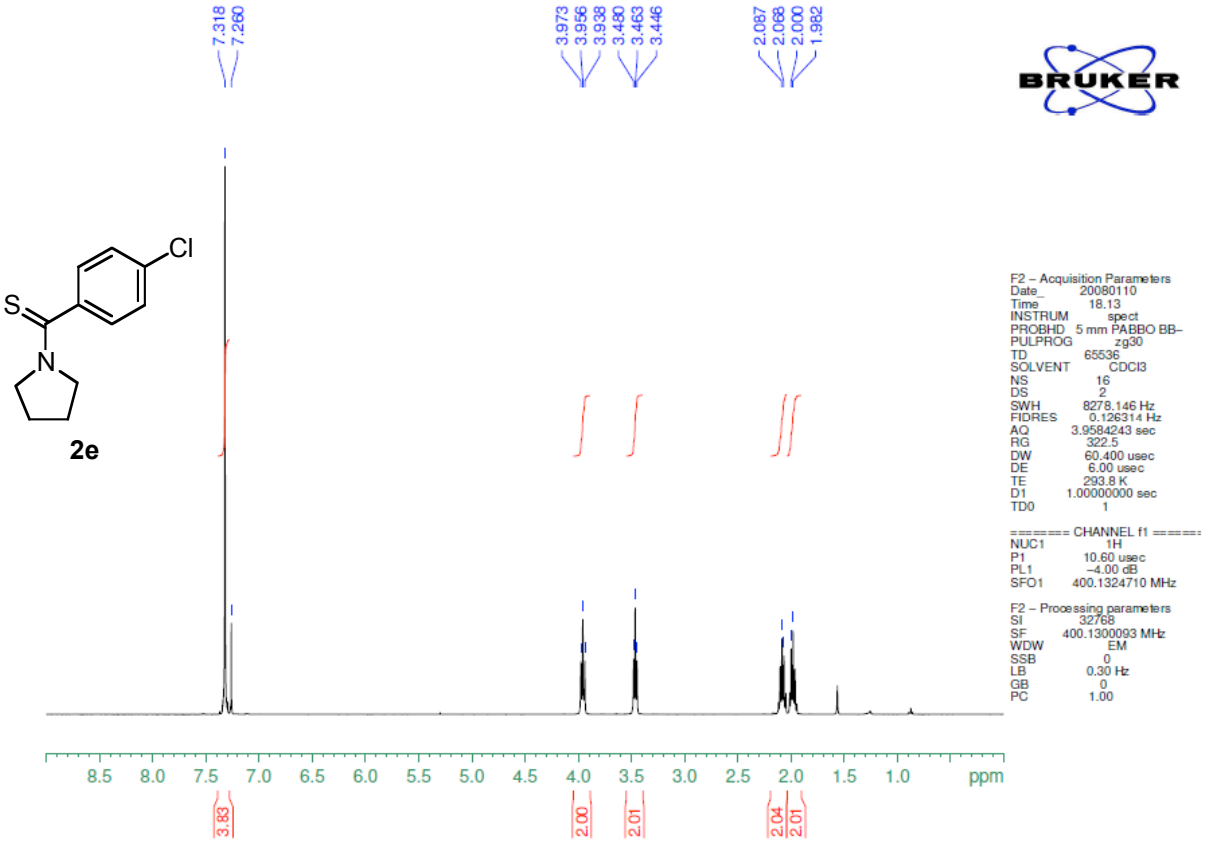

197.66
150.95
131.45
128.10
110.87
77.32
77.00
76.68
54.17
53.91
40.24
26.60
24.72
NMe2
S
N
2b
F2 – Acquisition Parameters
Date_ 20080804
Time 17.14
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2580.3
DW 20.850 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm


7.389
7.382
7.377
7.365
7.360
7.353
7.260
6.874
6.866
6.861
6.850
6.844
3.989
3.971
3.953
3.817
3.551
3.534
3.517
2.096
2.079
2.060
2.044
1.996
1.980
1.963
1.946
1.561
BRUKER
OMe
S
N
2c
F2 – Acquisition Parameters
Date_ 20080109
Time 18.12
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.96
1.97
2.01
3.00
2.05
2.03
2.05


197.06
160.02
136.44
127.68
113.36
77.32
77.00
76.68
55.32
53.94
53.67
26.50
24.65
BRUKER
OMe
S
N
2c
F2 – Acquisition Parameters
Date_ 20080804
Time 17.25
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2580.3
DW 20.850 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm


7.285
7.280
7.276
7.265
7.260
7.156
7.155
7.135
7.134
3.984
3.967
3.949
3.507
3.490
3.473
2.345
2.092
2.075
2.056
2.041
2.039
1.992
1.990
1.975
1.957
1.941
1.600
BRUKER
Me
S
N
2d
F2 – Acquisition Parameters
Date_ 20080804
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 161.3
DW 60.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.12
1.97
2.00
2.01
3.00
2.02
2.01


197.46
141.16
138.78
128.78
125.71
77.32
77.00
76.68
53.77
53.43
26.43
24.63
21.22
BRUKER
Me
S
N
2d
F2 – Acquisition Parameters
Date_ 20080804
Time 17.35
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ===
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ===
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

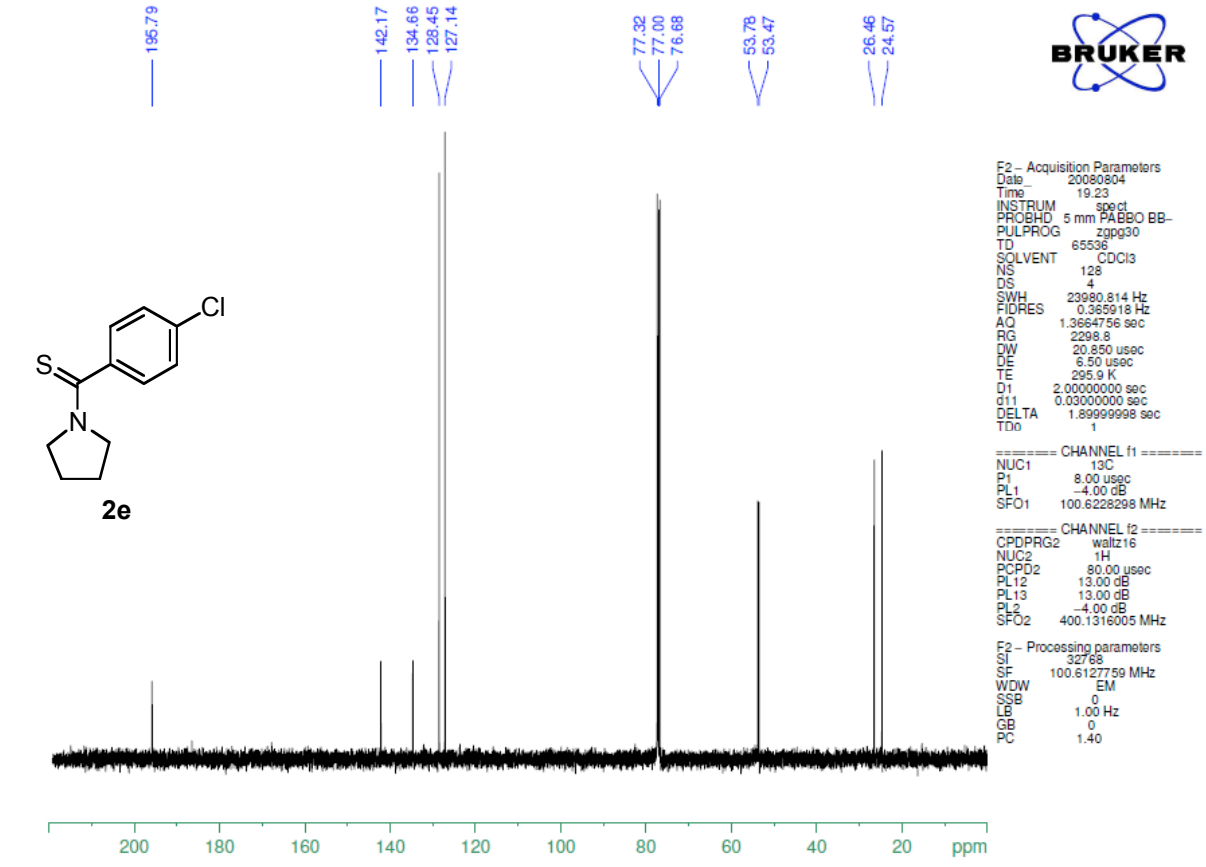


BRUKER

F2 – Acquisition Parameters
Date_ 20080110
Time 18.13
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz

F2 – Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



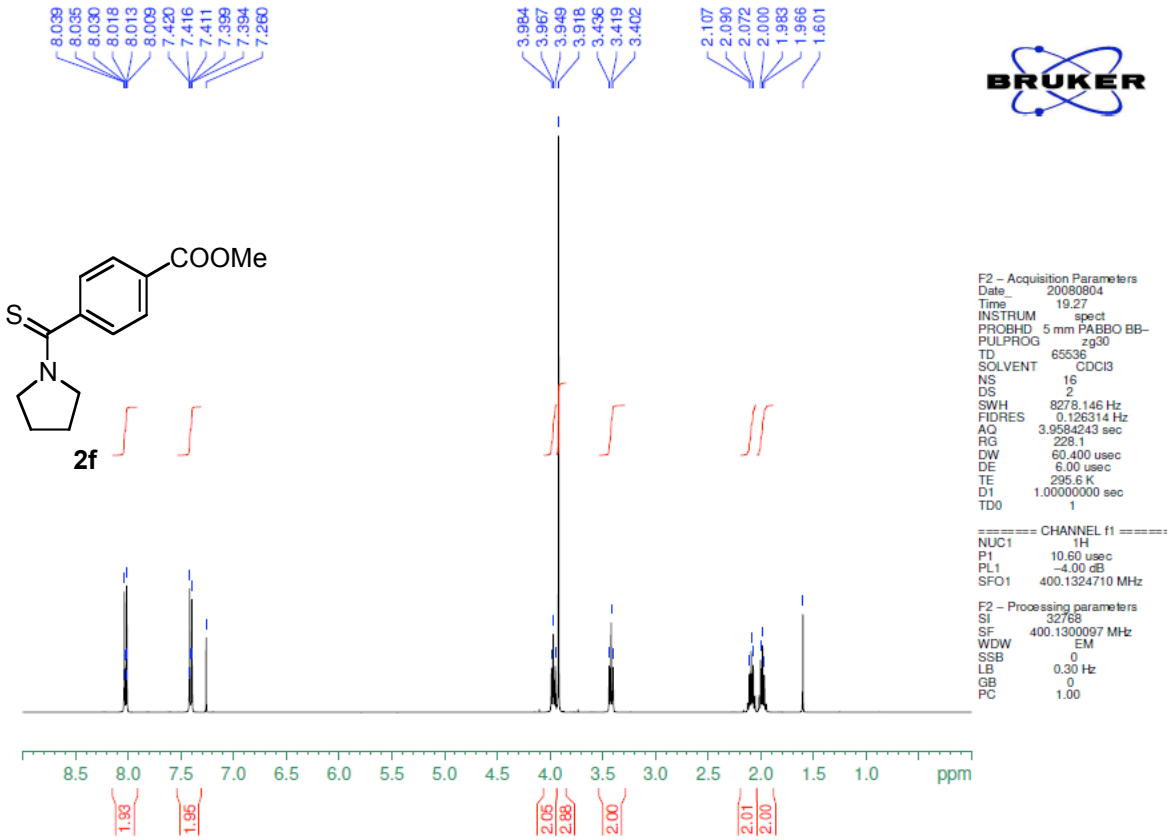
BRUKER

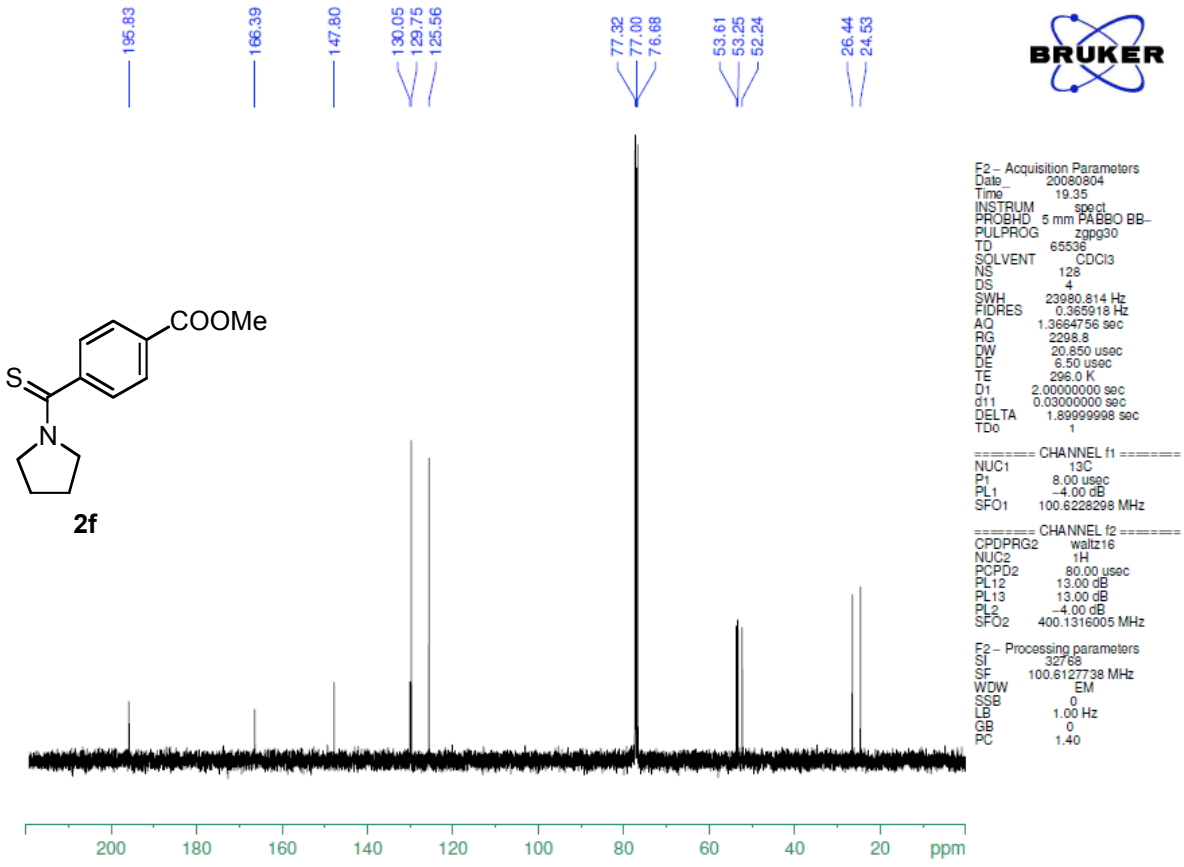
F2 – Acquisition Parameters
Date_ 20080804
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

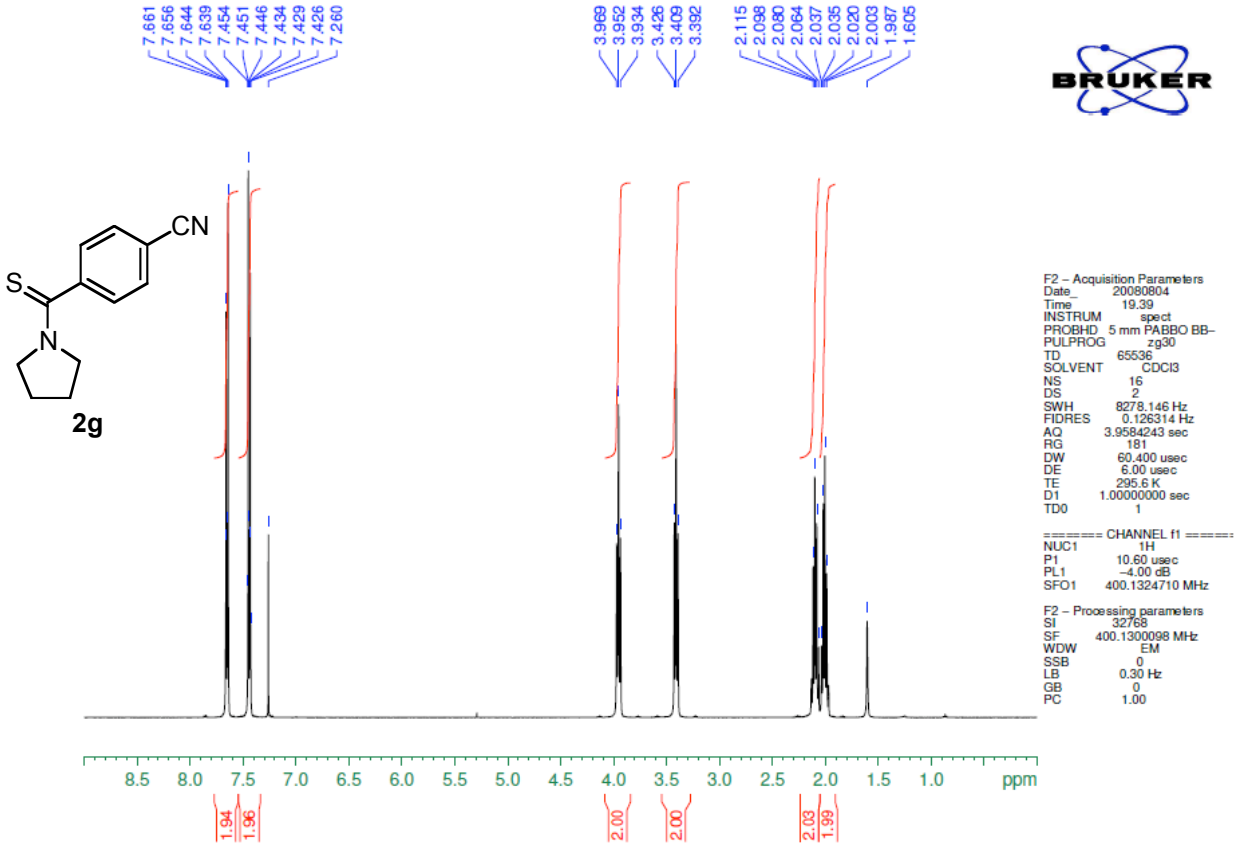
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz

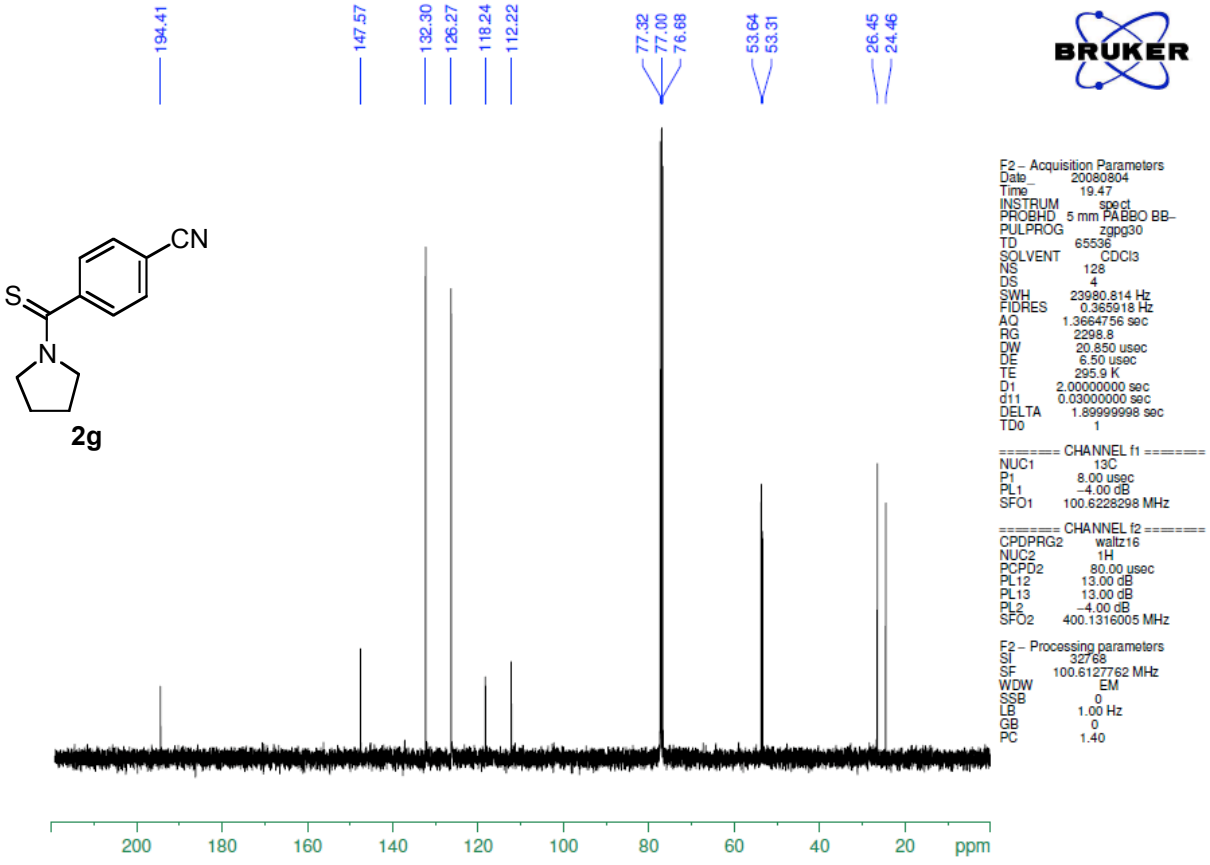
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz

F2 – Processing parameters
SI 32768
SF 100.6127759 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


8.039
8.035
8.030
8.018
8.013
8.009
7.420
7.416
7.411
7.399
7.394
7.260
3.984
3.967
3.949
3.918
3.436
3.419
3.402
2.107
2.090
2.072
2.000
1.983
1.966
1.601
BRUKER
COOMe
S
N
2f
F2 – Acquisition Parameters
Date_ 20080804
Time 19.27
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 228.1
DW 60.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.93
1.95
2.05
2.88
2.00
2.01
2.00


195.83
166.39
147.80
130.05
129.75
125.56
77.32
77.00
76.68
53.61
53.25
52.24
26.44
24.53
BRUKER
COOMe
S
N
2f
F2 – Acquisition Parameters
Date_ 20080804
Time 19.35
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127738 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm


7.661
7.656
7.644
7.639
7.454
7.451
7.446
7.434
7.429
7.426
7.260
3.969
3.952
3.934
3.426
3.409
3.392
2.115
2.098
2.080
2.064
2.037
2.035
2.020
2.003
1.987
1.605
BRUKER
CN
S
N
2g
F2 – Acquisition Parameters
Date_ 20080804
Time 19.39
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
SFO1 400.1324710 MHz
F2 – Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.94
1.96
2.00
2.00
2.03
1.99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BRUKER
CN
S
N
2g
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Time 19.47
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
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NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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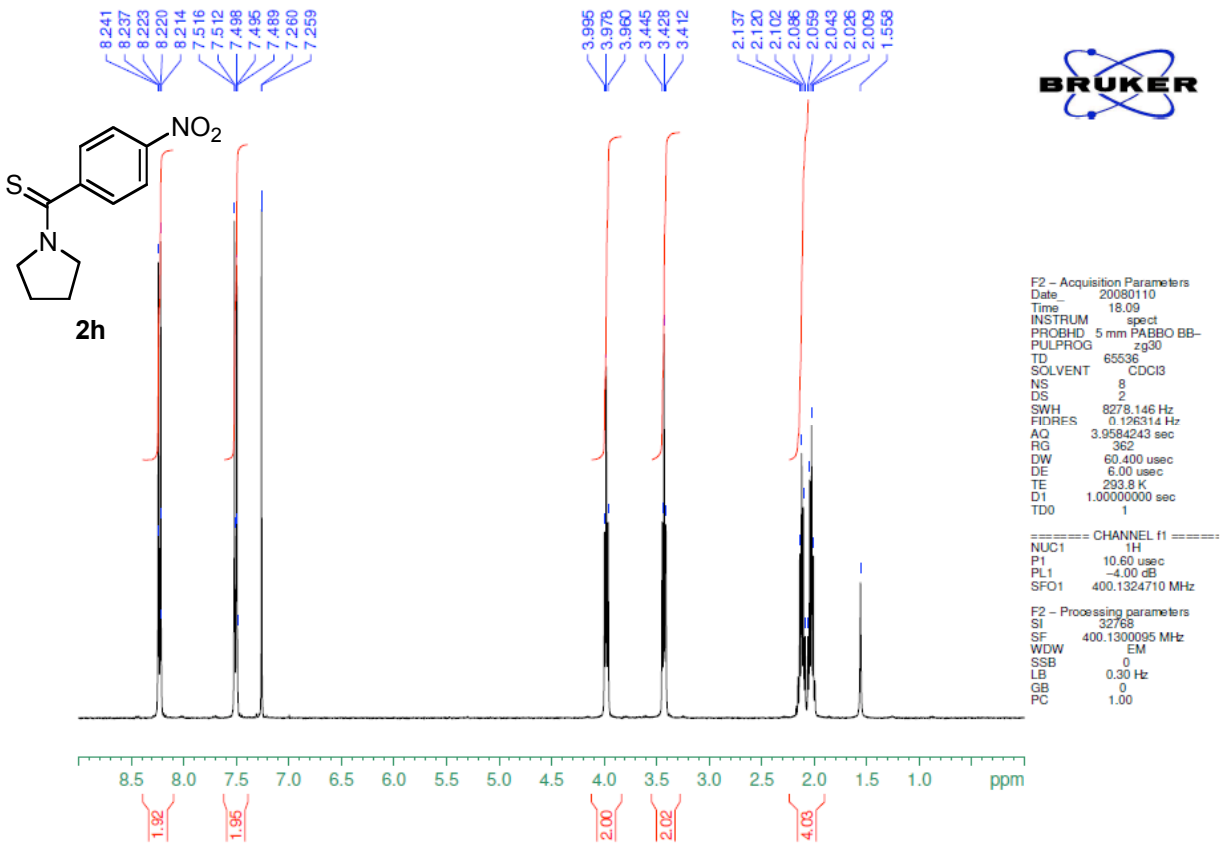

BRUKER

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PULPROG zg30
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SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ======
NUC1 1H
P1 10.60 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 – Processing parameters
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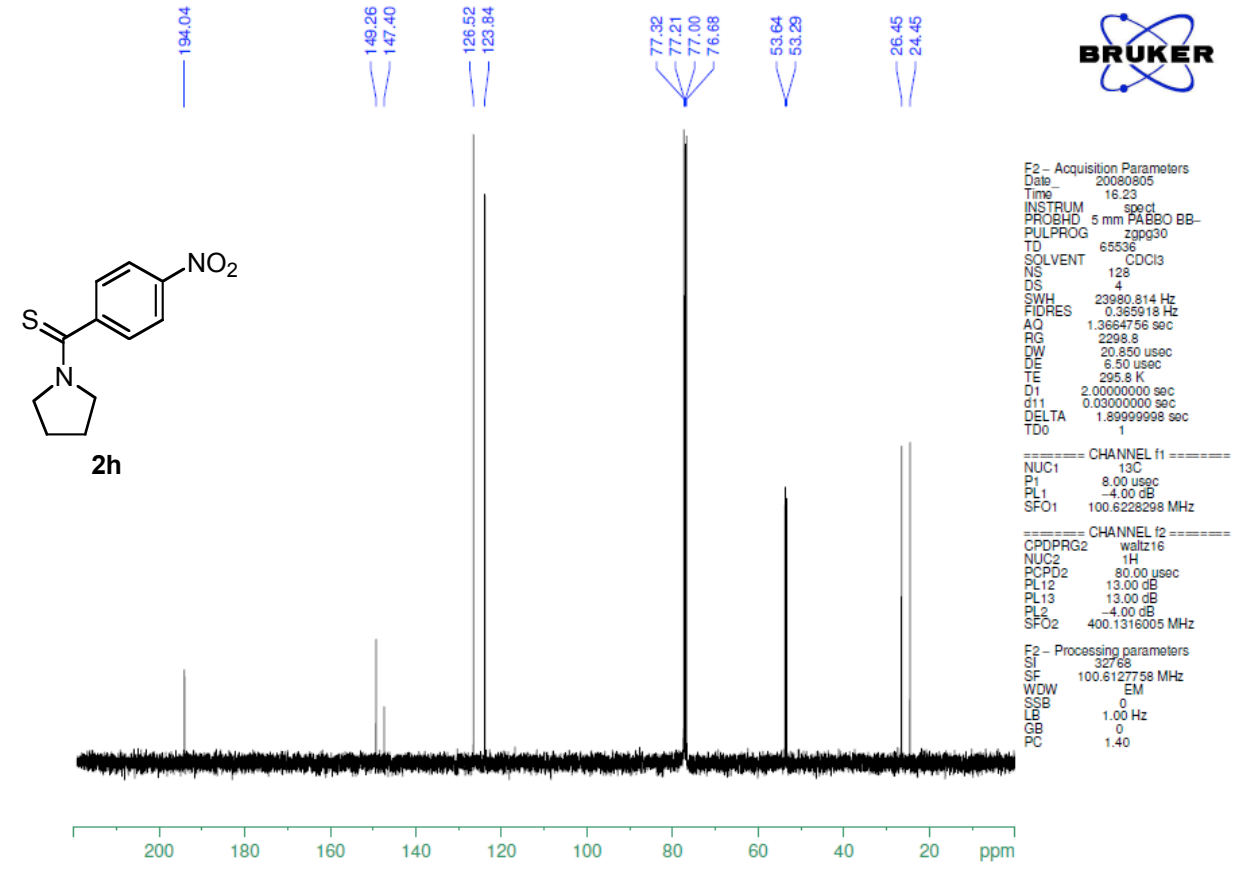
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -4.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 -4.00 dB
SFO2 400.1316005 MHz

F2 – Processing parameters
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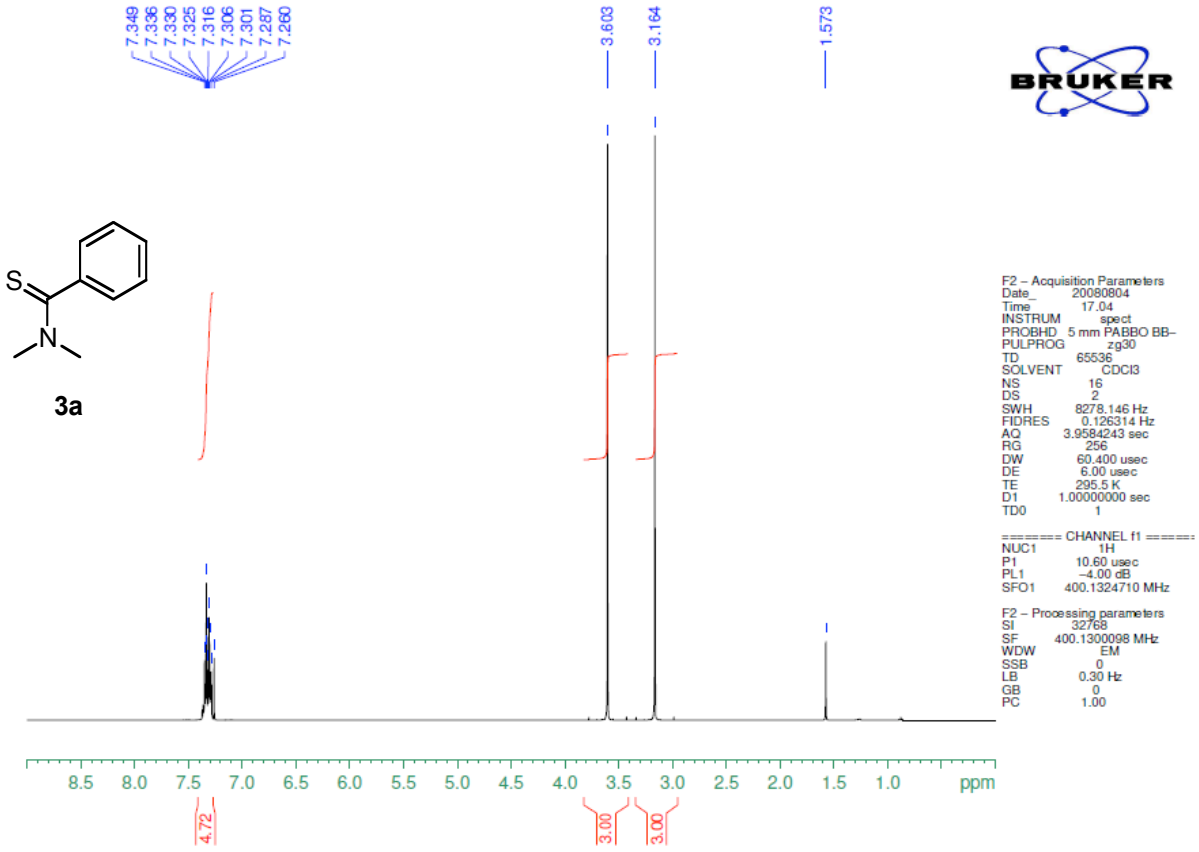
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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3.164
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N
3a
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.72
3.00
3.00
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PULPROG zg30
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SOLVENT CDCl3
NS 16
DS 2
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FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.60 usec
PL1 –4.00 dB
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F2 – Processing parameters
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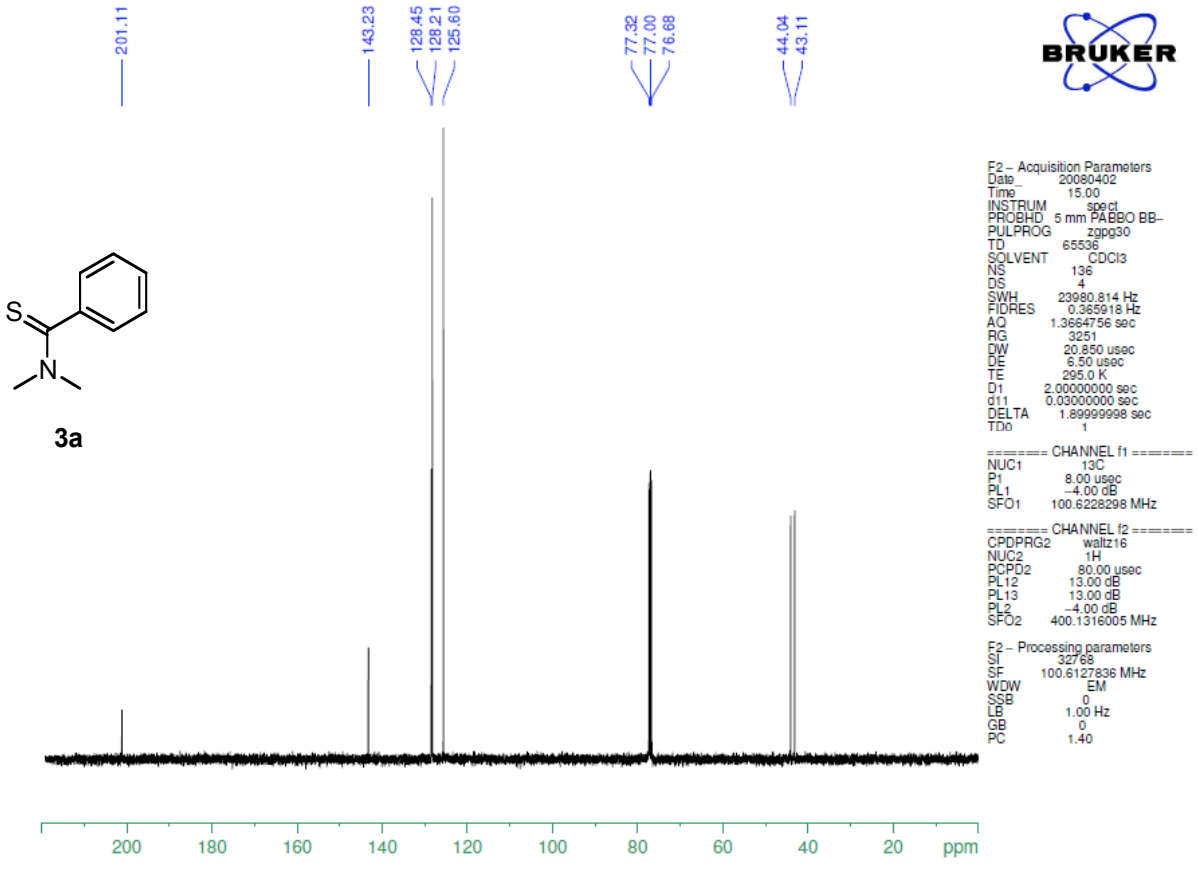
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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128.21
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44.04
43.11
S
N
3a
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Time 15.00
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 136
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3251
DW 20.850 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 –4.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 13.00 dB
PL13 13.00 dB
PL2 –4.00 dB
SFO2 400.1316005 MHz
F2 – Processing parameters
SI 32768
SF 100.6127836 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2. Crystallographic Data

Single-Crystal X-Ray Diffraction Data of 1a.

Empirical formula	C13 H15 N S	
Formula weight	217.32	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 11.0169(17) Å	α= 90°.
	b = 14.654(2) Å	β= 90°.
	c = 28.298(5) Å	γ = 90°.
Volume	4568.4(13) $Å^3$	
Z	16	
Density (calculated)	1.264 Mg/m^3	
Absorption coefficient	0.249 mm^{-1}	
F(000)	1856	
Crystal size	0.40 x 0.30 x 0.30 mm	
Theta range for data collection	1.44 to 28.32°.	
Index ranges	-14<=h<=14, -18<=k<=16, -28<=l<=36	
Reflections collected	26399	
Independent reflections	5517 [R(int) = 0.0724]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5517 / 0 / 271	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1071	
R indices (all data)	R1 = 0.0763, wR2 = 0.1263	
Largest diff. peak and hole	0.321 and -0.284 $e.Å^{-3}$	

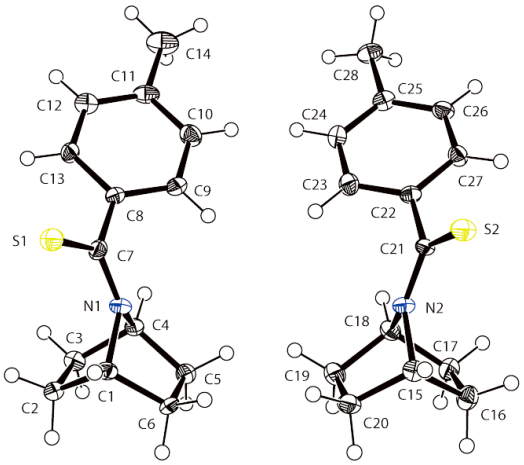
Single-Crystal X-Ray Diffraction Data of 1b.

Empirical formula	C15 H20 N2 S	
Formula weight	260.39	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 7.6862(8) Å	α= 90°.
	b = 7.7203(8) Å	β= 91.162(2)°.
	c = 22.579(2) Å	γ = 90°.
Volume	1339.6(2) $Å^3$	
Z	4	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.226 mm^{-1}	
F(000)	560	
Crystal size	0.39 x 0.31 x 0.21 mm	
Theta range for data collection	1.80 to 28.29°.	
Index ranges	-6<=h<=10, -9<=k<=10, -29<=l<=26	
Reflections collected	7942	
Independent reflections	3168 [R(int) = 0.0326]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3168 / 0 / 165	
Goodness-of-fit on F^2	1.107	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.1010	
R indices (all data)	R1 = 0.0457, wR2 = 0.1066	
Largest diff. peak and hole	0.319 and -0.263 e.$Å^{-3}$	

Single-Crystal X-Ray Diffraction Data of 1d.

Empirical formula	C14 H17 N S	
Formula weight	231.35	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 7.789(2) Å	α= 90°.
	b = 17.671(5) Å	β= 90°.
	c = 17.796(5) Å	γ = 90°.
Volume	2449.2(12) $Å^3$	
Z	8	
Density (calculated)	1.255 Mg/m^3	
Absorption coefficient	0.236 mm^{-1}	
F(000)	992	
Crystal size	0.50 x 0.05 x 0.05 mm	
Theta range for data collection	1.62 to 28.29°.	
Index ranges	-10<=h<=10, -22<=k<=19, -16<=l<=22	
Reflections collected	14609	
Independent reflections	5730 [R(int) = 0.0962]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5730 / 0 / 292	
Goodness-of-fit on F^2	0.992	
Final R indices [I>2sigma(I)]	R1 = 0.0657, wR2 = 0.1362	
R indices (all data)	R1 = 0.1163, wR2 = 0.1600	
Absolute structure parameter	0.04(12)	
Extinction coefficient	0.0139(16)	
Largest diff. peak and hole	0.431 and -0.375 $e.Å^{-3}$	

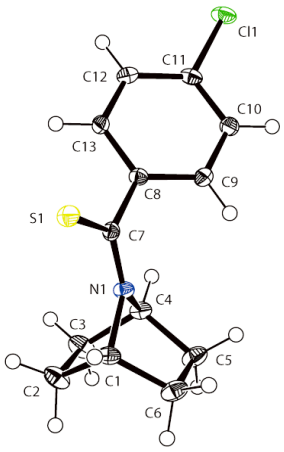
Figure S1. ORTEP Diagram of 1d showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 1e.

Empirical formula	C13 H14 Cl N S	
Formula weight	251.76	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 6.2373(8) Å	α= 90°.
	b = 18.052(2) Å	β= 102.110(2)°.
	c = 11.0263(14) Å	γ = 90°.
Volume	1213.9(3) $Å^3$	
Z	4	
Density (calculated)	1.378 Mg/m^3	
Absorption coefficient	0.457 mm^{-1}	
F(000)	528	
Crystal size	0.30 x 0.20 x 0.20 mm	
Theta range for data collection	2.20 to 28.26°.	
Index ranges	-8<=h<=6, -23<=k<=23, -12<=l<=14	
Reflections collected	7370	
Independent reflections	2861 [R(int) = 0.0456]	
Completeness to theta = 25.00°	99.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2861 / 0 / 145	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0942	
R indices (all data)	R1 = 0.0483, wR2 = 0.1013	
Largest diff. peak and hole	0.460 and -0.240 $e.Å^{-3}$	

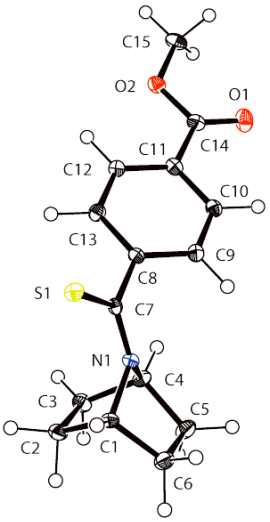
Figure S2. ORTEP Diagram of 1e showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 1f.

Empirical formula	C15 H17 N O2 S	
Formula weight	275.36	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pccn	
Unit cell dimensions	a = 26.056(3) Å	α= 90°.
	b = 7.7067(8) Å	β= 90°.
	c = 13.5969(15) Å	γ = 90°.
Volume	2730.3(5) $Å^3$	
Z	8	
Density (calculated)	1.340 Mg/m^3	
Absorption coefficient	0.234 mm^{-1}	
F(000)	1168	
Crystal size	0.29 x 0.28 x 0.07 mm	
Theta range for data collection	1.56 to 28.30°.	
Index ranges	-31<=h<=34, -10<=k<=10, -11<=l<=18	
Reflections collected	15375	
Independent reflections	3334 [R(int) = 0.0586]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3334 / 0 / 173	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.0954	
R indices (all data)	R1 = 0.0471, wR2 = 0.1016	
Largest diff. peak and hole	0.423 and -0.215 $e.Å^{-3}$	

Figure S3. ORTEP Diagram of 1f showing the thermal ellipsoids at 30% probability.



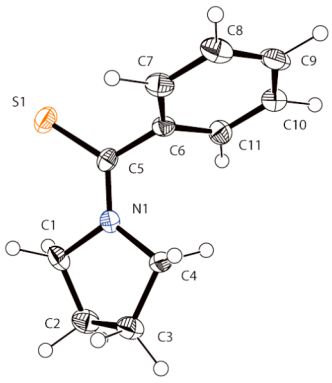
Single-Crystal X-Ray Diffraction Data of 1h.

Empirical formula	C13 H14 N2 O2 S	
Formula weight	262.32	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 7.9612(16) Å	α= 90°.
	b = 6.8315(14) Å	β= 98.845(3)°.
	c = 23.039(5) Å	γ = 90°.
Volume	1238.1(4) $Å^3$	
Z	4	
Density (calculated)	1.407 Mg/m^3	
Absorption coefficient	0.257 mm^{-1}	
F(000)	552	
Crystal size	0.50 x 0.24 x 0.20 mm	
Theta range for data collection	1.79 to 28.26°.	
Index ranges	-9<=h<=10, -4<=k<=9, -29<=l<=28	
Reflections collected	7277	
Independent reflections	2935 [R(int) = 0.0386]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2935 / 0 / 163	
Goodness-of-fit on F^2	1.065	
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0924	
R indices (all data)	R1 = 0.0402, wR2 = 0.0970	
Largest diff. peak and hole	0.330 and -0.286 $e.Å^{-3}$	

Single-Crystal X-Ray Diffraction Data of 2a.

Empirical formula	C11 H13 N S	
Formula weight	191.28	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna21	
Unit cell dimensions	a = 18.069(4) Å	α= 90°.
	b = 5.9249(14) Å	β= 90°.
	c = 9.399(2) Å	γ = 90°.
Volume	1006.3(4) $Å^3$	
Z	4	
Density (calculated)	1.263 Mg/m^3	
Absorption coefficient	0.273 mm^{-1}	
F(000)	408	
Crystal size	0.50 x 0.35 x 0.30 mm	
Theta range for data collection	2.25 to 28.25°.	
Index ranges	-23<=h<=17, -7<=k<=7, -11<=l<=12	
Reflections collected	5558	
Independent reflections	2247 [R(int) = 0.0465]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2247 / 1 / 118	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.1002	
R indices (all data)	R1 = 0.0412, wR2 = 0.1023	
Largest diff. peak and hole	0.319 and -0.156 $e.Å^{-3}$	

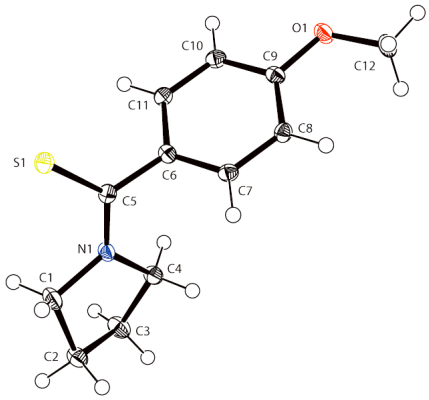
Figure S4. ORTEP Diagram of 2a showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 2c.

Empirical formula	C12 H15 N O S	
Formula weight	221.31	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 5.6481(11) Å	α= 90°.
	b = 13.449(3) Å	β= 90°.
	c = 14.691(3) Å	γ = 90°.
Volume	1116.0(4) $Å^3$	
Z	4	
Density (calculated)	1.317 Mg/m^3	
Absorption coefficient	0.262 mm^{-1}	
F(000)	472	
Crystal size	0.50 x 0.20 x 0.18 mm	
Theta range for data collection	2.77 to 28.28°.	
Index ranges	-7<=h<=7, -17<=k<=15, -17<=l<=18	
Reflections collected	6818	
Independent reflections	2608 [R(int) = 0.0380]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2608 / 0 / 137	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0778	
R indices (all data)	R1 = 0.0343, wR2 = 0.0790	
Absolute structure parameter	-0.07(7)	
Largest diff. peak and hole	0.248 and -0.176 $e.Å^{-3}$	

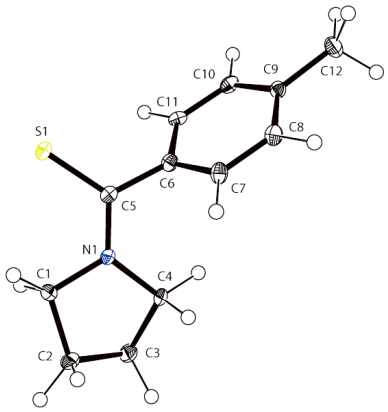
Figure S5. ORTEP Diagram of 2c showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 2d.

Empirical formula	C12 H15 N S	
Formula weight	205.31	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 14.5885(18) Å	α= 90°.
	b = 8.2099(10) Å	β= 90°.
	c = 18.071(2) Å	γ = 90°.
Volume	2164.3(5) $Å^3$	
Z	8	
Density (calculated)	1.260 Mg/m^3	
Absorption coefficient	0.258 mm^{-1}	
F(000)	880	
Crystal size	0.50 x 0.20 x 0.16 mm	
Theta range for data collection	2.25 to 28.29°.	
Index ranges	-19<=h<=15, -8<=k<=10, -23<=l<=23	
Reflections collected	12277	
Independent reflections	2618 [R(int) = 0.0585]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2618 / 0 / 128	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0992	
R indices (all data)	R1 = 0.0595, wR2 = 0.1138	
Largest diff. peak and hole	0.391 and -0.280 $e.Å^{-3}$	

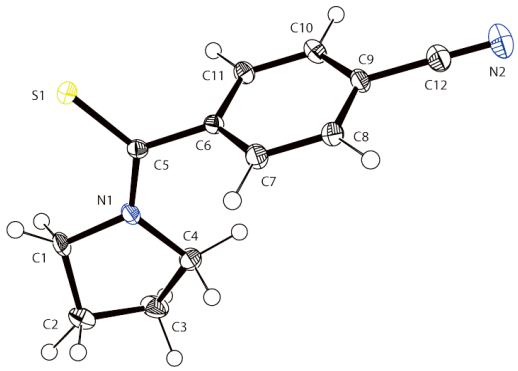
Figure S6. ORTEP Diagram of 2d showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 2g.

Empirical formula	C12 H15 N S	
Formula weight	205.31	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 14.5885(18) Å	α= 90°.
	b = 8.2099(10) Å	β= 90°.
	c = 18.071(2) Å	γ = 90°.
Volume	2164.3(5) $Å^3$	
Z	8	
Density (calculated)	1.260 Mg/m^3	
Absorption coefficient	0.258 mm^{-1}	
F(000)	880	
Crystal size	0.50 x 0.20 x 0.16 mm	
Theta range for data collection	2.25 to 28.29°.	
Index ranges	-19<=h<=15, -8<=k<=10, -23<=l<=23	
Reflections collected	12277	
Independent reflections	2618 [R(int) = 0.0585]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2618 / 0 / 128	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0992	
R indices (all data)	R1 = 0.0595, wR2 = 0.1138	
Largest diff. peak and hole	0.391 and -0.280 $e.Å^{-3}$	

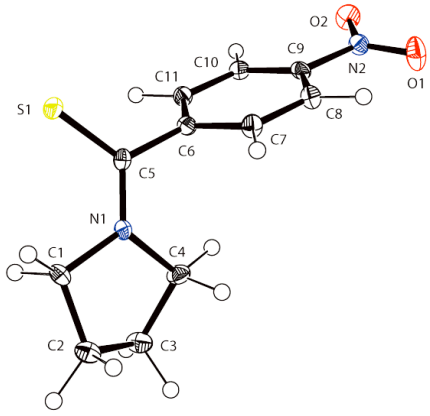
Figure S7. ORTEP Diagram of 2g showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 2h.

Empirical formula	C11 H12 N2 O2 S	
Formula weight	236.29	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 6.5884(8) Å	α= 90°.
	b = 22.658(3) Å	β= 108.060(2)°.
	c = 7.8877(10) Å	γ = 90°.
Volume	1119.5(2) $Å^3$	
Z	4	
Density (calculated)	1.402 Mg/m^3	
Absorption coefficient	0.275 mm^{-1}	
F(000)	496	
Crystal size	0.48 x 0.41 x 0.28 mm	
Theta range for data collection	1.80 to 28.30°.	
Index ranges	-8<=h<=8, -29<=k<=29, -4<=l<=10	
Reflections collected	6716	
Independent reflections	2640 [R(int) = 0.0404]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2640 / 0 / 145	
Goodness-of-fit on F^2	1.127	
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.1114	
R indices (all data)	R1 = 0.0438, wR2 = 0.1241	
Largest diff. peak and hole	0.389 and -0.395 $e.Å^{-3}$	

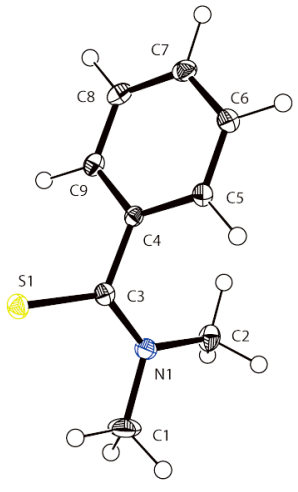
Figure S8. ORTEP Diagram of 2h showing the thermal ellipsoids at 30% probability.



Single-Crystal X-Ray Diffraction Data of 3a.

Empirical formula	C9 H11 N S	
Formula weight	165.25	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 5.8821(8) Å	α= 90°.
	b = 12.6936(17) Å	β= 99.402(2)°.
	c = 12.0076(16) Å	γ = 90°.
Volume	884.5(2) $Å^3$	
Z	4	
Density (calculated)	1.241 Mg/m^3	
Absorption coefficient	0.299 mm^{-1}	
F(000)	352	
Crystal size	0.30 x 0.30 x 0.20 mm	
Theta range for data collection	2.35 to 28.26°.	
Index ranges	-7<=h<=6, -16<=k<=13, -15<=l<=15	
Reflections collected	5316	
Independent reflections	2086 [R(int) = 0.0315]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2086 / 0 / 102	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0877	
R indices (all data)	R1 = 0.0436, wR2 = 0.0927	
Largest diff. peak and hole	0.311 and -0.262 $e.Å^{-3}$	

Figure S9. ORTEP Diagram of 3a showing the thermal ellipsoids at 30% probability.



3. Dynamic NMR.

Figure S10. Relationship between Rotational Barriers $\Delta G^{\ddagger}_{c}$ (kcal/mol) of Thioamides and Hammett's σ_p^+ Values of the Corresponding Substituents on the Benzene Ring.

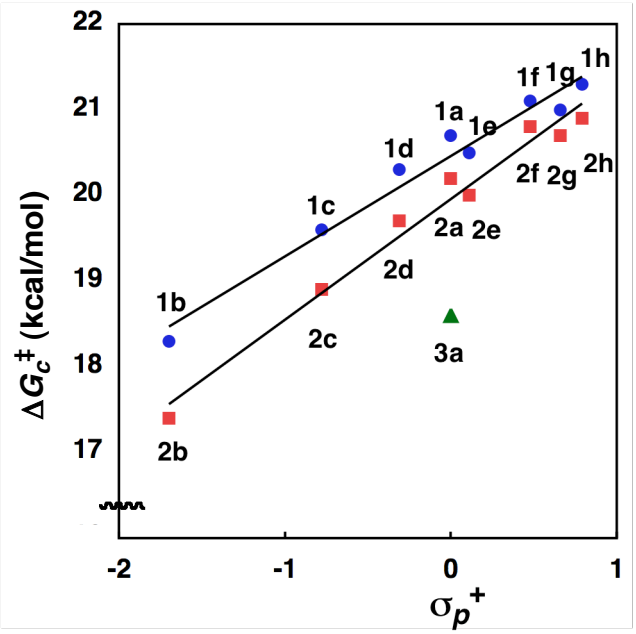
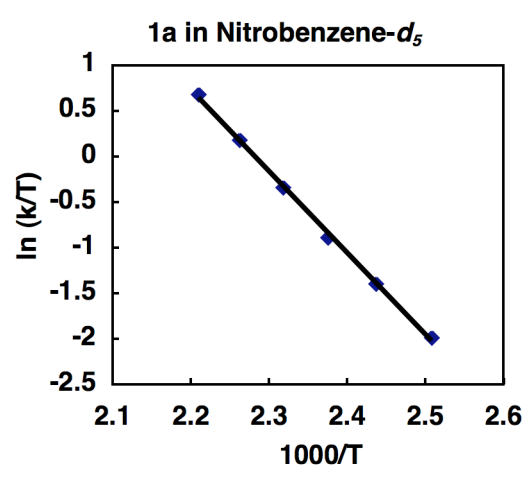
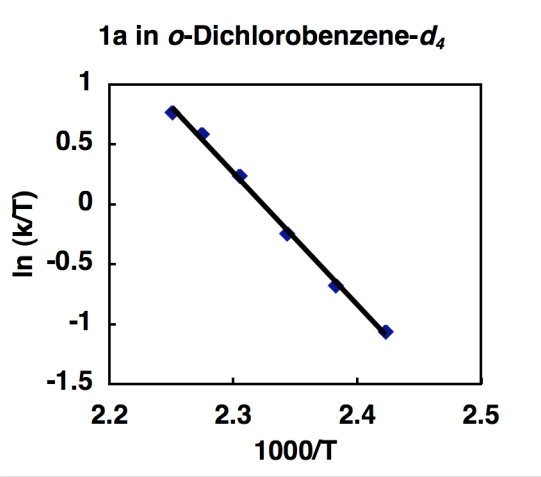


Figure S11. Eyring Plots of Representative Compounds.



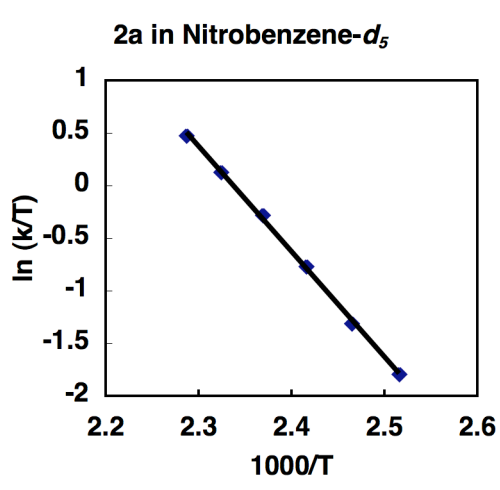
$y = -8.94x + 20.4$

$R^2=0.999$



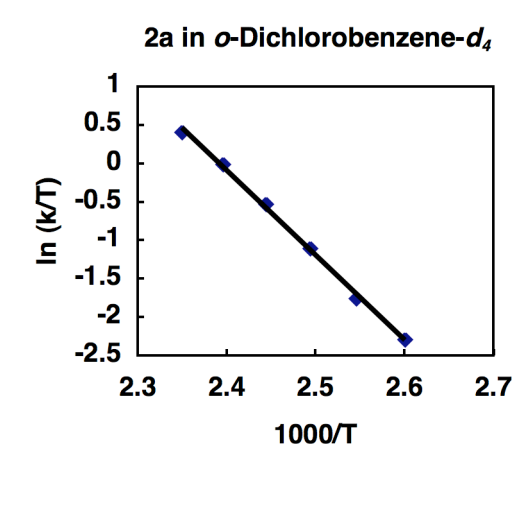
$y = -11.0x + 25.5$

$R^2 = 0.997$



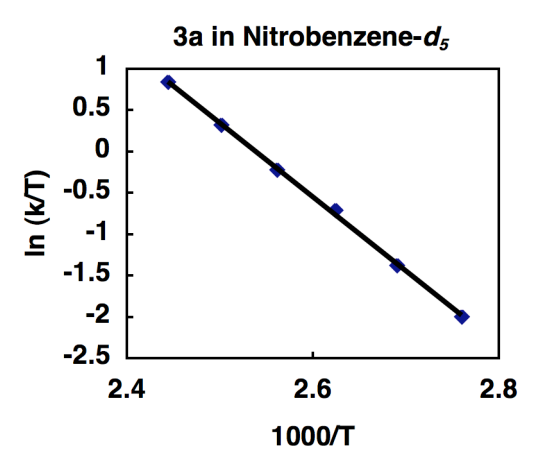
$y = -9.99x + 23.4$

$R^2 = 0.999$



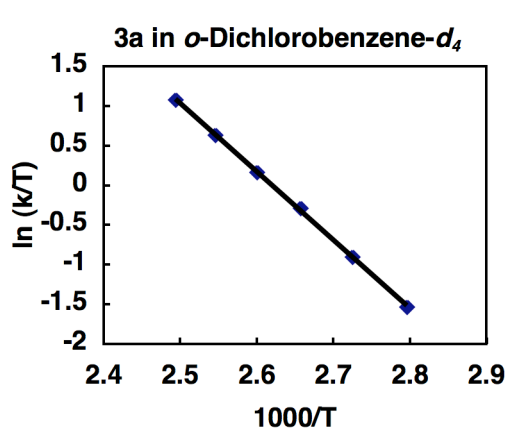
$y = -11.0x + 26.4$

$R^2 = 0.998$



y = -8.95x + 22.7

R^2= 0.999



y = -8.61x + 22.6

R^2= 1.000

4. Calculations

All conformations of each molecule were optimized in the Gaussian 03 program [26] at the B3LYP/6-31G(d) level of theory to find the global minimum and lowest-energy transition state. Ground and transition states were confirmed by the number of imaginary frequencies and, for transition states, by observing the related vibration motion of the imaginary frequency to ensure that it corresponds to C-N rotation. It was confirmed that the rate-determining step of the proton exchange is a rotation process around the thioamide bond, not an inversion process. Zero-point energy corrections were applied with the appropriate scaling. Single-point energies were obtained by B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6) // B3LYP/6-31G(d) level.

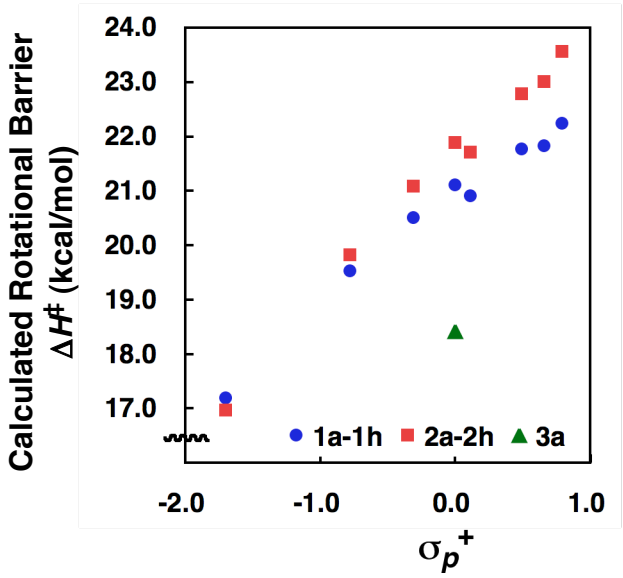
Table S1. Calculated Geometrical Parameters of the Ground States of Thioamides.

	N-C(S) bond	θ	α	|τ|
1a	1.350	352.9	158.1	13.2
1b	1.357	351.5	156.0	16.1
1c	1.353	352.4	157.2	15.0
1d	1.351	352.9	158.1	13.8
1e	1.349	353.3	158.8	13.4
1f	1.348	354.0	159.8	11.5
1g	1.347	354.1	160.1	12.1
1h	1.345	354.5	160.7	11.4
2a	1.348	359.1	171.5	7.3
2b	1.353	358.7	169.5	9.0
2c	1.351	358.9	170.3	8.3
2d	1.349	359.1	171.2	7.6
2e	1.348	359.1	171.3	7.4
2f	1.347	359.3	172.0	6.6
2g	1.346	359.2	172.0	6.7
2h	1.345	359.3	172.5	6.3
3a	1.357	358.6	169.0	13.0

Table S2. Calculated Rotational Barriers.

Compound	$\Delta H^{\ddagger}$(kcal/mol)
1a	21.11
1b	17.19
1c	19.53
1d	20.51
1e	20.91
1f	21.77
1g	21.82
1h	22.24
2a	21.88
2b	16.97
2c	19.83
2d	21.09
2e	21.71
2f	22.79
2g	23.01
2h	23.57
3a	18.42

Figure S12. Hammett Plot of Calculated Rotational Barriers.



4.1 The Details of Optimized Geometries

1a

Total Energy (a.u.) = -957.5335509 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.255296 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.176745	-1.954237	-0.434059
2	6	0	1.194283	-1.206678	0.491663
3	6	0	2.405590	0.461472	-0.365764
4	6	0	3.023018	-0.785939	-1.035950
5	1	0	2.778334	-2.680219	0.121403
6	1	0	1.637021	-2.496729	-1.216579
7	1	0	4.090815	-0.872605	-0.813413
8	1	0	2.909537	-0.735431	-2.122867
9	6	0	1.958950	-0.671409	1.730563
10	1	0	1.253920	-0.307232	2.484336
11	1	0	2.569980	-1.452239	2.195046
12	6	0	2.802838	0.498549	1.129722
13	1	0	2.519206	1.459258	1.568119
14	1	0	3.880402	0.365863	1.267798
15	1	0	0.267602	-1.730691	0.713615
16	1	0	2.525091	1.399825	-0.901967
17	7	0	0.985699	0.049626	-0.280804
18	6	0	-0.087460	0.869019	-0.300684
19	6	0	-1.416496	0.208115	-0.121698
20	6	0	-2.386813	0.784232	0.711691
21	6	0	-1.735072	-0.966678	-0.823097
22	6	0	-3.636361	0.186082	0.858271
23	1	0	-2.148604	1.704962	1.234012
24	6	0	-2.994320	-1.551535	-0.691276
25	1	0	-1.002989	-1.400914	-1.498071
26	6	0	-3.945709	-0.981683	0.156259
27	1	0	-4.373987	0.637350	1.516316
28	1	0	-3.233271	-2.448786	-1.256038
29	1	0	-4.925408	-1.439668	0.262798
30	16	0	0.012331	2.519626	-0.588920

1a-TS

Total Energy (a.u.) = -957.499076 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.254445 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554906	-2.576303	-0.781904
2	6	0	-1.554906	-1.064077	-1.105290
3	6	0	-1.554906	-1.064077	1.105290
4	6	0	-1.554906	-2.576303	0.781904
5	1	0	-2.426322	-3.083144	-1.209034
6	1	0	-0.656234	-3.057710	-1.178332
7	1	0	-2.426322	-3.083144	1.209034
8	1	0	-0.656234	-3.057710	1.178332
9	6	0	-2.958366	-0.491320	-0.777817
10	1	0	-3.071648	0.522345	-1.167973
11	1	0	-3.750720	-1.113342	-1.208580
12	6	0	-2.958366	-0.491320	0.777817
13	1	0	-3.071648	0.522345	1.167973
14	1	0	-3.750720	-1.113342	1.208580
15	1	0	-1.161561	-0.803200	-2.089960
16	1	0	-1.161561	-0.803200	2.089960
17	7	0	-0.663356	-0.597466	0.000000
18	6	0	-0.119549	0.721096	0.000000
19	6	0	1.366153	0.740999	0.000000
20	6	0	2.087623	1.954077	0.000000
21	6	0	2.095147	-0.465549	0.000000
22	6	0	3.476283	1.956650	0.000000
23	1	0	1.537678	2.888604	0.000000
24	6	0	3.488436	-0.459553	0.000000
25	1	0	1.544612	-1.397625	0.000000
26	6	0	4.184577	0.749483	0.000000
27	1	0	4.012352	2.901823	0.000000
28	1	0	4.030776	-1.401264	0.000000
29	1	0	5.271476	0.755150	0.000000
30	16	0	-1.017145	2.118928	0.000000

1b

Total Energy (a.u.) = -1091.5419321 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.328698 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.839599	-2.246738	-0.211545
2	6	0	1.996710	-1.248810	0.609394
3	6	0	3.488023	0.085786	-0.372683
4	6	0	3.878375	-1.309485	-0.908774
5	1	0	3.303929	-3.002351	0.429807
6	1	0	2.219132	-2.768357	-0.947152
7	1	0	4.914641	-1.560137	-0.661545
8	1	0	3.773939	-1.346301	-1.997232
9	6	0	2.833086	-0.735666	1.810662
10	1	0	2.197461	-0.174892	2.503144
11	1	0	3.287666	-1.561066	2.368707
12	6	0	3.879870	0.196510	1.120885
13	1	0	3.774842	1.231114	1.458154
14	1	0	4.914127	-0.117135	1.294877
15	1	0	0.991273	-1.578373	0.859872
16	1	0	3.777815	0.932301	-0.990558
17	7	0	2.017440	-0.059481	-0.287724
18	6	0	1.113277	0.948852	-0.370483
19	6	0	-0.310941	0.563037	-0.208290
20	6	0	-1.222965	1.421177	0.427295
21	6	0	-0.820529	-0.633611	-0.740816
22	6	0	-2.562807	1.091418	0.560102
23	1	0	-0.861340	2.366378	0.818746
24	6	0	-2.164134	-0.968880	-0.635738
25	1	0	-0.158895	-1.296703	-1.291173
26	6	0	-3.075074	-0.121847	0.038787
27	1	0	-3.218333	1.788520	1.067987
28	1	0	-2.506410	-1.887535	-1.096909
29	16	0	1.552747	2.536974	-0.714475
30	7	0	-4.409051	-0.462808	0.182777
31	6	0	-4.929784	-1.633337	-0.502607
32	1	0	-5.979028	-1.768098	-0.233153
33	1	0	-4.863551	-1.550744	-1.599076
34	1	0	-4.390769	-2.538432	-0.197808
35	6	0	-5.350418	0.519978	0.694523
36	1	0	-5.409766	1.419416	0.062360
37	1	0	-6.343954	0.070590	0.743717
38	1	0	-5.079168	0.835944	1.709184

1b-TS

Total Energy (a.u.) = -1091.5137782 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.32793 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.157745	-2.046523	0.781940
2	6	0	2.816661	-0.572463	1.103814
3	6	0	2.816675	-0.572431	-1.103819
4	6	0	3.157756	-2.046500	-0.781982
5	1	0	4.121259	-2.343894	1.208913
6	1	0	2.390339	-2.718040	1.178440
7	1	0	4.121274	-2.343860	-1.208952
8	1	0	2.390355	-2.718006	-1.178512
9	6	0	4.059233	0.298464	0.778023
10	1	0	3.941256	1.312046	1.166366
11	1	0	4.970490	-0.131607	1.208637
12	6	0	4.059244	0.298487	-0.777987
13	1	0	3.941271	1.312079	-1.166302
14	1	0	4.970505	-0.131572	-1.208601
15	1	0	2.375286	-0.405846	2.088704
16	1	0	2.375314	-0.405785	-2.088710
17	7	0	1.846226	-0.317296	-0.000006
18	6	0	1.013849	0.847323	0.000007
19	6	0	-0.417390	0.530767	-0.000006
20	6	0	-1.411273	1.537535	0.000003
21	6	0	-0.873514	-0.806397	-0.000028
22	6	0	-2.758062	1.237403	-0.000009
23	1	0	-1.095494	2.575373	0.000020
24	6	0	-2.220295	-1.125007	-0.000040
25	1	0	-0.133142	-1.596672	-0.000036
26	6	0	-3.209844	-0.110336	-0.000031
27	1	0	-3.472636	2.051851	0.000000
28	1	0	-2.508215	-2.169614	-0.000057
29	16	0	1.584686	2.417691	0.000027
30	7	0	-4.550371	-0.414266	-0.000043
31	6	0	-4.984044	-1.802653	0.000106
32	1	0	-6.074350	-1.837949	0.000071
33	1	0	-4.626296	-2.340077	-0.888695
34	1	0	-4.626291	-2.339898	0.889013
35	6	0	-5.544965	0.647592	-0.000033

36	1	0	-5.457729	1.286866	-0.888972
37	1	0	-6.541790	0.204268	-0.000264
38	1	0	-5.458021	1.286635	0.889108

1c

Total Energy (a.u.) = -1072.0933513 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.288036 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.676939	-2.122766	-0.384945
2	6	0	1.745244	-1.268720	0.500420
3	6	0	3.176494	0.250015	-0.289309
4	6	0	3.675337	-1.057699	-0.942997
5	1	0	3.167281	-2.912076	0.193217
6	1	0	2.114476	-2.601424	-1.192755
7	1	0	4.716204	-1.267043	-0.678011
8	1	0	3.613083	-0.991536	-2.033252
9	6	0	2.509272	-0.827620	1.776714
10	1	0	1.817854	-0.382511	2.498992
11	1	0	3.002428	-1.674769	2.264502
12	6	0	3.511230	0.235383	1.221924
13	1	0	3.325273	1.221665	1.655579
14	1	0	4.558407	-0.025705	1.404270
15	1	0	0.756348	-1.684788	0.678210
16	1	0	3.427600	1.170456	-0.810877
17	7	0	1.716733	0.005164	-0.271628
18	6	0	0.747960	0.949173	-0.314263
19	6	0	-0.652810	0.449038	-0.231129
20	6	0	-1.621254	1.156697	0.491713
21	6	0	-1.058365	-0.711153	-0.919590
22	6	0	-2.942808	0.719394	0.558337
23	1	0	-1.327718	2.065800	1.006072
24	6	0	-2.374709	-1.146532	-0.879169
25	1	0	-0.336917	-1.254312	-1.522976
26	6	0	-3.327924	-0.437989	-0.131638
27	1	0	-3.659831	1.287302	1.139835
28	1	0	-2.694700	-2.027085	-1.427374
29	16	0	1.070913	2.585021	-0.528415
30	8	0	-4.589850	-0.949723	-0.146409

31	6	0	-5.607242	-0.259610	0.564685
32	1	0	-5.389927	-0.217313	1.639951
33	1	0	-5.744040	0.760341	0.183015
34	1	0	-6.522924	-0.831375	0.404383

1c-TS

Total Energy (a.u.) = -1072.0615601 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.287356 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.002485	-1.927576	0.781837
2	6	0	2.546619	-0.485402	1.104543
3	6	0	2.546619	-0.485399	-1.104543
4	6	0	3.002485	-1.927575	-0.781838
5	1	0	3.986387	-2.146984	1.209064
6	1	0	2.290828	-2.657663	1.178320
7	1	0	3.986386	-2.146982	-1.209069
8	1	0	2.290826	-2.657661	-1.178322
9	6	0	3.715173	0.481932	0.778005
10	1	0	3.518304	1.482922	1.167425
11	1	0	4.657581	0.125543	1.208558
12	6	0	3.715173	0.481934	-0.778002
13	1	0	3.518302	1.482925	-1.167421
14	1	0	4.657581	0.125546	-1.208555
15	1	0	2.093242	-0.355020	2.089412
16	1	0	2.093243	-0.355018	-2.089413
17	7	0	1.557601	-0.307310	0.000000
18	6	0	0.641318	0.788396	0.000000
19	6	0	-0.770298	0.359057	0.000000
20	6	0	-1.830144	1.289216	0.000000
21	6	0	-1.111822	-1.013940	0.000000
22	6	0	-3.157899	0.886156	0.000000
23	1	0	-1.591997	2.347375	0.000001
24	6	0	-2.431758	-1.429953	0.000000
25	1	0	-0.309871	-1.741038	-0.000001
26	6	0	-3.469799	-0.484484	0.000000
27	1	0	-3.941012	1.635621	0.000001
28	1	0	-2.691615	-2.483922	-0.000001
29	16	0	1.082402	2.394822	0.000000

30	8	0	-4.729270	-0.988177	0.000000
31	6	0	-5.827225	-0.084052	0.000000
32	1	0	-5.823865	0.550104	0.895262
33	1	0	-5.823865	0.550106	-0.895260
34	1	0	-6.723489	-0.706279	0.000000

1d

Total Energy (a.u.) = -996.8615915 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.282683 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.322524	-2.108036	-0.444628
2	6	0	1.417986	-1.267620	0.481587
3	6	0	2.813681	0.266250	-0.344450
4	6	0	3.294585	-1.032410	-1.028695
5	1	0	2.837956	-2.899441	0.108293
6	1	0	1.734038	-2.582758	-1.235990
7	1	0	4.345594	-1.238836	-0.804530
8	1	0	3.191552	-0.955831	-2.115160
9	6	0	2.224067	-0.834231	1.734015
10	1	0	1.556775	-0.398649	2.484189
11	1	0	2.737760	-1.683221	2.196540
12	6	0	3.201412	0.238333	1.153859
13	1	0	3.027886	1.219428	1.604306
14	1	0	4.255430	-0.019874	1.296165
15	1	0	0.437581	-1.690090	0.688655
16	1	0	3.040775	1.193018	-0.865720
17	7	0	1.356683	0.013346	-0.275893
18	6	0	0.380211	0.946830	-0.294258
19	6	0	-1.015189	0.435624	-0.149983
20	6	0	-1.944656	1.116453	0.651178
21	6	0	-1.446229	-0.702599	-0.849007
22	6	0	-3.251952	0.656102	0.765587
23	1	0	-1.626895	2.009433	1.179378
24	6	0	-2.764323	-1.144893	-0.745844
25	1	0	-0.752630	-1.225136	-1.501800
26	6	0	-3.689772	-0.478633	0.065924
27	1	0	-3.950414	1.191293	1.405185
28	1	0	-3.079725	-2.019183	-1.310953

29	16	0	0.671516	2.581952	-0.545346
30	6	0	-5.122982	-0.944333	0.164910
31	1	0	-5.490515	-0.894811	1.196188
32	1	0	-5.786696	-0.315740	-0.443468
33	1	0	-5.235689	-1.975275	-0.185654

1d-TS

Total Energy (a.u.) = -996.8281637 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.281927 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.621314	-1.941851	-0.781783
2	6	0	-2.177304	-0.496124	-1.104816
3	6	0	-2.177301	-0.496126	1.104815
4	6	0	-2.621311	-1.941851	0.781783
5	1	0	-3.603347	-2.169035	-1.209137
6	1	0	-1.903705	-2.666018	-1.178284
7	1	0	-3.603341	-2.169037	1.209142
8	1	0	-1.903699	-2.666018	1.178280
9	6	0	-3.353136	0.462083	-0.778008
10	1	0	-3.164852	1.464653	-1.167780
11	1	0	-4.292675	0.098337	-1.208512
12	6	0	-3.353134	0.462082	0.778011
13	1	0	-3.164849	1.464651	1.167784
14	1	0	-4.292672	0.098335	1.208517
15	1	0	-1.724852	-0.362289	-2.089627
16	1	0	-1.724845	-0.362290	2.089625
17	7	0	-1.189397	-0.309996	-0.000001
18	6	0	-0.282885	0.791854	-0.000001
19	6	0	1.138918	0.374349	0.000000
20	6	0	2.191332	1.316725	0.000000
21	6	0	1.485711	-0.990724	0.000000
22	6	0	3.515002	0.907859	0.000000
23	1	0	1.946251	2.373170	0.000000
24	6	0	2.818973	-1.392711	0.000000
25	1	0	0.689276	-1.724022	0.000000
26	6	0	3.858554	-0.456542	0.000000
27	1	0	4.304477	1.656291	0.000000
28	1	0	3.056126	-2.454110	0.000000

29	16	0	-0.732551	2.392541	0.000000
30	6	0	5.304860	-0.885319	0.000000
31	1	0	5.833014	-0.500115	-0.881252
32	1	0	5.832989	-0.500193	0.881303
33	1	0	5.401513	-1.975225	-0.000046

1e

Total Energy (a.u.) = -1417.15689 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.245515 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.537820	-2.168069	-0.467563
2	6	0	1.671429	-1.297743	0.467333
3	6	0	3.156257	0.174400	-0.317863
4	6	0	3.572726	-1.135947	-1.022253
5	1	0	3.003741	-2.996689	0.074379
6	1	0	1.932499	-2.595135	-1.273277
7	1	0	4.608568	-1.403113	-0.792202
8	1	0	3.485300	-1.034012	-2.107938
9	6	0	2.487965	-0.931941	1.734414
10	1	0	1.838545	-0.476522	2.488429
11	1	0	2.951508	-1.816198	2.183197
12	6	0	3.526108	0.098171	1.183129
13	1	0	3.400463	1.078320	1.651315
14	1	0	4.563412	-0.217961	1.329923
15	1	0	0.667555	-1.670314	0.658064
16	1	0	3.437465	1.096954	-0.819983
17	7	0	1.687023	-0.001021	-0.265689
18	6	0	0.761285	0.980469	-0.289138
19	6	0	-0.661416	0.539173	-0.163269
20	6	0	-1.557796	1.256054	0.642864
21	6	0	-1.142899	-0.561848	-0.889642
22	6	0	-2.891479	0.871217	0.746739
23	1	0	-1.198891	2.124605	1.184791
24	6	0	-2.480687	-0.945195	-0.811389
25	1	0	-0.471895	-1.105299	-1.548260
26	6	0	-3.343392	-0.228666	0.016428
27	1	0	-3.577478	1.421390	1.381806
28	1	0	-2.851567	-1.784674	-1.389768

29	16	0	1.129199	2.600568	-0.526992
30	17	0	-5.028299	-0.713160	0.134852

1e-TS

Total Energy (a.u.) = -1417.1228322 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.24477 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.871513	-2.010549	0.781732
2	6	0	2.492134	-0.546906	1.105617
3	6	0	2.492137	-0.546904	-1.105618
4	6	0	2.871515	-2.010548	-0.781732
5	1	0	3.842467	-2.280513	1.209151
6	1	0	2.123189	-2.702705	1.178611
7	1	0	3.842471	-2.280511	-1.209149
8	1	0	2.123193	-2.702705	-1.178615
9	6	0	3.707588	0.359284	0.778021
10	1	0	3.564594	1.369112	1.168340
11	1	0	4.630154	-0.045250	1.208340
12	6	0	3.707590	0.359285	-0.778019
13	1	0	3.564597	1.369113	-1.168338
14	1	0	4.630157	-0.045249	-1.208337
15	1	0	2.046010	-0.393350	2.090403
16	1	0	2.046013	-0.393349	-2.090404
17	7	0	1.511964	-0.317254	0.000000
18	6	0	0.658353	0.823951	0.000000
19	6	0	-0.783922	0.469492	0.000000
20	6	0	-1.790286	1.458429	0.000000
21	6	0	-1.186167	-0.880927	0.000000
22	6	0	-3.135319	1.118309	0.000000
23	1	0	-1.498610	2.502848	0.000000
24	6	0	-2.531911	-1.236088	0.000000
25	1	0	-0.420011	-1.645593	0.000000
26	6	0	-3.498603	-0.232065	0.000000
27	1	0	-3.901172	1.886479	0.000000
28	1	0	-2.830196	-2.279108	0.000000
29	16	0	1.172858	2.402763	0.000000
30	17	0	-5.197650	-0.666543	0.000000

1f

Total Energy (a.u.) = -1185.4844494 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.298366 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.914146	-2.342634	-0.311252
2	6	0	2.142161	-1.325145	0.555399
3	6	0	3.779928	-0.074070	-0.307847
4	6	0	4.058387	-1.466199	-0.917119
5	1	0	3.284287	-3.179803	0.288337
6	1	0	2.270696	-2.752422	-1.096000
7	1	0	5.057723	-1.825776	-0.653774
8	1	0	3.991514	-1.429243	-2.008390
9	6	0	2.988544	-0.966966	1.804400
10	1	0	2.387883	-0.400597	2.522821
11	1	0	3.356538	-1.864702	2.311251
12	6	0	4.130170	-0.086450	1.199872
13	1	0	4.101379	0.930804	1.600146
14	1	0	5.129179	-0.494730	1.381150
15	1	0	1.103010	-1.574655	0.757597
16	1	0	4.160174	0.777115	-0.867523
17	7	0	2.300270	-0.089351	-0.259709
18	6	0	1.480418	0.973322	-0.378976
19	6	0	0.020525	0.695831	-0.205868
20	6	0	-0.769851	1.534020	0.595759
21	6	0	-0.591071	-0.374742	-0.879934
22	6	0	-2.129999	1.290453	0.740746
23	1	0	-0.303974	2.376813	1.095214
24	6	0	-1.957639	-0.607218	-0.752564
25	1	0	0.005709	-1.008438	-1.529461
26	6	0	-2.735506	0.219430	0.068432
27	1	0	-2.746107	1.925138	1.368920
28	1	0	-2.425109	-1.425130	-1.289151
29	16	0	2.001770	2.517412	-0.776428
30	6	0	-4.198868	0.012702	0.258891
31	8	0	-4.905409	0.706149	0.964057
32	8	0	-4.667843	-1.045834	-0.442547
33	6	0	-6.074361	-1.296644	-0.301452
34	1	0	-6.654370	-0.436701	-0.646848

35	1	0	-6.278638	-2.171101	-0.920063
36	1	0	-6.325985	-1.496360	0.743571

1f-TS

Total Energy (a.u.) = -1185.4487746 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.297357 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.294859	-2.179489	-0.781829
2	6	0	-3.063706	-0.685443	-1.105907
3	6	0	-3.063706	-0.685443	1.105907
4	6	0	-3.294859	-2.179490	0.781829
5	1	0	-4.233914	-2.545756	-1.209003
6	1	0	-2.480818	-2.792899	-1.178706
7	1	0	-4.233912	-2.545757	1.209005
8	1	0	-2.480817	-2.792898	1.178704
9	6	0	-4.362295	0.095954	-0.777829
10	1	0	-4.318965	1.115129	-1.167674
11	1	0	-5.240776	-0.396711	-1.208642
12	6	0	-4.362295	0.095954	0.777829
13	1	0	-4.318966	1.115128	1.167675
14	1	0	-5.240776	-0.396713	1.208640
15	1	0	-2.635212	-0.487795	-2.090639
16	1	0	-2.635212	-0.487795	2.090639
17	7	0	-2.110172	-0.360164	0.000000
18	6	0	-1.373973	0.859513	0.000000
19	6	0	0.100717	0.653147	0.000000
20	6	0	0.999875	1.741281	0.000000
21	6	0	0.635468	-0.650838	0.000000
22	6	0	2.369497	1.531340	0.000000
23	1	0	0.602518	2.749909	0.000000
24	6	0	2.010538	-0.863014	0.000000
25	1	0	-0.051214	-1.487456	0.000000
26	6	0	2.888926	0.227112	0.000000
27	1	0	3.061778	2.366622	0.000000
28	1	0	2.406552	-1.872315	0.000000
29	16	0	-2.041787	2.378707	0.000000
30	6	0	4.372010	0.065878	0.000000
31	8	0	5.162151	0.989270	0.000000

32	8	0	4.750907	-1.232186	0.000000
33	6	0	6.169649	-1.454848	0.000000
34	1	0	6.627081	-1.013634	0.889528
35	1	0	6.294986	-2.537952	0.000000
36	1	0	6.627081	-1.013634	-0.889528

1g

Total Energy (a.u.) = -1049.805028 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.253642 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.422120	-2.152990	-0.504047
2	6	0	1.550519	-1.309737	0.451182
3	6	0	3.033840	0.187287	-0.293619
4	6	0	3.456330	-1.104386	-1.028414
5	1	0	2.888164	-2.994367	0.017489
6	1	0	1.820265	-2.560160	-1.322476
7	1	0	4.491720	-1.374105	-0.799939
8	1	0	3.373903	-0.975965	-2.111598
9	6	0	2.363098	-0.973225	1.728641
10	1	0	1.711037	-0.540890	2.493827
11	1	0	2.829737	-1.867107	2.154165
12	6	0	3.398061	0.075317	1.206292
13	1	0	3.266612	1.042646	1.699084
14	1	0	4.436368	-0.239094	1.348768
15	1	0	0.547047	-1.690131	0.629175
16	1	0	3.312363	1.122721	-0.772850
17	7	0	1.564869	0.005123	-0.248554
18	6	0	0.632598	0.976315	-0.279400
19	6	0	-0.788983	0.524536	-0.155469
20	6	0	-1.677180	1.207945	0.689148
21	6	0	-1.270179	-0.549844	-0.922417
22	6	0	-3.005453	0.813813	0.788704
23	1	0	-1.313179	2.055865	1.259149
24	6	0	-2.603169	-0.938889	-0.845398
25	1	0	-0.600055	-1.063661	-1.604816
26	6	0	-3.478974	-0.264158	0.020195
27	1	0	-3.684687	1.337786	1.453194
28	1	0	-2.973007	-1.758700	-1.452713

29	16	0	0.973463	2.599381	-0.528280
30	6	0	-4.850147	-0.671532	0.115909
31	7	0	-5.961523	-1.006214	0.196293

1g-TS

Total Energy (a.u.) = -1049.7695006 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.25288 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.752859	-2.008695	-0.781659
2	6	0	-2.366244	-0.547358	-1.106328
3	6	0	-2.366241	-0.547360	1.106327
4	6	0	-2.752857	-2.008697	0.781656
5	1	0	-3.725094	-2.273208	-1.209226
6	1	0	-2.008434	-2.704874	-1.178634
7	1	0	-3.725091	-2.273210	1.209229
8	1	0	-2.008429	-2.704876	1.178627
9	6	0	-3.575439	0.366206	-0.778008
10	1	0	-3.427644	1.375171	-1.169026
11	1	0	-4.500297	-0.032802	-1.208214
12	6	0	-3.575436	0.366204	0.778012
13	1	0	-3.427641	1.375168	1.169032
14	1	0	-4.500294	-0.032805	1.208218
15	1	0	-1.919272	-0.396513	-2.091120
16	1	0	-1.919267	-0.396518	2.091119
17	7	0	-1.383644	-0.322467	0.000000
18	6	0	-0.527202	0.813379	0.000000
19	6	0	0.919452	0.452180	0.000000
20	6	0	1.928042	1.438520	0.000000
21	6	0	1.311040	-0.901151	0.000000
22	6	0	3.269214	1.090296	0.000000
23	1	0	1.639508	2.483509	0.000000
24	6	0	2.653583	-1.260750	0.000000
25	1	0	0.538760	-1.659267	0.000000
26	6	0	3.644134	-0.266667	0.000000
27	1	0	4.035956	1.858111	0.000000
28	1	0	2.942287	-2.306882	0.000000
29	16	0	-1.027187	2.394148	0.000000
30	6	0	5.030440	-0.630899	0.000000

31	7	0	6.155382	-0.927336	0.000000

1h

Total Energy (a.u.) = -1162.1019424 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.257757 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.719899	-2.202130	-0.381014
2	6	0	1.864969	-1.287655	0.522208
3	6	0	3.401969	0.125853	-0.276736
4	6	0	3.789796	-1.211526	-0.945882
5	1	0	3.155903	-3.029382	0.186891
6	1	0	2.113924	-2.632128	-1.184463
7	1	0	4.814905	-1.501474	-0.696794
8	1	0	3.718251	-1.132079	-2.034509
9	6	0	2.673802	-0.914719	1.791502
10	1	0	2.027841	-0.424214	2.526194
11	1	0	3.106256	-1.800892	2.266334
12	6	0	3.748041	0.073203	1.231089
13	1	0	3.645344	1.066470	1.676882
14	1	0	4.773682	-0.268928	1.398763
15	1	0	0.848068	-1.627910	0.705592
16	1	0	3.713827	1.028748	-0.796221
17	7	0	1.927714	-0.008977	-0.238481
18	6	0	1.024469	0.982889	-0.338351
19	6	0	-0.410929	0.579445	-0.200210
20	6	0	-1.276083	1.316072	0.624369
21	6	0	-0.922700	-0.504134	-0.935092
22	6	0	-2.616756	0.966597	0.736479
23	1	0	-0.886180	2.169218	1.168606
24	6	0	-2.267003	-0.852031	-0.847662
25	1	0	-0.267403	-1.058904	-1.599343
26	6	0	-3.094026	-0.115016	-0.003251
27	1	0	-3.294631	1.516331	1.377572
28	1	0	-2.680749	-1.674298	-1.418222
29	16	0	1.406452	2.578121	-0.684965
30	7	0	-4.512501	-0.487858	0.107790
31	8	0	-5.221826	0.180317	0.859417
32	8	0	-4.904605	-1.448286	-0.555381

1h-TS

Total Energy (a.u.) = -1162.065662 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.256896 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.080034	-2.033202	0.781622
2	6	0	2.727393	-0.563478	1.106676
3	6	0	2.727394	-0.563477	-1.106676
4	6	0	3.080035	-2.033202	-0.781623
5	1	0	4.045978	-2.320000	1.209121
6	1	0	2.319924	-2.712084	1.178792
7	1	0	4.045983	-2.319996	-1.209116
8	1	0	2.319930	-2.712085	-1.178799
9	6	0	3.956358	0.322651	0.778004
10	1	0	3.831321	1.334780	1.168893
11	1	0	4.872013	-0.096735	1.208427
12	6	0	3.956359	0.322654	-0.778004
13	1	0	3.831320	1.334782	-1.168889
14	1	0	4.872013	-0.096731	-1.208430
15	1	0	2.283796	-0.402591	2.091425
16	1	0	2.283797	-0.402590	-2.091425
17	7	0	1.749214	-0.316193	0.000000
18	6	0	0.920257	0.839151	0.000000
19	6	0	-0.536846	0.512182	0.000000
20	6	0	-0.958010	-0.832584	0.000000
21	6	0	-1.520965	1.523452	0.000000
22	6	0	-2.309388	-1.162976	0.000000
23	1	0	-0.203143	-1.607785	0.000000
24	6	0	-2.871599	1.208145	0.000000
25	1	0	-1.208112	2.561214	0.000000
26	6	0	-3.248431	-0.135916	0.000000
27	1	0	-2.642410	-2.193521	0.000000
28	1	0	-3.633698	1.977478	0.000000
29	16	0	1.454761	2.407878	0.000000
30	7	0	-4.681600	-0.476797	0.000000
31	8	0	-4.984496	-1.669492	0.000000
32	8	0	-5.488472	0.452035	0.000000

2a

Total Energy (a.u.) = -880.1100266 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.2193 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.263284	0.808099	-0.116512
2	6	0	-1.097735	0.190065	-0.051943
3	6	0	-2.017567	0.613557	0.918885
4	6	0	-1.497115	-0.773302	-0.991598
5	6	0	-3.297682	0.065281	0.964271
6	1	0	-1.718915	1.379714	1.627070
7	6	0	-2.786923	-1.303301	-0.958464
8	1	0	-0.806152	-1.083696	-1.770423
9	6	0	-3.687829	-0.892752	0.025176
10	1	0	-3.996237	0.394495	1.728784
11	1	0	-3.088102	-2.033706	-1.704730
12	1	0	-4.690745	-1.310012	0.054980
13	16	0	0.429625	2.474593	-0.228313
14	6	0	2.705162	0.462725	-0.208260
15	6	0	1.286985	-1.468970	0.247610
16	6	0	3.564820	-0.804064	-0.103018
17	1	0	2.895880	1.169082	0.609178
18	1	0	2.834975	1.016503	-1.142509
19	6	0	2.706183	-1.741998	0.759561
20	1	0	1.071815	-2.076917	-0.640356
21	1	0	0.505711	-1.664412	0.984972
22	1	0	3.722761	-1.242990	-1.095719
23	1	0	4.547849	-0.597817	0.329695
24	1	0	2.982618	-2.796577	0.667422
25	1	0	2.783401	-1.462588	1.817101
26	7	0	1.318807	-0.030945	-0.103815

2a-TS

Total Energy (a.u.) = -880.0742642 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.218391 (B3LYP/6-31G(d))

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.150330	0.734873	-0.000004
2	6	0	1.196023	0.125359	0.000000
3	6	0	2.365021	0.915426	0.000000
4	6	0	1.334163	-1.277612	0.000003
5	6	0	3.620644	0.322446	0.000002
6	1	0	2.265123	1.995476	-0.000004
7	6	0	2.595678	-1.868397	0.000007
8	1	0	0.434140	-1.880500	0.000004
9	6	0	3.741910	-1.072301	0.000006
10	1	0	4.510859	0.945417	0.000002
11	1	0	2.684022	-2.951462	0.000009
12	1	0	4.726477	-1.532747	0.000009
13	16	0	-0.421736	2.369532	-0.000008
14	6	0	-2.129463	-0.153754	1.168458
15	6	0	-2.129457	-0.153779	-1.168457
16	6	0	-3.263808	-1.118622	0.777937
17	1	0	-2.513077	0.868142	1.317598
18	1	0	-1.592474	-0.453268	2.074366
19	6	0	-3.263777	-1.118668	-0.777931
20	1	0	-1.592459	-0.453289	-2.074362
21	1	0	-2.513093	0.868108	-1.317609
22	1	0	-3.064722	-2.124022	1.161069
23	1	0	-4.219503	-0.791088	1.198528
24	1	0	-3.064626	-2.124081	-1.160993
25	1	0	-4.219470	-0.791204	-1.198584
26	7	0	-1.227579	-0.213973	-0.000003

2b

Total Energy (a.u.) = -1014.117915 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.292967 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495958	0.830383	-0.195874
2	6	0	0.058311	0.463205	-0.089530
3	6	0	-0.817693	1.228394	0.696858
4	6	0	-0.499764	-0.590948	-0.829949
5	6	0	-2.171115	0.936334	0.774995

6	1	0	-0.419437	2.072898	1.249955
7	6	0	-1.858417	-0.879141	-0.784690
8	1	0	0.130016	-1.173399	-1.496385
9	6	0	-2.733903	-0.134230	0.038860
10	1	0	-2.796993	1.555974	1.405769
11	1	0	-2.238049	-1.681147	-1.406128
12	16	0	1.955942	2.430682	-0.445115
13	6	0	3.850261	0.084469	-0.251995
14	6	0	2.154520	-1.527687	0.424834
15	6	0	4.501872	-1.278433	0.016856
16	1	0	4.156752	0.844493	0.477105
17	1	0	4.061583	0.494135	-1.244060
18	6	0	3.517390	-1.949727	0.986267
19	1	0	1.846182	-2.208721	-0.378810
20	1	0	1.355256	-1.504489	1.168519
21	1	0	4.573763	-1.860075	-0.910530
22	1	0	5.511513	-1.177132	0.425333
23	1	0	3.624803	-3.037595	1.037108
24	1	0	3.647830	-1.548264	1.998409
25	7	0	2.404112	-0.168891	-0.106334
26	7	0	-4.083794	-0.438675	0.122518
27	6	0	-4.654497	-1.413621	-0.791326
28	1	0	-5.712906	-1.544985	-0.558250
29	1	0	-4.568748	-1.111274	-1.847316
30	1	0	-4.167750	-2.389738	-0.677808
31	6	0	-4.983227	0.478624	0.803125
32	1	0	-5.994793	0.068807	0.780038
33	1	0	-4.699733	0.599371	1.855427
34	1	0	-5.004756	1.477442	0.339584

2b-TS

Total Energy (a.u.) = -1014.0897761 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.291844 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.405284	0.829293	-0.000003
2	6	0	0.017759	0.509011	-0.000002
3	6	0	1.015984	1.510819	0.000001
4	6	0	0.460836	-0.832525	-0.000005

5	6	0	2.360286	1.200669	0.000003
6	1	0	0.704861	2.550360	0.000003
7	6	0	1.805039	-1.160235	-0.000004
8	1	0	-0.288912	-1.614925	-0.000008
9	6	0	2.801294	-0.151221	0.000000
10	1	0	3.081627	2.009068	0.000005
11	1	0	2.086687	-2.206482	-0.000006
12	16	0	-2.017775	2.379459	0.000000
13	6	0	-3.166261	-0.442493	1.166791
14	6	0	-3.166266	-0.442496	-1.166789
15	6	0	-4.087175	-1.613818	0.778123
16	1	0	-3.745444	0.482691	1.316369
17	1	0	-2.580970	-0.628448	2.073508
18	6	0	-4.087189	-1.613812	-0.778112
19	1	0	-2.580979	-0.628461	-2.073507
20	1	0	-3.745443	0.482693	-1.316372
21	1	0	-3.692531	-2.560224	1.160683
22	1	0	-5.089186	-1.483051	1.198585
23	1	0	-3.692568	-2.560222	-1.160687
24	1	0	-5.089206	-1.483026	-1.198552
25	7	0	-2.270743	-0.322558	-0.000007
26	6	0	5.141766	0.589978	0.000005
27	1	0	6.135252	0.139336	-0.000077
28	1	0	5.059269	1.229645	-0.889047
29	1	0	5.059370	1.229556	0.889132
30	7	0	4.139310	-0.464686	0.000001
31	6	0	4.563417	-1.856234	-0.000002
32	1	0	4.201986	-2.390898	-0.888907
33	1	0	5.653417	-1.898959	0.000000
34	1	0	4.201970	-2.390910	0.888891

2c

Total Energy (a.u.) = -994.669612 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.252227 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.125362	0.841423	0.130921
2	6	0	0.294178	0.382181	0.133187
3	6	0	1.226544	0.965452	-0.733427

4	6	0	0.754999	-0.585353	1.045567
5	6	0	2.567234	0.583608	-0.723688
6	1	0	0.892301	1.735574	-1.420941
7	6	0	2.091430	-0.957204	1.083254
8	1	0	0.065484	-1.024841	1.760455
9	6	0	3.008200	-0.381946	0.190810
10	1	0	3.255102	1.049871	-1.419691
11	1	0	2.453126	-1.686304	1.801489
12	16	0	-1.491004	2.480624	0.202629
13	6	0	-3.518046	0.230136	0.134411
14	6	0	-1.883704	-1.532790	-0.268769
15	6	0	-4.230658	-1.121098	-0.008735
16	1	0	-3.749272	0.914268	-0.691305
17	1	0	-3.747680	0.763253	1.061535
18	6	0	-3.242575	-1.950755	-0.842795
19	1	0	-1.644284	-2.127494	0.621889
20	1	0	-1.054820	-1.634833	-0.972304
21	1	0	-4.376488	-1.584242	0.974851
22	1	0	-5.213545	-1.018832	-0.477512
23	1	0	-3.406888	-3.030147	-0.771142
24	1	0	-3.306711	-1.667301	-1.900170
25	7	0	-2.083147	-0.110516	0.091018
26	8	0	4.293537	-0.822049	0.296947
27	6	0	5.273509	-0.252788	-0.558714
28	1	0	6.215570	-0.738069	-0.297592
29	1	0	5.047209	-0.445551	-1.615585
30	1	0	5.366191	0.829474	-0.400872

2c-TS

Total Energy (a.u.) = -994.6370854 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.251278 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.017499	0.794067	0.000000
2	6	0	0.380681	0.347735	0.000000
3	6	0	1.453183	1.262687	0.000004
4	6	0	0.695734	-1.031522	-0.000007
5	6	0	2.773612	0.837173	0.000003
6	1	0	1.229998	2.324392	0.000009

7	6	0	2.008446	-1.468838	-0.000008
8	1	0	-0.121968	-1.742014	-0.000011
9	6	0	3.061547	-0.539175	-0.000003
10	1	0	3.569886	1.572510	0.000007
11	1	0	2.252230	-2.526585	-0.000013
12	16	0	-1.485180	2.388814	0.000007
13	6	0	-2.881355	-0.318367	1.167545
14	6	0	-2.881360	-0.318355	-1.167546
15	6	0	-3.898263	-1.406596	0.777975
16	1	0	-3.378849	0.653315	1.315469
17	1	0	-2.314338	-0.553496	2.074262
18	6	0	-3.898322	-1.406538	-0.777967
19	1	0	-2.314352	-0.553520	-2.074261
20	1	0	-3.378815	0.653343	-1.315486
21	1	0	-3.585978	-2.382863	1.161056
22	1	0	-4.885198	-1.190277	1.198519
23	1	0	-3.586165	-2.382806	-1.161150
24	1	0	-4.885273	-1.190097	-1.198414
25	7	0	-1.978018	-0.276021	-0.000006
26	8	0	4.312089	-1.063511	-0.000005
27	6	0	5.425823	-0.178483	0.000000
28	1	0	6.310938	-0.816385	-0.000002
29	1	0	5.433405	0.455484	-0.895326
30	1	0	5.433400	0.455481	0.895327

2d

Total Energy (a.u.) = -919.438051 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.246823 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745015	0.842884	-0.117064
2	6	0	-0.672271	0.372304	-0.057963
3	6	0	-1.553706	0.899702	0.898404
4	6	0	-1.172340	-0.550962	-0.987145
5	6	0	-2.883181	0.493253	0.935868
6	1	0	-1.183746	1.634507	1.606259
7	6	0	-2.512997	-0.934668	-0.958008
8	1	0	-0.519022	-0.948932	-1.758741
9	6	0	-3.390987	-0.426872	0.005882

10	1	0	-3.543945	0.905951	1.695212
11	1	0	-2.882214	-1.637952	-1.701079
12	16	0	1.087494	2.483391	-0.221522
13	6	0	3.138354	0.243332	-0.205363
14	6	0	1.524648	-1.527910	0.249327
15	6	0	3.859287	-1.107187	-0.101240
16	1	0	3.401027	0.923152	0.614606
17	1	0	3.327723	0.782994	-1.137695
18	6	0	2.906962	-1.947925	0.763098
19	1	0	1.247816	-2.113048	-0.636749
20	1	0	0.726144	-1.637649	0.985966
21	1	0	3.967457	-1.560809	-1.094001
22	1	0	4.859522	-1.006388	0.329520
23	1	0	3.070797	-3.025997	0.673484
24	1	0	3.012986	-1.675599	1.819988
25	7	0	1.707707	-0.102166	-0.105361
26	6	0	-4.845732	-0.832166	0.033979
27	1	0	-5.168921	-1.096050	1.047827
28	1	0	-5.492801	-0.013121	-0.306101
29	1	0	-5.034981	-1.692856	-0.615276

2d-TS

Total Energy (a.u.) = -919.4035073 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.245868 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.636484	0.793250	0.000000
2	6	0	0.768973	0.349433	0.000000
3	6	0	1.840124	1.269853	0.000000
4	6	0	1.080594	-1.024053	-0.000001
5	6	0	3.153593	0.830103	0.000000
6	1	0	1.616699	2.331385	0.000000
7	6	0	2.404154	-1.456158	-0.000001
8	1	0	0.263687	-1.735614	-0.000002
9	6	0	3.464319	-0.542572	0.000000
10	1	0	3.961070	1.558992	0.000000
11	1	0	2.618218	-2.522378	-0.000002
12	16	0	-1.101987	2.385278	0.000000
13	6	0	-2.497724	-0.321944	1.167993

14	6	0	-2.497724	-0.321944	-1.167993
15	6	0	-3.512149	-1.412275	0.777951
16	1	0	-2.997471	0.648533	1.316431
17	1	0	-1.929836	-0.556269	2.074314
18	6	0	-3.512149	-1.412275	-0.777950
19	1	0	-1.929837	-0.556269	-2.074314
20	1	0	-2.997471	0.648533	-1.316430
21	1	0	-3.197772	-2.387802	1.161077
22	1	0	-4.499486	-1.197950	1.198478
23	1	0	-3.197773	-2.387801	-1.161077
24	1	0	-4.499486	-1.197949	-1.198477
25	7	0	-1.594656	-0.277117	-0.000001
26	6	0	4.900596	-1.003764	0.000000
27	1	0	5.437031	-0.630211	-0.881248
28	1	0	5.437018	-0.630251	0.881271
29	1	0	4.973056	-2.095496	-0.000002

2e

Total Energy (a.u.) = -1339.7334429 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.209676 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.134241	0.853479	-0.115206
2	6	0	-0.305403	0.451000	-0.059848
3	6	0	-1.156947	1.011220	0.903554
4	6	0	-0.847371	-0.434009	-1.004212
5	6	0	-2.508061	0.677777	0.944532
6	1	0	-0.751831	1.720178	1.618050
7	6	0	-2.203297	-0.757739	-0.989377
8	1	0	-0.213299	-0.851134	-1.781079
9	6	0	-3.021685	-0.205050	-0.006049
10	1	0	-3.159929	1.105179	1.698872
11	1	0	-2.621111	-1.426974	-1.733883
12	16	0	1.546409	2.476332	-0.219031
13	6	0	3.495023	0.140785	-0.198162
14	6	0	1.796726	-1.553609	0.247376
15	6	0	4.150028	-1.243213	-0.097709
16	1	0	3.786966	0.804406	0.625169
17	1	0	3.711397	0.674011	-1.128268

18	6	0	3.156670	-2.041075	0.761194
19	1	0	1.493532	-2.121088	-0.641605
20	1	0	0.993610	-1.627917	0.983564
21	1	0	4.238815	-1.697114	-1.092172
22	1	0	5.152640	-1.191997	0.335932
23	1	0	3.268647	-3.125220	0.666685
24	1	0	3.273164	-1.779208	1.819541
25	7	0	2.048950	-0.136650	-0.102227
26	17	0	-4.729255	-0.620311	0.031336

2e-TS

Total Energy (a.u.) = -1339.6978357 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.208649 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.032876	0.814862	-0.000002
2	6	0	-0.397823	0.447807	-0.000001
3	6	0	-1.414261	1.425878	0.000000
4	6	0	-0.778905	-0.908781	-0.000002
5	6	0	-2.754386	1.067754	0.000001
6	1	0	-1.133428	2.473562	0.000000
7	6	0	-2.119782	-1.280823	-0.000001
8	1	0	0.000705	-1.660803	-0.000003
9	6	0	-3.098833	-0.288067	0.000000
10	1	0	-3.531187	1.824826	0.000002
11	1	0	-2.405818	-2.327235	-0.000002
12	16	0	1.578761	2.378814	-0.000001
13	6	0	2.827421	-0.401489	-1.168998
14	6	0	2.827421	-0.401486	1.168999
15	6	0	3.782414	-1.543829	-0.777960
16	1	0	3.377585	0.540994	-1.318148
17	1	0	2.247545	-0.606050	-2.074854
18	6	0	3.782420	-1.543821	0.777965
19	1	0	2.247544	-0.606047	2.074855
20	1	0	3.377581	0.541000	1.318148
21	1	0	3.417068	-2.501397	-1.160946
22	1	0	4.779513	-1.381711	-1.198456
23	1	0	3.417085	-2.501390	1.160963
24	1	0	4.779520	-1.381692	1.198451

25	7	0	1.927665	-0.306867	-0.000003
26	17	0	-4.791701	-0.744414	0.000001

2f

Total Energy (a.u.) = -1108.0611172 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.262401 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.864581	0.827225	-0.200933
2	6	0	0.395692	0.572377	-0.069108
3	6	0	-0.357577	1.260428	0.894903
4	6	0	-0.259599	-0.310151	-0.942943
5	6	0	-1.727157	1.049672	0.998295
6	1	0	0.142330	1.965021	1.551414
7	6	0	-1.635332	-0.503588	-0.856436
8	1	0	0.307312	-0.823682	-1.714183
9	6	0	-2.377872	0.168603	0.123018
10	1	0	-2.316096	1.567046	1.748324
11	1	0	-2.137080	-1.172907	-1.546126
12	16	0	2.416049	2.381822	-0.500417
13	6	0	4.143355	-0.118279	-0.252151
14	6	0	2.300328	-1.583589	0.392418
15	6	0	4.661599	-1.545850	-0.032542
16	1	0	4.526046	0.588250	0.494871
17	1	0	4.380080	0.298627	-1.235138
18	6	0	3.621264	-2.157748	0.918547
19	1	0	1.911373	-2.194788	-0.431824
20	1	0	1.519067	-1.507633	1.151696
21	1	0	4.675968	-2.096361	-0.980958
22	1	0	5.676894	-1.555738	0.373649
23	1	0	3.622677	-3.251705	0.922615
24	1	0	3.796270	-1.815018	1.945242
25	7	0	2.681140	-0.238368	-0.095938
26	6	0	-3.849235	-0.008161	0.274984
27	8	0	-4.525130	0.542977	1.121666
28	8	0	-4.365046	-0.860933	-0.641361
29	6	0	-5.782533	-1.069590	-0.552058
30	1	0	-6.318598	-0.126097	-0.684551
31	1	0	-6.026374	-1.765957	-1.355024

32	1	0	-6.048324	-1.494100	0.419826

2f-TS

Total Energy (a.u.) = -1108.0237523 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.261331 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.734970	0.825786	-0.000014
2	6	0	-0.294129	0.484211	-0.000008
3	6	0	0.702948	1.482135	-0.000010
4	6	0	0.108440	-0.866885	-0.000002
5	6	0	2.047827	1.143680	-0.000004
6	1	0	0.401268	2.523773	-0.000015
7	6	0	1.456188	-1.206343	0.000003
8	1	0	-0.658567	-1.631414	0.000000
9	6	0	2.435837	-0.206452	0.000002
10	1	0	2.805620	1.918776	-0.000006
11	1	0	1.771032	-2.244595	0.000008
12	16	0	-2.306918	2.379319	-0.000021
13	6	0	-3.507012	-0.422274	1.169366
14	6	0	-3.506999	-0.422327	-1.169350
15	6	0	-4.439914	-1.582696	0.777971
16	1	0	-4.075440	0.509236	1.320025
17	1	0	-2.922575	-0.616658	2.074496
18	6	0	-4.439748	-1.582850	-0.777952
19	1	0	-2.922550	-0.616633	-2.074488
20	1	0	-4.075531	0.509126	-1.319985
21	1	0	-4.056038	-2.532939	1.160887
22	1	0	-5.439999	-1.439749	1.198333
23	1	0	-4.055546	-2.533077	-1.160582
24	1	0	-5.439768	-1.440225	-1.198576
25	7	0	-2.610271	-0.309747	-0.000011
26	6	0	3.866839	-0.630108	0.000008
27	8	0	4.239152	-1.786909	0.000013
28	8	0	4.715806	0.421217	0.000006
29	6	0	6.111389	0.081960	0.000011
30	1	0	6.642898	1.033884	0.000009
31	1	0	6.363964	-0.500935	0.889663
32	1	0	6.363967	-0.500944	-0.889633

2g

Total Energy (a.u.) = -972.3818499 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.217846 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.002585	0.846548	-0.107500
2	6	0	-0.436628	0.437620	-0.055002
3	6	0	-1.278935	0.953379	0.942069
4	6	0	-0.980022	-0.408834	-1.034811
5	6	0	-2.625425	0.613416	0.977605
6	1	0	-0.867243	1.631495	1.681995
7	6	0	-2.331572	-0.736599	-1.020961
8	1	0	-0.346824	-0.788980	-1.830792
9	6	0	-3.162777	-0.234607	-0.006707
10	1	0	-3.269831	1.006098	1.757379
11	1	0	-2.749753	-1.376859	-1.790972
12	16	0	1.392660	2.472745	-0.215398
13	6	0	3.365938	0.145710	-0.185551
14	6	0	1.670583	-1.560415	0.235039
15	6	0	4.024640	-1.237740	-0.101530
16	1	0	3.654628	0.800807	0.645744
17	1	0	3.580091	0.690092	-1.109599
18	6	0	3.031500	-2.052075	0.742380
19	1	0	1.368176	-2.113398	-0.663291
20	1	0	0.868023	-1.647728	0.970595
21	1	0	4.119036	-1.676665	-1.102047
22	1	0	5.025225	-1.189332	0.336796
23	1	0	3.146534	-3.134022	0.629764
24	1	0	3.145278	-1.807935	1.805158
25	7	0	1.920530	-0.137772	-0.093331
26	6	0	-4.552976	-0.583127	0.021789
27	7	0	-5.680155	-0.870391	0.046864

2g-TS

Total Energy (a.u.) = -972.3441083 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.216759 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.898876	0.804653	0.000000
2	6	0	0.535181	0.428309	0.000000
3	6	0	1.555355	1.402173	0.000000
4	6	0	0.903345	-0.931623	-0.000001
5	6	0	2.890956	1.033900	0.000000
6	1	0	1.279382	2.450839	0.000002
7	6	0	2.240439	-1.310217	-0.000002
8	1	0	0.116623	-1.675823	-0.000002
9	6	0	3.244563	-0.329201	0.000000
10	1	0	3.669863	1.789315	0.000001
11	1	0	2.515207	-2.360038	-0.000002
12	16	0	-1.427260	2.371856	0.000002
13	6	0	-2.699185	-0.400527	1.169963
14	6	0	-2.699187	-0.400524	-1.169964
15	6	0	-3.660276	-1.537202	0.777909
16	1	0	-3.243765	0.545008	1.319627
17	1	0	-2.120086	-0.609114	2.075288
18	6	0	-3.660289	-1.537190	-0.777909
19	1	0	-2.120089	-0.609118	-2.075288
20	1	0	-3.243759	0.545015	-1.319628
21	1	0	-3.300579	-2.496713	1.161046
22	1	0	-4.656293	-1.369121	1.198323
23	1	0	-3.300618	-2.496701	-1.161068
24	1	0	-4.656311	-1.369085	-1.198300
25	7	0	-1.798827	-0.309755	0.000000
26	6	0	4.625545	-0.713404	0.000000
27	7	0	5.746137	-1.025821	-0.000001

2h

Total Energy (a.u.) = -1084.6787815 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.221879 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.403385	0.853069	-0.150525
2	6	0	-0.047080	0.487293	-0.082507

3	6	0	-0.870111	1.051637	0.905248
4	6	0	-0.614555	-0.369926	-1.040281
5	6	0	-2.226197	0.750323	0.954315
6	1	0	-0.437561	1.736580	1.626568
7	6	0	-1.974477	-0.662642	-1.015209
8	1	0	0.006888	-0.787618	-1.826477
9	6	0	-2.760395	-0.104097	-0.009821
10	1	0	-2.873047	1.168547	1.715538
11	1	0	-2.431385	-1.308978	-1.754356
12	16	0	1.832699	2.460001	-0.348797
13	6	0	3.746092	0.083325	-0.175654
14	6	0	1.998851	-1.551538	0.313872
15	6	0	4.363919	-1.312809	-0.018590
16	1	0	4.050182	0.771443	0.622794
17	1	0	3.979813	0.573054	-1.125189
18	6	0	3.341563	-2.057848	0.854121
19	1	0	1.686011	-2.135013	-0.561346
20	1	0	1.189629	-1.582222	1.046678
21	1	0	4.454001	-1.801879	-0.995935
22	1	0	5.361884	-1.271471	0.426311
23	1	0	3.425813	-3.146668	0.792594
24	1	0	3.455059	-1.767998	1.905365
25	7	0	2.292627	-0.153208	-0.076819
26	7	0	-4.194987	-0.422975	0.032898
27	8	0	-4.866770	0.084363	0.930826
28	8	0	-4.638221	-1.181269	-0.830094

2h-TS

Total Energy (a.u.) = -1084.6401455 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.220781 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.305781	0.828016	-0.000013
2	6	0	-0.140720	0.492893	0.000000
3	6	0	-1.131838	1.496753	-0.000063
4	6	0	-0.545249	-0.856997	0.000076
5	6	0	-2.479072	1.167772	-0.000051
6	1	0	-0.826381	2.537017	-0.000122
7	6	0	-1.893336	-1.199900	0.000089

8	1	0	0.220527	-1.622496	0.000124
9	6	0	-2.841404	-0.180645	0.000026
10	1	0	-3.249681	1.928537	-0.000098
11	1	0	-2.217650	-2.233177	0.000148
12	16	0	1.876758	2.379316	-0.000100
13	6	0	3.070025	-0.428677	-1.170354
14	6	0	3.070144	-0.428484	1.170394
15	6	0	3.997844	-1.592475	-0.777965
16	1	0	3.641450	0.500879	-1.320152
17	1	0	2.485049	-0.620775	-2.075553
18	6	0	3.998852	-1.591644	0.777873
19	1	0	2.485264	-0.621124	2.075538
20	1	0	3.640971	0.501393	1.320411
21	1	0	3.609858	-2.541310	-1.160059
22	1	0	4.997962	-1.453749	-1.199323
23	1	0	3.612807	-2.540625	1.161559
24	1	0	4.999368	-1.451058	1.197667
25	7	0	2.172474	-0.311685	0.000057
26	7	0	-4.271696	-0.535454	0.000040
27	8	0	-5.087195	0.385726	-0.000017
28	8	0	-4.562715	-1.731010	0.000108

3a

Total Energy (a.u.) = -802.6644047 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))
Number of Imaginary Frequencies = 0 (B3LYP/6-31G(d))
Zero-point energy (a.u.) = 0.182221 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.922546	0.326037	-0.052800
2	6	0	-0.558359	0.116543	-0.016803
3	6	0	-1.370226	0.932051	0.785176
4	6	0	-1.165536	-0.844753	-0.841739
5	6	0	-2.754379	0.773358	0.779359
6	1	0	-0.903782	1.692892	1.402564
7	6	0	-2.552863	-0.986075	-0.862581
8	1	0	-0.548100	-1.464199	-1.486719
9	6	0	-3.350842	-0.183091	-0.046074
10	1	0	-3.369980	1.404920	1.414095
11	1	0	-3.009310	-1.721134	-1.520134
12	1	0	-4.431464	-0.296652	-0.058000

13	16	0	1.531910	1.855581	-0.369727
14	7	0	1.713726	-0.762363	0.124005
15	6	0	1.278286	-2.000303	0.774022
16	1	0	0.228408	-1.941898	1.050767
17	1	0	1.425272	-2.860035	0.109153
18	1	0	1.873386	-2.161819	1.681921
19	6	0	3.159558	-0.654051	-0.057405
20	1	0	3.378387	-0.075145	-0.955797
21	1	0	3.629252	-0.145479	0.793988
22	1	0	3.572179	-1.662506	-0.151165

3a-TS

Total Energy (a.u.) = -802.6343398 (B3LYP/6-311+G(d,p) SCRF=PCM (ε=35.6))

Number of Imaginary Frequencies = 1 (B3LYP/6-31G(d))

Zero-point energy (a.u.) = 0.181498 (B3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.827579	0.320324	0.000000
2	6	0	0.632790	0.099780	0.000000
3	6	0	1.541637	1.179575	0.000000
4	6	0	1.149052	-1.212227	0.000000
5	6	0	2.911284	0.952149	0.000000
6	1	0	1.150587	2.191268	0.000000
7	6	0	2.524049	-1.435581	0.000000
8	1	0	0.448524	-2.038337	0.000000
9	6	0	3.408984	-0.356536	0.000000
10	1	0	3.597483	1.794566	0.000000
11	1	0	2.904871	-2.453273	0.000000
12	1	0	4.481900	-0.530286	0.000000
13	16	0	-1.538221	1.815368	0.000000
14	7	0	-1.609537	-0.893187	0.000000
15	6	0	-2.418614	-1.039880	-1.215221
16	1	0	-1.774339	-0.959668	-2.096032
17	1	0	-2.870568	-2.037642	-1.209689
18	1	0	-3.216620	-0.284621	-1.293012
19	6	0	-2.418610	-1.039880	1.215223
20	1	0	-1.774333	-0.959667	2.096032
21	1	0	-3.216618	-0.284624	1.293016
22	1	0	-2.870562	-2.037644	1.209690

5. Reference

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